

INVESTIGATION OF THE PHOTOENHANCED REDUCTION OF NITROGEN DIOXIDE  
(NO<sub>2</sub>) ON ORGANIC FILMS AND ABOVE SOILS AS THE MISSING SOURCE OF  
DAYTIME TROPOSPHERIC NITROUS ACID (HONO)

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## ABSTRACT

Recent observed unpredictably high HONO daytime concentrations, demanding its ordinarily proposed heterogeneous source to proceed > 60 times faster at noon than during the night, prompted this study, concerning the effect of UV-A radiation on the uptake kinetics of gas-phase  $\text{NO}_2$  on various phenolic-containing organic films using a wetted-wall flow tube (WWFT) photoreactor.

Experimental methods are discussed in detail. A time-dependent model for non-equilibrium conditions incorporating both the chemistry and diffusion for predicting a best-fit reaction probability,  $\gamma_{\text{best-fit}}$ , as a function of the experimental parameters is detailed.

Emphasis is placed on the kinetics of the photoenhanced  $\text{NO}_2$  uptake reaction under acidic conditions for humic acids (HA), a ubiquitous group of environmental compounds. The linear correlation of HONO production rate with  $[\text{NO}_2]_0$  ( $k_1 = 6.7 \times 10^{-3} \text{ s}^{-1}$ ) for commercial HA suggest  $\text{NO}_2^-$  particles only diffuse throughout the surface layer depth, as experimentally verified.

In general, the pH-dependent results were qualitatively coherent with those of Stemmler et al. (2006), monitoring increases in the photoenhanced HONO formation with pH, owing to increases in reactivity in the reaction with  $\text{NO}_2$  with several carboxyl groups within the commercial HA with deprotonation, however centred on more authentic pH conditions of anaerobic humic soils (between pH 1.5 and 4.3).

A value of  $k_{\text{rxn}} = 2.70 \times 10^{-3} \text{ s}^{-1}$  at pH 3 was obtained, indicative that there was no competition with the hydrolysis reaction, for the tested conditions. Assuming that  $\gamma_{\text{rxn}}$  was rate-limiting,  $\gamma_{\text{diffusion}}$  was estimated to account for ~ 19% of the total uptake, consistent with the model results.

The humification-generated bacteria likely functioned as multicellular aggregates on the acidic HA substrate, producing a biofilm containing numerous chromophoric sensitizer units capable of photochemically reducing  $\text{NO}_2$  to HONO, defending the observed exponential dependence of HONO yield on irradiance under the tested conditions.

The datasets presented for the photoenhanced reaction of  $\text{NO}_2$  on acidic HA films provide a rather complete kinetic 'picture' of an important surface reaction ( $\gamma_{\text{best-fit, max}}$  of  $10^{-8}$  at pH 4 under the tested conditions). The scaling up assessments of the kinetic results for the small-scale photoreactor to that of both urban and rural scales are discussed.

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# 1 INTRODUCTION

## 1.1 SOURCES OF HONO

In the polluted urban atmosphere, it has long been recognized that the photolysis of nitrous acid (HONO), (R1),



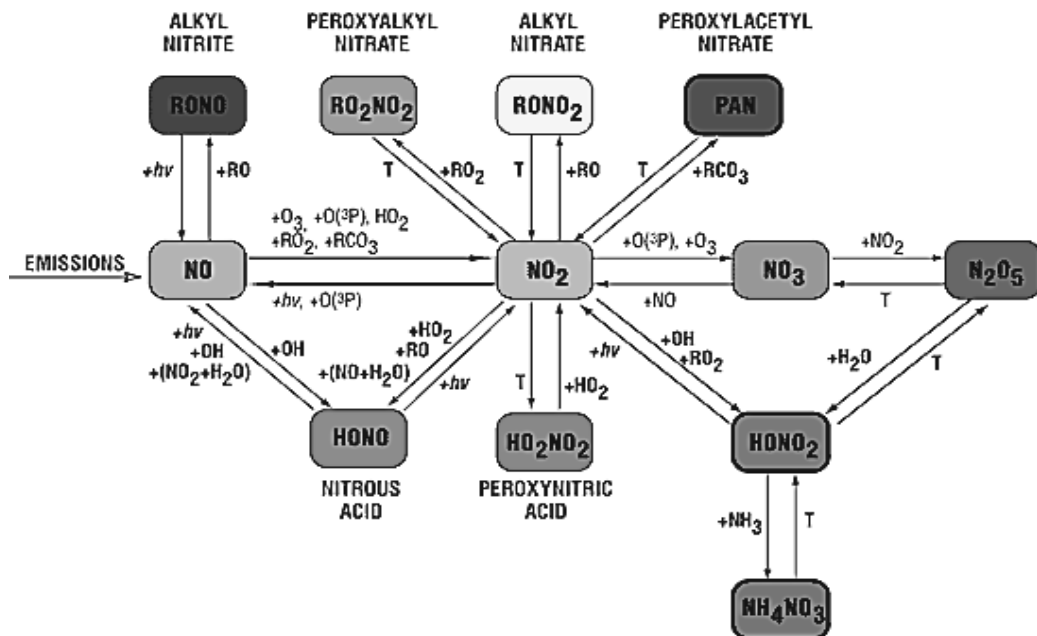
is a potentially important production mechanism for the hydroxyl radical ( $\bullet\text{OH}$ ), the most important oxidizing species in the daytime atmosphere (see **Figure 1**), in the polluted urban atmosphere (Harris et al., 1982), contributing to 60% of the integrated OH yield (Alicke et al., 2002, 2003; Zhou et al., 2002a; Aumont et al., 2003; Ren et al., 2003; Vogel et al., 2003; Kleffmann et al., 2005). Note that the typical lifetime of HONO at noon is around 15 min, but at higher zenith angles, or during periods of mild to moderate cloud cover, the lifetime can be considerably longer (Wall et al., 2006). This direct hydroxyl radical source is of most importance during early morning when HONO concentrations may be high after night-time accumulation (nighttime levels ranging from 1–15 ppb of HONO have been reported – for instance, HONO concentrations of up to 15 ppb were observed by Winer and Biermann (1994) in the California South Coast Air Basin), and when OH $\bullet$  production rates from other sources (see **Figure 2**), including the photolysis of ozone ( $\text{O}_3$ ), and formaldehyde, (HCHO), are slow (Harris et al., 1982).

The chemical consequences of the rapid photolysis of HONO imply that the significance of HONO surpasses that anticipated from its relative low abundance,  $f_{\text{HONO}}$  (Alicke et al., 2002; and Aumont et al., 2003):

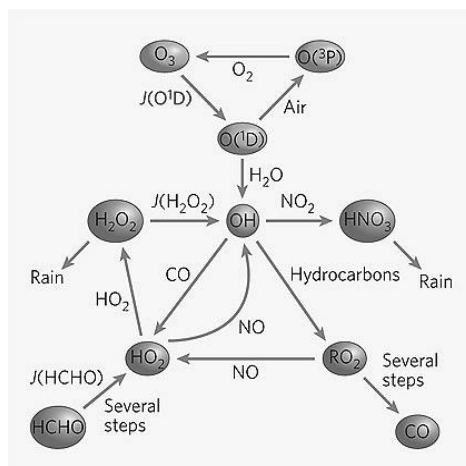
$$f_{\text{HONO}} = [\text{HONO}]/[\text{NO}_2] < 0.1$$

The newest tropospheric chemistry models specify that ozone mixing ratios are about three times more sensitive to HONO than to  $\text{NO}_2$  inputs (Jenkin et al., 2008). Referring to the photochemical smog cycle detailed in **Figure 3**, it is evident that as  $J_3 \sim 100(J_1)$ , under hazy/foggy conditions (high humidity and reduced insolation), the “HONO cycle” may well overtake the ‘ $\text{O}_3$  cycle’ generating ‘smog without ozone’ (Acker et al., 2006). Furthermore, the large discrepancies between detected and predicted  $\text{HO}_x$  ( $\bullet\text{OH} + \text{HO}_2\bullet$ ) concentrations at higher  $\text{NO}_x$  levels and high solar zenith angles are likely due to the more efficient



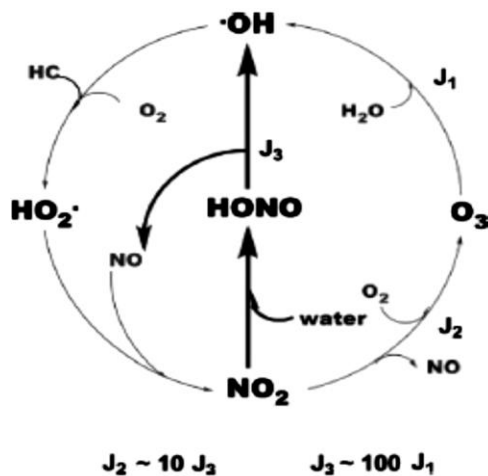


**Figure 1.** Chemical transformations of nitrogen oxides in the troposphere. The *hydroxyl radical* and trace hydrocarbons react with nitrogen oxides through the sequence of reactions shown, producing oxidants, the final product of photochemical smog. Ozone and oxygen atoms are generated from the photodissociation of nitrogen dioxide ( $\text{NO}_2$ ). Water reacts with oxygen atoms producing *hydroxyl radicals* – these radicals, in succession, react with hydrocarbons to form hydrocarbon radical. Aldehydes result from oxidation of hydrocarbons by the *hydroxyl radical* – they can undergo further oxidation forming aldehyde peroxides and aldehyde peroxyacids. From: Foust.



**Figure 2.** The main route for hydroxyl-radical production. Ozone is broken up by UV(A) light to form atomic oxygen in the 1D excited electronic state, occurring with a frequency denoted by  $J(\text{O}^1\text{D})$ . The excited oxygen atoms react with water vapour to form OH radicals. Alternatively, the excited atoms may be recycled back to ozone, via the 3P electronic ground state. In the lower atmosphere, recycling with NO is the mechanism responsible for the formation of ozone in the lower atmosphere.  $J(\text{H}_2\text{O}_2)$  and  $J(\text{HCHO})$  are the first-order rate constants (in  $\text{time}^{-1}$ ) for the solar photolysis of  $\text{H}_2\text{O}_2$  and HCHO, respectively. Note that R represents any hydrocarbon chain. From: Wennberg (2006).

than formerly assumed HONO cycle (Olson et al., 2006), but may, too, be attributed to direct •OH production from electronically excited NO<sub>2</sub> (+ H<sub>2</sub>O) (Li et al., 2008).



**Figure 3.** The “HONO (photochemical smog) cycle”.  $J_1$ ,  $J_2$ , and  $J_3$  are the first-order rate constants (in time<sup>-1</sup>) for the solar photolysis of O<sub>3</sub>, NO<sub>2</sub>, and HONO, respectively. HC stands for reactive hydrocarbons, and “water” represents fog or cloud droplets. From: Haagen-Smit (1952).

### 1.1.1 HOMOGENEOUS SOURCES

Several early modelling studies (e.g. Aumont et al., 1999; and Staffelbach et al., 1997) have conclusively demonstrated that observed daytime HONO concentrations cannot be explained by its principal homogeneous source reaction, (R2) (the reverse of its photolysis reaction),



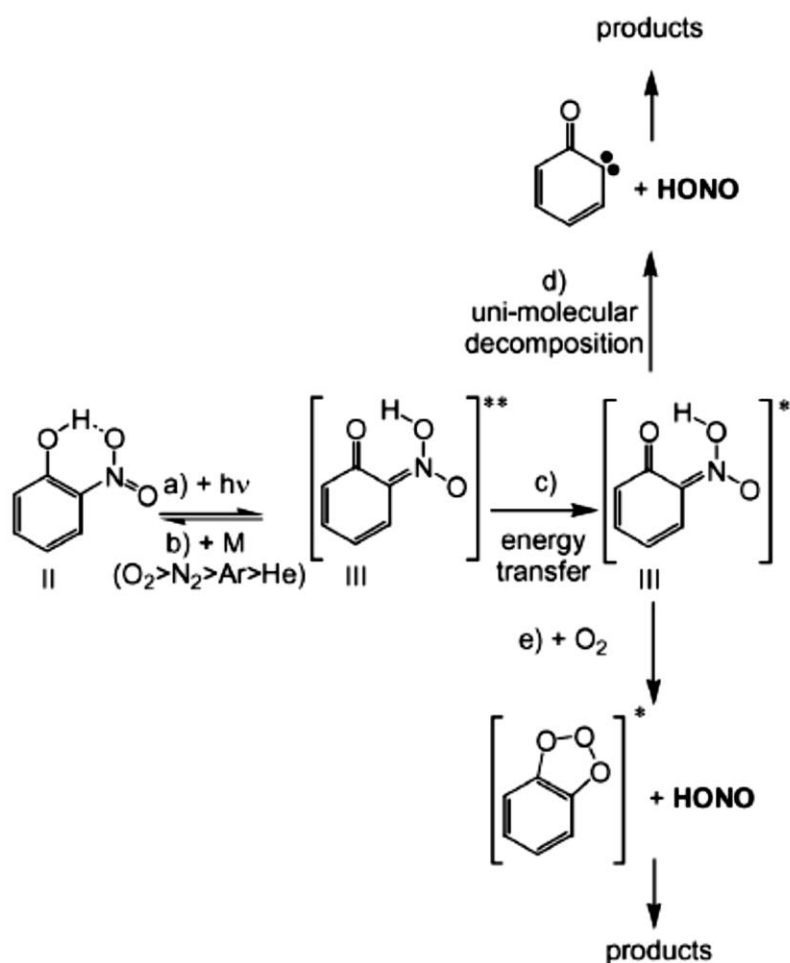
alone, however, this reaction does become significant during the day when OH and NO concentrations are high). Accordingly, pure gas-phase chemistry, too, drastically underestimates observed night-time HONO concentrations. Thus, in the absence of direct HONO sources, we expect a steady-state HONO (noon-time) HONO concentration in the ppt range for urban areas (Alicke et al., 2002b). Other homogeneous reactions involving nitrogen oxides and water have also been shown to be too slow to be of any significance in the atmosphere (Kaiser and Wu, 1977). Finally, with regards to automobile emissions, recent tunnel measurements by Ackermann (2000) indicate HONO/NO<sub>x</sub> conversion ratios of

0.65% for both cars with catalytic converters and diesel engines, while a previous traffic tunnel study in the United States presents smaller values of 0.3% (Kirchstetter et al., 1996), ruling out emissions as a significant HONO source. Note that differences in the fleet compositions and engine technologies are likely account for the discrepancies in the observed ratios.

Recently, the gas-phase production of HONO was observed resulting from the photolysis of different *ortho*-nitrophenols (Bejan et al., 2006). The proposed mechanism is detailed in **Figure 4**. Amid the diverse types of aromatic hydrocarbons (HC), nitrophenols (NPs) are of unique interest due to their phytotoxic properties which might be a contributing cause to forest decline (Harrison et al., 2005). In the environment, the presence of nitrophenols is related to both natural processes and anthropogenic activity. In particular, the *ortho*-nitrophenols, 2-nitrophenol (2-NP) and 4-nitrophenol (4-NP) are generated from the reaction of phenol with nitrite ions in water. The reactions proceed in a wide range of acidities (pH values) under the influence of UV radiation (Patnaik and Khoury, 2004; and Vione et al., 2004). In the atmosphere, environmental reactions, too, lead to the production of nitrophenols. The reaction of phenol, nitrite ions and the hydroxyl radical results in the formation of 2-NP (and other nitrated compounds) (Harrison et al., 2005) – this and other atmospheric nitrophenol species are usually measured in low concentration levels ( $\text{ng dm}^{-3}$ ), although in heavily polluted areas, concentrations up to  $320 \text{ ng dm}^{-3}$  have been observed (Flox et al., 2005). Nitrophenol levels in fog water have been detected as high as  $40 \mu\text{g L}^{-1}$  in North East Bavaria (for 4-NP, Richartz et al., 1990). During the generation and degradation of pesticides including 2-buthyl-4,6-dinitrophenol (Dinoseb) and 4,6-dinitro-2-methylphenol (DNOC) (these compounds are also used as components and precursors in polymers and drug production; Pocerull et al., 1996), nitrophenols are also produced. Finally, nitrated phenols are utilized in the production of dyes, solvents, plastics, as well as, explosives (Furuta et al., 2004) and formed due to metallurgic, electronic, and electric activity (US EPA, 1980).

Based on experimental data obtained for 3-methyl-2-nitrophenol (3M2NP), a (noontime) photolytic HONO production rate of  $100 \text{ pptv h}^{-1}$  was estimated by Bejan et al. (2006) for urban conditions in the presence of 1 ppbv of the selected NP, which cannot be neglected when compared to the observed production in the atmosphere. However, this estimate requires verification from experimentation under atmospheric conditions, as well as, further investigations on the wavelength dependencies of the photolysis processes.

Additionally, the gas-phase photolysis of methyl-substituted nitroaromatics was very recently demonstrated (Bejan et al., unpublished results; in Kleffmann, 2007) as a HONO source. The photolysis of other nitrogen-containing organic species should be studied in the future since they may also be of importance for atmospheric HONO production. Furthermore, strong photochemical gas-phase sources might help to explain the absence of daytime HONO/NO<sub>x</sub> gradients.



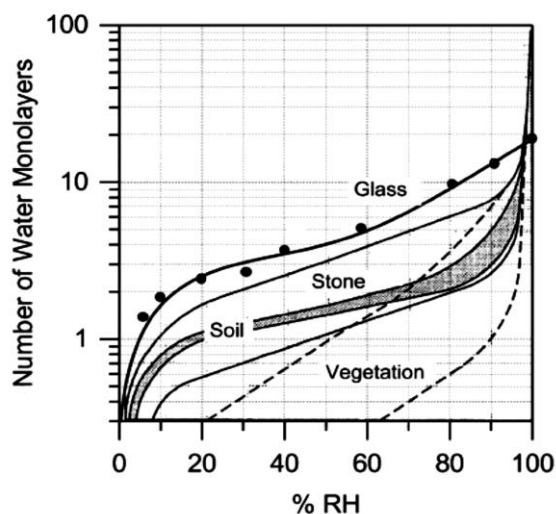
**Figure 4.** Proposed mechanism (Bejan et al., 2006) for HONO production resulting from the photolysis of gas-phase *ortho*-nitrophenols. The further reaction, (e) was recommended in order to explain the decrease in HONO formation that Bejan et al. (2006) observed on switching from synthetic air to pure oxygen (O<sub>2</sub>). For relatively low oxygen concentrations (synthetic air), the concentrations of (excited state) III<sup>\*\*</sup> and II<sup>\*</sup> will decrease significantly as a result of efficient quenching of III<sup>\*\*</sup> (b), so that (e) will be less critical. Note that the mechanism is still highly theoretical, requiring validation via further product and spectroscopic studies.

Finally, in the (tropospheric relevant) wavelength range > 290 nm, the photolysis of gas phase nitric acid is also proposed to be a minor source of HONO (Huber, 2004).

### 1.1.2 HETEROGENEOUS SOURCES

Airborne particulate matter (PM) and ground level surfaces (e.g., soils, buildings) provide unique solid-air interfaces which can support heterogeneous chemistry, as well as, impact tropospheric photochemical cycles (Ravishankara, 1997). Such types of surfaces have been suggested in the past as important substrates for heterogeneous  $\text{NO}_2$  hydrolysis (see for example, Lammel and Cape, 1996; Lammel, 1999) and may, too, be critical in other processes including renoxification of nitric acid (Saliba et al., 2001; and Rivera-Figueroa et al., 2003). A thorough understanding of these solid-air interfaces, nevertheless, requires the incorporation of heterogeneous and photochemical reactivity of surface-adsorbed organics (Perreau et al., 2001). For example, mineral (Falkovich et al., 2004) aerosols attain organic coatings during production processes, as well as, from adsorption of semi-volatile compounds during transport. Organic aerosols are generated from both biogenic and anthropogenic emissions (Pio et al., 2001; Simoneit, 2002; Robinson et al., 2006; and Huang et al., 2006) – note that these emissions also contribute to the organic content of inorganic aerosols. Urban surfaces (buildings and windows), too, contain surface films composed of complex mixtures of organic and inorganic compounds (Lam et al., 2005), while rural surfaces including soils are abundant in degraded biomolecules (Beck et al., 1993). The area concerning reactions in thin films on surfaces, (with SURFACE assigned the appropriate parameterization, **SURFACE** = Surfaces, Urban and Remote: Films As a Chemical Environment) (Finlayson-Pitts et al., 2003), which has not yet attracted much interest, may contribute significantly to the chemistry of the Earth's boundary layer. Since this chemistry occurs in the physical setting in which people are subjected to air pollutants, the consequential impacts can be sizeable.

Water uptake isotherms for some common materials (soil, vegetation, stone and glass) found in the boundary layer (Lammel, 1999) are presented in **Figure 5**. It is clear that although vegetation takes up less water, a monolayer or more is present at relative humidities (RH) higher than 50%. Hence, in urban areas where significant  $\text{NO}_2$  levels are present (Finlayson-Pitts et al., 2003), all of these common surfaces are expected to participate in HONO (and NO) formation.



**Figure 5.** Water uptake isotherms for some common materials found in the boundary layer. Labels for water uptake isotherms: (●) glass; (– unshaded) stone; (– shaded) soil; and (---) vegetation. To account for porosity (outer surfaces may grow and when pores are filled with condensing water, inner surfaces can shrink under the influence of water uptake), wetness types (%) and surface area indices (SAI = total surface/cross section) were attributed to the various ground types as a function of ambient humidity. Adapted by Finlayson-Pitts et al. (2003) in Lammel (1999).

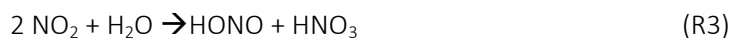
### 1.1.2.1 Ground SURFACES

#### 1.1.2.1.1 Indoors

In a number of studies, nitrous acid has been detected indoors (e.g., see refs. Park et al., 2008; Khoder, 2002; and Jarvis et al., 2005). Though HONO is a product of combustion, for instance, in gas stoves and space heaters (Park et al., 2008), it is evident that the heterogeneous hydrolysis of NO<sub>2</sub> on materials inside of homes represents a significant source. Formation of nitrous acid is expected in commercial facilities such as ice skating rinks (Wolfson et al., 2012), as well due to high levels of nitrogen dioxide that are often found inside. The uptake of NO<sub>2</sub> on various materials used inside and outside buildings has been examined by Spicer et al. (1989), who observed that wallboard, cement blocks, wool carpets, brick and masonite had the highest uptake rates (larger than window glass by more than an order of magnitude), possibly reflecting their ability to adsorb water (due to higher porosities,  $p$ , compared to glass, as given in Folkerts et al., 1984) and form a surface film.

#### 1.1.2.1.2 Humic Acid (HA)

Recent unexpectedly high HONO daytime concentrations have been observed that, consequently, demand the heterogeneous disproportionation of NO<sub>2</sub> with water given in Reaction (R3),



to proceed greater than 60 times faster at noon than during the night (Kleffmann, 2007; and Acker et al., 2008). This result evokes two important consequences: (i) it reminds HONO researchers of the persistent discrepancies between observed and under/overestimated ( $\bullet\text{OH}/\text{HO}_2\bullet$ ) levels in atmospheres with greater than 100 ppt NO<sub>x</sub> (Faloona et al., 2000; Olson et al., 2006; and Kanaya et al., 2008); and (ii) awakens unanswered issues concerning (R3) (Aumont et al., 2003).

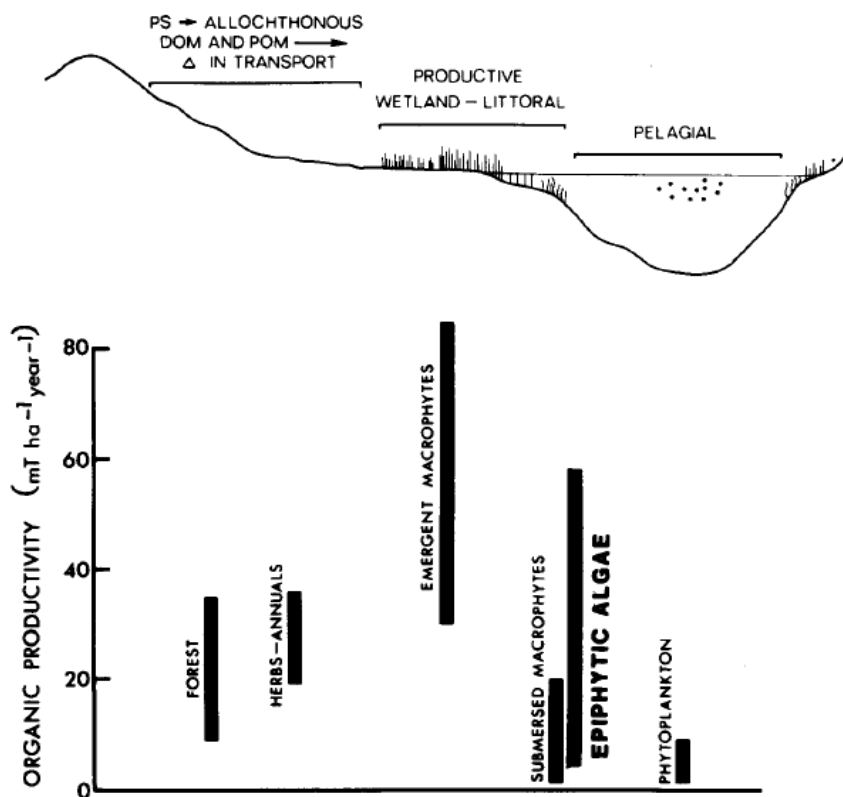
While the heterogeneous hydrolysis reaction of NO<sub>2</sub> (R3) was first proposed based on smog chamber experiments (Finlayson-Pitts et al., 2003), more novel studies suggest that the heterogeneous reduction of NO<sub>2</sub> with adsorbed hydrocarbons (R4) is, too, of importance under atmospheric conditions (Gutzwiller et al., 2002; and Ammann et al., 2005):



There is an expanding body of proof that the heterogeneous reactive loss of gas-phase NO<sub>2</sub> at surfaces containing photoactive compounds can be significantly enhanced under illumination (George et al., 2005; Stemmler et al., 2006; Stemmler et al., 2007; Jammoul et al., 2008; and Nieto-Gligorovski et al., 2008). The photosensitized reaction of NO<sub>2</sub> with organic material is one possible conversion pathway leading to HONO formation. A good fraction of the enhancement is owing to the heterogeneous reduction of the gas-phase reactant (NO<sub>2</sub>) to HONO, followed by photoexcitation of the substrate (George et al., 2005; Stemmler et al., 2006; and Stemmler et al., 2007). Substrates that act as photosensitizing or photoreducing agents demonstrate this effect to the greatest extent (George et al., 2005). This reduction has been verified to occur on pure organic substrates including humic substances at wavelengths not only in the UV-A spectral region, but also in the visible region under atmospheric conditions (Stemmler et al., 2006).

Humic substances (HS) represent the main carbon reservoir in the biosphere, estimated at  $1600 \times 10^{15}$  g C (Hedges et al. 2000). This assembly of organic “leftovers” contributes vital properties to soils, including

sequestration, mobilization, and oxidative or reductive transformation of organic xenobiotic molecules, trace gases, and trace metal contaminants (Sutton and Sposito, 2005). Humic substances are formed by secondary synthesis reactions (humification) during the decay process and transformation of biomolecules originating from plants and other dead organisms (Stevenson, 1994). In nature, humic substances, mainly humic acids (HA) (insoluble under acidic conditions below pH 1) and humin (fraction which is insoluble in water at any pH value) (Malcolm, 1990), are extremely resistant to biodegradation (highly refractory), with mean residence times in soil varying from ca. 800 to >3000 years (Stevenson, 1994). The humic substances found in soils, oceans, and deep lakes are generally autochthonous (produced within the system), while those in streams and shallow lakes are more often allochthonous (produced outside the system) (see **Figure 6**). Flowing surface and ground water are responsible for their distribution throughout the hydro- and lithosphere. Differences in origin, age, and genesis lead to a high degree of chemical and morphological complexity that makes the compounds difficult to characterize (von Wandruszka, 2000).



**Figure 6.** The lake ecosystem, with the drainage basin of terrestrial synthesis (PS) of OM, movement of nutrients and dissolved organic matter (DOM) and particulate organic matter (POM) in surface and groundwater flows toward



the lake basin. Also displayed are the chemical and biotic alteration of these materials en route, specifically as they pass through the productive and metabolically active wetland-littoral zones of the lake *per se* (net organic productivity in metric tons per hectare per year). From: Wetzel (1992).

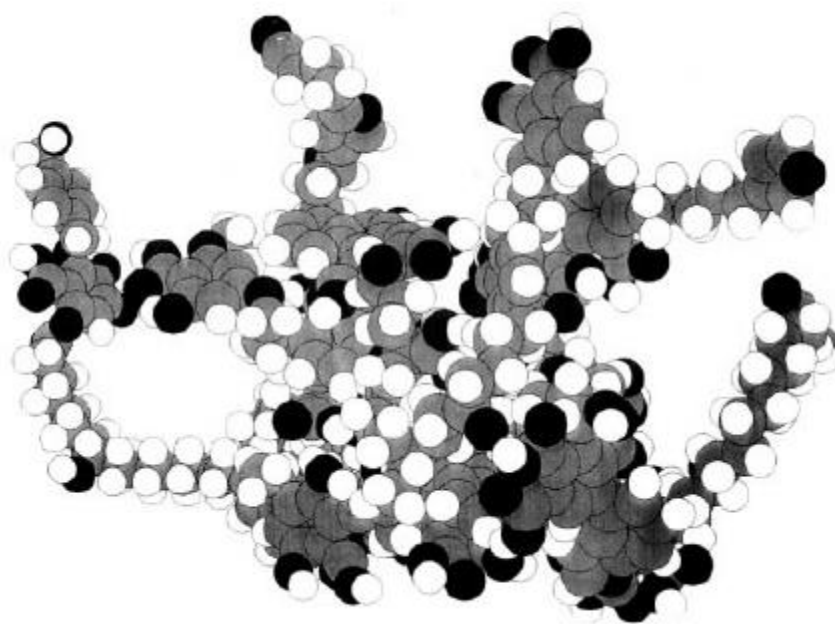
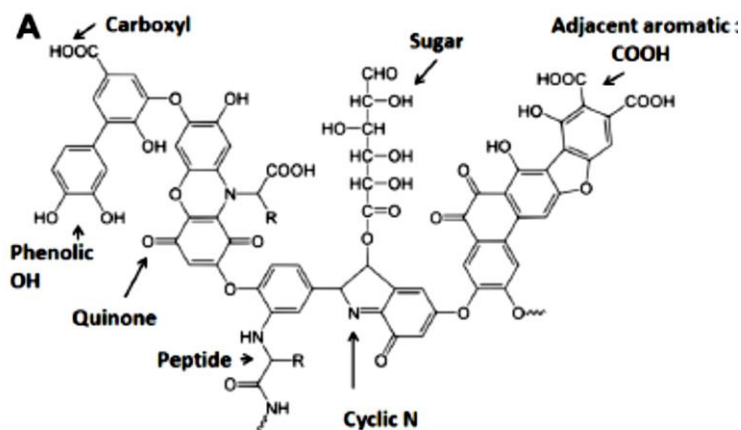
A new concept of humic substances has thus emerged, that of the **supramolecular** association, in which many relatively small and chemically diverse organic molecules form clusters linked by hydrogen bonds (H-bonds) and hydrophobic interactions (Piccolo, 2001; Simpson et al., 2002). A corollary to this model is the concept of **micellar** structure (see **Figure 7**), i.e., an arrangement of organic molecules in aqueous solution to form hydrophilic exterior regions shielding hydrophobic interiors from contact with vicinal water molecules (von Wandruszka et al., 1999). Reviews of current research regarding the composition of the individual fragments of humic material produced through the degradation of biomolecules and, therefore, which are relevant to the supramolecular association model of humic substances (see **Figure 8 A & B** for proposed 2- and 3-D model structures). These biomolecules are derived primarily from lipids,



**Figure 7.** Representation of the humic micelle. From: von Wandruszka (2000) (adapted from: Wershaw, 1986).

lignin, nonlignin aromatic species, carbohydrates, and proteins (e.g. Brown et al., 1998; Fan et al., 2000; González-Vila et al., 2001; Mao et al., 2001; Simpson et al., 2001; Hertkorn et al., 2002; and Mao et al., 2002). Heteroatomic functionalities include phenols and other alcohols, ketones/quinones, aldehydes, carboxylic acids, amino- and nitro-groups, and sulfur containing entities such as mercaptans, sulfates, and sulfonates (von Wandruszka, 2000). The average molecular weights (MW) of humic substances, HA and, in particular, humin, are still under debate. A small minority of researchers state that HAs are relatively small humic molecules that only self-assemble into apparently high- MW material held together by weak

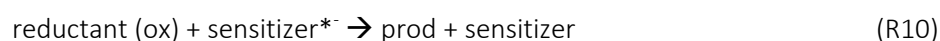
dispersive forces, such as van der Waals, *p-p* and CH-*p* interactions (Piccolo, 2001; Sutton & Sposito, 2005). Most of the research community, however, claims that HAs are comprised of macromolecules ranging mainly from about 5,000 to 100,000 Da (e.g. De Nobili & Chen, 1999; Stevenson, 1994). To support the latter hypothesis, lignin, a major source for HS, can be taken as an example. Lignin is a high-MW macromolecule degraded by microorganisms (mainly fungi) through oxidative reactions (Grinhut et al., 2007). The high-MW transformation products of lignin degradation are likely to be macromolecules (Filip and Tesarova, 2004).



**Figure 8.** (A) 2-D structure of a model humic acid<sup>a</sup>. (B) 3-D computer generated model of humic acid. Using semi empirical calculations and known chemical features of HAs, Schulten (1995) arrived at this set of open structures

containing numerous voids. Note that the computer generated model indicates that the individual HA polymers can assume configurations which incorporate all the essential attributes critical of the pseudomicellar arrangement. <sup>a</sup> From: Briones (2012) (adapted from: Stevenson, 1994). <sup>b</sup> From: Schulten (1995).

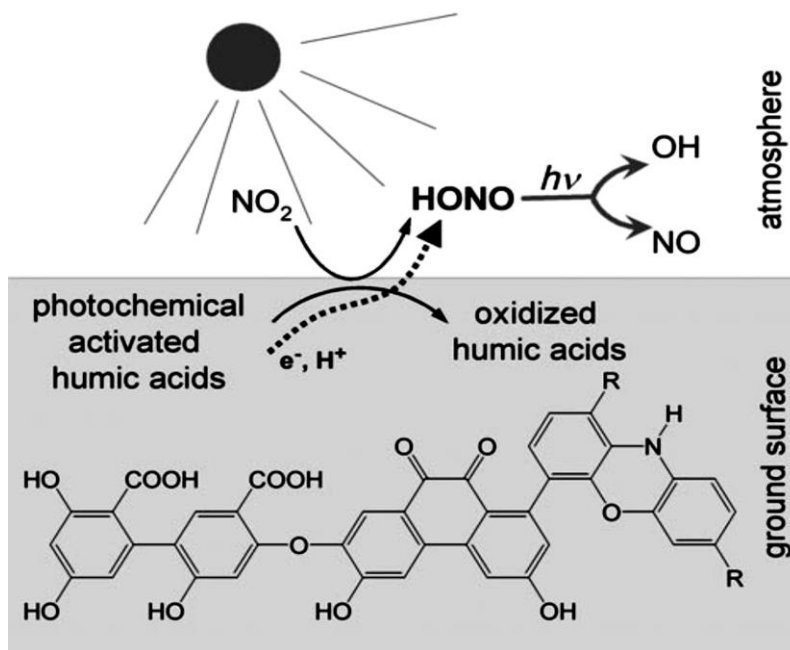
Fundamental to the schematic photosensitized NO<sub>2</sub> reaction mechanism, (M1), seen below (George et al., 2005) is a light absorbing sensitizer (R5), which in its excited state will initiate a series of possible reaction pathways, potentially involving a reducing agent to generate a reduced sensitizer radical species, via (R6). After the adsorption of NO<sub>2</sub> from the gas-phase, (R7), this intermediate radical species will either react with react with NO<sub>2</sub> to form nitrite, (R8) (which is in equilibrium depending on the acidity, (R9)). Alternatively, in (R10) the sensitizer radical intermediate can react with the oxidant radical species, yielding the second reaction product of step (R6). Note that this path does not lead to the production of HONO.



The simplified mechanism, (M1), for the photosensitized HONO formation on a representative structure of humic acid is shown in **Figure 9**. For the net reaction, NO<sub>2</sub> is reduced to HONO, while the aromatic hydrocarbon is oxidized, producing high yields of HONO in the laboratory (up to nearly 100 %) (George et al., 2005). The noted rate of HONO formation (estimated to be  $\sim 5 \times 10^{10}$  molecules cm<sup>-2</sup> s<sup>-1</sup> (Stemmler et al., 2006) (scaling for lamp intensities) (Donaldson et al., 2010) for a moderately polluted atmosphere ( $\sim 20$  ppb NO<sub>2</sub>, a typical urban concentration) and representative midday solar irradiances (300-700 nm  $\sim 400$  Wm<sup>-2</sup>) could account for the recently observed high daytime concentration of HONO in the boundary layer, with a predicted significant contribution of up to 60% to the hydroxyl radical production of the lowest hundred (to a few hundred) meters of the atmosphere.

Later, this mechanism was also used to explain experiments with real soil surfaces (Stemmler et al., 2006). Based on the kinetic results obtained for the soil surfaces, it was possible to explain daytime HONO formation in the atmosphere, at least for conditions with several ppbv of NO<sub>2</sub> (Stemmler et al.,

2006). This mechanism is, unable to explain daytime HONO formation in a rural area for very low  $\text{NO}_2$  concentrations, however (see Kleffmann, 2007). Thus, if these measurements were unaffected by artefacts (as recently observed for polar regions; Liao et al., 2006), other mechanisms are necessary to explain the high measured HONO concentrations in remote regions.



**Figure 9.** Simplified mechanism for the formation of HONO in the heterogeneous reaction of  $\text{NO}_2$  on photosensitized humic acid (representative structure shown here). From: George et al. (2005) and Stemmler et al. (2006) in Kleffmann (2007).

### 1.1.2.1.3 Soil

Recent studies have suggested that the reduction of N(IV) in  $\text{NO}_2$  to N(III) in HONO can proceed on ground surfaces (Stemmler et al., 2007; Monge et al., 2010), consistent with field data indicating that HONO is indeed released from the ground (Zhang et al., 2009; Sörgel et al., 2001). In soil, the dominant sources of N(III), however, include biological nitrification and denitrification processes (Canfield et al., 2010), which generate nitrite ions ( $\text{NO}_2^-$ ) from ammonium ( $\text{NH}_4^+$ ) (by nitrifying microbes), as well as from nitrate ( $\text{NO}_3^-$ ) (by denitrifying microbes). Due to the high water solubility of nitrites, they may undergo the following reversible acid-base reaction, (R11), and partition between air and the aqueous phase of humid soil:



Molecular nitrous acid in the aqueous-phase (aq), represented by  $\text{HNO}_2$ , can reversibly dissociate into  $\text{H}^+$  and  $\text{NO}_2^-$  ions or partition to the gas phase (g). The equilibrium gas-phase concentration over an aqueous solution of nitrous acid, termed  $[\text{HONO}]^*$ , is determined by the acidity (pH value) and nitrite solution concentration (Su et al., 2011). The exchange of HONO between the gas- and aqueous- phases is controlled principally by  $[\text{HONO}]^*$ : when  $[\text{HONO}]^*$  is greater than the true gas-phase concentration,  $[\text{HONO}]$ , nitrous acid will be released from the aqueous-phase; otherwise, gas-phase HONO will be deposited.

In addition to the magnitude of the missing source, HONO release from soil nitrite can account for the characteristic diurnal course observed in field measurements (Su et al., 2011). The release of HONO from soil nitrite might largely increase in the course of global change, because of enhanced fertilizer use and soil acidification in developing countries (Guo et al., 2010), resulting in an amplified oxidizing capacity of the lower troposphere. Nitrite production and HONO release is likely significant in natural environments, too, including forests and boreal soils, due to intensifying N deposition (Reay et al., 2008) and acid deposition, and the ubiquity of (de)nitrifying microbes. As soils in boreal and tropical forests are normally moderately acidic (pH  $\approx$  4 to 5), even very low soil nitrite concentrations can lead to a sizeable release of HONO in such environments (Su et al., 2011). Further studies of HONO release from soil nitrite are recommended in view of the potentially important influence on atmospheric chemistry.

#### **1.1.2.1.4 Plants**

Of late, Schimang et al. (2006) investigated the uptake of gas-phase HONO by several plant species; however, their data suggest a quick metabolism of HONO by the plants that is limited by the diffusion of HONO through the plant stomata. Their data imply that plant surfaces therefore represent a sink for HONO, eliminating these boundary layer materials as potential SURFACES.

#### **1.1.2.1.5 Urban Grime**

The coating on impermeable surfaces in an urban environment (urban organic films or window grime) is another SURFACE which contains a moderate mass fraction of organics that is exposed to the urban

atmosphere (Diamond et al., 2000; Gingrich et al., 2001; Lam et al., 2005; and Simpson et al., 2006). In the same manner as particle surfaces, the films may function as sequestering agents (for any compounds associated with them) (Donaldson et al., 2005), and, too, act as a substrate for chemical reaction (Kahan et al., 2006). Several of the identical organic compounds as found in aerosol particles (Simpson et al., 2006), including polycyclic aromatic hydrocarbons (PAHs), are observed in such surface films; thus, the heterogeneous oxidation processes are expected to be similar.

Recently, HONO was detected as a gas-phase product in the heterogeneous reaction between gaseous  $\text{NO}_2$  and solid pyrene/ $\text{KNO}_2$  films; such films were employed as a simplified proxy for urban grime (Ammar et al., 2010). As a conservative estimate, Ammar et al. (2010) expect a HONO production rate of 130 pptv/hr., assuming that only 1% of a street canyon surface with 10 m street width and 20 m building height is covered by pyrene/nitrate films. Brigante et al. (2008) measured the uptake coefficient for  $\text{NO}_2$  loss on films of solid pyrene over a range of gas-phase concentrations and atmospherically relevant conditions under near-UV illumination, to find that the uptake coefficient depends inversely on the  $\text{NO}_2$  concentration, implying a Langmuir-Hinshelwood kinetic mechanism (Adamson and Gast, 1997) ( $\text{NO}_2$  is in rapid equilibrium between the surface and the gas-phase and the reaction takes place between the adsorbed pyrene and co-adsorbed  $\text{NO}_2$ ). By analogy to similar results on other organic films, Brigante et al. (2008) observed that photoexcited pyrene can reduce  $\text{NO}_2$  to HONO and NO, with yields of ca. 15% and 30%, respectively.

### **1.1.2.2 Polar SURFACES**

#### **1.1.2.2.1 Ice**

Ice surfaces provide an interesting model for the study of  $\text{NO}_2$ -water interactions in a two-dimensional water environment – the speed of a reaction is greatly reduced on a cold ice surface, in comparison to a liquid water surface at room temperature, and often the reaction intermediates can be isolated on the ice surface resulting via kinetic trapping (Kang, 2005; Günster et al., 2005; Park et al., 2003; and Kim et al., 2009). Below the surface premelting regime (140 K), Kim and Kang (2010) observed efficient conversion of  $\text{NO}_2$  into nitrous acid on the ice surface. Their recent results yield that the reaction occurs through interactions of isolated  $\text{NO}_2$  adsorbates with water, disputing a reaction mechanism involving  $\text{NO}_2$ - $\text{NO}_2$  intermediates. In its early stage, in accordance with observations, the  $\text{NO}_2$  hydrolysis mechanism occurs

only to the formation of nitrous acid, and nitric acid is not yet formed. A probable reaction mechanism at this stage may be:



The reaction mechanism, however, is expected to be more complex than represented by these simple chemical formula – nitrous acid and the hydroxyl radical may not be generated as isolated molecular species, but certainly, may be part of a larger molecular structure on the ice surface connected via hydrogen bonds (Kim and Kang, 2010).

Since  $\text{NO}_2$  hydrolysis is efficient on cold ice surfaces, it is expected that (R12) will readily occur under atmospheric conditions at the SURFACES of water films, aerosols, and icy particles, which offer higher molecular mobility, solvation efficiency, and thermal energy than the cold ice surface of the laboratory experiment (Kim and Kang, 2010). Furthermore, due to its very small activation energy, the reaction can readily occur with thermal energy in the absence of any additional energy input, such as the absorption of sunlight. Thus, nitrous acid is expected to be generated efficiently during the night via the heterogeneous hydrolysis of  $\text{NO}_2$  on surfaces containing condensed atmospheric moisture, in agreement with field measurements (Lammel and Cape, 1996).

#### 1.1.2.2.2 Snow

In polar regions, one would expect OH production to be low as the rate of OH production from  $\text{O}_3$  photolysis is reduced due to higher solar zenith angles (SZA) and lower water partial pressures. However, measurements of HONO concentrations within the last decade at the South Pole (Mauldin et al., 2002) are nearly 10 times higher than predicted by gas-phase chemistry models (Chen et al., 2001; Grannas et al., 2002a; and Yang et al., 2002), suggesting a substantial influence of the snowpack. Snow pack emissions of photolabile species including HONO and HCHO can have pronounced influences as they remain restricted to a thin layer close to the surface, due to poor vertical mixing in the polar lower atmosphere.

There exists increasing evidence that humic-like substances, as well as electron-rich phenolic and polyaromatic light-absorbing substrates, resembling those proposed by George et al. (2005), are ubiquitously found even in polar snow (Grannas et al., 2007). Additionally, the other reactant,  $\text{NO}_2(\text{g})$ , is generated during the photolysis of nitrate in snow (Honrath et al., 2000), predominantly producing  $\text{O}^-$  and  $\text{NO}_2$  at the air-ice interface. Accordingly, the proposed mechanism, (M1), might be an efficient pathway to resolve high HONO mixing ratios seen in the polar atmosphere.

Humic acid, doped to an ice film, has been observed by Thorsten Bartels-Rausch et al. (2010) to effectively photosensitize the  $\text{NO}_2$  reduction, likely due to its moieties, some which can act as the sensitizer, as well as others that act as the reductant. The results of their extrapolation of expected HONO fluxes with increasing  $\text{NO}_2$  concentration at different photolytically active organic matter content of surface snow indicate a strong dependence on both organic and  $\text{NO}_2$  concentration. Extrapolation to 100 ppt ( $3 \times 10^9$  molecules  $\text{cm}^{-3}$ ) typical for the interstitial air of polar snow-packs (Honrath et al., 2002; and Grannas et al., 2007), and an organic matter content of approximately  $10 \mu\text{g C L}^{-1}$  (Grannas et al., 2004), yields a light-driven HONO flux of around  $1 \times 10^{13}$  molecules  $\text{m}^{-2} \text{s}^{-1}$  (Thorsten Bartels-Rausch et al., 2010), indicative that the conversion of  $\text{NO}_2$  to HONO on humic substances in snow, sensitized in the VIS, can readily explain the overall HONO flux. Future studies focusing on the content, specification and location of organic compounds in environmental snow samples, however, are desired, including mountain sites where preferable conditions for the light-driven  $\text{NO}_2$  reduction typically prevail during winter (Thorsten Bartels-Rausch et al., 2010).

### ***1.1.2.3 Aerosol Particles***

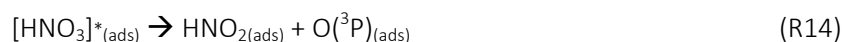
In urban areas, aerosol particles have a complex composition and can function as condensation nuclei for fog and cloud formation. In fact, several field studies report evidence for the production of HONO in both aerosols and clouds (e.g. see refs.: Acker et al., 2005; and Acker et al., 2006).

#### ***1.1.2.3.1 Inorganic Aerosol***

##### **1.1.2.3.1.1 Photolysis of adsorbed $\text{HNO}_3$ /nitrate**



On the basis of field measurements in polar (Zhou et al., 2001; Beine et al., 2001; Dibb et al., 2002; Honrath et al., 2002; Beine et al., 2002; and Beine et al., 2003) and rural (Zhou et al., 2002) regions, and on the observation of HONO formation in an irradiated glass sampling manifold (Zhou et al., 2002b), the photolysis of adsorbed nitrate or nitric acid at wavelengths around 300 nm was proposed as a significant daytime source of HONO, with the reaction 1-2 orders of magnitude more rapid than in the gas and aqueous phase (Zhou et al., 2002b, 2003). The reaction mechanism (M2) proceeds via the following reactions (R13) – (R15):

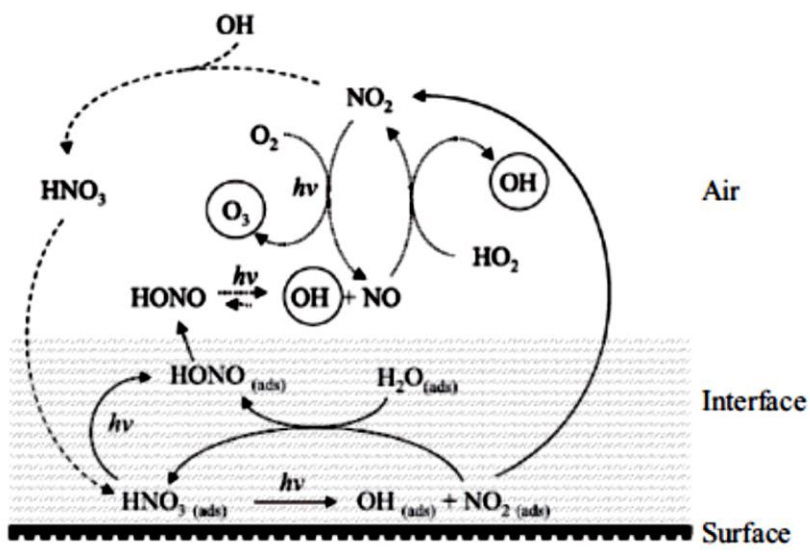


Under humid conditions, the  $\text{NO}_{2(\text{ads})}$  produced on the surface can react further with  $\text{H}_2\text{O}_{(\text{ads})}$  to generate  $\text{HONO}_{(\text{ads})}$ , which through (R3) may be released into the gas phase. This mechanism had previously been proposed to account for the background radical formation in smog chambers (Killus and Whitten, 1990). Other conceivable mechanisms include:

- (i) Photolysis of adsorbed organic nitrates, nitro compounds (Bejan et al., 2006), etc., produced from the heterogeneous reactions of nitric acid with organic impurities, as suggested in a simulation chamber study (Rohrer et al., 2005); or
- (ii) A reduction of nitric acid to HONO by photosensitized organic impurities, analogous to a mechanism observed for the reaction of  $\text{NO}_2$  with organic substrates (George et al., 2005; and Stemmler et al., 2006). Organic impurities are normally present on photoreactor surfaces, if not chemically cleaned. Additionally, organics, including HAs may be expected on surfaces of glass sampling manifolds in field campaigns (Zhou et al., 2002) and have been measured in polar snow (Grannas et al., 2004). Furthermore, such a photochemistry may, too, explain the elevated HONO/ $\text{NO}_x$  ratios observed over snow surfaces (Beine et al., 2001).

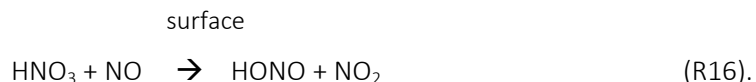
Modeling has indicated that an  $\text{HNO}_3$  photolysis mechanism was of significance for HONO production during the 2001 Northeast Oxidant and Particle Study (Sarwar et al., 2008). A new source of photochemically reactive nitrogen species, i.e., HONO and  $\text{NO}_x$ , would be supplied by the heterogeneous photolysis of  $\text{HNO}_3$ , significantly impacting the chemistry of the remote low- $\text{NO}_x$  atmospheric boundary layer via the transformation of the radical pool, as elucidated in **Figure 10**. As an example, incorporation

of renoxification processes on surfaces increased HONO concentrations significantly (by an order of magnitude), and enhanced O<sub>3</sub> model performance in the South Coast Air Basin of California (Knipping and Dabdub, 2002). Further studies are required to clarify the mechanism of photochemical formation of HONO on surfaces treated with nitric acid.



**Figure 10.** Effects of the photolytic remobilization of HNO<sub>3</sub> (“re-NOxification”) on ground surfaces on the chemistry of the above atmosphere. Solid arrows indicate processes accountable for surface HNO<sub>3</sub> remobilization; dashed arrows designate removal of oxidized nitrogen from the atmosphere to ground surfaces by deposition; and dotted arrows specify gas-phase reactions resulting in the production of O<sub>3</sub> and OH radicals (in circles). From: Zhou et al. (2003).

An additional mechanism of HONO formation includes the reaction of HNO<sub>3</sub> with NO (Rivera-Figueroa et al., 2003) on hydrated glass surfaces, (R16), via a non-photochemical heterogeneous pathway:



More recent laboratory work has indicated that the dissolved nitrate ion (NO<sub>3</sub><sup>-</sup>), not merely adsorbed HNO<sub>3</sub>, contributes to HONO (and NO<sub>2</sub>) production on organic films (Handley et al., 2007).

Several researchers have observed that surface nitrate may be generated on Al<sub>2</sub>O<sub>3</sub> through heterogeneous reactions with NO<sub>2</sub> and HNO<sub>3</sub>, while photolysis of adsorbed nitrate yields only NO<sub>2</sub>, NO and N<sub>2</sub>O (Schuttlefield et al., 2008; Rubasinghege and Grassian, 2009; and Chen et al., 2011). Additionally, the formation of adsorbed HNO<sub>3</sub> on SiO<sub>2</sub> was detected when gaseous NO<sub>x</sub> reacts with SiO<sub>2</sub> (Goodman et al., 1999; Liu et al., 2012; and Ma et al., 2011b). As mineral dust consists of approximately

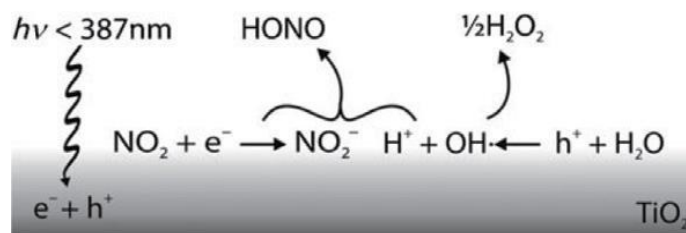
60% SiO<sub>2</sub> (Usher et al., 2003), the photolysis of adsorbed nitric acid on mineral dust or glass surfaces might be a significant source of atmospheric HONO. Further studies are required, however, to assess the relevance of this HONO source.

#### 1.1.2.3.1.2 TiO<sub>2</sub>-containing SURFACES

It is common knowledge that windstorms can transport airborne dust particles extensive distances, and, thus, may impact chemistry on a global scale, for instance, in the elimination of oxides of nitrogen such as N<sub>2</sub>O<sub>5</sub> which otherwise might precede the formation of ozone (Kitada et al., 2007). Silicates and a number of other components, including Fe<sub>2</sub>O<sub>3</sub>, Al<sub>2</sub>O<sub>3</sub>, and TiO<sub>2</sub> are common components of such particles (Laskina et al., 2013).

It is adequately known that, in the anatase configuration, titanium dioxide (TiO<sub>2</sub>) nanoparticles are effective photocatalysts for the destruction of atmospheric pollutants including toxic volatile organic compounds (VOCs) (Ao et al., 2003) and oxides of nitrogen (NO<sub>x</sub> = NO + NO<sub>2</sub>) (Dalton et al., 2002; Devahasdin et al., 2003; Maggos et al., 2007, 2008; Wang et al., 2007). Recently, a line of commercial building material products have emerged exploiting these properties: one prototype is self-cleaning window glass, which is coated by a thin layer of TiO<sub>2</sub> that destroys adsorbed organic dirt; other examples include TiO<sub>2</sub> materials including cements, paving stones and indoor/outdoor paints which have been instituted precisely for NO<sub>x</sub> abatement applications in polluted urban areas (Frazer, 2001; Maggos et al., 2007). In spite of the seeming promise of these materials, comprehensive trials by authorities across Japan and Europe have produced relatively little solid proof in support of their effectiveness for NO<sub>x</sub> removal, yet, nonetheless, further interest in their widespread use continues to develop (Berdahl and Akbari, 2008).

Recently, the anti-polluting quality of TiO<sub>2</sub>-containing materials was challenged (Langridge et al., 2009; Monge et al., 2010; and Ndour et al., 2009). Under UV-irradiation, Ndour et al. (2009) have demonstrated that nitrate ions adsorbed onto mixed TiO<sub>2</sub>/SiO<sub>2</sub> and pure TiO<sub>2</sub> are converted into gas-phase NO and NO<sub>2</sub>. Furthermore, it has been proven that the interaction of NO<sub>2</sub> with TiO<sub>2</sub> (Monge et al., 2010) and commercial self-cleaning TiO<sub>2</sub>-containing window glass (Langridge et al., 2009) terminates in the production of gas-phase nitrous acid. The proposed mechanism, (M3) is shown in **Figure 11**.



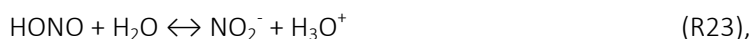
**Figure 11.** Proposed mechanism, (M3) for the photocatalytic formation of nitrous acid on UV-illuminated  $\text{TiO}_2$  (Beaumont et al., 2009).

Monge et al. (2010a), who studied the reaction of  $\text{NO}_2$  on irradiated  $\text{TiO}_2$  (x%)/ $\text{SiO}_2$  films as proxies for  $\text{NO}_x$  de-polluting materials, observed  $\text{NO}$ ,  $\text{HONO}$ , and nitrate anions generated as a result of the  $\text{NO}_2$  loss on UV-illuminated  $\text{TiO}_2$  films. The proposed mechanism, (M4), for the observed gas-phase products is detailed below (where the subscripts **vb** and **cb** denote valence band and conduction band, respectively):



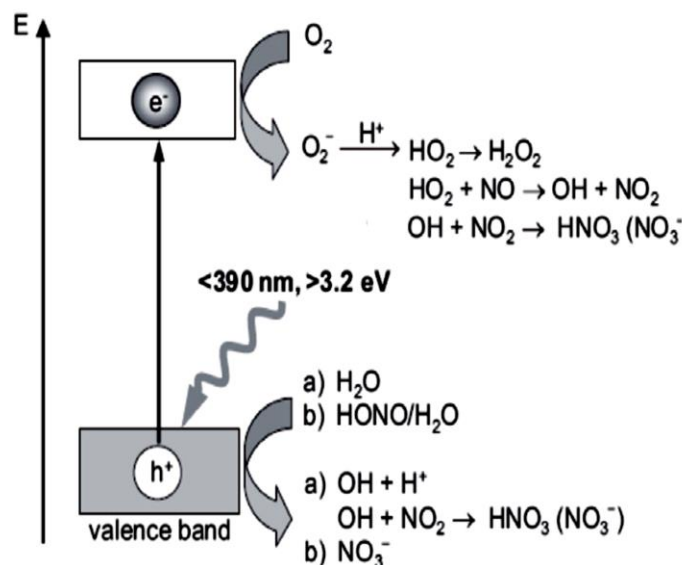
In opposition to the above-mentioned studies, Laufs et al. (2010), who studied  $\text{TiO}_2$ -doped commercial paints, observed an efficient decomposition of  $\text{HONO}$  on the photolytic samples (mechanism, (M5) shown in **Figure 12**), and thus, ruled that the paint surfaces do not represent a source of  $\text{HONO}$ .

The solution of  $\text{NO}_2^-$  in a film of adsorbed water (rather than gas-phase  $\text{HONO}$ ) was proposed



with (R23) strongly dependent on pH. The lack of gas-phase  $\text{HONO}$  formation observed by Laufs et al. (2010) can be explained by the alkaline surface properties (pH 8.0 – 8.5) of the paints used. The more

acidic surface properties of pure TiO<sub>2</sub> and glass materials when compared to the paints tested by Laufs et al. (2010) shift (R23) to the left side, resulting in low decomposition of HONO.



**Figure 12.** Suggested mechanism, (M5) for the photocatalytic reaction of NO, NO<sub>2</sub> and HONO on photoactive paint surfaces containing TiO<sub>2</sub>. From: Laufs et al. (2010).

Although being a small component of mineral dust particles (Karagulian et al., 2006), titanium dioxide was shown, of late, to be accountable for the photochemical activity of atmospheric mineral aerosols (Ndour et al., 2008). These authors, researching the interaction of NO<sub>2</sub> with irradiated mixed TiO<sub>2</sub>/SiO<sub>2</sub>, Sahara dust, and Arizona Test Dust films, did observe HONO formation for all tested samples, though with varying yields. These results, in line with the previously discussed data (Monge et al., 2010; Ndour et al., 2008; and Beaumont et al., 2009) yields evidence for photochemical HONO formation on the surface of mineral aerosols in the atmosphere, which may contribute to daytime HONO production, partly supplying the remaining deficit of the daytime HONO sources. However, additional kinetic studies under atmospherically relevant conditions are required to have a greater understanding of the photochemistry of NO<sub>y</sub> in the atmosphere.

### **1.1.2.3.2 Organic Aerosol**

#### **1.1.2.3.2.1 Soot Aerosol**

Soot aerosol, is ubiquitous in the atmosphere, consisting mainly of elemental carbon with a variable fraction of organic materials. It embodies about 10% - 50% of the total tropospheric particulate matter and may afford a significant fraction of accessible reaction surface owing to its fractal morphology (Chameides and Bergin, 2002; and Zhang et al., 2008). It is important to note, however, that only a small fraction of a typical total surface density consists of pure and externally mixed soot, with the purely emitted soot being rapidly transformed via coagulation and condensation of sulphuric acid into internally mixed soot (Riemer et al., 2003).

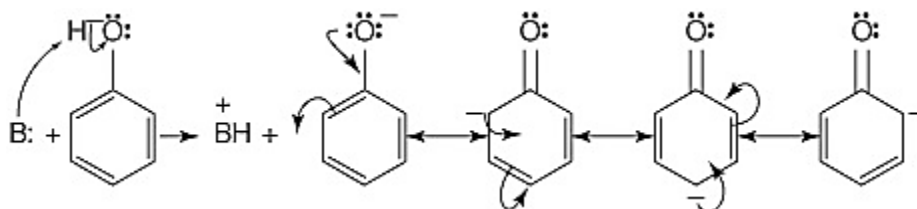
Soot aerosol has been identified as a probable reaction surface for HONO generation by (R4) (Ammann et al., 1998), and is regarded as likely nighttime source of HONO (Aumont et al., 1999). Due to its atmospheric relevance, the heterogeneous conversion of NO<sub>2</sub> to HONO has been comprehensively studied in the laboratory for a wide range of NO<sub>2</sub> concentrations on various carbonaceous materials, including spark discharge soot (Ammann et al., 1998; Kalberer et al., 1999), hydrocarbon flame soot (Gerecke et al., 1998; Kleffmann et al., 1999; Al-Abadleh and Grassian, 2000; Stadler and Rossi, 2000; Salgado and Rossi, 2002; Lelièvre et al., 2004; Kleffmann and Wiesen, 2005; Aubin and Abbatt, 2007; and Khalizov et al., 2010), commercial black carbon (Kleffmann et al., 1999; Kleffmann and Wiesen, 2005) and diesel soot (Arens et al., 2001). The published uptake coefficients ( $\gamma$ ) range over seven orders of magnitude, from 10<sup>-1</sup> to 10<sup>-8</sup>, with HONO yields varying from a few percent to around 100%, however, depending on the measurement method, type of soot, assumed surface area, and initial concentration of NO<sub>2</sub> employed.

Although the HONO production rate appears to be rapid within the first minute of exposure to NO<sub>2</sub>, a passivation of the surface quickly retards the formation (Kleffmann et al., 1999), leading to the knowledge that soot influences the tropospheric concentration of HONO only in a minor way. Recently, Monge et al. (2010b) observed that the conversion of NO<sub>2</sub> to HONO on soot particles was markedly enhanced in the presence of artificial solar radiation, leading to persistent reactivity over time scales comparable to the lifetime of atmospheric soot. Based on their results, (as a lower limit value), a HONO production rate of 25 pptv hr<sup>-1</sup> would be expected for an urban environment, challenging the existing view of the negligible

significance of tropospheric soot chemistry due to its rapid surface deactivation in the dark. Nevertheless, only the interaction between soot and UV-A radiation has been studied as of yet, while the effect of visible light has still not been quantified. Thus, more studies on soot photochemistry are necessary in the near future.

### 1.1.2.3.2 Phenolic Aerosol

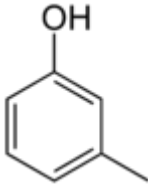
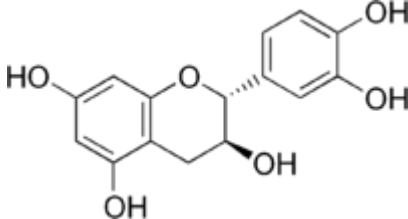
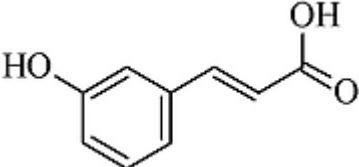
By and large, the multiphase or heterogeneous chemistry of aromatic compounds is, even now, uncertain – the vast number of polar aromatic species found in aerosols is inexact, as they have several sources including primary emissions, as well as both gas- and particle-phase oxidation processes. Phenolic compounds, which are ubiquitous in particulate matter (PM) (Nakao et al., 2011), and in the SURFACE environment, have been shown to be generated in elevated concentrations in both the gas- and condensed-phases (owing to their very low volatility) via wood combustion (Gonçalves et al., 2011), as well as biomass combustion, which releases a variety of guaiacols, catechols and syringols (mainly from lignin pyrolysis) (Keiluweit et al., 2010). In addition, photooxidation of aromatic compounds in the gas phase may produce hydroxybenzenes as intermediates (Shakya and Griffin, 2010). Finally, due to microbial decomposition of vegetation a large number of polyphenols (along with their acid and aldehyde derivatives) are released primarily in the form of **soil organic matter (SOM)** in significant concentrations (Zhang et al., 2013).



**Figure 13.** Due to the resonance in phenol, the oxygen atom acquires a positive charge, weakening the oxygen-hydrogen bond and facilitating the release of a proton. Deprotonation of phenol, (M6) results in the phenoxide ion, or phenate, which also exists as a resonance structure. From: <http://chemistry.tutorvista.com/organic-chemistry/phenols.html>.

Semi-volatile species from diesel engine exhaust, have been shown quite recently to undergo transfer to the condensed phase under atmospheric conditions, and subsequently react (specifically, in an **electron transfer** reaction) in the aqueous phase with  $\text{NO}_2$  to form nitrite, or HONO if sufficiently acidic conditions are employed (Gutzwiller et al., 2002b). Some of these semi-volatile condensed species include hydroxy-

substituted aromatics (Alfassi et al., 1986), aromatic amines (Saltzman, 1954) or alcohol amines (Levaggi et al., 1974). NO<sub>2</sub> may, too, undergo electron transfer reactions with phenoxide ions. The kinetics of such reaction has been studied in the past for methylphenols and hydroxybenzenes (Alfassi et al., 1986; Gutzwiller et al., 2002), catechins (Miao et al., 2001), and hydroxycinnamic acid derivatives (Zhan et al., 1998). The electron transfer reaction displays strongly pH dependent overall kinetics (Gutzwiller et al., 2002a), resultant from the deprotonated species (the **phenoxide ion**). The deprotonation mechanism, (M6) of phenol is shown in **Figure 13**, with primary reaction products comprising the corresponding **phenoxy type radical** (or the corresponding radical cations) and the **nitrite ion** - the nitrite ion may be subsequently protonated and released to the gas phase as HONO<sub>(g)</sub> in an acidic environment (Gutzwiller et al., 2002b). Refer to **Table 1** for the chemical structures and acid dissociation constants of some phenol-derived biomolecules.

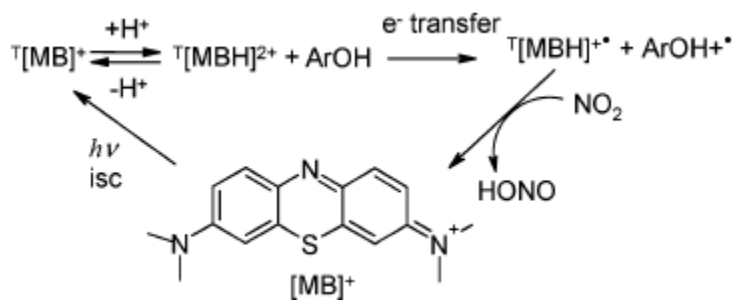
Organic Species	Chemical Structure	pK <sub>a</sub>
<i>m</i> -methylphenol ( <i>m</i> -cresol)		10.08 <sup>a</sup>
(±)-catechin (cyanidanol)		8.77 <sup>b</sup> , 9.97 <sup>b</sup> , 11.99 <sup>b</sup>
3-hydroxycinnamic acid ( <i>m</i> -coumaric acid)		9.4

**Table 1.** Chemical structures and acid dissociation constants (pK<sub>a</sub>) for selected phenol-derived biomolecules. <sup>a</sup> From experimental MOPAC database. <sup>b</sup> From: Herrero-Martinez et al. (2005). <sup>c</sup> From: ChemAxonMolconvert database.

Photoenhanced reduction of NO<sub>2</sub> to HONO on representative organic films constituting a mixture of synthetic phenols with an aromatic UV absorbing photosensitizer (aromatic ketones and their derivatives) was recently proven to be a credible candidate for the missing HONO source at the ground (George et al., 2005). As presented by Canonica et al., (1995), the excited triplet state of a photosensitizer may undergo



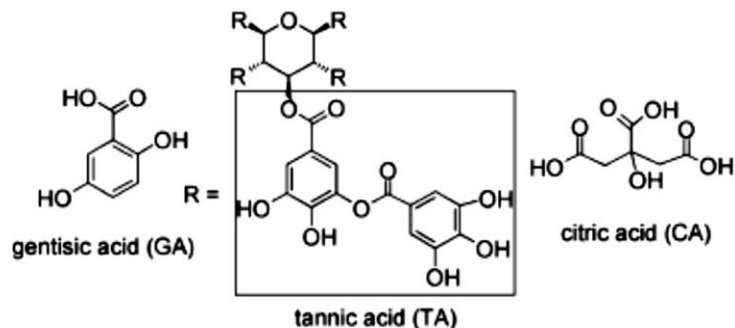
an electron or proton transfer reaction with an electron-donating phenol in its ground state, ensued by the reaction of the diphenylketyl radical intermediate with  $\text{NO}_2$ . The overall mechanism of this light-induced  $\text{NO}_2 \rightarrow \text{HONO}$  conversion has also been proposed for HA coatings, where chromophoric centres hold the role of the sensitizer, with the phenolic moieties acting as the electron donor (Stemmler et al., 2006; 2007). The results attained by Sosedova et al. (2011) were used to establish a kinetic and photochemical model that allowed estimation of the importance of this chemistry for atmospheric conditions. For an  $\text{NO}_2$  mixing ratio of 20 ppbv, representative of biomass burning plume, an actinic flux of  $1.7 \times 10^{21}$  photons  $\text{m}^{-2} \text{s}^{-1}$  (model clear sky flux in the 300 – 750 nm range, 40 degrees SZA) and RH varied between 20 to 60%, the uptake coefficient was in the order of  $\gamma_{\text{rxn}} = 1.6 \times 10^{-6}$  for the  $\text{NO}_2$  to conversion on a phenolic aerosol similar in reactivity to the gentisic acid (GA)/methylene blue (MB) and tannic acid (TA)/methylene blue (MB) investigated by Sosedova et al. (2011) (see **Figure 14** for mechanism, (M7)). The chemicals used for preparation of these organic films are shown in **Figure 15**.



**Figure 14.** Proposed mechanism, (M7) of the  $\text{NO}_2$  to  $\text{HONO}$  conversion (adapted from George et al., 2005) by replacing the aromatic ketone by methylene blue (MB) of relevance in the study of Sosedova et al. (2011). Triplet MB is generated via intersystem crossing (denoted isc) upon absorption of light, followed by an electron transfer reaction with a substituted phenol ( $\text{ArOH}$ ), and finally recycling to ground-state MB via reaction with  $\text{NO}_2$ . From: Sosedova et al. (2011).

Methylene blue (3,7-bis(dimethylamino)phenazathionium chloride) was selected as a model photosensitizer absorbing in the visible part of the solar spectrum with a high yield of the triplet state (Redmond and Gamlin, 1999), with the aim of using the synthetic photosensitizer to represent naturally occurring environmental chromophoric material (Sosedova et al., 2011). Under the assumption that all biomass burning aerosol consists of phenolic compounds (for a representative aerosol surface concentration of  $10^{-3} \text{ m}^{-1}$  in a plume), a  $\text{HONO}$  formation rate between 10.6 and 12.6 pptv  $\text{h}^{-1}$  is estimated. These calculated  $\text{HONO}$  formation rates on phenolic aerosol should be regarded as upper limits, which when compared to the observed formation rates of 57 pptv  $\text{h}^{-1}$  in the free troposphere and

of 110-180 pptv h<sup>-1</sup> in the upper boundary layer at noontime (Zhang et al., 2009), likely indicates that it is only a minor source to the observed HONO, in comparison to the photochemical HONO production on the ground, yet possibly via similar processes.



**Figure 15.** Chemicals used for preparation of organic films in the study of Sosedova et al. (2011) using typical mass ratios of 10:1 of GA:CA or TA:CA.

### 1.1.2.3.2.3 Humic Acid Aerosol

Recently, Stemmler et al. (2007) investigated the light-induced heterogeneous conversion of NO<sub>2</sub> into HONO on submicron humic acid aerosol. Under simulated atmospheric conditions with respect to the actinic flux, relative humidity (RH) and initial NO<sub>2</sub> concentration ([NO<sub>2</sub>]<sub>0</sub>), Stemmler et al. (2007) observed reactive uptake coefficients,  $\gamma_{rxn}$  for the photoenhanced conversion on the aerosol between less than 10<sup>-7</sup> (in the dark) and 6×10<sup>-6</sup> (under illumination), which were inversely correlated with [NO<sub>2</sub>]<sub>0</sub> (ranged from 2.7 to 280 ppb), with slight deductions in values of  $\gamma_{rxn}$  for values of RH < 20 and > 60%. By extrapolation to typical surface concentrations (10<sup>2</sup> – 10<sup>3</sup> μm<sup>2</sup> cm<sup>-3</sup>), Stemmler et al. (2007) estimated a HONO formation rate of 1.2 ppt h<sup>-1</sup> and 17 ppt h<sup>-1</sup> for aerosol surfaces in rural and urban environments, respectively, assuming that the aerosol is entirely composed of HAs.

It is important to note, however, that rural/urban continental aerosol is actually only composed of about 20-30% of its mass due to organic matter (OM). It must be indicated, however, that the humic acid material employed in these studies (the commercial standard readily available from Aldrich) may have a higher photoreactivity than environmental humic substances. In addition, HA generally has a higher photoreactivity than that of fulvic acid (FA), which has been suggested as a substitute of oxidized atmospheric organic matter (**H**Umic-Like **S**ubstances or **HULIS**, coined by Havers et al. (1998)). Accordingly, the measured uptake coefficients of Stemmler et al. (2007), which must be considered as

upper limits, are too low to explain the formation rates observed for forested or rural sites of 170 – 500 ppt h<sup>-1</sup> (Acker et al., 2006b; Kleffmann et al., 2005; and Zhou et al., 2002) or in urban environments of up to 2 ppb h<sup>-1</sup> (Acker et al., 2006a; Ren et al., 2003; and Ren et al., 2006). Thus, Stemmler et al. (2007) conclude that the processes leading to HONO formation on the Earth's surface will have a much larger impact on the HONO formation in the lowermost layer of the troposphere than humic material potentially occurring in airborne particles.

## 1.2 Objectives

Although nighttime levels of HONO may credibly be explained by the heterogeneous conversion of NO<sub>2</sub> on humid surfaces as previously considered (Vogel et al., 2003), recently observed high daytime HONO concentration indicate strong photochemical sources, the mechanisms of which (previously discussed herein), to this time, are still the subject of controversial deliberation.

Additional laboratory studies on the photochemical formation of HONO are compulsory to better interpret and predict daytime atmospheric HONO production. The contribution of principal sources to the concentration of HONO needs verification, i.e., Sarwar et al. (2008) recommended that heterogeneous reactions and surface photolysis reactions justified nearly 86% of the predicted HONO, while gas-phase reactions explained only 14% of the forecasted HONO using the Community Multiscale Air Quality modeling system. Up until recently, most climate models have not examined the effect of light on the heterogeneous reactivity of atmospheric trace gases on ground/aerosol sources. Accordingly, the contribution of atmospheric heterogeneous photochemistry must be included in these models. Of course, it is important to note that the performance of any model including heterogeneous reactions are limited by the data depicting the surface involved and that future improvements would require a more detailed representation of the ground, i.e., (S/V) ratio of the urban canopy and aerosol surfaces (constructed using size distribution and chemical composition data).

Currently, it is still under examination whether heterogeneous HONO production happens mainly on the surface of aerosols or on ground surfaces. Although some of the known gradient measurements indicate a ground surface source (Harrison and Kitto, 1994; Veitel et al., 2002), combined HONO and aerosol observations suggest that aerosol might be the principal HONO source (Notholt et al., 1992; Reisinger,

2000). In a recent field study, however, in which gradients of HONO, NO<sub>x</sub> and particles were simultaneously measured for the first time (Kleffmann et al., 2003); production on particles was shown to be of little importance. This is in agreement with recent kinetic investigations humid/aqueous surfaces (Finlayson-Pitts et al., 2003; Kim and Kang, 2010), and organic particles, including: soot (i.e., Kleffmann and Wiesen, 2005; Khalizov et al., 2010), phenolic (Sosedova et al., 2011) and humic (Stemmler et al., 2007), for which either deactivation or small uptake coefficients infer a minor significance of aerosols for the heterogeneous HONO production in the atmosphere.

Consequently, the main objective of this project is to add to the compendium of experimental studies on the photochemical formation of HONO on ground sources in aid of affording equally easier analysis and modelling of daytime atmospheric HONO production. In assessing the contribution of HONO to the HO<sub>x</sub> (OH + HO<sub>2</sub> + RO<sub>2</sub>) budget, such ambiguities are key, and therefore critical to the entire VOC/NO<sub>x</sub>/O<sub>3</sub> chemistry involved in photochemical pollution.

(I) This area of research, concerning the effect of ultraviolet-A radiation on the uptake kinetics of gas-phase NO<sub>2</sub> onto various phenolic-containing (constantly renewed) organic films (taken as proxies for SURFACES encountered in the troposphere) will be undertaken using a wetted-wall flow tube (WWFT) photoreactor (i.e., see Danckwerts, 1970 for details on the WWFT). This will be specifically designed and constructed for this project, to provide the following functions:

- (i) The WWFT dimensions and the corresponding gas and liquid flows needs to be designed and chosen suitably in order to obtain: non-turbulent flows, and thus, prevent rippling; a well-defined liquid surface that can be *rapidly* renewed; a suitable gas-liquid reaction time; and, finally, testing of, and likely, modification, to the recommending cleaning procedure described by Fickert et al. (1998) is necessary to achieve highly reproducible films for the experiments to follow. Dimensioning the WWFT correctly is of utmost importance, as the uniformly covered glass surface obtained by such a cleaning procedure, will provide direct verification of the correctness of the geometry of our in-house WWFT.
- (ii) Online simultaneous sampling of WWFT effluent products (HONO<sub>(g)</sub> and NO<sub>2</sub><sup>-</sup><sub>(aq)</sub>) during NO<sub>2</sub> uptake experiments on selected organic films via previously characterized analytical

techniques. It is, of course, an ideal goal to conduct online product analysis for both the gas- and liquid-phases.

- (iii) Finally, the photoreactor itself should be suitably designed so as to minimize heating, and thus, decrease evaporation of the tested liquid film.

(III) Considering that nitrophenols are understood to strongly absorb UV light in the 300-400 nm range (Harrison et al., 2005; Ishag and Moseley, 1977; and Alif et al., 1991), and may react directly through photochemical reactions, they are of significance for environmental photochemistry. Thus, a minor portion of the laboratory experiments will be centered on:

- (i) The kinetics of the uptake of  $\text{NO}_2$  (including photolysis,  $[\text{NO}_2] = 0$  ppbv) on films of *ortho*-nitrophenols at an environmentally relevant concentration for typical urban  $\text{NO}_2$  levels. Such experimentation is necessary using our WWFT photoreactor since there exists the possibility of photochemical conversion of  $\text{NO}_2$  into nitrous acid on organic surfaces containing phenoxy-type compounds (Ammann et al., 2005).
- (ii) Analysis of the reaction kinetics in (i) directly above will allow assessment of the importance as a daytime HONO source of the photochemical conversion of  $\text{NO}_2$  on aqueous-phase *ortho*-nitrophenols into nitrous acid. This is an important objective, as no such research is yet available in the literature.

(IV) In particular, the bulk of the laboratory experiments are focused on studying the kinetics of the photosensitized reduction of  $\text{NO}_2$  on environmentally realistic (renewable) films of humic acid. Since these materials are ubiquitously found in the environment, the photochemical  $\text{NO}_2$  conversion on such SURFACES needs to be investigated – it is a potentially important HONO source that could explain the recently observed high daytime nitrous acid concentrations in the boundary layer (BL). Furthermore, the photoreactivity of such surfaces may significantly impact our understanding of the chemical processes occurring in the lowermost troposphere. The impetus, of course, for this study, was the earlier work done by Stemmler et al. (2006) on solid films of humic acid, however, obtained for only a single acidic pH value at a single HA solution concentration.

- (i) With little exception, the studies of kinetics of reactions of NO<sub>2</sub> with the previously-described phenol-derived biomolecules were conducted at only a single pH (Alfassi et al., 1996; Gutzwiller et al., 2002; Miao et al., 2001; and Zhan et al., 1998), ignoring the fact that the reaction kinetics are strongly pH-dependent due to the acidic nature of phenols. It is clear that such reaction kinetics need to be studied over a larger range of pH, more suitable to the natural environment under consideration. Hence, to better understand the occurring photochemistry at hand, the study of NO<sub>2</sub> interaction with renewable films with different acidic properties would be very useful, and, as such, is a major goal of this experiment subset.
- (ii) Analogously, for the HA solution concentration, the reaction kinetics need to be examined over an environmentally relevant HA concentration range typical for the acidic, anaerobic conditions of wetland soils (Histosols).
- (iii) The reaction order with respect to NO<sub>2</sub> requires determination over a set of typical urban NO<sub>2</sub> levels to provide insight into the reaction mechanism.
- (iv) A comparison study of the reaction kinetics of NO<sub>2</sub> with acidic (renewable) HA films of two types, commercial and natural HA standards, is a necessary sub-goal in order to assess the photoreactivity of the recommended commercial standard.
- (v) An examination of the reaction kinetics of NO<sub>2</sub> with variation in the intensity of UV light (i.e., the number of lamps) is useful for hypothesizing a photochemical mechanism, and henceforth, is a worthwhile sub-goal.
- (vi) Finally, the atmospheric implications of the photosensitized reduction of NO<sub>2</sub> on the studied environmentally realistic (renewable) films of humic acid will be discussed based on the predicted best-fit reaction probabilities obtained from the data sets as a collective whole, thus, allowing an assessment of the overall importance of this reaction as a daytime HONO source.

## 2 EXPERIMENTAL METHODS

### 2.1 WETTED WALL FLOW TUBE TECHNIQUE (WWFT)

The rate of mass transfer of trace gases into an aqueous phase is limited by several processes including gas-phase diffusion, surface saturation and reaction in the liquid phase in addition to the interfacial resistance (represented by the mass accommodation coefficient,  $\alpha$ ). It is usually impossible to directly measure the mass accommodation coefficient experimentally — the surface reaction probability ( $\gamma_{\text{expt}}$ ), defined as the net fraction of gas-condensed phase collisions that leads to the reversible uptake of the gas due to chemical reaction (Finlayson-Pitts and Pitts, 2000), is usually measured instead. This overall uptake ( $\gamma_{\text{expt}}$ ) of gas molecules into the liquid, is considered as a sequence of resistances: transport to the interface ( $\gamma_{\text{diffusion}}$ ); mass accommodation ( $\alpha$ ); liquid-phase reaction ( $\gamma_{\text{rxn}}$ ); and/or solvation ( $\gamma_{\text{solvation}}$ ) of the trace gas

$$\left( \frac{1}{\gamma_{\text{expt}}} \right) = \left( \frac{1}{\gamma_{\text{diffusion}}} \right) + \left( \frac{1}{\alpha} \right) + \left( \frac{1}{\gamma_{\text{solvation}} + \gamma_{\text{rxn}}} \right) \quad (\text{E1})$$

where the mass accommodation coefficient,  $\alpha$ , represents the fraction of molecules that penetrate into the bulk of the liquid upon striking the surface (i.e., the probability for a molecule to cross the interface) (Davidovits et al., 1995).

For the simple case where the surface concentration of  $\text{NO}_2$  (aq.) is in equilibrium with the gas-phase concentration, the liquid-phase diffusion can be neglected under such experimental conditions (slow liquid-phase reactions), and the experimental uptake, defined as the net fraction of gas-condensed phase collisions that leads to the irreversible uptake of the gas due to chemical reaction (Finlayson-Pitts and Pitts, 2000), is simply

$$\gamma_{\text{expt}} = \left( \frac{2rk_1}{w} \right) \quad (\text{E2}),$$

where  $r$  is the radius of the tube,  $w$  is the average molecular velocity of the gas, and  $k_1$  is the experimentally determined (first-order) rate coefficient for the reaction (Fickert et al., 1998). If, however,

the liquid-phase reaction becomes fast enough compared to the diffusion of NO<sub>2</sub> in the solution, then the reaction will not take place across the entire liquid film, but rather in a **surface layer**, that is, the uptake becomes **diffusion-limited**. As a result, a concentration gradient builds up from the film's surface to the inner tube walls.

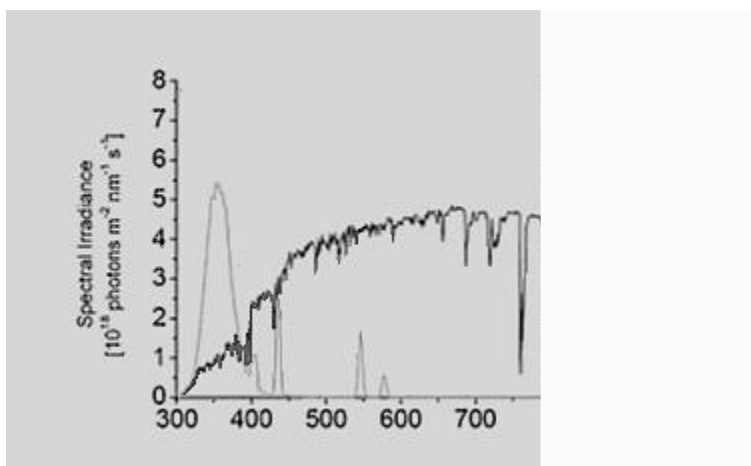
The well-established wetted wall flow tube (WWFT) technique (Danckwerts, 1970; Murphy et al., 1987; Hanson et al., 1994; Scheer et al., 1997; Fickert et al., 1998; Finlayson-Pitts and Pitts, 2000) is used for this work concerning the uptake of gaseous NO<sub>2</sub> onto a constantly renewed liquid surface. The wetted-wall flow tube technique has several advantages including: only a small volume of liquid is required; the liquid is renewed; the liquid surface area is known accurately (Danckwerts, 1970); the data analysis is straightforward (Howard, 1979; and Brown, 1978) and atmospherically relevant reactant gas concentrations can be used (Hanson and Lovejoy, 1996). The main limitation of the technique is that gas-phase diffusion complicates precise measurements of large reaction probabilities (Hanson and Ravishankara, 1991; and Hanson and Ravishankara, 1995).

The in-house WWFT photoreactor, based on the design by Fickert et al. (1998; original design by Danckwerts) consists of a vertically mounted Pyrex glass tube in an aluminum housing surrounded by six fluorescent lamps at a distance of approximately 3 cm in a cylindrical arrangement, four of which were typically used in the experiments. The lamps used are Phillips Cleo Compact tanning lamps (24 in. × 2.6 cm, Microlites Scientific), which emit light as a continuous band in the 300 – 420 nm, ( $\lambda_{\text{max}} = 354$  nm) spectral region (90% of the light power) and in the discrete Hg-lines at 436 nm, 546 nm, and 578 nm (9.8% of the light power). The spectral irradiance of the light source used in this study, along with a standard solar spectral irradiance for a solar zenith of 48° (under clear sky conditions) for comparison, are displayed in **Figure 16** (Stemmler et al., 2006). As evident from this comparison, the UV-A lamp utilized in this study shares significant spectral overlap with the standard solar spectral irradiance typical of a cloudless midday atmosphere.

As the Eppley radiometer was unavailable for laboratory use during the course of this project, the irradiance at the reactor surface under typical irradiation conditions (4 lamps) was estimated at approximately 85.7 W m<sup>-2</sup>, based on scaling the measured value of 150 W m<sup>-2</sup> (for 7 lamps) in a similar arrangement (50 cm × 0.8 cm i.d. Duran glass tube in an air-cooled aluminum housing holding seven fluorescence lamps in a circular arrangement, about 3 cm away from the thermostated flow tube) used by George et al. (2005) and Stemmler et al. (2006).



Although the setup was not thermostated, a small fan (Comair Rotron, 12 V) was installed in the aluminum housing (midway between the two sets of lamps in use) in order to avoid excessive evaporation of the liquid film due to the temperature increase (1.5°C) from the lamps. Controlling humidity in the WWFT is necessary to avoid any potential evaporation from the falling liquid film that could result in cooling.



**Figure 16.** Light gray line: Spectral irradiance of the light source used in this study, 300-420 nm, (90% of the total light power),  $\lambda_{\text{max}} = 354$  nm. For comparison a standard solar spectral irradiance for solar zenith of 48° and clear sky is shown (dark gray line) (American Society for Testing and Materials, ASTM). Modified from Stemmler et al. (2006).

Prior to the  $\text{NO}_2$  uptake experiments, the WWFT photoreactor required thorough cleaning, since one of the major difficulties in studying gas/liquid interactions is to obtain a well-defined liquid surface that can be rapidly renewed. The quality (i.e., uniformity) of the liquid film was visually monitored in the WWFT using a light-emitting diode by wrapping a piece of white card around the entire length of the WWFT reaction zone surface and examining this for discontinuities where the film is not covering the glass surface evenly. Initial efforts involving thorough cleaning of the WWFT with 37% hydrochloric acid ( $\sim 12$  M) were unsuccessful in obtaining a uniformly covered glass surface. Subsequently, the procedure described by Fickert et al. (1998) consisting of cleaning of the tube with a mixture of deionized water, 2-propanol, and potassium hydroxide (5-M), followed by thorough rinsing with deionized water was employed. The exact details of the cleaning procedure consisted of two repetitions of the following list of volumes of cleaning solvents in order: 10-mL water; 15-mL 2-propanol; 10-mL 5-M NaOH; 15-mL isopropyl alcohol; 15-mL water; 10-mL 5-M NaOH; 15-mL isopropyl alcohol; 30-mL water. The uniformly covered glass surface obtained by this cleaning procedure, verifies the correctness of the geometry of the WWFT.

Following immediate thorough drying of the WWFT using zero-air at typically  $3.8 \text{ L min}^{-1}$  (for greater than 30 min.), the reactant  $\text{NO}_2$  (g), flowing typically between  $8.0$  to  $50 \text{ mL min}^{-1}$  ( $50 \text{ mL min}^{-1}$  MFC), from a cylinder with  $5.0 \text{ ppm}$  in  $\text{N}_2$  certified accurate to  $2\%$  (Air Liquide), is diluted in zero air at  $3.8 \text{ L min}^{-1}$  (using a  $30 \text{ L min}^{-1}$  MFC) to atmospherically relevant mixing ratios in the concentrations range of  $10$  to  $72 \text{ ppb}$ , (derived based on a dilution calculation using the respective MFCs) and is introduced into the WWFT via a moveable  $45\text{-cm}$  long glass inlet ( $0.25 \text{ in. o.d.}$ ) at atmospheric pressure. Note that all mass flow controllers (MFC) were calibrated using the Gilian Gilibrator-2 Air Flow Calibrators ranging from  $1 \text{ mL min}^{-1}$  to  $30 \text{ L min}^{-1}$  (Sensidyne). Aqueous organic solutions of environmental relevance are transported via a peristaltic pump (Ismatec, 4-channel) into a  $10\text{-cm}$  long reservoir at the top of the WWFT ( $1.4 \text{ cm i.d.}$ ) at  $0.24 (\pm 8.1 \times 10^{-4}) \text{ mL min}^{-1}$ . This entrance section is separated from the  $56\text{-cm}$  long reaction zone ( $1.2 \text{ cm i.d.}$ ,  $S/V = 3.4 \text{ cm}^{-1}$ ) by a ground glass piece which is partially plugged by a glass cone with a  $1\text{-mm}$  vertical groove on either side that allows for a little reservoir of solution to be formed just above the reaction zone. The liquid then flows in a film, under the influence of gravity, covering the walls of the reaction zone and reacts with the diluted  $\text{NO}_2$  for a typical reaction time,  $t_{\text{reac}}$ , of  $1 \text{ s}$  for the experimental conditions (derivation of this quantity is given on p. 37).

When the film has attained its terminal velocity-distribution, the velocity  $\mathbf{u}$  at any depth  $\mathbf{x}$  beneath the surface is

$$u = \frac{3}{2} \left( \frac{u}{\pi d} \right)^{2/3} \left( \frac{g\rho}{3\mu} \right)^{1/3} \left( 1 - x^2 \left[ \frac{\pi g d \rho}{3\mu u} \right]^{2/3} \right) \quad (\text{E3}),$$

where:  $\mathbf{u}$  is the volumetric liquid flow rate;  $\mathbf{d}$  is the diameter of the tube on which the film flows (i.e., the diameter of the reaction zone);  $\mathbf{\rho}$  is the density, and  $\mathbf{\mu}$  is the dynamic viscosity of the liquid of interest; and  $\mathbf{g}$  is the gravitational constant (Danckwerts, 1970).

The film thickness,  $\mathbf{f}$  is derived upon the fact that the velocity  $u$  is zero at the wall, where  $x = f$  (Danckwerts, 1970). Thus, from (E3),  $f$  is simply:

$$f = \left( \frac{3\mu u}{\pi g d \rho} \right)^{1/3} \quad (\text{E4}).$$

Now (E3) can be expressed as

$$\mathbf{u} = \mathbf{u}_s \left( 1 - \left[ \frac{x^2}{f^2} \right] \right) \quad (\text{E5}),$$

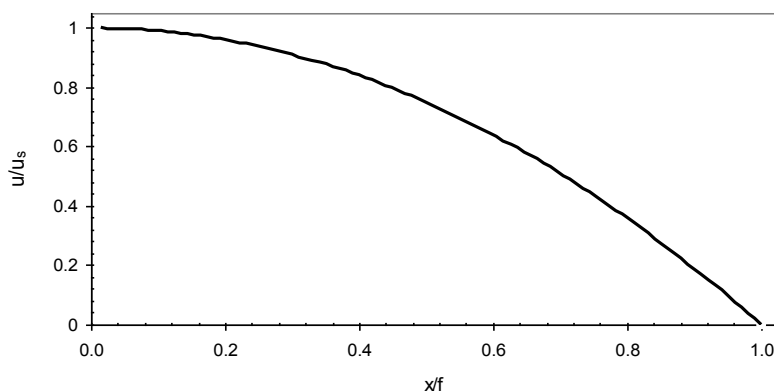
where the velocity at the surface ( $x = 0$ ),  $\mathbf{u}_s$ , is:

$$\mathbf{u}_s = \frac{3}{2} \left( \frac{\nu}{\pi d} \right)^{2/3} \left( \frac{g\rho}{3\mu} \right)^{1/3} = \frac{3}{2} \frac{\nu}{\pi d f} \quad (\text{E6})$$

(Danckwerts, 1970). Thus, the velocity at point  $x$  as a fraction of the surface velocity is:

$$\left( \frac{\mathbf{u}}{\mathbf{u}_s} \right) = \left( 1 - \frac{x^2}{f^2} \right) \quad (\text{E7}).$$

The parabolic velocity profile for a liquid flowing in a film under the influence of gravity, as predicted by laminar theory is given in **Figure 17**. Since the velocity of the newly-formed surface at the upper end of the column is zero, and the terminal velocity is achieved asymptotically further down the reaction zone, there is a readjustment of velocities between the exit of the annular gap and the film in the reaction zone (Danckwerts, 1970). Thus, an ‘entrance effect’ error is thus introduced by assuming that the surface has the terminal velocity at all points (Danckwerts, 1970). Wilkes and Nedderman (1962) have analyzed this effect in detail and the error has shown to be negligible (less than 1%; Roberts and Danckwerts, 1962) if the WWFT is suitably designed – that is, the width of the annular gap (0.15 cm in the tested design) must be greater than that of the film thickness ( $f = 3.32 \times 10^{-2}$  cm for a typical solution of phenol; see **Table 2**), i.e. the mean velocity in the gap will be greater than that in the film (Danckwerts, 1970).



**Figure 17.** Parabolic velocity profile for liquid flowing in a film under the influence of gravity, as predicted by laminar theory.

The time of exposure of any element of (film) surface to the gas,  $t_{\text{renewal}}$  is computed from  $u_s$  as:

$$t_{\text{renewal}} = \left( \frac{h}{u_s} \right) = \left( \frac{2h}{3} \right) \left( \frac{3\mu}{g\rho} \right)^{1/3} \left( \frac{\pi d}{v} \right)^{2/3} \quad (\text{E8})$$

(Danckwerts, 1970), where  $h$  is the height of the reaction column. For the uptake experiments reported herein, the computed renewal time,  $t_{\text{renewal}}$ , dictates the time period,  $t_{\text{delay}}$ , between subsequent measurements of HONO produced and/or  $\text{NO}_2$  remaining in the reacted effluent gas using the appropriate detector.

The gas-liquid reaction (contact) time,  $t_{\text{rxn}}$  (or  $t_{\text{reac}}$ ) is simply:

$$t_{\text{rxn}} = \left( \frac{V_{\text{rxn.zone}}}{F_g} \right) = \left( \frac{V_g}{F_g} \right) = \left( \frac{\pi r^2 h}{F_g} \right) \quad (\text{E9}),$$

where  $F_g$  is the volumetric gas flow rate through the volume of gas ( $V_g$ ) in the reaction column,  $V_{\text{rxn.zone}}$ .

Parameter	Computed value	Units
$f$	$3.32 \times 10^{-2}$	cm
$u_s$	0.48	$\text{cm s}^{-1}$
$t_{\text{renewal}} (= t_{\text{delay}})$	1.94 (~ 2)	min
$t_{\text{rxn}}$	0.97 (~ 1)	s

**Table 2.** Summary of computed values of the film flow dynamics parameters  $f$ ,  $u_s$ ,  $t_{\text{renewal}} (= t_{\text{delay}})$ , and  $t_{\text{rxn}}$  for a solution of phenol at 293 K for the experimental setup, with:  $\rho = 1.08 \text{ g cm}^{-3}$ ;  $\mu = 1.22 \times 10^{-2} \text{ g cm}^{-1} \text{ s}^{-1}$ ;  $v = 4.0 \times 10^{-3} \text{ cm}^3 \text{ s}^{-1}$  ( $= 0.24 \text{ mL min}^{-1}$ );  $F_g = 64.7 \text{ cm}^3 \text{ s}^{-1}$ ;  $V_g = 63.3 \text{ cm}^3$ ;  $h = 56 \text{ cm}$  (injector position = 0);  $d = 1.2 \text{ cm}$ ; and  $g = 981 \text{ cm s}^{-2}$ .

The expressions for film flow dynamics are only applicable if the aqueous and gas-phase flows are laminar, that is, non-turbulent. We must consider each phase separately.

When the Reynolds number,  $N_{\text{Re}}$ , defined as

$$N_{\text{Re}} = \left( \frac{v\rho}{\pi d\mu} \right) \quad (\text{E10})$$

exceeds a value between 250 – 400 for the aqueous film ( $N_{RE, film}$ ), turbulence (rippling) sets in, and the flow will no longer be laminar (Brauer, 1958; Hobler, 1966; and Wilkes and Nedderman, 1962). When the film flow is non-laminar, ripples will appear generally on the film on the lower part of the column, making it impossible to interpret measured kinetic rates (Lynn et al., 1955; Stirba and Hurt, 1955; and Emmert and Pigford, 1954). When ripples occur, they can be eliminated via the addition of surface-active agents, if the chemical situation permits, such as Lubrol W (I.C.I.), a polyhydric alcohol (Roberts and Danckwerts, 1962).

For the gas-phase, the assumption of laminar flow at a volumetric flow rate  $Q$  in the tube of area,  $A (= \pi r^2)$ , requires that two conditions be met. First, the Reynolds number,  $N_{RE, gas}$  defined as

$$N_{RE, gas} = \left( \frac{r \rho \nu}{\mu} \right), \nu = \left( \frac{Q}{A} \right) \quad (E11)$$

must be smaller than  $\sim 2300$  (Holman, 2002), where:  $\nu$  is the linear velocity of the gas; and  $(\rho/\mu)$  is the inverse of the gas' kinematic viscosity,  $\nu$ . Finally,  $(r/\lambda) \geq \sim 2100$ , where  $r$  is the tube radius, and  $\lambda$  the molecular mean free path. Expressed as a lower limit on the reaction zone pressure  $p$ , the second condition restated assumes that  $(rp) \geq \sim 0.07$  cm kPa (or 0.5 cm Torr) (Bird et al., 1960; Murphy and Fahey, 1987). As seen from the computed values of the Reynolds numbers for the film and gas-phases (as well as  $(rp)$ ) in **Table 3**, the flow in both phases is indeed, laminar, as desired.

Parameter	Computed value	Laminar transport?
$N_{RE, film}$	$\sim 0.1 \ll (250 - 400)$	Yes
(i) $N_{RE, gas}$ (ii) $(rp)_{(cm\ torr)}$	$454 < 2300$ $456 \geq 0.5_{(cm\ torr)}$	Yes

**Table 3.** Summary of computed values of Reynolds number,  $N_{RE}$  for film and gas-phases, respectively, as well as  $(rp)$  (for the gas-phase) used for determination of laminar or turbulent flow. Computed values are compared with the respective turbulent regime limits. Experimental parameters used for computations:  $Q = 64.67 \text{ cm}^3 \text{ s}^{-1}$  ( $3.88 \text{ L min}^{-1}$ ) in the tube of area,  $A = \pi r^2 = 1.13 \text{ cm}^2$ ;  $u = 57.18 \text{ cm s}^{-1}$ ;  $\nu = 15.11 \times 10^{-2} \text{ cm}^2 \text{ s}^{-1}$  for dry air at 293 K and atmospheric pressure (The Engineering Toolbox);  $r = 0.6 \text{ cm}$ ; and  $p = 1 \text{ atm}$  (760 torr).

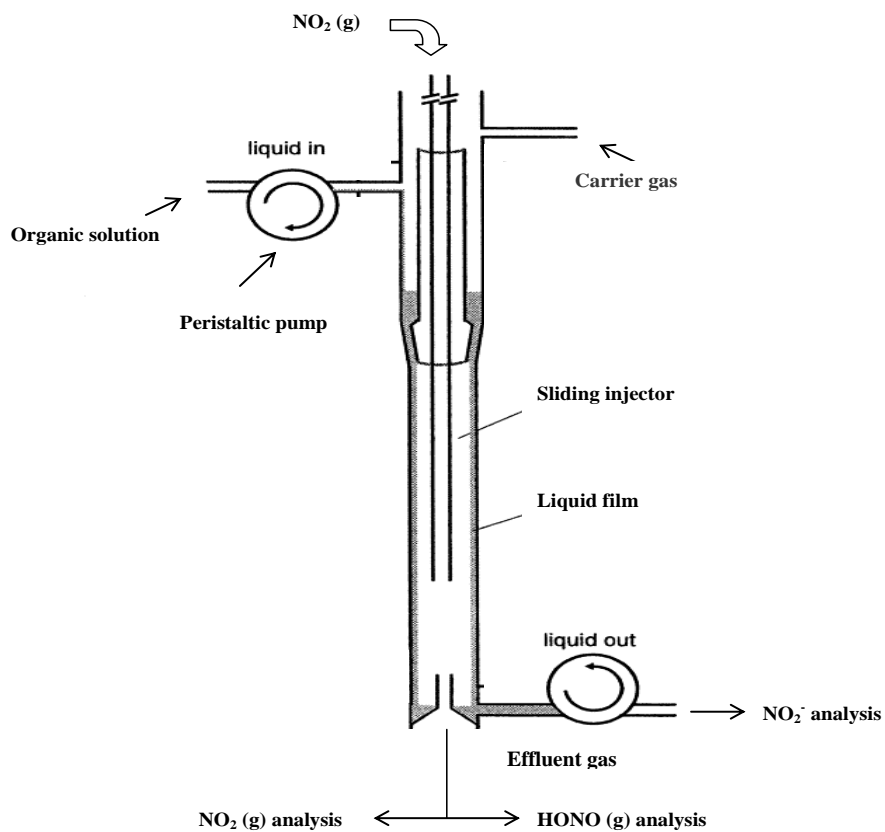
The outlet of the WWFT is designed so that the liquid flows between the glass tube and the Teflon glass outlet tube, and is pumped out of the flow tube to prevent contamination of the gas outlet with the liquid (Behnke et al., 1997).

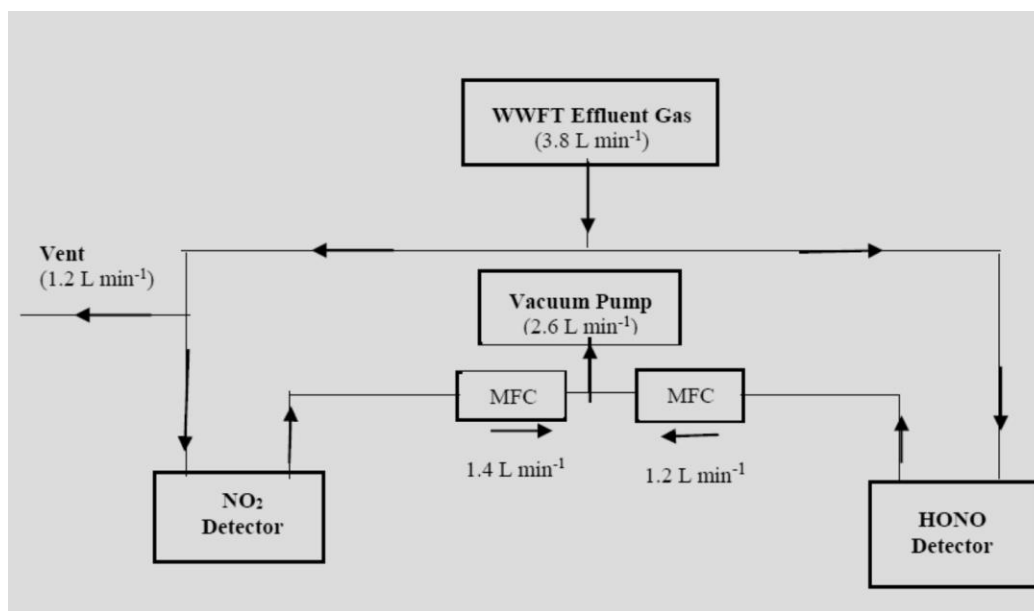
Following interaction with the liquid film, the reacted (effluent) gas (flowing at  $3.8 \text{ L min}^{-1}$ ), saturated with water vapour from the aqueous organic solution of interest (at near 100% relative humidity), can be simultaneously sampled online for gas-phase HONO and  $\text{NO}_2$  using the appropriate detector (derivatization or chemiluminescence). See **Figure 18** for schematic of the WWFT experimental setup as described. A vacuum pump (KNF Neuberger) draws off a total flow rate of  $2.6 \text{ L min}^{-1}$  of the WWFT effluent gas, with the excess flow rate of  $1.2 \text{ L min}^{-1}$  being vented off to the laboratory air. The HONO (derivatization) detector samples  $1.2 \text{ L min}^{-1}$  of the  $2.6 \text{ L min}^{-1}$  effluent flow rate (using a  $5 \text{ L min}^{-1}$  MFC), with the remainder of the flow rate ( $1.4 \text{ L min}^{-1}$ ) sampled by the  $\text{NO}_2$  (chemiluminescence) detector (via a  $2 \text{ L min}^{-1}$  MFC), as illustrated in **Figure 19**.

After approximately 20 minutes of gas-film equilibration time, the liquid film has been completely renewed about *ten* times, and the first measurement of gas-phase HONO and/or  $\text{NO}_2$  in the effluent gas is made. Depending upon chromatographic interferences from organic compound of interest, the effluent liquid at the exit of the tube is removed at  $0.24 \pm 8.1 \times 10^{-4} \text{ mL min}^{-1}$  and analyzed online via the HONO detector by bypassing the scrubbing coil sampler utilized for gas-phase sampling (see **Section 2.2** for details of this detector). Subsequent HONO and/or  $\text{NO}_2$  measurements are made with a time delay,  $t_{\text{delay}}$ , of approximately 2 min, corresponding to the computed film renewal time.

The percentage evaporation of the liquid film in the WWFT photoreactor due to the heating from the 4 lamps was quantified by measuring the flow rate of a deionized water film (pH 6, unadjusted pH) at the effluent exit with and without zero-air ( $3.88 \text{ L min}^{-1}$ ) flowing through the tube (injector position =  $0 = t_{\text{max}}$ ). Under these conditions, evaporation of the liquid film is found to be ( $6.85 \pm 0.0029 \%$ ,  $n = 3$ ) for the experimental setup. The precision obtained was excellent (3.15%) and thus the value obtained can be used to correct the  $\text{NO}_2^-$  concentrations measured at the effluent exit of the WWFT during uptake

**Figure 18.** Detailed schematic of the experimental setup for online simultaneous sampling of HONO and  $\text{NO}_2$  (in the effluent gas) during  $\text{NO}_2$  uptake experiments on selected organic films via the respective detectors (HONO and  $\text{NO}_2$ ). [Modified from: Fickert et al. (1998)].





**Figure 19.** Detailed schematic of the experimental setup permitting online simultaneous sampling of HONO and NO<sub>2</sub> in the effluent gas of the WWFT during NO<sub>2</sub> uptake experiments on selected organic films of interest. Direction of gas flows are indicated by the arrows. Gas-sampling flow rates are also given in units of L min<sup>-1</sup>.

experiments for organic films using deionized water as the diluent. This included the selected compounds: 4-BBA, and the commercial humic acid (HA), the main compound of interest in this thesis.

The commercial humic acid (technical grade) readily available from Aldrich was used without purification (due to time constraints) for all experiments to follow. Very recent structural (elemental and/or <sup>13</sup>C-NMR) characterization of Aldrich HA, both in the unpurified and purified form, (see Table 4) compares well with that of representative environmental HA samples for locations differing in geology and vegetation (Albers et al., 2008 and Albers and Hansen, 2010), thus, justifying the use of the commercial HA as an HA standard. Descriptions of environmental HA soil samples used for comparison include: *Forest*, sampled from the lower part of a 10-cm-thick coniferous forest organic O-horizon; *Clay*, A horizon of a clay rich agricultural soil; and *Sand*, A horizon of a very sandy agricultural soil. The differences in the compositional



data (in Table 4) suggest that the purification procedure may have physically altered the composition of the Aldrich HA, a point in favour of opting out of a purification procedure.

HS	Origin (horizon)	<sup>a</sup> C	<sup>a</sup> H	<sup>a</sup> N	<sup>a</sup> S	<sup>a</sup> O	<sup>b</sup> Structural groups						
							<sup>b</sup> C=O	<sup>b</sup> COOH	<sup>b</sup> Amide or ester	<sup>b</sup> Arom.	<sup>b</sup> Carbohy. acid	<sup>b</sup> Amino αC	<sup>b</sup> Aliph.
ForO-HA	Forest (O)	53.9	4.8	2.2	<1/2	39.0	1	13	5	53	11	4	12
Aldunpur-HA	Lignite	53.3	4.3	0.7	3.7	37.9	–	–	–	–	–	–	–
Aldpur-HA	Lignite	54.7	4.3	0.7	3.5	36.8	1	13	<1	65	<1/2	<1/2	19
ClayA-HA	Clayey field (A)	54.4	4.6	4.9	<1/2	36.1	<1/2	13	<1	54	8	6	18
SandA-HA	Sandy field (A)	54.8	4.5	3.0	<1/2	37.7	1.5	17	<1	52	9	3	18

**Table 4.** Main structural characteristics of humic substances as determined by <sup>a</sup>CHNS-analysis in mass (%) for ash-content and <sup>b</sup>liquid-state <sup>13</sup>C-NMR. The structural groups are presented as the carbon present in the groups in percentage of total carbon. ArO and ArH represent O-substituted and non-substituted aromatic carbons, respectively. From: Albers et al. (2008). Note that the HA samples were extracted largely according to the International Humic Substances Society standards procedure, with minor modifications (see Albers et al., 2008).

Note that unpurified Aldrich HA (**Aldunpur-HA**) was not suitable for the NMR analysis performed by Albers et al. (2008) due to a large quantity of iron and other inorganic impurities. Most of the major inorganic impurities (in units of mg g<sup>-1</sup>) in the unpurified Aldrich HA: Al, Ca, Fe, Mg, Na, and Si, respectively (see Table 5), can be effectively removed with 0.1 M HCl/HF, followed by dialysis (Albers et al., 2008). The high sodium content remaining (~ 2.5 mg g<sup>-1</sup>) in the purified commercial HA as observed by (Pompe et al., 2000) (see Table 5), is likely due to incomplete elimination of Na by dialysis. Although the sodium content in the unpurified commercial form seems unacceptably high, that is [Na<sup>+</sup>]<sub>AldunpurHA</sub> ~ 75 mg g<sup>-1</sup> or

Impurity (mg g <sup>-1</sup> )	AldunpurHA <sup>a</sup>	AldpurHA <sup>b</sup>
Al	2.95	0.078 (±0.009)
Ca	9.93	0.126 (±0.095)
Fe	12.21	3.651 (±0.224)
Mg	0.70	0.010 (±0.005)
Na	75.12	2.465 (±0.418)
Si	3.33	0.372 (±0.187)

**Table 5.** Inorganic impurities in units of mg g<sup>-1</sup> in the two forms of Aldrich humic acid: unpurified (AldunpurHA) and purified (AldpurHA). <sup>a</sup>From: Rajec et al. (1999). No uncertainty given. <sup>b</sup>From: Pompe et al. (2000). The Aldrich HA was washed several times with 0.1 M HCl, followed by dialysis.

7.5% mass, it is negligible when compared with the known proton or cation exchange capacity (CEC) of the (purified) commercial humic acid (see Table 6) for the (dissociated) carboxyl group (with pK<sub>a</sub> values up

to 7; Hayes and Swift, 2001) in the pH range of interest ( $\sim 1.5$  to  $4.3$ ), i.e.,  $\frac{CEC_{\text{carboxyl}}}{[Na^+]_{\text{AldunpurHA}}} = \frac{4.8 \times 10^{-3} \text{ mg g}^{-1}}{75 \text{ mg g}^{-1}}$  or  $6.4 \times 10^{-3} \%$ .

	Proton exchange capacity (meq/g)		
	Total (Ba(OH) <sub>2</sub> exchange)	Carboxyl groups (Ca-acetate exchange)	Phenol groups (Difference between total and carboxyl)
Aldrich-HA	7.06 ± 0.67	4.80 ± 0.21	2.26 ± 0.72

**Table 6.** Proton exchange capacities of total, carboxyl and phenol groups as well as by direct titration in units of meq g<sup>-1</sup>. Purification of Aldrich HA with 0.1 M HCl, followed by dialysis. The total proton exchange capacity was measured by the Baryta adsorption methods (Stevenson, 1982), which allows the HA to react with excess Ba(OH)<sub>2</sub>, followed by titration of unused base with standard acid. The Ca-acetate exchange method, where Ca exchanges in acetate medium (Stevenson, 1982), was used for the determination of the carboxyl group capacity. Finally, the phenol group (or acidic OH) capacity was obtained from the difference between the total and the carboxyl group capacities. From: Kim et al., (1990).

The lower extent of concentration reduction of iron ( $\sim 30\%$ ), which is present as a higher oxidation state in solution ( $Z = 3+$ ), infers its strong complexation affinity towards HA (David et al., 2010). Iron may also act as a possibly photochemically interfering impurity, as follows according to the photo-Fenton reaction mechanism (M8), (R24) through (R25) (Zepp et al. 1992):



As a result of spiking their HA sample solutions ( $0.5$  and  $1.0 \text{ g L}^{-1}$ , respectively) used to generate their solid films by additional 1.2% and 3.6% mass portions of iron(III), Stemmler et al. (2006) found that it did not significantly alter the reactivity of the HA coatings. Although the gas-liquid interaction time is twice as long as that used by Stemmler et al. (2006), only 57% of their total lamp power is used, so that iron is likely not a photochemically interfering impurity for the NO<sub>2</sub> uptake experiments to follow.

Due to the hygroscopic properties of humic acids (Badger et al., 2006), the commercial HA sample, as well as the isolated samples: **Elliot Soil** HA, **Leonardite** HA, and **Pahokee Peat** HA, for comparison, available from the International Humic Substances Society (IHSS), were stored in a desiccator under vacuum. Official series descriptions and geographic extent maps as provided by the USDA-NRCS Soil Survey

Division (Soil Survey Staff) (when available), along with IHSS extraction procedures for the preparation of the HA sample from the bulk soil sample, are provided in **Appendix A** for the reader's reference. The soil source for the IHSS Leonardite HA was obtained from the Gascoyne Mine in Bowman County, North Dakota, U.S.A. that produces Leonardite from the natural oxidation of exposed lignite, a low-grade coal ([www.humicsubstances.org/sources.html](http://www.humicsubstances.org/sources.html)). Chemical properties, including elemental and acidic functional group compositions, along with  $^{13}\text{C}$ -NMR estimates of carbon distribution for the selected IHSS HA standards are given in **Section 5.5**.

Effective colloidal dispersion/dissolution of the HA samples, was achieved using 2 mM sodium hydroxide, as per the recommendations of Ritchie and Perdue (2003). The concentrations of commercial HA solutions,  $[\text{HA}]_{\text{solution}}$  (0.50, 0.67, 0.76, 0.84, and 1.00 g L<sup>-1</sup>, respectively) used to generate the corresponding  $[\text{HA}]_{\text{film}}$  of (3.46, 4.63, 5.25, 5.80, and 6.91  $\mu\text{g cm}^{-2}$ ) in the HA concentration-dependent NO<sub>2</sub> uptake kinetics study were freshly prepared by dissolving a set quantity (0.50, 0.67, 0.76, 0.84, and 1.00 g, respectively) of the isolated commercial HA sample (Aldrich) in approximately 990 mL of 2 mM NaOH, followed by pH adjustment to 3 with concentrated HCl to 1L final volume. The selected HA standard samples are readily available from the IHSS, however, in small quantities (100 mg vials). Accordingly, for comparison with NO<sub>2</sub> reactivity data on the commercial HA film, the studied  $[\text{HA}]_{\text{solution}}$  of 0.76 g L<sup>-1</sup> used to generate the corresponding  $[\text{HA}]_{\text{film}}$  of 5.25  $\mu\text{g cm}^{-2}$  was newly made by dissolving 0.038 g of the respective IHSS HA standard samples in approximately 49 mL of 2 mM NaOH, followed by adjustment of acidity to 10<sup>-3</sup> M with concentrated HCl to 50 mL total volume. Finally, for the (film) pH-dependent (pH range: 1.5 to 4.3) NO<sub>2</sub> uptake kinetics study, the examined concentration of unpurified Aldrich  $[\text{HA}]_{\text{film}}$  of 5.80  $\mu\text{g cm}^{-2}$  (corresponding to  $[\text{HA}]_{\text{solution}}$  of 0.84 g L<sup>-1</sup>) was freshly prepared via dissolution of 0.84 g of the HA sample in approximately 990 mL of 2 mM NaOH (solution pH ~ 10.5), followed by pH adjustment to the individual studied acidities, respectively (with concentrated HCl to 1 L total volume) using a pH meter accurate to  $\pm 0.01$  pH units (Eutech Instruments).

Due to the poor water solubility of *ortho*-nitrophenols (i.e., 2-NP: 1.2 g/L water solubility at 293 K; Boehncke et al., and references therein), and the minimal expected chromatographic interference from methanol, the latter solvent of choice, **methanol** was chosen as the optimum diluent for solutions used to generate the *ortho*-nitrophenol films. Since significant evaporative cooling of the liquid film is expected using methanol (in lieu of deionized water) as solvent, due to its markedly higher vapour pressure ( $P_{\text{vap, methanol}} \approx 125$  mm Hg compared to  $P_{\text{vap, water}} = 23.8$  mm Hg) (Lange's Handbook of Chemistry), the

evaporation of the liquid film in the WWFT needed quantification, and, as such, was achieved via measurement of the liquid flow rate at the exit of the WWFT with and without zero-air ( $3.88 \text{ L min}^{-1}$ ) flowing through the tube (injector position =  $0 = t_{\text{max}}$ ) for the following tested solvent compositions: (i) 100% MeOH, (ii) 5% MeOH, and (iii) 1% MeOH, with the balance of the compositions in (ii) and (iii) being deionized water.

	Percentage (%) MeOH of total solvent volume				
	(i) 100	(ii) 5		(iii) 1	
%Evaporation (avg)	78.8	11.9	17.9	22.2	33.1
$\pm 1\sigma$ (%)	0.001	0.004	0.003	0.0007	0.001
No. of replicates, n	3	3	3	3	3

**Table 7.** Measured evaporative cooling (%) for the following tested solvent compositions given as percentage (%) MeOH of total solvent volume: (i) 100% MeOH, (ii) 5 % MeOH, and (iii) 1% MeOH, using the WWFT photoreactor and a  $t_{\text{reac}}$  of 1 s. Experimental results shaded in gray performed with no light source, while remaining data obtained from experiments with 4 lamps on. Propagated uncertainty given is  $\pm 1\sigma$ .

Using pure methanol as the solvent, evaporation of the film volume is severe (nearly 80%, see **Table 7 (i)**), and thus, is discarded as a plausible solvent composition for the *ortho*-nitrophenol uptake experiments. The 5% MeOH composition (in purified water) (refer to **Table 7 (ii)**) yielded the smallest film volume loss due to evaporation of approximately 12% (with excellent precisions), possibly due to an optimal viscosity, with an additional loss of approximately 6% when the light source was turned on due to heating ( $1.5^\circ\text{C}$ ) from the 4 lamps, and thus was chosen as the optimal solvent composition for  $\text{NO}_2$  photochemistry experiments on the selected *ortho*-nitrophenol films to follow (see **Section 4.3**).

It follows that it is quite simple to accurately estimate the temperature decrease of the film due to the (quantified) film evaporation. Using the Clausius-Clapeyron equation, it is possible to solve for the change in the saturation vapour pressure,  $e_s$ , as a function of temperature,

$$\frac{de_s}{dT} = \frac{L_v}{T(V_v - V_w)} \quad (\text{E11})$$

where  $L_v$  is the latent heat of vaporization ( $2.5 \times 10^6 \text{ J kg}^{-1}$ ), and  $V_v$  and  $V_w$  are the volumes of water vapour and liquid water, respectively. Realizing that the volume of water vapour, is much greater than that for liquid water, (E11) can be further simplified by substituting the equation of state for water vapour, yielding

$$\frac{de_s}{e_s} = \frac{L_v dT}{R_v T(T)} \quad (\text{E12}),$$

where  $R_v$  is the gas constant for water vapour ( $461 \text{ J kg}^{-1} \text{ K}^{-1}$ ).

From the definition of saturation specific humidity,  $q_s$ , the saturation vapour pressure,  $e_s$  can be substituted:

$$\frac{dq_s}{q_s} = \frac{L_v dT}{R_v T(T)} \quad (\text{E13}).$$

Finally, integration results in an equation which relates the saturation specific humidity,  $q_s$ , to temperature:

$$q_s = q_s^0 e^{\left(\frac{L_v}{R_v}\right)\left(\frac{1}{T_0} - \frac{1}{T}\right)} \quad (\text{E14}),$$

where:  $T_0$  is the reference temperature of the (fluid) film, for typical conditions, 295 K;  $T$  is the temperature of the film resulting from condensation in units of K;  $q_s^0$  is the reference saturation specific humidity ( $\text{kg kg}^{-1}$ );  $q_s$  is the saturation specific humidity after cooling ( $\text{kg kg}^{-1}$ ); and the parameters  $L_v$  and  $R_v$  have been previously defined. Since the ratio of the reference saturation specific humidity to the saturation specific humidity is defined as the relative humidity, (E14) also simplifies to the following expression:

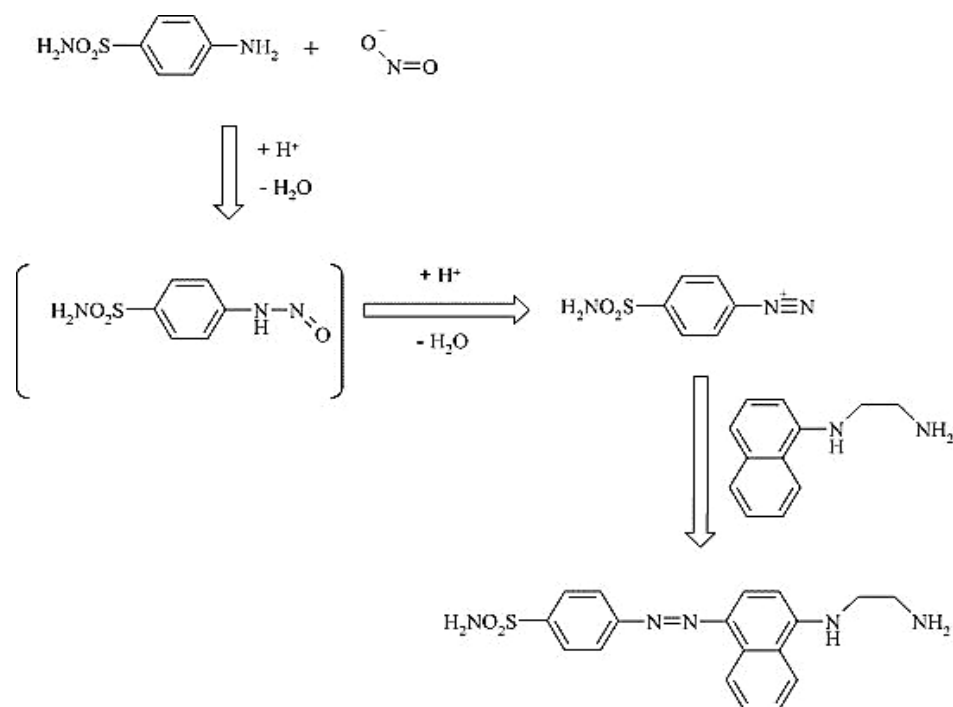
$$\text{RH} = e^{\left(\frac{L_v}{R_v}\right)\left(\frac{1}{T_0} - \frac{1}{T}\right)} \quad (\text{E15})$$

Using the experimentally determined evaporation percentage of ( $6.85 \pm 0.0029$ )% for the water (diluent) film, the average relative humidity of the effluent film is simply  $(100 - 6.85)\%$  or 93.1%. Thus, substitution of the experimental values in (E15) yields a temperature decrease due to condensation of approximately  $1.3^\circ\text{C}$ . Therefore, the estimate indicates that the temperature increase of the WWFT reaction zone due to the 4 lamps ( $1.5^\circ\text{C}$ ) is nearly entirely compensated by the cooling due to condensation. The unaccounted temperature difference of about  $0.2^\circ\text{C}$  is compensated by the variability in the room temperature of the laboratory (often,  $1 - 2^\circ\text{C}$  above the norm). Thus, it can be stated with confidence that the film evaporation does not affect either the gas or film profiles during uptake experiments when deionized water is the organic film diluent. Switching the concern to the  $\text{NO}_2$  reaction kinetics on *ortho*-nitrophenols in the WWFT photoreactor, the mean RH of the effluent film is now

markedly decreased to approximately 82.1%, based on the empirically determined evaporation percentage of  $(17.9 \pm 0.003)^\circ\text{C}$  for the 5% MeOH (diluent) film. Again, substitution of the experimental parameters in (E15) results in a temperature drop due to condensation of nearly  $3.1^\circ\text{C}$ , not entirely offset by heating from the lamps in combination with variability in the laboratory room temperature. Hence, when 5% MeOH is the organic film diluent, it is expected that film evaporation has a minor effect on either the gas or film profiles during kinetic experiments.

## 2.2 HONO AND $\text{NO}_2$ DETECTORS

The highly sensitive technique for the measurement of gas-phase nitrous acid developed by Huang et al. (2002) is utilized to quantify the HONO produced during  $\text{NO}_2$  uptake experiments. The technique is



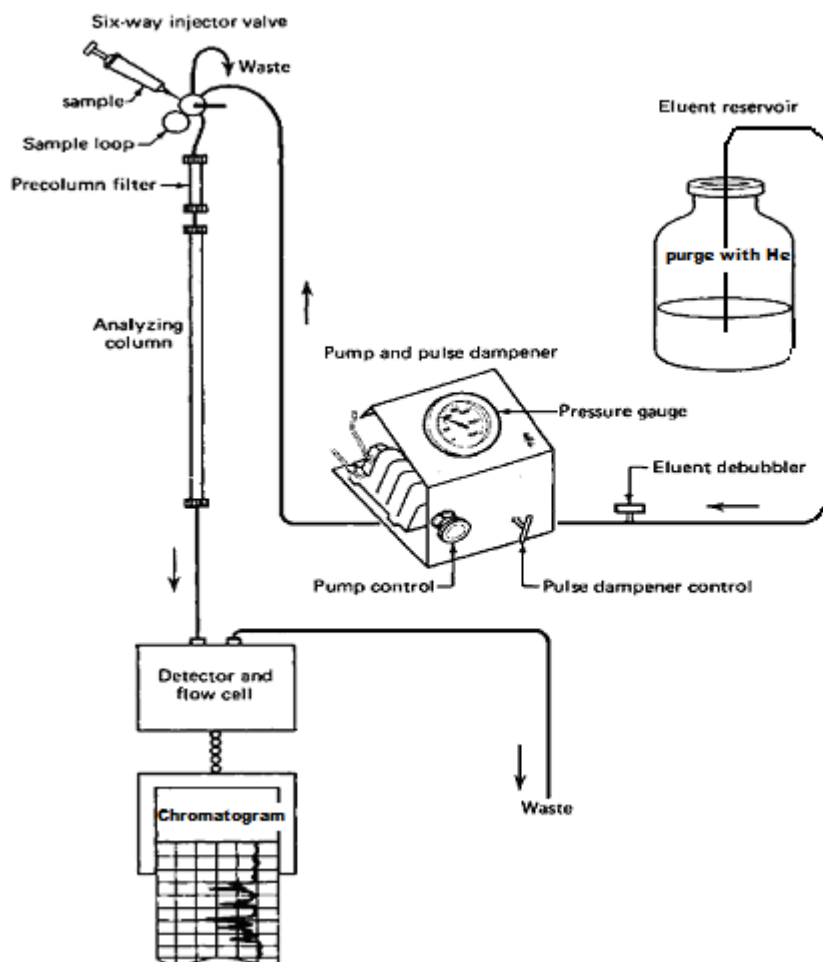
**Figure 20.** The modified, currently most commonly used Griess reaction, (R26). Under acidic conditions nitrite reacts with the amino group of sulfanilamide to form the diazonium cation, which couples to N-(1-naphthyl)ethylenediamine in para-position to form the corresponding azo dye. From: Tsikas (2007).

based on the aqueous scrubbing of HONO in a neutral buffer (pH 7), followed by derivatization of aqueous-phase nitrite ( $\text{NO}_2^-$ ) to a highly light-absorbing azodye via reaction with sulfanilamide (SA) and

(1-naphthyl)-ethylenediamine dihydrochloride (NED) in acidic solution via the most commonly used Griess reaction, (R26) (see **Figure 20**).

The reagents sulfanilamide (SA) ( $\geq 99\%$ , Aldrich) and N-1-naphthylethylene dihydrochloride (NED) ( $\geq 99\%$ , Fluka) contain significant impurities requiring further purification. The purification procedure consists of recrystallizing the reagents twice in 0.05 M hydrochloric acid (HCl) diluted from 37% v/v (ACS reagent grade), followed by Büchner filtration and washing with cold deionized water purified with a Millipore Milli-Q water system (resistivity  $\geq 18 \text{ M}\Omega$ ). For the optimized in-house technique (Wall et al., 2006), sampled air is drawn (typically at  $1.2 \text{ L min}^{-1}$ ) by a vacuum pump (KNF Neuberger) through a scrubbing coil.

Quantitative collection of nitrite is achieved using a neutral phosphate buffer solution (45-mM): sodium

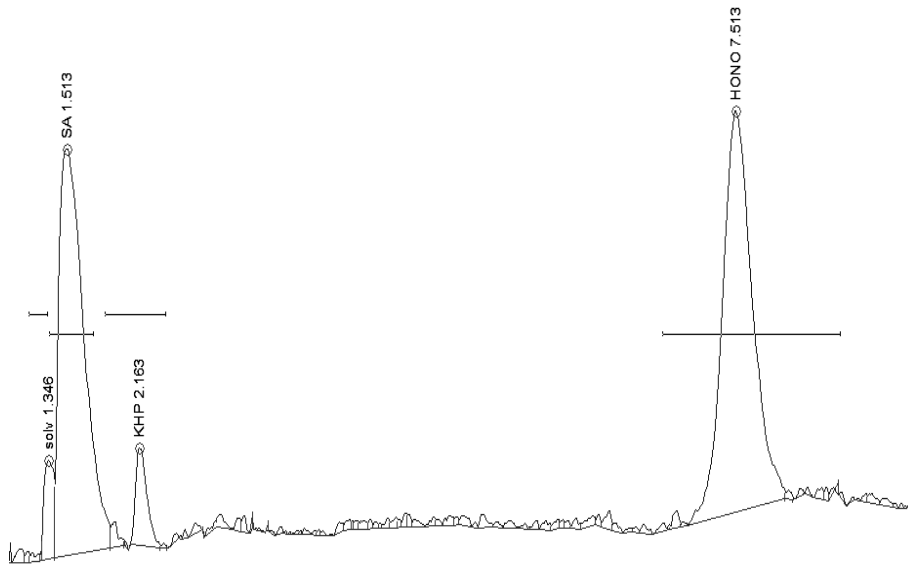


**Figure 21.** Block diagram of the HPLC system. Adapted from HP Liquid Chromatography Manual.

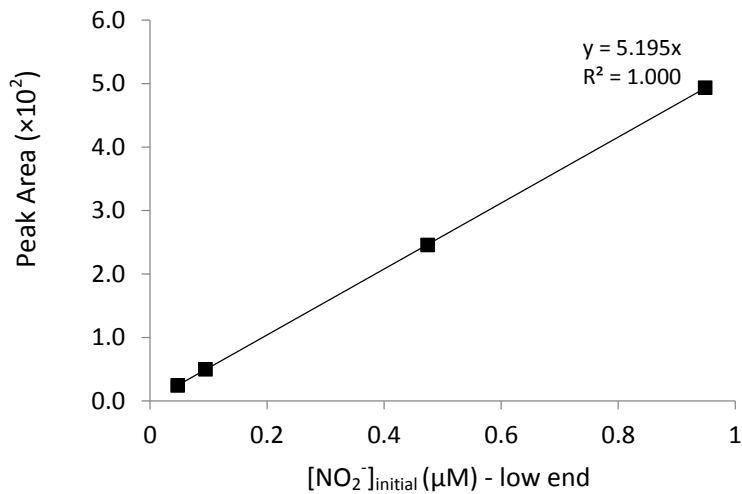
dihydrogen phosphate (99%, Aldrich) / sodium phosphate dibasic (ACS reagent grade, Aldrich). Via a peristaltic pump (Ismatec, 8-channel), the scrubbing solution is mixed with fresh SA/NED working reagent solution, and the mixture is passed through a reaction coil with a volume of approximately 2.5 ml, allowing a derivatization time of approximately 5 minutes (i.e., measured liquid flow rate =  $0.24 \pm 8.1 \times 10^{-4}$  mL min<sup>-1</sup>). To correct for volume loss during scrubbing, which can be as much as 20% at 1.5 L min<sup>-1</sup> sampling rate, potassium hydrogen phthalate (KHP, > 99.95%, Aldrich), was added to the scrubbing solution as an internal standard. Purification of reagent grade KHP was required due to the presence of metallic impurities (<100 ppm), and consists of recrystallization in deionized water, followed by Büchner filtration and washing with cold deionized water. A block diagram of the HPLC system is given in **Figure 21**. The derivatized solution is loaded onto a 100- $\mu$ L sample loop (Rheodyne Inc.) using a 6-port electrically actuated auto-injection valve (Rheodyne Inc.). The sample is then separated on a C<sub>18</sub> reverse-phase column (5  $\mu$ m, 4.0 $\times$ 150 mm analytical column, Waters) and detected using a variable wavelength UV-VIS detector (Varian 9050) at 540 nm. Isocratic elution is accomplished with 25% acetonitrile (CH<sub>3</sub>CN, HPLC grade, Caledon) in 15-mM hydrochloric acid at a flow rate of 1.0 mL min<sup>-1</sup> using an HPLC pump (Varian 9010). Chromatographic data acquisition and system automation is achieved using a PeakSimple chromatography data system (Version 3.29 Software, SRI Instruments), with sampling time limited by the chromatographic run-time of approximately 8 minutes. A typical chromatogram is shown in **Figure 22** below for a derivatized nitrite sample. Advantages specific to the optimized technique over the similar **LOngPathAbsorptionPhotometer** technique (Heland et al., 2001) include: correction for evaporation during scrubbing using an internal standard, and quantitative high-resolution separation of all absorbing species (Wall et al., 2006).

Prior to uptake experiments, aqueous-phase calibration of the HONO detector was performed by bypassing the scrubbing coil sampler, derivatizing fresh SA/NED working reagent solution (4-mM SA/0.4-mM NED) with freshly prepared calibration standards of NaNO<sub>2</sub> (> 99.99%, Aldrich) (in pH 7 phosphate buffer; 45-mM, containing 0.5-mM KHP) in the concentration range of 0.05 – 150  $\mu$ M, followed by separation and analysis using the optimized technique.

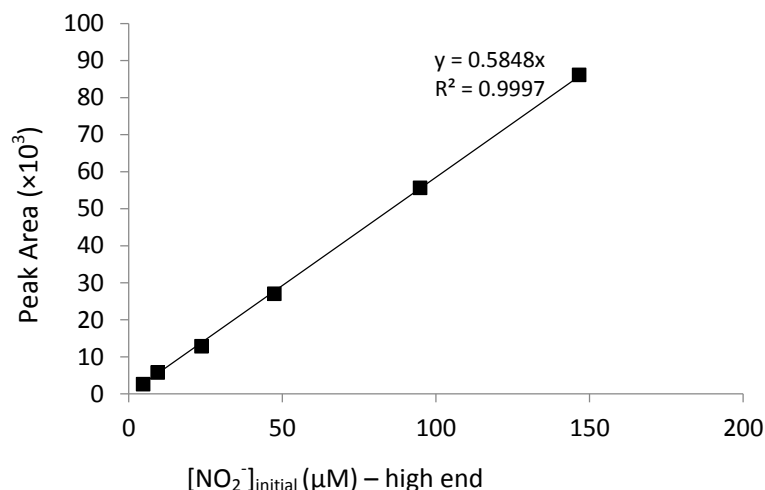




**Figure 22.** Typical chromatogram of a 50% v/v mixture of the working SA/NED reagent solution (4-mM SA/0.4-mM NED) and an aqueous nitrite calibration standard solution. Identification of peaks: (1) solvent; (2) SA; (3) KHP (0.5-mM); (4) azo-dye (0.6  $\mu$ M). Retention times are shown in minutes. Quantitative high-resolution separation of all absorbing species is achieved in < 8 minutes. Noise level shown is typical during uptake experiments.



(Figure 23, top)



(Figure 23, bottom)

**Figure 23.** Aqueous-phase nitrite ( $\text{NO}_2^-$ ) calibration of the HONO detector for measurement of scrubbed nitrite in WWFT experiments. Plotted nitrite calibrated standards ( $\mu\text{M}$ ) were prepared in pH 7 phosphate buffer solution. The solid (—) line (top) represents the linear regression to the four data points below  $0.95 \mu\text{M}$   $\text{NO}_2^-$ , while the dashed line (---) represents the linear regression for high nitrite concentrations (between  $4.75$  and  $150 \mu\text{M}$ ). Error bars represent one standard deviation of the averages. Solution flow rates:  $(0.24 \pm 8.1 \times 10^{-4}) \text{ mL min}^{-1}$ . Derivatization temperature:  $295 \text{ K}$ .

Division of the calibration data for the optimized HONO detector into two regions ( $0.05 - 0.95 \mu\text{M}$ ; and  $4.75 - 150 \mu\text{M}$ ), reveals a 12.6 % difference in slope for the corresponding observed highly linear responses ( $R^2 > 0.999$ ) (see **Figure 23**). This is due to increased peak tailing at higher nitrite concentrations, as observed in the corresponding chromatograms. The precision of the instrument was excellent with an average RSD of approximately 3% over all nitrite concentrations. During  $\text{NO}_2$  uptake experiments, a single point instrument calibration was performed by monitoring the stability of the HONO detector response to  $0.45 \mu\text{M}$   $\text{NaNO}_2$ , a concentration which falls on the linear regression of the instrument calibration curve, where heightened tailing is not an issue. The day-to-day variations in sensitivity were well within the typical precision attained for this tested  $\text{NaNO}_2$  concentration during calibration ( $\sim 1.5 \%$ ). It is important to note that the regressions presented in **Figure 23** (—) & (---) were obtained using the concentrations of nitrite in the calibration standards ( $[\text{NO}_2^-]_{\text{cal.std.}}$ ). Since the sampled azodye solution is a 50% v/v composition of SA/NED working solution and nitrite calibration standard, the concentration of nitrite in the injected azodye ( $[\text{NO}_2^-]_{\text{sampled}}$ ) is:

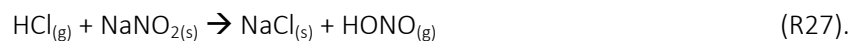
$$[\text{NO}_2^-]_{\text{sampled}} = [\text{NO}_2^-]_{\text{cal.std.}} \times \left(\frac{1}{2}\right) \quad (\text{E16}).$$

Under optimum chromatographic conditions, the detection limit ( $3\sigma_{\text{blank}}$ ) for the HONO detector is found to be approximately 1 nM (or  $1 \times 10^{-3}$   $\mu\text{M}$ )  $\text{NO}_2^-$  (aq.) using the neutral buffer as the solvent, however, is generally around a factor of 5 times larger for the average baseline noise encountered.

The empirical collection efficiency,  $\beta$  (%), of the scrubbing coil sampler, was previously determined (Wall et al., 2006) to be unity ( $\sim 100\%$  or quantitative collection) using a neutral phosphate buffer solution (45-mM) by connecting the scrubbing coil sampler and an impinger in series, and measuring the amount of HONO collected by each scrubber according to

$$\beta = 100\% \cdot \frac{c_1}{c_1 + c_2 (=c_{\text{total}})} \quad (\text{E17}),$$

where  $c_1$  and  $c_2$  are the concentrations of HONO collected in the scrubbing coil sampler and the impinger, respectively; and  $c_{\text{total}}$  is the concentration of sampled HONO. Of course, it is preferential to utilize a highly stable HONO output source, such as the one based on the system developed by Febo et al. (1995) where HONO is produced by passing a flow of humidified  $\text{HCl}_{(\text{g})}$  over a  $\text{NaNO}_{2(\text{s})}$  bed, resulting in the near 100% production of HONO from the HCl via reaction (R27):

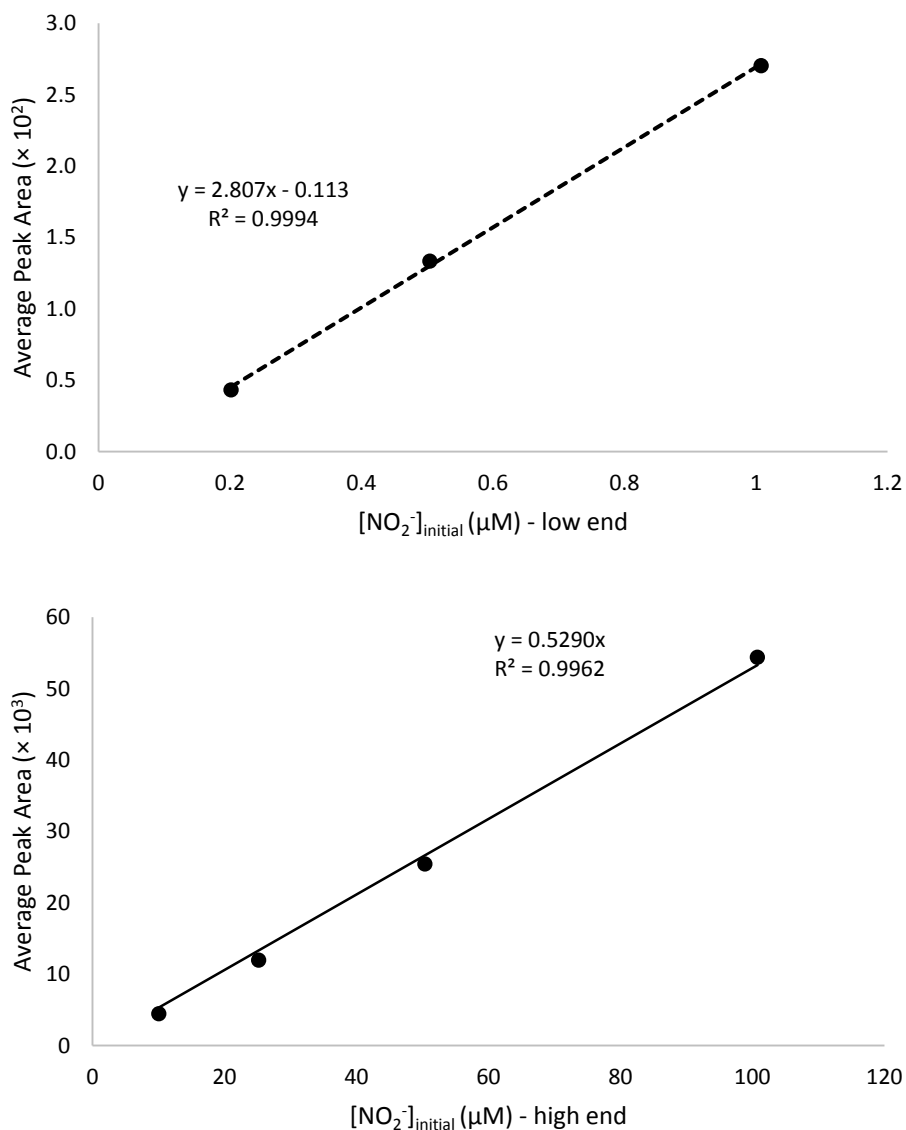


Note that the generated nitrous acid is easily quantified by collecting it into a sufficiently basic solution (pH 8.5 NaOH), followed by subsequent analysis of the nitrite and chloride contents by Ion Chromatography (IC). For experimental details of the ion chromatographic method used, refer to Wall et al. (2006). However, since the highly pure ( $\sim 98\%$ ), highly stable HONO generation system ( $122.4 \pm 1.4$   $\text{ng min}^{-1}$  HONO over several months) based on the one developed by Febo et al. (1995) had been out of commission for several months, calibration could only be achieved using solutions of  $\text{NaNO}_2$ . Since quantitative collection of nitrite is achieved in the scrubbing coil sampler using a neutral buffer solution during gas-phase sampling (Wall et al., 2006), the corresponding sampled gas-phase HONO concentration,  $[\text{HONO}]_{\text{sampled}}$  (pptv), produced at the exit of the WWFT during uptake experiments can be calculated based on the aqueous-phase nitrite calibration data via the following formula,

$$[\text{HONO}]_{\text{sampled}} = [\text{NO}_2^-]_{\text{sampled}} \times \left( \frac{F_1}{F_g} \right) \times \left( \frac{N_A}{n_{\text{air}}} \right) \times E_{\text{collection}} \quad (\text{E18}),$$

where  $[\text{NO}_2^-]$  is the measured scrubbed nitrite concentration in  $\text{mol L}^{-1}$  as calculated from (E16);  $F_l$  is the sampled liquid flow rate ( $0.24 \times 10^{-3} \text{ L min}^{-1}$ );  $F_g$  is the gas-phase sampling rate ( $1.20 \text{ L min}^{-1}$ );  $N_A$  is Avogadro's number ( $6.022 \times 10^{23} \text{ molecules mol}^{-1}$ );  $n_{\text{air}}$  is the number density of air at STP ( $2.46 \times 10^{10} \text{ molecules/L/pptv}$ ); and  $E_{\text{collection}}$  is the collection efficiency of gas-phase HONO in the scrubbing coil sampler (quantitative;  $E_{\text{collection}}$  is unity). Thus, the corresponding converted gas-phase HONO detection limit is  $\sim 2.4 \text{ pptv}$  for WWFT experiments under optimum chromatographic conditions. The optimized HONO detector is about an order of magnitude more sensitive than the original one developed by Huang et al. (2002) due to the following improvements: purification of derivatization reagents SA and NED; correction for evaporation during gas-phase sampling via the use of an internal standard; and a 20% higher gas-phase sampling rate.

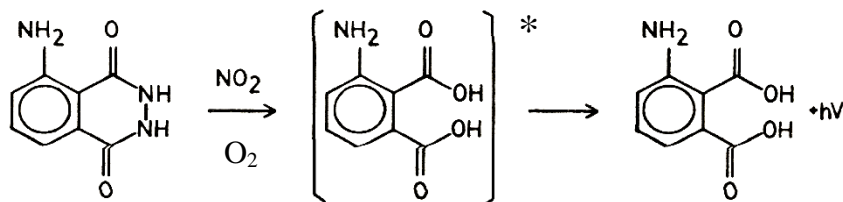
In order to quantify the nitrite remaining in the effluent liquid (organic film) during uptake experiments, a ten-point aqueous-phase calibration using calibration standards of  $\text{NaNO}_2$  ( $0.2 - 100 \mu\text{M}$ ) in deionized water (unadjusted pH of approximately 6) was performed. Since the  $\text{pK}_a$  of HONO is 3.3 (Al-Obaidi and Moodie, 1985), at pH 6 we can expect all the nitrite to remain in the liquid film. Online effluent analysis via the HONO detector is preferred over offline analysis by ion chromatography, since offline analysis would require freezing the samples for a few days, consequently resulting in possible oxidation to nitrate (Takenaka et al., 1998). Deionized water is chosen as the optimal solvent for the organic (phenolic-containing) films as opposed to the neutral phosphate buffer solution (45-mM, containing 0.5-mM KHP) or organic solvents, in order to avoid possible undesirable chromatographic peaks. A highly linear response ( $R^2 = 0.9962$ ) over a large dynamic range (2 orders of magnitude) is obtained (see **Figure 24**, solid line). The precision is excellent with an average RSD of approximately  $< 6\%$  over all nitrite concentrations. The sensitivity is reduced by a factor of two (i.e. an optimal detection limit of  $\sim 2 \text{ nM}$ ) for the lower nitrite concentrations ( $0.2 - 1 \mu\text{M}$ ) (refer to **Figure 24**, dashed line) compared to that obtained for the standards prepared in the neutral phosphate buffer. This is most likely due to decreased stability and/or solubility of nitrite in (pH 6) deionized water compared to that in the neutral buffer at very low concentrations.



**Figure 24.** Aqueous-phase nitrite ( $\text{NO}_2^-$ ) calibration of the HONO detector for possible effluent film analysis. Nitrite standards were prepared in (pH 6) deionized water. The solid (–) line (bottom) represents the linear regression to the four data points above  $10 \mu\text{M}$   $\text{NO}_2^-$ , while the dashed line (top) represents the reduced linear response of the instrument at low  $\text{NO}_2^-$  concentrations (between  $0.2$  and  $1.0 \mu\text{M}$ ). Error bars represent one standard deviation of the averages. Solution flow rates:  $(0.24 \pm 8.1 \times 10^{-4}) \text{ mL min}^{-1}$ . Derivatization temperature:  $295 \text{ K}$ .

The loss of  $\text{NO}_2$  was measured *only* during the uptake experiments for the first two simple organic compounds, that is, water (may have organic contaminants) and 4-benzoylbenzoic acid, respectively. Following these experiments, the  $\text{NO}_2$  chemiluminescence detector was removed from the experimental setup for online simultaneous sampling of ambient HONO and  $\text{NO}_2$  at the York University Keele campus, as the spare Luminox detector required substantial repairs. The LMA-3 Luminox system (Scintrex) detects

the chemiluminescence produced in the  $\lambda = 425$  nm region (refer to **Figure 25**) when  $\text{NO}_2$  encounters a surface wetted with a specially formulated *luminol* solution. The advantage that this system provides is that, unlike other chemiluminescent  $\text{NO}_x$  detectors, the LMA-3 Luminox measures the  $\text{NO}_2$  directly, without prior conversion of the  $\text{NO}_2$  to  $\text{NO}$ .

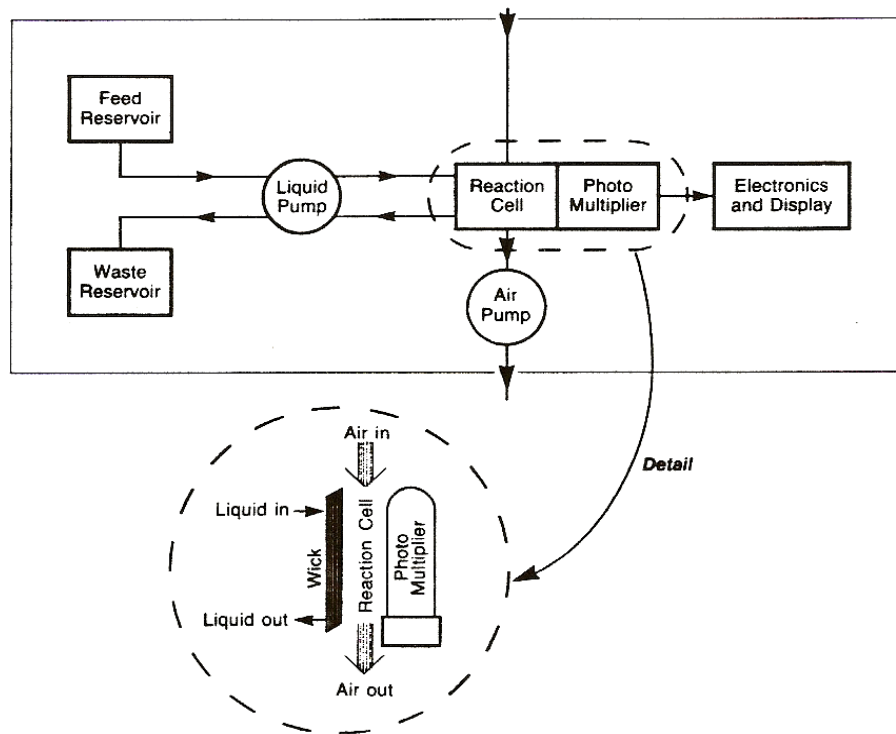


**Figure 25.** Mechanism (M9) of the luminol oxidation reaction (R28) in the presence of  $\text{NO}_2$  ( $\lambda \approx 425$  nm). From: LMA-3 Luminox Scintrex Manual.

The schematic of the instrument is detailed in **Figure 26**. Sampled air (the effluent gas), which is drawn through the instrument in-house by a vacuum pump at approximately  $1.4 \text{ L min}^{-1}$ , flows across a fabric wick wetted with the luminol solution: 0.1-mM luminol (3-aminophthalhydrazide, > 97%, Aldrich) / 0.1-M sodium sulphite ( $\text{NaSO}_3$ , 98.0%, Analar) / 0.01-M sodium hydroxide ( $\text{NaOH}$ , 99.998%, Aldrich) / 0.01-M 2-propanol (> 95%, BDH). The solution is continuously replenished at  $(0.056 \pm 3.1 \times 10^{-4}) \text{ mL min}^{-1}$  (2 rpm) at the top of the wick and removed at the bottom via a small peristaltic pump. The photomultiplier tube (PMT) views the central portion of the wick (with a time constant of 3.0 s). Thus, the signal from the PMT is proportional to the mixing ratio of the  $\text{NO}_2$  in the sampled air.

The linear range of the luminol detector was established by a laboratory calibration (nine point) spanning the (atmospherically relevant) range from sub-ppbv to over 100 ppbv, achieved by sampling typically between 1 to 50  $\text{mL min}^{-1}$  (50  $\text{mL min}^{-1}$  MFC) of  $\text{NO}_2$ , 5 ppm in  $\text{N}_2$  (certified accurate to 2%, Air Liquide) diluted into zero air, typically at 3.8 or 6.6  $\text{L min}^{-1}$  (using a 30  $\text{L min}^{-1}$  MFC). Fresh luminol solution was prepared prior to calibration. A time constant of 3.0 s, as opposed to the 0.3 or 1.0 s settings was employed since it is desirable to damp out noise in the signal originating from fluctuations in the  $\text{NO}_2$  concentration, or from the instrument when measuring very low  $\text{NO}_2$  mixing ratios.

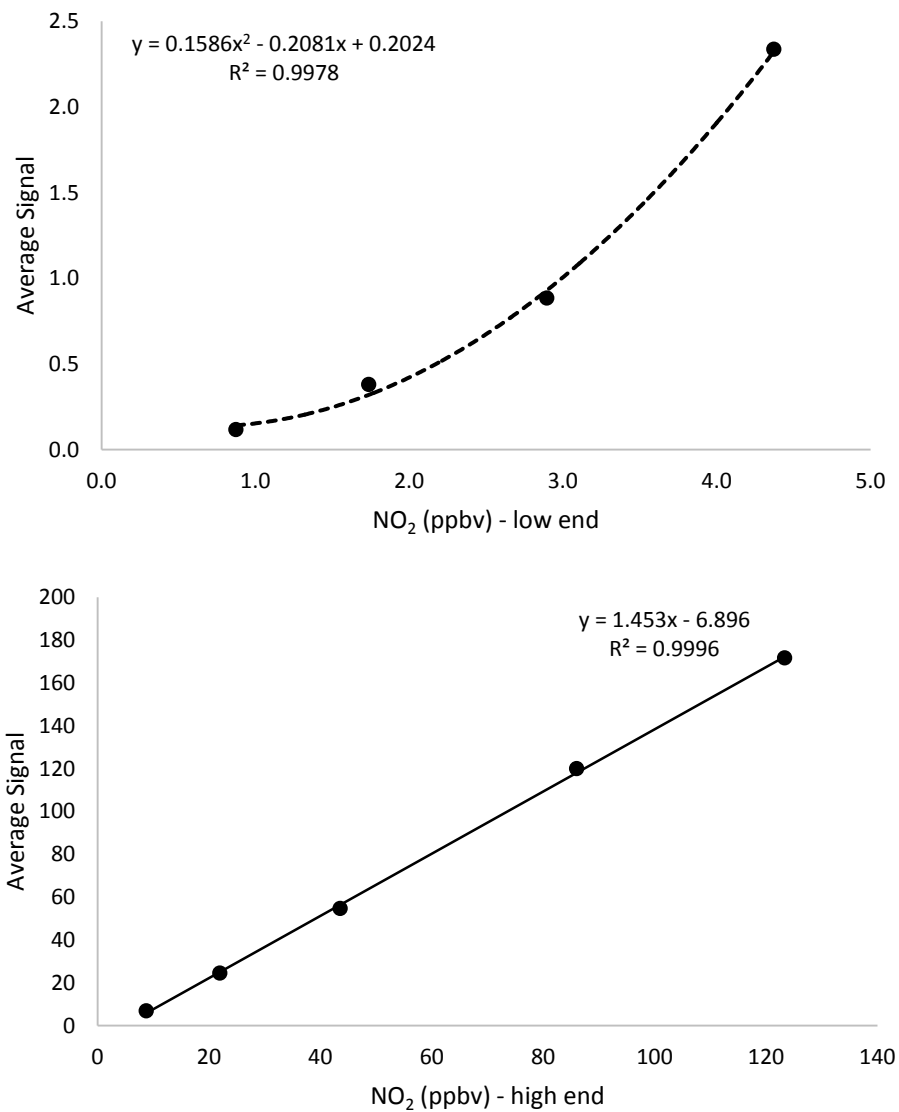
The calibration plot (**Figure 27**) is divided into two regions in order to account for the non-linear response of the LMA-3  $\text{NO}_2$  detector as described by Heitlinger et al. (1995). For  $\text{NO}_2$  mixing ratios between 9.0 and 125 ppbv, a highly linear response ( $R^2 = 0.9996$ ) of  $\text{NO}_2$  detector is obtained (see **Figure 27**, solid line).



**Figure 26.** Schematic diagram of the LMA-3 Luminol instrument (Scintrex/Unisearch).

At very low NO<sub>2</sub> mixing ratios between 1.0 and 4.0 ppbv, the instrument response is quadratic (refer to **Figure 27**, dashed line) as expected (Heitlinger et al., 1995), with a correlation coefficient ( $R^2$ ) of 0.9978. The precision of the instrument is excellent, with a value of < 2% over all NO<sub>2</sub> mixing ratios (1.0 – 125 ppbv). During NO<sub>2</sub> uptake experiments, fresh luminol solution was prepared daily, and single point instrument calibrations were performed by monitoring the stability of the luminol NO<sub>2</sub> detector response to 45 ppbv NO<sub>2</sub>, a concentration which falls on the linear regression of the instrument calibration curve. The day-to-day variations in sensitivity were well within ~ 10%, which is considered typical of the precision which may be attained with frequent attention to the luminol solution (Kelly et al., 1990).

An upper limit of 1.0 ppbv is, thus, assigned as the detection limit of the LMA-3 detector. This detection limit corresponds to the smallest measurable loss of NO<sub>2</sub> during uptake experiments with the LMA-3 detector. For a typical initial mixing ratio of 36 ppbv utilized in uptake experiments, this corresponds to a minimum measurable NO<sub>2</sub> loss of about 3%.



**Figure 27.** Gas-phase NO<sub>2</sub> calibration of the in-house luminol detector illustrating the linear and non-linear response regions of the luminol instrument. The solid (—) line (bottom) represents the linear regression to the five data points above 9 ppbv NO<sub>2</sub>, while the dashed line (top) represents the quadratic response of the instrument at very low NO<sub>2</sub> mixing ratios (between 1 and 4 ppbv). Error bars represent one standard deviation of the averages. Typical operating conditions: air sampling rate: 1.4 L min<sup>-1</sup>; solution flow rate: (0.056 ± 3.1×10<sup>-4</sup>) mL min<sup>-1</sup> (2 rpm); time constant: 3.0 s; derivatization temperature: 295 K.

Prior to the uptake experiments, the photolysis of gaseous NO<sub>2</sub> and HONO, respectively, needed to be considered, since significant concentrations of these species may be removed when the wetted wall flow



tube is exposed to UV irradiation ( $\lambda_{\max} = 354$  nm for the 4 lamps) during the typical gas-liquid reaction time,  $t_{\text{reac}}$ , of 1 s. The  $\text{NO}_2$  loss rate via photodissociation in the WWFT photoreactor is:

$$\frac{d[\text{NO}_2]}{dt} = -j_{\text{NO}_2}[\text{NO}_2]_0 \quad j_{\text{NO}_2} = 0.024 (\pm 0.007) \text{ s}^{-1} \quad (\text{E19}),$$

where the experimentally determined  $j_{\text{NO}_2}$  value (George et al., 2005) by the photolysis of  $\text{NO}_2$  in air and the subsequent measurement of the reaction product NO is used as a ‘maximum’ estimate for the irradiation conditions due to time and experimental restrictions (i.e., a non-functional HONO generation system). It is important to note that the experimental setup employed by George et al. (2005) and Stemmler et al. (2006) is similar to the one used for this project (*recall*: 50 cm  $\times$  0.8 cm i.d. Duran glass tube in an air-cooled aluminum housing holding 7 fluorescence lamps in a circular arrangement, 3 cm away from the flow tube), and, thus, the radiation in the setup was estimated by scaling appropriately.

Under the speculation that all the  $\text{NO}_2$  reacts instantaneously in the WWFT photoreactor to produce HONO with a 100% conversion yield, the maximum HONO loss rate via photodissociation is calculated as

$$\frac{d[\text{HONO}]}{dt} = j_{\text{HONO}}[\text{NO}_2]_0 \quad j_{\text{HONO}} = 0.0055 \text{ s}^{-1} \quad (\text{E20}),$$

with  $j_{\text{HONO}}$  calculated by George et al. (2005), using the actinic flux in the reactor derived as four times the measured  $2\pi$ -spectral irradiance (neglecting any influence of the glass reactor walls) (Madronich, 1987) for the Philips Cleo Compact Fluorescence lamps ( $\lambda_{\max} = 354$  nm) and the IUPAC recommendations for the cross-sections and quantum yields (Atkinson et al., 2004) under the assumption of isotropic radiation in the reactor. Using the actinic flux derived in this manner and the IUPAC recommendations for the cross-sections and quantum yields, George et al. (2005), compute photolysis frequencies,  $j_{\text{NO}_2} = 0.046 \text{ s}^{-1}$  and  $j_{\text{HONO}} = 0.011 \text{ s}^{-1}$ , for the respective gaseous species. As their model appears to overestimate the actual actinic fluxes by roughly a factor of two (and thus the corresponding  $j$  values), possibly due to the simplified representation of the radiation conditions in the reactor (George et al., 2005); the  $j_{\text{HONO}}$  value used as a maximum estimate for the irradiation conditions in (E20) has been scaled accordingly.

For the gas-liquid interaction time in the WWFT reactor,  $t_{\text{reac}}$ , which is typically 1 s during uptake experiments, and an initial  $\text{NO}_2$  mixing ratio ( $[\text{NO}_2]_0$ ) of 72 ppbv (highest mixing ratio used), this would result in a maximum  $\text{NO}_2$  loss of approximately 1.7 ppbv (i.e., 2.3 % loss, thus,  $L_{\text{NO}_2} = 2.3\%$ ). Since the precision of the  $\text{NO}_2$  detector ranges from approximately (0.9 – 2.0) % for very small (changes in)  $\text{NO}_2$  mixing ratios (< 2.0 ppbv), the photolysis of  $\text{NO}_2$  can be considered unimportant for the highest level of

NO<sub>2</sub> (72 ppbv) in the WWFT photoreactor. For the same  $t_{\text{reac}}$  and highest level of [NO<sub>2</sub>]<sub>0</sub>, this results in a maximum HONO loss of about 0.4 ppbv (i.e., 0.6% loss, so that  $L_{\text{HONO}} = 0.6\%$ ). The precision for the HONO detector in this ( $\Delta[\text{HONO}]$ ) concentration range varies from approximately (1.6 – 3.7) %, so that in the uptake experiments, the HONO photodissociation process can also be considered negligible. For uptake experiments using extreme NO<sub>2</sub> input conditions, i.e., approximately 1.0 ppmv, and same  $t_{\text{reac}}$ , the loss in initial NO<sub>2</sub> and HONO concentrations, respectively, are  $\Delta[\text{NO}_2] = 23$  and  $\Delta[\text{HONO}] = 5.5$  in units of ppbv (again, corresponding to  $L_{\text{NO}_2} = 2.3$  and  $L_{\text{HONO}} = 0.6$  in percentage units). Since these loss percentages are within the precisions of the NO<sub>2</sub> detector and the HONO detector, the photolysis of NO<sub>2</sub> and HONO can, too, be ruled unimportant during uptake experiments with extreme NO<sub>2</sub> conditions.

### 3 MODEL FOR PREDICTING $y_{\text{best-fit}}$ FROM EXPERIMENTAL DATA

*In this Chapter, a fully functional time-dependent model for predicting a  $y_{\text{best-fit}}$  from experimental data is developed based on the Henry's Law equilibrium between the partial pressure of the acidic product gas, HONO, and the concentration of nitrite. It is numerically shown that well-mixed conditions do not apply to the WWFT photoreactor for the film acidities tested in this study. A relatively straightforward equation is derived for the observed HONO mixing ratio for a conveniently chosen fraction of the reaction time (or time step), based on the simple Henry's Law expression and the acid dissociation expression for HONO, with the total number of moles of N(III) represented by both the number of NO<sub>2</sub> collisions and the reaction probability (the fitting parameter). The equation is complicated by its film volume parameter – in order to solve for this variable, the problem of diffusion in a semi-infinite medium is considered for the cylindrical reactor geometry. It is shown that the moles of partitioned reaction products are easily calculated using the acid dissociation expression for HONO for the first time step, continued iteratively until the elapsed reaction time. Next, the chapter addresses the issue of computation of film pH, as it was not measured during the experiments. The percentage of reactant (NO<sub>2</sub>(g)) remaining at  $t_{\text{reac}}$  is easily calculated (iteratively) using the moles of initial reactant (at each time step) and a few conversion*

factors. As a definitive verification that the model is valid, an internal consistency check is presented. By the end of the chapter, the model presented allows for meaningful results to be extracted ( $\gamma_{best-fit}$ ) from experimental parameters/data (film pH, reactant  $[NO_2]$  and  $[HONO]_{treac}$ ).

### 3.1 DERIVATION OF MODEL EQUATIONS

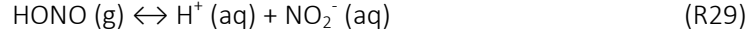
It would have been ideal to conduct product analysis for both the gas- and liquid-phases. The use of the in-house ion chromatographic method for nitrite product analysis was one straightforward option for consideration, however, its rather large detection limit (about 0.5  $\mu$ M), coupled with the offline nature of the analysis, made it a non-ideal method for such analysis. The current HONO measurement (HPLC) method also ruled out its use for online nitrite analysis. Significant effort would have been required to develop a method such as that used by Susic and Boto (1989), which involves eluting the sodium or calcium complex of HA as a single sharp peak on a glass-lined reversed-phase column (the retention mechanism is unknown) coupled with fluorescence detection, achieving a d.l. at the nanogram level.

Due to the discussed complications with the available LC techniques, liquid-phase product analysis was not possible in the scope of this project. This setback provided the motivation for the development of the following time-dependent model for non-equilibrium conditions incorporating both chemistry (partitioning of the total uptake product) and diffusion on the respective time-scales for predicting a best-fit reaction probability,  $\gamma_{best-fit}$  as a function of the following experimental input parameters:  $NO_2$  concentration, film pH, and the corresponding observed HONO production rate at a single set of conditions. This described model that immediately follows will easily allow predicted best-fit reaction probabilities ( $\gamma_{best-fit}$ ) to be fitted from the collected experimental data.

For the WWFT photoreactor, wherein the acidic product gas, HONO, is dissolved in a continuously renewed film, the situation is quite complicated. In a given droplet, the molar concentration of dissolved HONO, denoted  $[HONO(aq)]$  is computed as

$$[HONO(aq)] = H_{HONO} P_{HONO} \quad (E21),$$

where  $H_{\text{HONO}}$  is the Henry's law constant of 49 ( $\pm 3$ ) M atm<sup>-1</sup> for gas-phase HONO (Park and Lee, 1988), and the partial pressure of HONO,  $P_{\text{HONO}}$ , in equilibrium with the concentration of nitrite (R29)



depends on the pH of the (film) solution. The equilibrium concentration of  $\text{NO}_2^-$ , denoted as,  $[\text{NO}_2^-]$  is simply

$$[\text{NO}_2^-] = \frac{K_a [\text{HONO(aq)}]}{[\text{H}^+]} = \frac{K_a H_{\text{HONO}} P_{\text{HONO}}}{[\text{H}^+]} \quad (\text{E22}),$$

where  $K_a$  is the acid dissociation constant for gas-phase HONO, that is  $10^{-3.3}$  (Al-Obaidi and Moodie, 1985). The concentration of the product species in the liquid-phase, denoted  $[\text{N(III)}]_l = [\text{HONO(aq)}] + [\text{NO}_2^-]$  (for these rapid acid-base equilibria) is evaluated as a function of pH as the sum of equations (E21) and (E 22):

$$[\text{N(III)}]_l = H_{\text{HONO}} \left( 1 + \frac{K_a}{[\text{H}^+]} \right) P_{\text{HONO}} \quad (\text{E23}).$$

But, since the partial pressure of HONO,  $P_{\text{HONO}}$ , is simply evaluated as:

$$P_{\text{HONO}} = [\text{HONO}]_{\text{treac}} RT \quad (\text{E24}),$$

where  $[\text{HONO}]_{\text{treac}}$  is the measured molarity of the product gas, HONO, at  $t_{\text{reac}}$  of 1s at the exit of the WWFT. Hence, (E23) can be re-expressed as:

$$[\text{N(III)}]_l = H_{\text{HONO}} [\text{HONO}]_{\text{treac}} RT \left( 1 + \frac{K_a}{[\text{H}^+]} \right) \quad (\text{E25}).$$

This molarity is easily converted to a rate for the aqueous-phase,  $\phi_l$ , in units of mol min<sup>-1</sup> using the film flow rate,  $F_l$ :

$$\phi_l = [\text{N(III)}]_l \times F_l = H_{\text{HONO}} [\text{HONO}]_{\text{treac}} RT F_l \left( 1 + \frac{K_a}{[\text{H}^+]} \right) \quad (\text{E26}).$$

The fraction of N(III) converted to the gas-phase (relative to the liquid-phase) is easily estimated as

$$\frac{\phi_g}{\phi_l} = \frac{F_g}{H_{\text{HONO}} RT F_l \left( 1 + \frac{K_a}{[\text{H}^+]} \right)} \quad (\text{E27}),$$

where (the numerator, before simplification)  $\phi_g$  is simply the product  $[\text{HONO}]_{\text{treac}} F_g$ . Note that for equilibrium (well-mixed) conditions to apply in the WWFT reactor, the following condition must be true:

$$\frac{\phi_g}{\phi_l} = \frac{F_g}{H_{\text{HONO}} RT F_l} \quad (\text{E28}),$$

(that is, at very high pH,  $\left(1 + \frac{K_a}{[H^+]}\right) = 1$ ), which does not apply for the film acidities tested herein, namely, pHs  $\leq 5$ .

For the usual gas-liquid reaction time of 1 s, the total time is divided into 100 time steps (**ts**), each 0.01 s in length ( $=t_{ts}$ ). The number of collisions of gaseous NO<sub>2</sub> occurring at the first time step, **s**,  $Z_{NO_2,s}$  (collisions)mol<sup>-1</sup> is easily calculated as

$$Z_{NO_2,s} \text{ (collisions)} = \frac{P(\text{Pa})}{\sqrt{2\pi m_{NO_2} k_B T}} \cdot SA_{\text{rxn zone},s} \cdot [NO_2] \quad (\text{E29}),$$

where:  $m_{NO_2}$  is the atomic mass of NO<sub>2</sub>(g), 46 amu or 7.636×10<sup>-26</sup> kg; P (Pa) is the pressure in the WWFT, atmospheric pressure or 1.013×10<sup>5</sup>Pa; T is the experimental temperature, i.e., 295 K for HA experiments;  $SA_{\text{rxn zone},s}$  is the surface area of the reaction zone for one ts, easily computed using the surface area of a cylinder,  $\left(\frac{2\pi rL}{100 t_s}\right)$ ,  $[NO_2]_s$  is the concentration of NO<sub>2</sub> in ppbv in the WWFT at the first ts; and  $k_B$  is the Boltzmann constant (1.38 × 10<sup>-23</sup> m<sup>2</sup> kg s<sup>-2</sup> K<sup>-1</sup>).

The observed mixing ratio of HONO (pptv) partitioned at the first time step, **s**,  $[HONO]_s$  is computed using the input test parameter,  $\chi_{\text{best-fit}}$  as follows

$$[HONO]_s = \frac{\left(\frac{Z_{NO_2,s} \chi_{\text{best-fit}}}{N_A}\right)}{\left(1 + \frac{K_a}{[H^+]_s}\right) \cdot H_{HONO} \cdot V_{\text{film,diff},s}} \cdot \frac{10^{12} \text{ pptv}}{\text{atm}} \quad (\text{E30}),$$

where:  $\left(\frac{Z_{NO_2,s} \chi_{\text{best-fit}}}{N_A}\right)$  represents the total number of moles of N(III)(= gas+liquid);  $N_A$  is Avogadro's number, 6.022×10<sup>23</sup> molecules mol<sup>-1</sup>;  $H_{HONO}$  is the Henry's law constant for HONO, with a value of 49 (±3) M atm<sup>-1</sup> (Park and Lee, 1988); and  $V_{\text{film,diff},s}$  is the film volume (L) at the first time step, taking into account diffusion. In order to compute the last parameter,  $V_{\text{film,diff},s}$  accurately, the problem of diffusion in a semi-infinite medium must be considered for the cylindrical photoreactor. This problem is resolved in **Section 3.2**.

The mixing ratio of HONO observed at the first time step,  $[HONO]_s$  is easily converted into the equivalent number of moles of HONO partitioned,  $\Phi_{HONO,s}$  using (E31)

$$\phi_{\text{HONO},s} = P_{\text{HONO(ppb)}} \cdot \left( \frac{N_{\text{air}} F_g t_{ts}}{N_A} \right) \cdot \frac{1 \text{ min}}{60s} \quad (\text{E31}),$$

where  $F_g$  is the typical gas flow rate,  $3.81 \text{ L min}^{-1}$ ;  $N_{\text{air}}$  represents the number density of air,  $2.46 \times 10^{10}$  molecules  $\text{cm}^{-3}$  ppbv $^{-1}$  at STP; and the terms  $N_A$  and  $t_{ts}$  (s) has been previously defined.

It follows that the number of moles of HONO partitioned into the aqueous-phase at the first time step,  $\phi_{\text{HONO(aq)},s}$  is easily computed as:

$$\phi_{\text{HONO(aq)},s} = \frac{\left( \frac{Z_{\text{NO}_2,s} Y_{\text{best-fit}}}{N_A} \right)}{\left( 1 + \frac{K_a}{[\text{H}^+]_s} \right)} \quad (\text{E32}).$$

Finally, the number of moles of nitrite at the first time step,  $\phi_{\text{NO}_2^-,s}$  is computed as:

$$\phi_{\text{NO}_2^-,s} = \left( \frac{K_a}{[\text{H}^+]_s} \right) \cdot \phi_{\text{HONO(aq)},s} \quad (\text{E33}).$$

Thus, the total product N(III) in moles partitioned in both the gas- and liquid-phases at the first time step,  $s$  ( $t_{ts} = 0.01 \text{ s}$ ) is

$$\begin{aligned} \phi_{\text{total},s} &= \phi_{\text{HONO},s} + \phi_{\text{HONO(aq)},s} + \phi_{\text{NO}_2^-,s} = \left( \frac{Z_{\text{NO}_2,s} Y_{\text{best-fit}}}{N_A} \right) \\ &= \frac{\left( \frac{Z_{\text{NO}_2,s} Y_{\text{best-fit}}}{N_A} \right)}{\left( 1 + \frac{K_a}{[\text{H}^+]_s} \right) \times H_{\text{HONO}} V_{\text{film,diff},s}} \cdot \left( \frac{N_{\text{air}} F_g t_{ts}}{N_A} \right) \cdot \left( \frac{10^{12} \text{ ppt}}{\text{atm}} \cdot \frac{1 \text{ min}}{60s} \right) + \frac{\left( \frac{Z_{\text{NO}_2,s} Y_{\text{best-fit}}}{N_A} \right)}{\left( 1 + \frac{K_a}{[\text{H}^+]_s} \right)} + \left[ \left( \frac{K_a}{[\text{H}^+]_s} \right) \cdot \phi_{\text{HONO(aq)},s} \right] \quad (\text{E34}). \end{aligned}$$

The partitioned reaction products,  $\text{HONO}_g$ ,  $\text{HONO}_{\text{aq}}$ , and  $\text{NO}_2^-_{\text{aq}}$ , are accumulated over the entire elapsed reaction time, i.e., At the second time step,  $s + 1$ , with an elapsed reaction time of  $0.02 \text{ s}$ , the moles of the products species are as follows,

$$\phi_{\text{HONO},s+1} = \phi_{\text{HONO},s} + \phi_{\text{HONO},s+1} \quad (\text{E35});$$

$$\phi_{\text{HONO(aq)},s+1} = \phi_{\text{HONO(aq)},s} + \phi_{\text{HONO(aq)},s+1} \quad (\text{E36});$$

$$\phi_{\text{NO}_2^-,s+1} = \phi_{\text{NO}_2^-,s} + \phi_{\text{NO}_2^-,s+1} \quad (\text{E37}),$$

continued iteratively until the end of the total gas-liquid reaction time ( $t_{\text{reac}} = 1 \text{ s}$ ).

It is important to note that the film pH *decreases* as HONO(aq) dissociates, and must be recalculated at each time step (i.e., iteratively until the final pH,  $\text{pH}_{\text{t}_{\text{reac}}}$ ), as it was not measured, according to the following formula (for the first ts),

$$[\text{H}^+]_s = [\text{H}^+]_0 + [\text{NO}_2^-]_s \quad (\text{E38}),$$

where the film hydronium ion concentration ( $\text{mol L}^{-1}$ ) at the first time step is denoted  $[\text{H}^+]_s$ . The initial film hydronium ion concentration is simply  $10^{-\text{pH}_{\text{film},0}}$ , with  $\text{pH}_{\text{film},0}$  representing the measured film pH corresponding to the time at which the HONO was measured in the effluent gas; and  $[\text{NO}_2^-]_s$  is the film nitrite concentration at the first time step derived as:

$$[\text{NO}_2^-]_s = \left( \frac{\phi_{\text{NO}_2, s}}{V_{\text{film}, \text{diff}, s}} \right) \quad (\text{E39}).$$

The number of moles of  $\text{NO}_2$  remaining (unreacted),  $\phi_{\text{NO}_2, s}$  and thus, the concentration, in units of ppb, at the end of the first time step are readily computed as follows

$$\phi_{\text{NO}_2, s} = \phi_{\text{NO}_2, 0} - \phi_{\text{total}, s} \quad (\text{E40}),$$

where the moles of  $\text{NO}_2$  that were introduced at the entrance of the WWFT,  $\phi_{\text{NO}_2, 0}$  is simply:

$$\phi_{\text{NO}_2, 0} = [\text{NO}_2]_0 (\text{ppb}) \cdot \left( \frac{N_{\text{air}} F_g t_{\text{reac}}}{N_A} \right) \cdot \left( \frac{1 \text{min}}{60 \text{s}} \cdot \frac{1000 \text{mL}}{\text{L}} \right) \quad (\text{E41}).$$

Finally, the gas-phase concentration of  $\text{NO}_2$  at each time step can be calculated (as it was not measured) using  $\phi_{\text{total}, s}$  iteratively, in order to estimate the percentage of  $\text{NO}_2$  remaining at the end of  $t_{\text{reac}}$  — this percentage is expected to be quite small, i.e., centred near the precision of the HONO detector. For the first time step, the following formulae for the concentration of  $\text{NO}_2$  unreacted ( $[\text{NO}_2]_s$ ), and the percentage of  $\text{NO}_2$  remaining, respectively are given:

$$[\text{NO}_2]_s = \phi_{\text{NO}_2, s} \cdot \left( \frac{N_A}{N_{\text{air}} F_g t_s} \right) \cdot \left( \frac{60 \text{s}}{\text{min}} \cdot \frac{1 \text{L}}{1000 \text{mL}} \right) \quad (\text{E42});$$

$$\% \text{NO}_{2, s} = \left( \frac{P_{\text{NO}_2, s}}{P_{\text{NO}_2, 0}} \right) \times 100\% \quad (\text{E43}).$$

The model formulae are programmed into a spreadsheet, so that the user need only input the initial film pH ( $\text{pH}_{\text{sol'n}}$ ) and initial  $\text{NO}_2$  concentration (*fixed* variables), and the **input test variable**,  $y_{\text{best-fit}}$  (reaction

probability), such that the model predicted gas-phase HONO concentration accumulated at 1 s reaction time best fits the experimentally observed mixing ratio. An internal consistency check of the model is automatically conducted at the first time step as a final verification that (E50) is valid:

$$\text{ABS} \left[ \left( \frac{\phi_{\text{total},s} - \left( \frac{Z_{\text{NO}_2,s} Y_{\text{best-fit}}}{N_A} \right)}{\phi_{\text{total},s}} \right) \cdot 100\% \right] \leq 0.1\% \quad (\text{E44}).$$

As a final note, the model output data is available for the reader's reference in **Appendix C** for the photoenhanced NO<sub>2</sub> uptake experiments on humic acid films experiments.

### 3.2 INCORPORATION OF DIFFUSION

In order to compute the last parameter,  $V_{\text{film,diff},s}$  accurately, the problem of diffusion in a semi-infinite medium,  $x > 0$  was considered, i.e., when the boundary is kept at a constant concentration,  $C_0$ , the initial concentration remains zero throughout the medium (Crank, 1975). Accordingly, this calls for a solution of

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \quad (\text{E45})$$

satisfying the boundary condition

$$C = C_0, \quad x = 0, \quad t > 0,$$

and the initial condition

$$C = 0, \quad x > 0, \quad t = 0.$$

Multiplication of both sides of (E45) by  $e^{-pt}$ , followed by integration with respect to  $t$  from 0 to  $\infty$ , yields:

$$\int_0^\infty e^{-pt} \frac{\partial^2 C}{\partial x^2} dt - \frac{1}{D} \int_0^\infty e^{-pt} \frac{\partial C}{\partial t} dt = 0. \quad (\text{E46}).$$

Accepting that the orders of differentiation and integration are able to be exchanged, and that this is valid for the functions of concerned, it follows that:

$$\int_0^\infty e^{-pt} \frac{\partial^2 C}{\partial x^2} dt = \frac{\partial^2}{\partial x^2} \int_0^\infty C e^{-pt} dt = \frac{\partial^2 \bar{C}}{\partial x^2} \quad (\text{E47}).$$

Moreover, via integration by parts, the following result arises

$$\int_0^\infty e^{-pt} \frac{\partial^2 C}{\partial x^2} dt = [C e^{-pt}]_0 + p \int_0^\infty C e^{-pt} dt = p \bar{C} \quad (\text{E48}),$$



as the term in the square bracket disappears at  $t = 0$  by reason of the initial condition, as well, at  $t = \infty$  owing to the exponential factor (Crank, 1975). Consequently, (E45) reduces to:

$$D \frac{\partial^2 \bar{C}}{\partial x^2} = \rho \bar{C} \quad (\text{E49}).$$

Analogous treatment of the boundary condition yields:

$$\bar{C} = \int_0^\infty C_0 e^{-pt} dt = \frac{C_0}{p} \quad (\text{E50}).$$

Therefore, the partial differential equation (E45) is reduced to the conventional differential equation (E49). It ensues that the solution of (E45) fulfilling (E49), and for which  $\bar{C}$  remains finite as  $x$  approaches infinity is

$$\bar{C} = \frac{C_0}{p} e^{-qx} \quad (\text{E51}),$$

where  $q^2 = \rho/D$ . The corresponding function, given by the transform in (E51) is

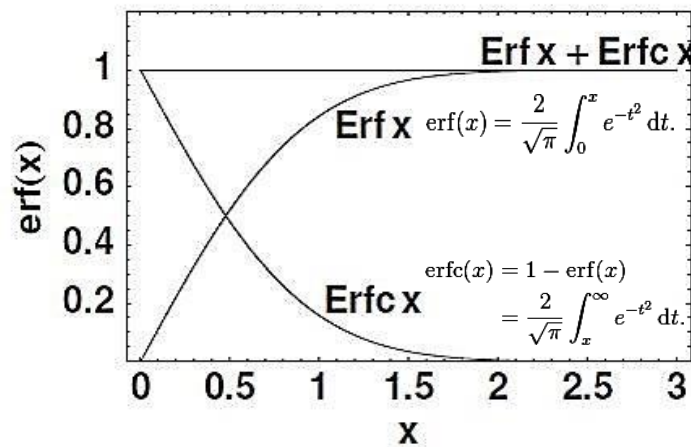
$$C = C_0 \operatorname{erfc} \frac{x}{2\sqrt{Dt}} \quad (\text{E52})$$

(Crank, 1975), where the **erfc x**, the complementary error function of  $x$  is defined as:

$$\operatorname{erfc} x = 1 - \operatorname{erf} x \quad (\text{E53}).$$

Both the error function (**erf x**) and the complementary error function (**erfc x**), are illustrated in **Figure 28**.

It is straightforward to demonstrate that (E52) satisfies (E45), the boundary condition and the initial condition (Crank, 1975), and therefore, that is the requisite solution of the diffusion problem for direct incorporation in the model.



**Figure 28.** The error and complementary error functions, defined and superimposed.

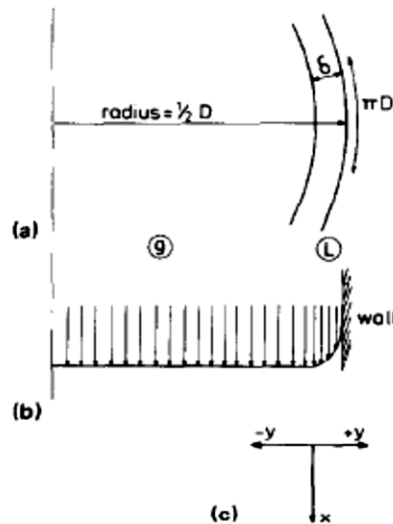
Expression (E52) shows that the solution of the problem of diffusion into a semi-infinite medium having initial concentration,  $C_0$ , and the surface of which is maintained constant (that is,  $C = C_0$ ), involves only the single dimensionless parameter,

$$\frac{x}{2\sqrt{Dt}} \quad (\text{E54}).$$

The **distance of penetration,  $x$** , of any concentration ( $C$ ) is thus computed as:

$$2\sqrt{Dt} \cdot \left(\frac{C}{C_0}\right) \quad (\text{E55}).$$

which holds in general in semi-infinite media, provided that the initial concentration is uniform and the surface concentration remains constant (Crank, 1975), that is,  $C/C_0$  does not decrease by more than a few percent over the reaction time. This is expected to be valid under the experimental conditions — and, is shown to be true for the HA experiments in **Sections 5.2, 5.4 and 5.5**. A physical representation of  $\pi D$  is given in **Figure 29 a** (with co-ordinates shown in **Figure 29 c**). For the typical gas-liquid reaction time employed in the experiments,  $t \approx 1$  s, and the diffusivity of  $\text{NO}_2^-$ ,  $D_{\text{NO}_2^-} = 1.91 \times 10^{-5} \text{ cm}^2 \text{ s}^{-1}$  (CRC Handbook), a penetration depth of  $6.22 \times 10^{-3} \text{ cm}$  is estimated. As the film thickness,  $f$  ( $3.32 \times 10^{-2} \text{ cm}$ ) ( $= x$ ) is about five times greater than the computed value of  $d_{\text{penetration}}$ , the gas-side resistance can be neglected for the experimental setup.



**Figure 29.** Wetted-wall column. (a) film thickness (represented by  $\delta$  here, instead of  $f$ ) with  $D$  representing the diffusivity of the reactant gas in solution; (b) velocity profile; (c) co-ordinates. Symbols  $g$  and  $L$  (encircled) represent gas and liquid-phases, respectively. From: Van Den Berg and Hoornstra (1977).

For the tested 56-long reaction zone ( $L_{\text{rxn zone}}$ ), the length of reaction zone at each time step,  $L_{\text{rxn zone,ts}}$  is simply

$$L_{\text{rxn zone,ts}} = \frac{L_{\text{rxn zone}}}{100 \text{ ts}} \quad (\text{E56}),$$

or 0.56 cm. Therefore, the corresponding diffusion time for the time step ( $t_{\text{diffusion,ts}}$ ) in seconds is

$$t_{\text{diffusion,ts}} = \frac{L_{\text{rxn zone,ts}}}{u_s} \quad (\text{E57}).$$

Recall that  $u_s$ , the surface velocity of the film is  $0.48 \text{ cm s}^{-1}$  for the typical experimental conditions. Substituting the specified parameters into (E55), yields the following expression for computation of the penetration distance at the first time step ( $x_{\text{penetration,s}}$ )

$$x_{\text{penetration,s}} = 2 \sqrt{D_{\text{NO}_2} t_{\text{diff,s}}} \times \left( \frac{[\text{NO}_2]_s}{[\text{NO}_2]_0} \right) \quad (\text{E58}).$$

The formula for  $[\text{NO}_2]_s$  (at first time step) was given previously on p. 64. Finally, the film volume at 0.01 s (incorporating diffusion),  $V_{\text{film,diff,s}}$  is simply derived as the product of the volume at the time step, with diffusion excluded ( $V_{\text{film,s}}$ ), and the fraction  $\frac{x_{\text{penetration,s}}}{f}$ , that is:

$$V_{\text{film,diff,s}} = V_{\text{film,s}} \times \frac{x_{\text{penetration,s}}}{f} \quad (\text{E59}).$$

Lastly, the parameter  $V_{\text{film,s}}$  is calculated as

$$V_{\text{film,s}} = \left( \frac{F_l}{L_{\text{rxn zone}}/u_s} \right) \times \frac{1}{100 \text{ ts}} \quad (\text{E60}),$$

where all parameters have been previously defined. The value of  $1.23 \times 10^{-6} \text{ L}$  obtained for  $V_{\text{film,diff,s}}$  using (E60) can now be substituted in (E30) to mathematically solve for the best-fit reaction probability.

## 4 EXPERIMENTS ON SIMPLE ORGANIC COMPOUNDS

*This preliminary results chapter begins with experiments on several ‘simple’ organic compounds. In **Section 4.1**, the heterogeneous hydrolysis reaction of  $\text{NO}_2$  on a borosilicate surface is discussed, with respect to its proposed reaction mechanism and its reaction order in gas-phase  $\text{NO}_2$ . This section continues with a discussion of impurity specifications for the purified water used for the study of the heterogeneous hydrolysis reaction of  $\text{NO}_2$  in the WWFT photoreactor ( $t_{\text{reac}} \sim 1$  s,  $85.7$   $\text{W}/\text{m}^2$  irradiance). To end Section 4.1, an upper limit for the model-predicted  $\gamma_{\text{best-fit, pH=2 water}}$  is given. The chapter continues in **Section 4.2** with an examination of a photosensitized electron transfer reaction involving  $\text{NO}_2$  and a simple benzophenone, (3,4)-dihydroxyphenylacetic acid (DOPAC) (pH 5, 1.4 mg/L). Details of the postulated reaction mechanism are given, along with a comparison of HONO yields observed by George et al. (2005) for a similar experiment. **Section 4.3** begins anew with a discussion of the proposed mechanism for the photohydrolysis of aqueous 2-nitrophenol (2-NP) in both acidic and basic conditions, including listings of chemical yields for identified intermediates produced, as available from most recent literature. Results from the studied photolysis experiments, which are the first to be performed under acidic conditions (pH 2) at environmentally realistic ortho-nitrophenol levels (5 mg/L in MeOH; 2-NP and 4M2NP, respectively) are presented for the reader. Next, HONO yield data is shown for (both urban and extreme levels)  $\text{NO}_2$  uptake experiments on these films and the individual data is used to estimate how uniformly the films are reproduced over  $N$  individual uptake experiments. Lastly, as an extension to 4.3, the possibility of analyzing the WWFT effluent following uptake experiments was examined. Photoenhancement data for the  $\text{NO}_2$  uptake on  $\text{DOPAC}_{\text{pH=5}}$  reaction obtained using the WWFT photoreactor is shown and compared with that of George et al. (2005) for a similar experiment. Finally, in the final section (4.4), the slight HONO production data presented for the  $\text{NO}_2$  uptake reaction on potassium hydrogen phthalate (KHP, pH 2, 0.5 mM) is shown as an example of general base catalysis.*

#### 4.1 WATER (MAY HAVE ORGANIC CONTAMINANTS)

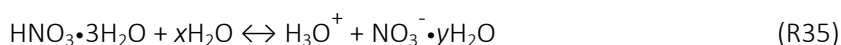
Within the last decade, Finlayson-Pitts et al. (2003) proposed a new reaction mechanism for the heterogeneous hydrolysis (of moderate acidity) reaction of  $\text{NO}_2$

surface



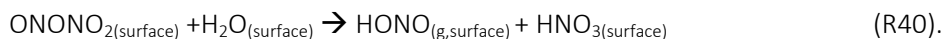
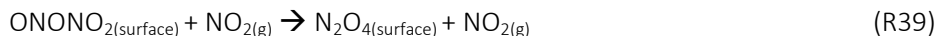
on a common laboratory surface, namely, borosilicate glass. Silicates, being major components of both building materials (Shao et al., 2013) and soils (Tarafder and Thakur, 2013), are atmospherically relevant, and thus, essential to the extrapolation of such processes in urban air sheds. Finlayson-Pitts et al. (2003) hypothesize that the symmetric form of the  $\text{NO}_2$  dimer,  $\text{N}_2\text{O}_4$ , is taken up on the surface, and isomerizes to the asymmetric form,  $\text{ONONO}_2$ . The asymmetric form auto-ionizes to  $\text{NO}^+\text{NO}_3^-$  which then reacts with water to produce HONO and surface-adsorbed  $\text{HNO}_3$ . As the WWFT column is composed of borosilicate glass (approximately 80% silica, 13% boric oxide, 4% sodium oxide, and 2-3% aluminum oxide; see Vogel, 1994), it is expected that the proposed mechanism by Finlayson-Pitts et al. (2003) for the  $\text{NO}_2$  hydrolysis reaction on the glass column will apply to the WWFT photoreactor.

Recently, Ramazan et al. (2006) have observed that the nitric acid formed during  $\text{NO}_2$  heterogeneous hydrolysis (at intermediate relative humidities typical of the tropospheric boundary layer) exists both as nitrite ions from the dissociation of nitric acid formed on the surface and as molecular nitric acid, with the ions and  $\text{HNO}_3$  complexed to water molecules in both cases. Plausible equilibria involved include the following (Ramazan et al., 2006):



Selective removal of water shifts the  $\text{NO}_3^- - \text{HNO}_3(\text{H}_2\text{O})_y$  equilibria towards more dehydrated forms of nitric acid, and eventually, to nitric acid dimers (Ramazan et al., 2006). Under  $\lambda = 300 - 400$  nm radiation (WWFT radiation conditions,  $\lambda_{\text{max}} = 354$  nm), the nitric acid–water film produces gas-phase nitrous oxide (NO) (Ramazan et al., 2006).

The mechanism, (M10) proposed by Finlayson-Pitts et al. (2003) predicts that HONO formation is **first-order** in gas-phase NO<sub>2</sub> in spite of N<sub>2</sub>O<sub>4</sub> being a major precursor to HONO. This is a result of the back reaction of asymmetric ONONO<sub>2</sub> with gas-phase NO<sub>2</sub>. Detailed below are the main reactions involved:



Finlayson-Pitts et al. (2003) derive the steady-state concentration of surface ONONO<sub>2</sub>, denoted [ONONO<sub>2</sub>]<sub>ss</sub>, provided that the rate of reaction of ONONO<sub>2</sub> with NO<sub>2</sub> to regenerate surface N<sub>2</sub>O<sub>4</sub> is faster than its reaction with water, that is,  $k_{39} [\text{NO}_2] \gg k_{40} [\text{H}_2\text{O}]$ :

$$[\text{ONONO}_2]_{\text{ss}} = \frac{k_{39}K_{36}K_{37} \cdot [\text{NO}_2][\text{NO}_2]}{k_{39} [\text{NO}_2]} = C [\text{NO}_2] \quad (\text{E61}),$$

where  $k_{38}$  and  $k_{39}$  are the respective rate constants for reactions (R38) and (R39),  $K_{36}$  and  $K_{37}$  are the equilibrium constants for reactions (R36) and (R37), and  $C$  is  $(k_{38}K_{36}K_{37}/k_{39})$ , the combination of the respective rate and equilibrium constants. Therefore, the rate of HONO generation for the proposed mechanism is:

$$\frac{d[\text{HONO}]}{dt} = k_{40}[\text{ONONO}_2][\text{H}_2\text{O}_{(\text{surface})}] = k_{40}C[\text{H}_2\text{O}_{(\text{surface})}][\text{NO}_2] \quad (\text{E62}),$$

which is first-order in NO<sub>2</sub>. Note: however, that the experimentally determined reaction order for loss of NO<sub>2</sub> is considerably higher, 1.6 (±0.2); the grounds for the inconsistency between this empirical value and the expected value of 1.0 are ambiguous.

The Type 1 (TOC = 1 ppbm) purified water (Milli-Pore, Total Organic Carbon determined via an online Milli-Pore TOC Analyzer) used for uptake experiments used without further purification contains inorganic as well as organic (volatile and semi-volatile) (Whitehead, 2009) as listed in **Table 8 (A) through (C)**.

Whitehead (2009) found that all inorganic elements (see **Table 8 (A)**) were effectively absent from the ultrapure water, most with detection limits of less than  $1 \text{ ng L}^{-1}$  (ppt) using the latest ICP-MS techniques. As Nash (1970) observed that “catalysis” via transition metal ions, namely  $\text{Fe}^+$  (ferrocyanide) was found to only have significant impact on the  $\text{NO}_2$  hydrolysis reaction (Lee and Schwartz, 1981) for rather concentrated aqueous solutions ( $\geq \sim 0.01 - 0.1 \text{ M}$  range), additional HONO production from catalysis by the inorganic impurities in the ultrapure water film is not expected.

Preliminary results of Nash (1970) indicate that nitrogen dioxide acts as an electrophilic reagent, reacting rapidly with phenoxide ions, less rapidly with aromatic bases, and not at all with aromatic amine cations or un-ionized phenols. **Electron transfer** reactions involving  $\text{NO}_2$  with the following organic species in solution have been studied (to date): methylphenols and hydroxybenzenes (Alfassi et al., 1986; and Gutzwiller et al., 2002), catechins (Miao et al., 2001), and hydroxycinnamic acid derivatives (Zhan et al., 1998). Thus, (additional) HONO generation from electron transfer reactions with  $\text{NO}_2$  involving the volatile and semi-volatile organic impurities (Whitehead, 2009) found in the Level 1 ultrapure water (refer to **Table 8 (B) and (C)**) may be expected. However, given the very low levels, ( $< 0.05 \text{ } \mu\text{g L}^{-1}$ ) for volatile and ( $< 0.025 \text{ } \mu\text{g L}^{-1}$ ) for semi-volatile organic impurities of these organic impurities (both below the limits of detection for the respective analytical measurement techniques; see Whitehead, 2009), it is expected that any additional HONO formation from such electron transfer reaction reactions with  $\text{NO}_2$  will not be significant.

In order to maximize its purity, soon after it was dispensed into a glass carboy (within 2 days), the ultrapure water was used for the  $\text{NO}_2$  hydrolysis experiments. A glass carboy was utilized for storage as opposed to plastic on the suggestion of Horikiri (2006) who observed di-*n*-octyl phthalate (among other impurities, analysis by LC-MS) at much lower levels in the ultrapure water stored in glass. The risk of contamination from an additional plasticizer, *n*-butyl benzene sulfonamide (chemical structure shown in **Figure 30**) which can leach into the Level 1 ultrapure water (Whitehead, 2009) was minimized by not affixing a length of flexible plastic tubing to the Milli-Pore purifier with the fixed tap dispenser (in order to improve the convenience of filling a large carboy).

A

Element	ICP-MS Result: ppt
Aluminium	<1
Antimony	<0.2
Arsenic	<2
Cadmium	<0.5
Calcium	<2
Chromium	<1
Copper	<2
Iron	<2
Lead	<0.2
Magnesium	<1
Manganese	<0.5
Mercury	<5
Nickel	<2
Potassium	<5
Sodium	<2
Tin	<0.5
Titanium	<0.5
Vanadium	<0.2
Zinc	<2
Bromide	<20
Chloride	<20
Fluoride	<30
Nitrate	<20



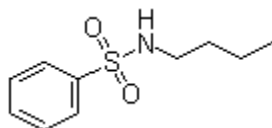
B

Volatile organic compounds by Purge & Trap GC-MS			
	Result		Result
	µg/l (ppb)		µg/l (ppb)
benzene	<0.05	1,3-dichloropropane	<0.05
bromobenzene	<0.05	2,2-dichloropropane	<0.05
bromochloromethane	<0.05	1,1-dichloropropene	<0.05
bromodichloromethane	<0.05	cis-1,3-dichloropropene	<0.05
bromoform	<0.05	trans-1,3-dichloropropene	<0.05
bromomethane	<0.05	ethylbenzene	<0.05
2-butanone (MEK)	<0.05	hexachlorobutadiene	<0.05
n-butylbenzene	<0.05	hexane	<0.05
sec-butylbenzene	<0.05	isopropyl alcohol	<0.05
tert-butylbenzene	<0.05	isopropylbenzene	<0.05
carbon tetrachloride	<0.05	isopropyltoluene	<0.05
chlorobenzene	<0.05	methyl tert-butyl ether	<0.05
chlorodibromomethane	<0.05	naphthalene	<0.05
chloroethane	<0.05	n-propylbenzene	<0.05
chloroform	<0.05	styrene	<0.05
chloromethane	<0.05	1,1,2-tetrachloroethane	<0.05
2-chlorotoluene	<0.05	1,1,2-tetrachloroethane	<0.05
4-chlorotoluene	<0.05	tetrachloroethane	<0.05
1,2-dibrom-3-chloropropane	<0.05	Toluene	<0.05
1,2-dibromomethane (EDB)	<0.05	1,2,3-trichlorobenzene	<0.05
dibromomethane	<0.05	1,2,4-trichlorobenzene	<0.05
1,2-dichlorobenzene	<0.05	1,3,5-trichlorobenzene	<0.05
1,3-dichlorobenzene	<0.05	1,1,1-trichloroethane	<0.05
1,4-dichlorobenzen	<0.05	1,1,2-trichloroethane	<0.05
dichlorodifluoromethane	<0.05	trichloroethene	<0.05
1,1-dichloroethane	<0.05	trichlorofluoromethane	<0.05
1,2-dichloroethane	<0.05	1,2,3-trichloropropane	<0.05
1,1-dichloroethane	<0.05	1,2,4-trimethylbenzene	<0.05
cis-1,2-dichloroethane	<0.05	1,2,5-trimethylbenzene	<0.05
trans-1,2-dichloroethane	<0.05	vinyl chloride	<0.05
dichloromethane	<0.05	o-xylene	<0.05
1,2-dichloropropane	<0.05	m-xylene & p-xylene	<0.05

C

Semi-volatile compounds by thermal-desorption GC-MS			
	Result		Result
	µg/l (ppb)		µg/l (ppb)
Acenaphthene	<0.025	Hexachlorobutadiene	<0.025
Acenaphthylene	<0.025	Hexachlorocyclopentadiene	<0.025
Anthracene	<0.025	Hexachloroethane	<0.025
Benidine	<0.025	Isophorone	<0.025
Benzo (a) anthracene	<0.025	2-methylnaphthalene	<0.025
Benzo (b) fluoranthene	<0.025	Naphthalene	<0.025
Benzo (k) fluoranthene	<0.025	2-nitroaniline	<0.025
Benzyl alcohol	<0.025	3-nitroaniline	<0.025
Butyl benzyl phthalate	<0.025	4-nitroaniline	<0.025
Bis(2-chloroethoxy)methane	<0.025	Nitrobenzene	<0.025
Bis(2-ethylhexyl)phthalate	<0.025	N-nitrosodimethylaniline	<0.025
Bis(2-chloroisopropyl)ether	<0.025	N-nitrosodiphenylaniline	<0.025
Bisphenol A	<0.025	Nonylphenol	<0.025
4-bromophenyl phenyl ether	<0.025	Phenanthrene	<0.025
Carbazole	<0.025	Pyrene	<0.025
4-chloroaniline	<0.025	Pyridine	<0.025
2-chloronaphthalene	<0.025	1,2,4-trichlorobenzene	<0.025
4-chlorophenyl phenyl ether	<0.025	Benzoic acid	<0.025
Chrysene	<0.025	4-chloro-3-methylphenol	<0.025
Dibenzofuran	<0.025	2-chlorophenol	<0.025
1,2-dichlorobenzene	<0.025	Cresols	<0.025
1,3-dichlorobenzene	<0.025	2,4-dichlorophenol	<0.025
1,4-dichlorobenzene	<0.025	2,4-dimethylphenol	<0.025
3,3'-dichlorobenzidine	<0.025	2,4-dinitrophenol	<0.025
Diethyl phthalate	<0.025	4,6-dinitro-2-methylphenol	<0.025
Dimethyl phthalate	<0.025	2-methylphenol	<0.025
Di-n-butyl phthalate	<0.025	4-methylphenol	<0.025
2,6-dinitrotoluene	<0.025	4-nitrophenol	<0.025
Di-n-octyl phthalate	<0.025	Pentachlorophenol	<0.025
Fluoranthene	<0.025	Phenol	<0.025
Fluorene	<0.025	2,4,5-trichlorophenol	<0.025
Hexachlorobenzene	<0.025		

**Table 8.** Impurity specifications of Type 1 ultrapure water (TOC = 1 ppb). (A) Elemental impurities analysed by ICP-MS in units of  $\text{ng L}^{-1}$  (ppt). (B) Volatile organic compounds (VOCs) analysed by purge & trap GC-MS. (C) Semi-volatile organic compounds analysed by thermal desorption GS-MS. Impurities in (B), (C), are also in units of  $\mu\text{g L}^{-1}$  (ppb). From: Whitehead (2006).

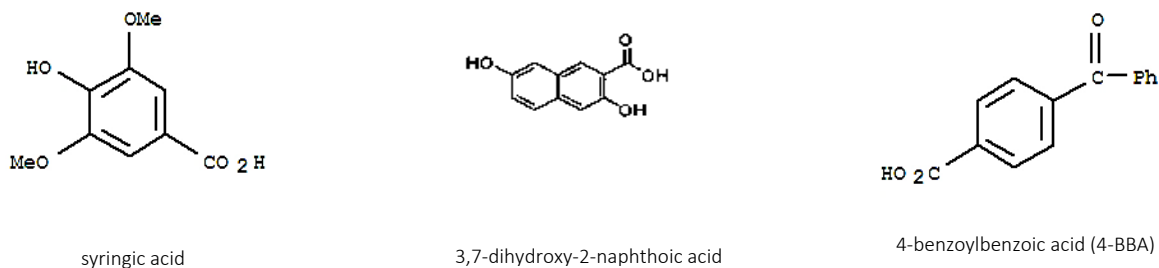


**Figure 30.** Chemical structure of plasticizer, *n*-butyl benzene sulfonamide.

The uptake of NO<sub>2</sub> on deionized water (at pH's 2 and 6), investigated using the WWFT photoreactor (t<sub>reac</sub> of 1 s) for NO<sub>2</sub> mixing ratios of 14, 42, and 71 ppbv (verified using the NO<sub>2</sub> detector) in the dark and under irradiation (4 lamps), and was found to be beyond the sensitivity (i.e., negligible, *n* = 3) of the WWFT and the HONO/NO<sub>2</sub><sup>-</sup> and NO<sub>2</sub> measurement techniques. Therefore, it can be concluded that in the dark and under irradiation, the uptake of NO<sub>2</sub> on a purified water film (pH's 2 and 6) due to the hydrolytic disproportionation of NO<sub>2</sub> on the borosilicate column (WWFT photoreactor) and/or an electron transfer reaction of NO<sub>2</sub> with an organic impurity (in the ultrapure water) is unimportant under the tested conditions. The exceedingly low probability of (R29) (hydrolytic disproportionation) observed (upper limit for model-predicted best-fit  $\gamma_{\text{pH}=2}$  of  $1.26 \times 10^{-10}$ ) is consistent with molecular dynamics (MD) calculations illustrating that the hydrophobic free radical NO<sub>2</sub> has a strong propensity for the surface of neutral clusters NO<sub>2</sub>(H<sub>2</sub>O)<sub>*n*</sub> (Bezrukov et al., 2004; and Yabushita et al., 2009).

#### 4.2 3,4-DIHYDROXYPHENYLACETIC ACID (DOPAC)

George et al. (2005) have recently observed enhanced NO<sub>2</sub> → HONO conversion during ultraviolet-A radiation for *solid* films of mixtures of synthetic phenols and an aromatic light absorber (a benzophenone), with organic substrates containing a combination of electron donors (i.e., phenols) and compounds yielding excited triplet states (i.e., aromatic ketones) found to show the highest reactivity (up to 100%) towards NO<sub>2</sub>. Refer to **Figure 31** for selected chemical structures of compounds tested by George et al. (2005), as well as to **Table 9** for the corresponding yields observed.



**Figure 31.** Selected chemical structures are given for syringic acid, (3,7)-dihydroxy-2-naphthoic acid, and 4-benzoylbenzoic acid (4-BBA).

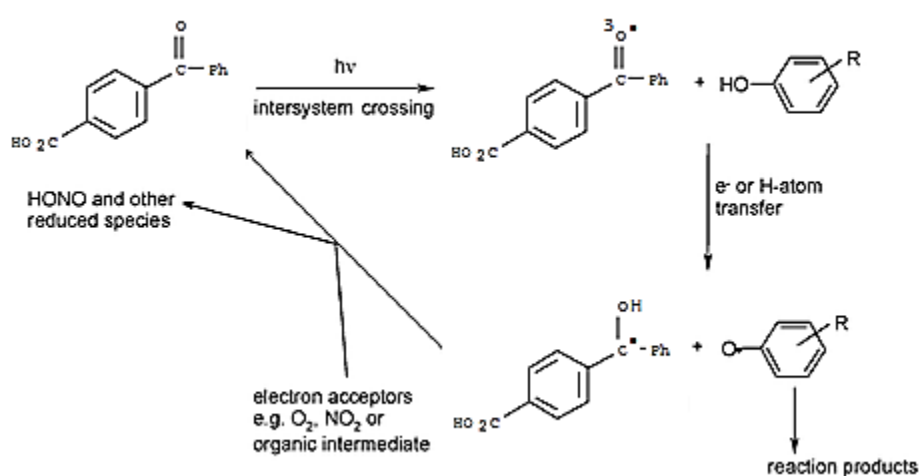
Type of organic coating and amount of organic compound used	Removal of initial [NO <sub>2</sub> ] by dark reaction <sup>b</sup> (%)	Yield of HONO per reacted NO <sub>2</sub> in dark reaction (%)	Removal of initial [NO <sub>2</sub> ] by light reaction <sup>cd</sup> (%)	Yield of HONO per reacted NO <sub>2</sub> in light reaction (%)
Sodium 4-benzoylbenzoate (1 mg)	4	7	20/17	45/48
4-benzoylbenzoic acid (1 mg)	2	n.a.	12/12	68/71
3,7-dihydroxy-2-napthoic acid (1 mg)	4	11	22/28/38 <sup>e</sup>	67/74/77
Perylene (0.5 mg)	3	n.a.	~ 0/0	n.a
Syringic acid (1 mg)	6	6	7/7	36/43
3,4-dihydroxyphenylacetic acid (1 mg)	6	n.a.	1/2	n.a
Potassium iodide (1 mg)	53	100	~ 0/0	n.a
External mixture <sup>a</sup> Sodium 4-benzoylbenzoate (1 mg) Syringic acid (0.5 mg)	4	4	36/36	61/70
External mixture <sup>a</sup> Sodium 4-benzoylbenzoate (1 mg) 3,4-dihydroxyphenylacetic acid (1 mg)	2	n.a.	42/38	91/90
External mixture <sup>a</sup> Sodium 4-benzoylbenzoate (1 mg) Potassium iodide (1 mg)	14	n.a	66/58	93/101
External mixture <sup>a</sup> Perylene (0.5 mg) 3,4-dihydroxyphenylacetic acid (1 mg)	2	n.a.	6/9	57/67
External mixture <sup>a</sup> Perylene (0.5 mg) Potassium iodide (1 mg)	20	> 80	7/10	n.a
Internal mixture <sup>a</sup> 4-benzoylbenzoic acid (1 mg) 3,4-dihydroxyphenylacetic acid (0.5 mg)	16	n.a	52/63	90/93
Internal mixture <sup>a</sup> 4-benzoylbenzoic acid (1 mg) 3,4-dihydroxyphenylacetic acid (1 mg)	7	n.a.	47/58	95/97

<sup>a</sup> The term external mixture is used when the reactor surface was coated first by the absorber molecule and subsequently by the phenol or potassium iodide. The term internal mixture is used when the reactor was coated from one solution containing both compounds. <sup>b</sup> The removal of NO<sub>2</sub> due to the dark reaction was measured by exposing the coated wall reactor to the NO<sub>2</sub>-mixture and measuring the decrease of the NO<sub>2</sub> concentration. <sup>c</sup> The removal of NO<sub>2</sub> due to the light reaction was measured by illuminating the NO<sub>2</sub>-mixture flowing through the coated wall reactor and comparing the NO<sub>2</sub> concentration before and during the irradiation. <sup>d</sup> Values after 5 and 10 min of irradiation, respectively. <sup>e</sup> Values after 5, 10 and 25 min of irradiation, respectively.

**Table 9.** Reactivity and HONO yields of the reaction of NO<sub>2</sub> (RH = 20%) with selected dried organic films (0.5 mL) of different compositions in the dark and under irradiation (300 – 420 nm) as found by George et al. (2005).

The mechanism (M11) proposed by George et al. (2005) (shown in **Figure 32**), for the *photosensitized electron transfer* reaction, with the primary electron donor (phenolic compound) coming from the synthetic organic film, is based on findings from photochemical experiments in solution (Murov and Hug, 1993), which conclude that the photoexcitation of benzophenones produces excited triplet states of benzophenone in near unity yield. Note that the high yields achieved by George et al. (2005) from the stoichiometry of formation of HONO from NO<sub>2</sub> in the presence of 4-BBA (especially when mixed with a

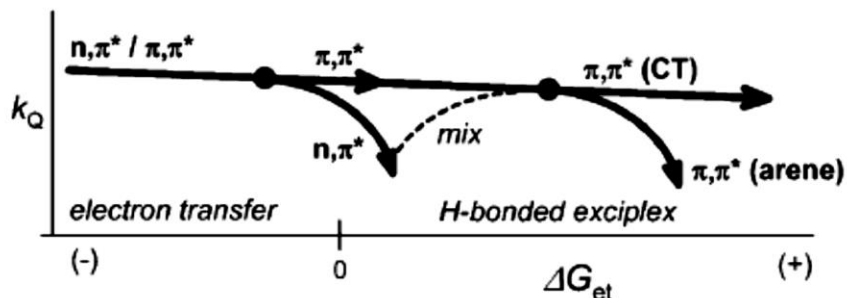
phenolic compound) revealed that the reaction cannot be explained as a catalyzed disproportionation of  $\text{NO}_2$  on wetted surfaces. Acting as one-electron oxidants, these triplet states react with electron donor-substituted phenols in near-diffusion controlled rates (Canonica et al., 2000), with the resultant products being phenoxy radicals and reduced benzophenones (diphenyl ketyl radicals) proceeding via a simple electron-transfer/proton-transfer mechanism. Reactive radical intermediates generated by this photosensitized reaction are thought to be reactive towards electrons acceptors such as  $\text{NO}_2$ , finally resulting in HONO (when  $\text{pH}_{\text{film}} < \text{pK}_{\text{a,HONO}}$ ) and other reduced species, with accumulation of the reduced benzophenone in the absence of  $\text{NO}_2$ .



**Figure 32.** Proposed reaction mechanism (M11) for the photoreduction of  $\text{NO}_2$  to HONO in the presence of 4-benzoylbenzoic acid (4-BBA) (absorbing photosensitizer) and a substituted phenol (electron donor). Modified from: George et al. (2005).

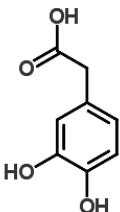
The results of a more recent study conducted by Lathioor and Leigh (2006) find a simple electron-transfer mechanism which applies to the  $n, \pi^*$  triplet ketones and those  $\pi, \pi^*$  triplets with particularly low reduction potentials, and a coupled electron-/proton-transfer mechanism (see **Figure 33**) involving the intermediacy of a hydrogen-bonded exciplex, which applies to the  $\pi, \pi^*$  ketone triplets. Lathioor and Leigh (2006) found that ketones with lowest charge-transfer  $\pi, \pi^*$  states exhibit rate constants which only vary slightly with triplet reduction potential over the range they studied as a result of the compensating effect of substituents on triplet state basicity and reduction potential (they both play a role in quenching by the H-bonded exciplex mechanism). Finally, ketones with arenoid  $\pi, \pi^*$  states displayed a fall-off in rate-constant typical of electron-transfer reactions, but for a much higher potential than would be

normally expected as a result of the effects of H-bonding on the rate of electron-transfer within the exciplex.



**Figure 33.** A coupled electron-/proton-transfer mechanism involving the intermediacy of a hydrogen-bonded exciplex, which applies to the (arene)  $\pi, \pi^*$  ketone triplets proposed by Lathioor and Leigh (2006). The subscript et indicates electron transfer.

One of the model electron donors employed in the study by George et al. (2005), namely, 3,4-dihydroxyphenylacetic acid (DOPAC), was selected for its ability to react directly with  $\text{NO}_2$  in a dark reaction yielding nitrite (when  $\text{pH}_{\text{film}} > \text{pK}_{\text{a,HONO}}$ ) or nitrous acid (when  $\text{pH}_{\text{film}} < \text{pK}_{\text{a,HONO}}$ ). The chemical structure, water solubility and one-electron reduction potential are given in **Table 10** for this compound.

Chemical structure	
Water solubility <sup>a</sup> (mg L <sup>-1</sup> )	$8.6 \times 10^4$
One-electron reduction potential <sup>b</sup> (mV)	21

**Table 10.** Chemical structure, water solubility and one-electron reduction potential for the model electron donor, DOPAC, employed in the study by George et al. (2005). <sup>a</sup> Water solubility at 25°C generated from the US Environmental Protection Agency's EPI Suite; from  $\text{Log } K_{\text{ow}} = 0.98$  (WSKOW v1.41, expkow database); <sup>b</sup> One-electron reduction potential obtained for an ionic strength,  $I = 0.5 \text{ M}$ ,  $\text{pH} = 13.5$ . Reference compound: DMAP; reference reduction potential = 174 mV, glycol as co-solute. Data from: Steenken and Neta (1982).

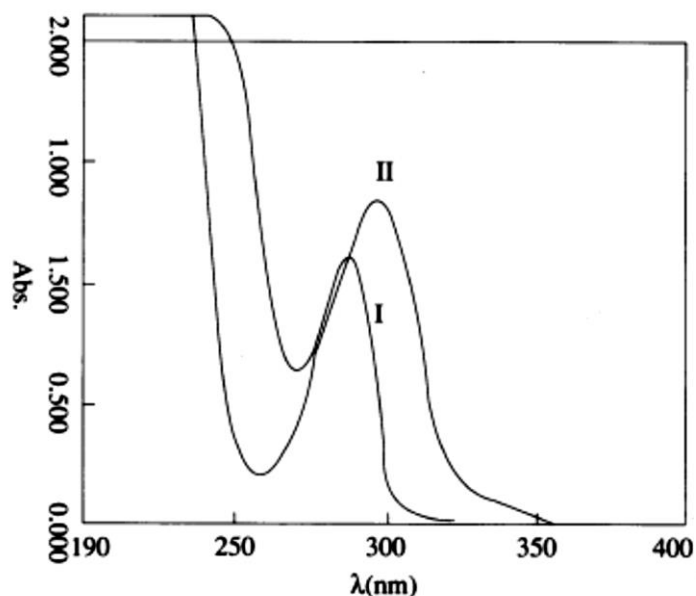
For a similar photoreactor tube, with a gas-film residence time of about 0.5 seconds (half of  $t_{\text{reac}}$  used in this study), George et al. (2005), observed a 6 % (no precision given) reactive loss of  $\text{NO}_2$  ( $[\text{NO}_2]_0 = 20 \text{ ppbv}$ ,  $\text{RH} = 20 \%$ ) for a  $1 \text{ mg mL}^{-1}$ -DOPAC solid film in the dark. Under typical experimental conditions, an

11 ( $\pm 0.07$ )% reactive loss of  $\text{NO}_2$  is observed, that is, 7.9 ( $\pm 0.03$ ) ppbv of the initial  $[\text{NO}_2]_0 = 75$  ppbv (verified using the  $\text{NO}_2$  detector) reacted in the dark for a fresh unbuffered  $1.4 \text{ mg L}^{-1}$  DOPAC solution (pH 5) and a  $t_{\text{reac}}$  of 1 s (see **Table 11**). However, the reaction was not significantly photoenhanced under typical irradiation conditions ( $\lambda_{\text{max}} = 354 \text{ nm}$ ), with 8.3 ( $\pm 0.4$ ) ppbv of the initial 75 ppbv  $\text{NO}_2$  reacted (corresponding to a  $12 \pm 0.1$  % reactive loss of  $\text{NO}_2$ ), and negligible HONO production occurred upon irradiation (refer to **Table 11**). The reference (blank) film (pH 5, deionized  $\text{H}_2\text{O}$ ), also yielded negligible HONO (and  $\text{NO}_2^-$ ) concentrations.

N	Dark Reaction		Light Reaction	
	Removal of initial $[\text{NO}_2]$ ( $\pm 1\sigma$ ) <sup>a</sup> (%)	Yield of HONO per reacted $\text{NO}_2$ ( $\pm 1\sigma$ ) (%)	Removal of initial $[\text{NO}_2]$ ( $\pm 1\sigma$ ) <sup>a</sup> (%)	Yield of HONO per reacted $\text{NO}_2$ ( $\pm 1\sigma$ ) (%)
1	11 ( $\pm 0.3$ )	n.a. <sup>b</sup>	11 ( $\pm 0.4$ )	n.a.
2	10 ( $\pm 0.3$ )	n.a. <sup>b</sup>	12 ( $\pm 0.3$ )	n.a.

**Table 11.** Reactivity and HONO (or  $\text{NO}_2^-$ ) yields of the reaction of  $\text{NO}_2$  ( $[\text{NO}_2]_0 = 71$  ppbv) with unbuffered DOPAC film ( $1.4 \text{ mg mL}^{-1}$  in deionized water,  $\text{pH}_{\text{film}} = 5$ ) in the dark and under irradiation (4 lamps) using the WWFT photoreactor and  $t_{\text{reac}}$  of 1 s. The removal of  $\text{NO}_2$  (%) represents the percentage decrease in the reactant  $\text{NO}_2$  concentration due to the  $\text{NO}_2(\text{g}) + \text{DOPAC}_{(\text{aq.})}$  reaction. <sup>a</sup>The precision obtained from 25 data points. <sup>b</sup>The term n.a. indicates that *negligible* HONO(g) and  $\text{NO}_2^-$  (aq) concentrations were observed resulting from the tested  $\text{NO}_2(\text{g}) + \text{DOPAC}_{(\text{aq.})}$  reaction ( $n = 3$ ).

For the moderately acidic film (pH 5) used in these most recent DOPAC experiments, it is expected that approximately 0.26% of the N(III) has partitioned into the gas-phase as HONO (or 21.58 pptv), and, thus, is assigned as an upper bound for N(III) conversion % (using (E27)), however, this was not what was observed. George et al., (2005) also observed no significant photoenhancement with a slight HONO production upon irradiation, thus providing confidence in the WWFT photoreactor method herein. This, is rather unexpected since DOPAC is scarcely absorbing under the tested light conditions (the absorption spectrum of DOPAC in the  $\lambda = 190$  to 400 nm region is given in **Figure 34**), and may be related to impurities present in the  $\geq 96\%$  purity standard used or on the reactor wall, or even possibly to absorbing species generated during the exposure of the compounds to the  $\text{NO}_2/\text{zero-air}$  mixture in the reactor (George et al., 2005). The former reason seems less likely as the selected experimental approach (WWFT photoreactor) prevents accumulation of impurities and/or reaction products via a rapidly renewed (in just under 2 min.) aqueous film.



**Figure 34.** Absorption spectrum of 3,4-dihydroxyphenylacetic acid (DOPAC) in the  $\lambda = 190$  to 400 nm region. *Curve I:* pH 5.16. *Curve II:* pH 9.85 (shown for comparison). From: Aydin and Özer (1997).

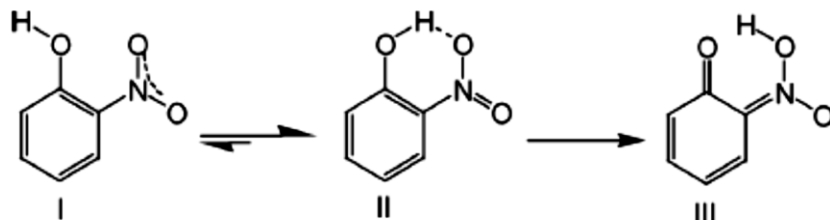
### 4.3 ORTHO-NITROPHENOLS

The kinetics of the uptake of  $\text{NO}_2$  (including photolysis,  $[\text{NO}_2] = 0$  ppbv) on films of the selected *ortho*-nitrophenols, 2-nitrophenol (2-NP, 98%, Aldrich), and its methylated analogue, 4-methyl-2-nitrophenol (4M2NP, 99%, Aldrich) at an environmentally relevant concentration ( $5 \text{ mg L}^{-1}$ , pH 2), required thorough experimental examination using the WWFT photoreactor since there exists the possibility of photochemical conversion of  $\text{NO}_2$  into nitrous acid on such organic surfaces containing phenoxy type compounds (Ammann et al., 2005). Working solutions ( $5 \text{ mg L}^{-1}$ , pH 2) of 2-NP and 4M2NP were freshly prepared in 5% MeOH from their respective stock solutions ( $100 \text{ mg L}^{-1}$  in 100% MeOH) prior to the experiments.

In the atmospherically relevant UV range of 300 – 400 nm, nitrophenols have a strong absorption, corresponding to the  $S_1 \leftarrow S_0$  transition as reported for the liquid-phase (Ishag and Moseley, 1977; Harrison et al., 2005, and references therein; Alif et al., 1991; and Bing et al., 2005), with its formation believed to be due to intramolecular interactions and solvent reactions. 2-nitrophenol (2-NP), with its OH and  $\text{NO}_2$  groups in ortho position to each other (see structure I in **Figure 35**), and its derivatives (i.e., 4-NP,



4M2NP, etc.), differ significantly from other nitrophenols in their physicochemical properties, given in **Table 12** (Sax and Lewis, 1987).



**Figure 35.** The strong intramolecular hydrogen bonding as seen in structure II can be considered the first step in a photon transfer process, (R9), leading to a nitronic acid structure III. From: Bejan et al. (2006).

Parameter	2-Nitrophenol	4-Nitrophenol
Molecular mass (g/mol)	139.11	139.11
Melting point (°C)	44–45 (1)(2)(3)	113–114 (1)(2)(3)
Boiling point (°C)	214–217 (1)	279 (decomposition)(3)
Vapour pressure (kPa)	$6.8 \times 10^{-3}$ (19.8 °C) (4)	$3.2 \times 10^{-6}$ (20 °C) (5)
Water solubility (g/litre)	1.26 (20 °C) (4)	12.4 (20 °C) (6)
<i>n</i> -Octanol/water partition coefficient (log $K_{ow}$ )	1.77–1.89 (7)	1.85–2.04 (7)
Dissociation constant (pK <sub>a</sub> )	7.23 (21.5 °C) (8)	7.08 (21.5 °C) (8)
Ultraviolet spectrum	• <sub>max</sub> (water): 230; 276 nm; log • <sub>max</sub> : 3.57; 3.80 (9)	• <sub>max</sub> (methanol): no absorption maxima • 290 nm (9)
Conversion factors	1 mg/m <sup>3</sup> = 0.173 ppmv 1 ppmv = 5.78 mg/m <sup>3</sup>	

References: (1) Budavari et al. (1996); (2) Booth (1991); (3) Verschuere (1983); (4) Koerdel et al. (1981); (5) Sewekow (1983); (6) Andrae et al. (1981); (7) BUA (1992); (8) Schwarzenbach et al. (1988); (9) Weast (1979)

**Table 12.** Physicochemical properties of 2- and 4-nitrophenol (NP). From: Boehncke et al.

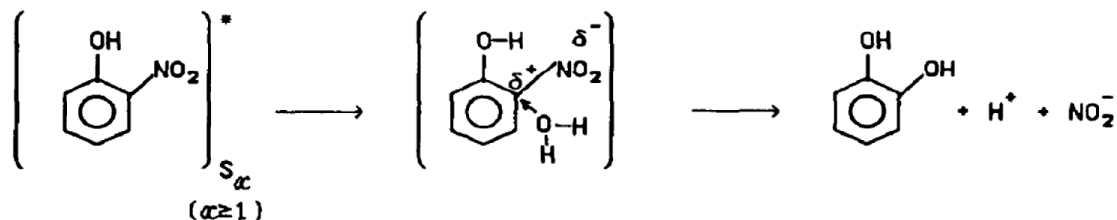
Strong intramolecular hydrogen bonding as seen in structure II (**Figure 35**) accounts for the significant difference (Kovács et al., 2000; Chen and Chieh, 2003). The strong intramolecular hydrogen bonding can be considered the first step in a photon transfer process, resulting in the nitronic acid structure III (in

**Figure 35)** (Bejan et al., 2006). Dissociation of structure III yielding HONO has been predicted based on theoretical calculations (Polášek et al., 2001).

Bing et al. (2005) have recently studied the direct photolysis of 2-nitrophenol, for a (non-renewable) *basic* solution of similar concentration (0.101 mM or 14.0 mg L<sup>-1</sup>), and determined a quantum yield,  $\Phi_{2\text{-NP}}$  in the wavelength range from  $\lambda = 200$  to 400 nm of  $1.44 (\pm 0.02) \times 10^{-3}$  (compare with the earlier value of  $7.8 \times 10^{-4}$  obtained by Alif (1991) for a 278 mg L<sup>-1</sup> 2-NP solution). Their research allowed identification of the major photoproducts (summarized in **Table 13**) including: nitrohydroquinone, and catechol, with photohydrolysis into catechol via proposed mechanism (M12) (see **Figure 36**), as well as oxalate (C<sub>2</sub>O<sub>4</sub><sup>2-</sup>) and total inorganic nitrogen,  $\text{IN} = (\text{NO}_2^- + \text{NO}_3^-)$  in basic solution. Nitrous acid is the main photoproduct observed in acidic solution (Bing et al., 2005).

Identified intermediates	<i>o</i> -NP
Nitrohydroquinone	7.8
Nitrocatechol	< 0.1
Catechol	1.3
Phenol	-
NO <sub>2</sub> <sup>-</sup>	3.0
NO <sub>3</sub> <sup>-</sup>	2.3
C <sub>2</sub> O <sub>4</sub> <sup>2-</sup>	5.9
Maleic acid	0.1
Formic acid	0.4

**Table 13.** Chemical yields for identified intermediates produced by direct photolysis of *o*-NP (2-NP) ( $\sim 0.1$  mmol L<sup>-1</sup>) aqueous *basic* solution after 15 min. of irradiation. Yields given as a percentage: yield (%) =  $100[\text{o-NP}]/[\text{o-NP}]_0$ . From: Bing et al. (2005).



**Figure 36.** Proposed heterolytic mechanism (M12) for the photohydrolysis of aqueous 2-NP into catechol (Alif et al., 1991), similar to that proposed for the phototransformation of 3-chlorophenol (Boule et al., 1982), chlorobenzene (Tissot et al., 1984), and 3- and 4- nitrophenol (Alif et al., 1990). At  $\lambda = 365$  nm, the corresponding excitation is for the transition  $S_0 \rightarrow S_1$ .

Although *no* HONO production ( $n = 4$ ) was observed as a result of phototransformation (4 lamps,  $\lambda = 354$  nm,  $t_{\text{reac}}$  of 1 s) of the acidic (pH 2) *ortho*-nitrophenol films at an environmentally relevant concentration ( $5 \text{ mg L}^{-1}$ ), aqueous 2-NP photolysis particulate product yield was successfully visually detected via the rapid formation of red-orange/copper particulate on the walls of the WWFT (identical  $t_{\text{reac}}$  and no. of lamps) for a considerably more concentrated ( $100 \text{ mg L}^{-1}$  in 100% MeOH with severe evaporation for this film,  $\sim 80\%$ ) and basic film (pH 11), likely attributed to nitrohydroquinone production (Bing et al., 2005). These photolysis experiments, which are the first to be performed under acidic conditions (pH 2) at environmentally realistic *ortho*-nitrophenol levels, *suggest* that the phototransformation of such compounds is not a significant source of atmospheric nitrous acid, however, this is *not* conclusive, as further studies with *ortho*-nitrophenol surfaces with different acidic properties (multi-pH study) and at other environmentally relevant concentrations would be necessary to justify this claim, as well as to better understand the occurring photochemistry. In addition, other *ortho*-nitrophenol species would need to be included in these future studies.

It is not surprising that the observed HONO production rates,  $P(\text{HONO})_{\text{ortho-nitrophenol}}$ , for the photolysis (4 lamps,  $\lambda_{\text{max}} = 354$  nm) of the acidified 2-NP and 4M2NP films ( $5 \text{ mg L}^{-1}$  in 5% MeOH), respectively, in the presence of 72 ppbv  $\text{NO}_2$  (summarized in **Table 14**), a typical urban  $\text{NO}_2$  level, are near the detection limit of the optimized HONO detector ( $\sim 10 - 15 \text{ pptv s}^{-1}$ ), since the film pH is considerably lower than their corresponding acid dissociation constants,  $\text{pK}_a$ 's (7.23 for 2-NP; Schwarzenbach et al., 1988), and, therefore, the selected *ortho*-nitrophenols are largely undissociated in solution. The data reveals a small HONO production rate,  $P(\text{HONO})$  ( $\sim 20 \text{ pptv s}^{-1}$ ) for both the blank film (5% MeOH, pH 2) and the examined *ortho*-nitrophenol films (labelled organic in **Table 14**), with individual precisions ranging from  $\sim 20 - 50\%$  deemed acceptable as the observed production rates are centred near the detection limit of the optimized HONO detector. Note that the mean HONO production rates for the tested *ortho*-nitrophenol films ( $P(\text{HONO})_{2\text{-NP}}$ ,  $P(\text{HONO})_{4\text{M2NP}}$ ) are *not* found to be statistically different ( $t_{\text{calc}} < t_{\text{table}}$ ,  $0.813 < 2.571$  for 5 *d.o.f.*).

Under simulated extreme  $\text{NO}_2$  conditions (1 ppmv), both the acidified (pH 2) blank (5% MeOH) and organic ( $5 \text{ mg L}^{-1}$  in 5% MeOH; 2-NP and 4M2NP, respectively) films exhibit significant HONO production rates, with  $P(\text{HONO})$  greater than  $600 \text{ pptv s}^{-1}$ , and individual precisions less than 10% (see **Table 14**). It is important to note, however, that since the  $\text{NO}_2$  level studied is environmentally irrelevant for typical

## (a) 2-NP

[NO <sub>2</sub> ](ppbv)	P <sub>HONO</sub> ± 1σ (pptv s <sup>-1</sup> )		RSD, % (n)		ΔP(HONO) <sub>2-NP</sub> (pptv s <sup>-1</sup> )
	Organic	Blank	Organic	Blank	
72	26.4 (±5.8)	25.0 (±7.8)	22 (4)	31 (3)	1.5 (±9.7)
1000	745.9 (±67.7)	622.8 (±7.0)	9.1 (3)	1.1 (3)	123.1 (±68.0)

## (b) 4M2NP

[NO <sub>2</sub> ](ppbv)	P <sub>HONO</sub> ± 1σ (pptv s <sup>-1</sup> )		RSD, % (n)		ΔP(HONO) <sub>4M2NP</sub> (pptv s <sup>-1</sup> )
	Organic	Blank	Organic	Blank	
72	21.2 (±11.4)	19.1 (±10.2)	54 (4)	54 (4)	2.1 (±15)
1000	750.0 (±50.9)	640.7 (±5.9)	6.8 (4)	0.9 (2)	109.3 (±51.3)

**Table 14.** HONO production rates, P(HONO) (pptv s<sup>-1</sup>) for the photolysis (4 lamps, λ<sub>max</sub> = 354 nm) of: (a) 2-NP and (b) 4M2NP, 5 mg L<sup>-1</sup> (pH 2, in 5% methanol), respectively, in the presence of 72 and 1000 ppbv NO<sub>2</sub> using the WWFT method photoreactor for a gas-liquid interaction time of ~ 1 s. Shaded columns (labelled as organic) correspond to the results obtained for the respective *ortho*-nitrophenol film, with the HONO yields for the reference (blank) film (5% MeOH, pH 2) displayed adjacent to the shaded values. The corresponding net HONO production rate, ΔP(HONO)<sub>*ortho*-nitrophenol</sub>, along with propagated uncertainty (± 1σ) is also given.

urban locales, the significance of the data set as a ‘realistic’ HONO source is minimized. The data set, can, however, be utilized to obtain an accurate estimate of the reproducibility, **R**, in percentage units, which, as a rule, is a good indicator of how uniformly the films are reproduced over *N* individual uptake experiments. This indicator, **R(%)**, can be easily estimated as

$$R(\%) = \left( \frac{e_{P(\text{HONO})_{\text{reference}}}}{P(\text{HONO})_{\text{reference},N}} \right) \times 100\% \quad (\text{E63}),$$

where  $e_{P(\text{HONO})_{\text{reference}}}$  is the total uncertainty in the averaged HONO production rate of the blank (or reference) film, with  $P(\text{HONO})_{\text{reference},N}$  is computed (over *N* individual experiments) as

$$P(\text{HONO})_{\text{reference},N} = \text{Average}[P(\text{HONO})_{\text{reference},1}, \dots, P(\text{HONO})_{\text{reference},N}] \quad (\text{E64}).$$

Thus, for the data summarized in **Table 14**, the calculated reproducibility, R is **1.44 %** over 2 experiments, with  $n = 5$ . The value obtained for the WWFT photoreactor is exceptional ( $< 5\%$ ), hence, providing much confidence in the reproducibility of the tested method.

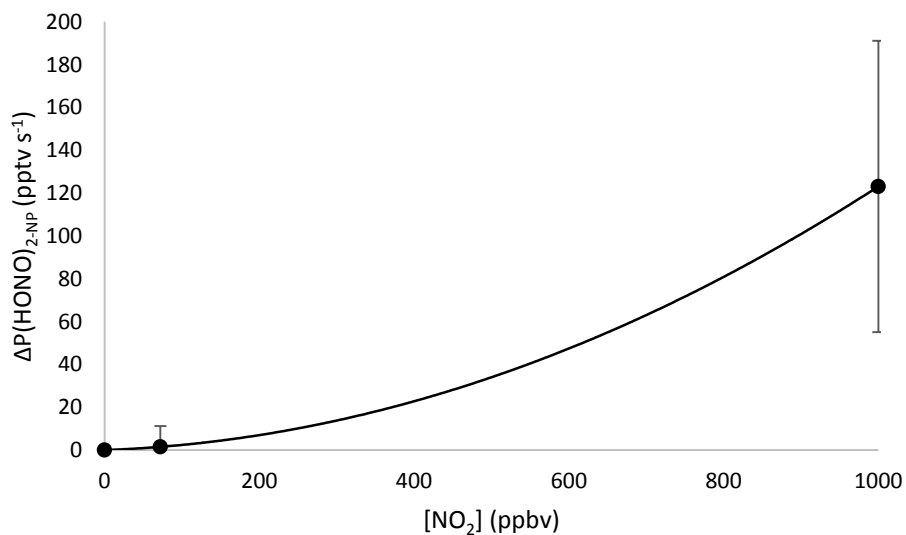
In general, the **net (average) HONO production rate**, for each tested organic (solution) film of interest, denoted  $\Delta P(\text{HONO})_{\text{organic film}}$  presented herein is simply computed by difference as:

$$\Delta P(\text{HONO})_{\text{organic film}} = P(\text{HONO})_{\text{organic film}} - P(\text{HONO})_{\text{reference film}} \quad (\text{E65})$$

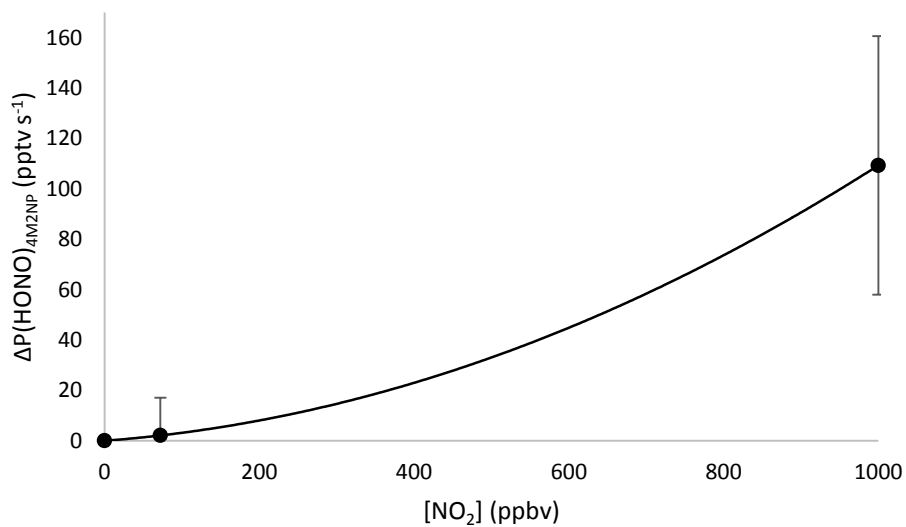
where the individual HONO production rates,  $P(\text{HONO})_{\text{organic film}}$  and  $P(\text{HONO})_{\text{reference film}}$  are averaged over  $n$  individual data points, with the reference (or blank) film HONO production rate corresponding to the respective solvent of choice. Note that  $P(\text{HONO})$  for the respective film of interest is simply the HONO production rate observed at the exit of the WWFT photoreactor, or  $[\text{HONO}]_{\text{treac}} \text{ s}^{-1}$ , since  $t_{\text{reac}} \sim 1 \text{ s}$ . Recall the relationship between  $P(\text{HONO})_s$  at the first time step (0.01 s) and  $\chi_{\text{best-fit}}$  as previously derived in (E30).

The dependence of net HONO production rate ( $\Delta P(\text{HONO})$ ) on  $[\text{NO}_2]_0$  produced using data from  $\text{NO}_2$  photochemistry experiments on acidic (pH 2, 5  $\text{mg L}^{-1}$  in 5% MeOH) *ortho*-nitrophenol (2-NP and 4M2NP) films over the entire tested  $[\text{NO}_2]_0$  concentration array (0, 72 and 1000 ppbv) were found to be *non-linear* for both *ortho*-nitrophenol species (see **Figure 37**). Although the small (net) HONO production rates obtained for typical urban  $\text{NO}_2$  levels, centred around the detection limit for the HONO detector in **Table 14** suggest that the uptake processes on the tested *ortho*-nitrophenols are unimportant as sources as HONO, further experiments using films with different acidic properties and at different environmentally relevant concentrations (as well as for other *ortho*-nitrophenol species) need to be performed in order to confirm this conclusion. Additionally, the considerably more significant HONO production rate observed for the reference (blank) film, 5% MeOH, ranging from about 100 to 600  $\text{pptv s}^{-1}$  for environmentally relevant to extreme  $\text{NO}_2$  conditions, indicates that the uptake of  $\text{NO}_2$  on the organic impurities in the HPLC grade MeOH including acetone, and dimethyl acetals of simple alkyl ketones (such as propanone, butanone, and pentanone in the range of 10 to 100 ppm), with a plausible chemical pathway of origin, (M8), illustrated in **Figure 38** (Guella et al., 2007), is kinetically *more favourable* than that on the selected *ortho*-nitrophenol films under the tested conditions.

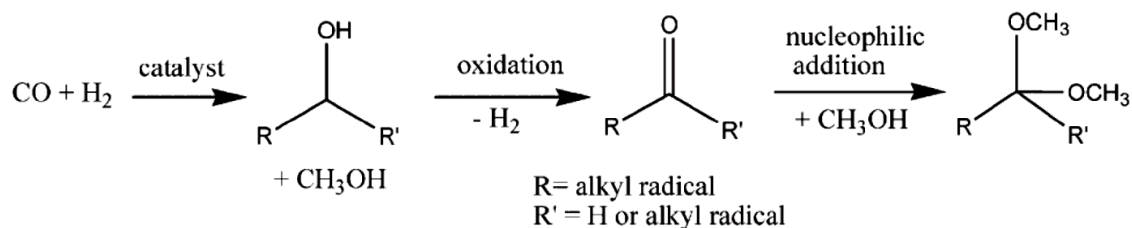
(a) 2-NP



(b) 4M2NP

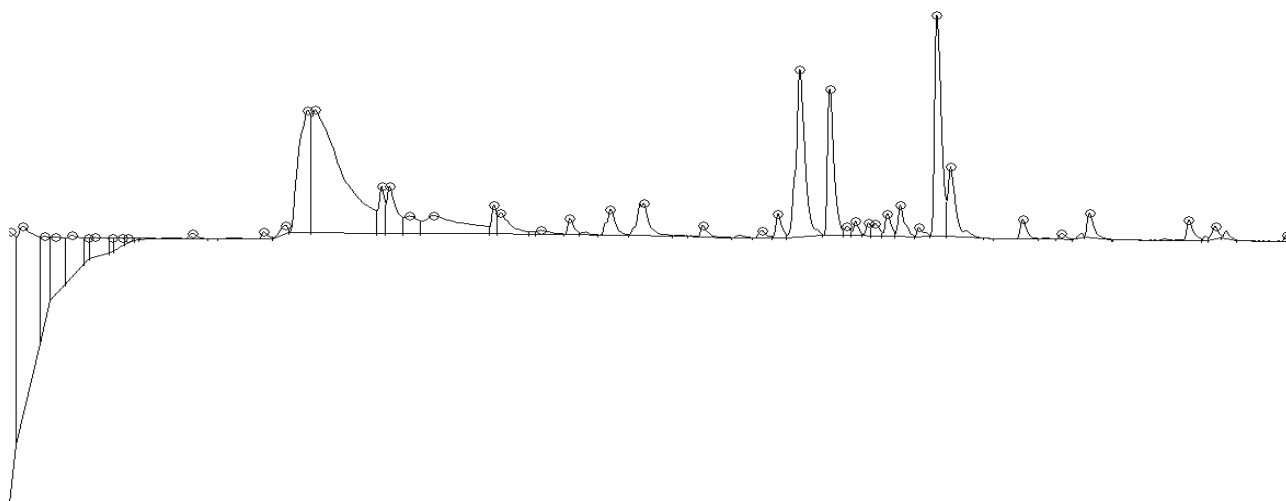


**Figure 37.** Non-linear correlation plots of tested NO<sub>2</sub> concentration (ppbv) against measured (net) HONO production rates  $\Delta P(\text{HONO})_{ortho\text{-nitrophenol}}$  (pptv s<sup>-1</sup>) for the selected *ortho*-nitrophenol films (a) 2-NP and (b) 4M2NP, 5 mg L<sup>-1</sup> (pH 2, in 5% methanol), respectively in the presence of 0 (photolysis), 72, and 1000 ppbv NO<sub>2</sub> using the WWFT photoreactor (4 lamps,  $\lambda_{\text{max}} = 354$  nm) for a gas-liquid interaction time of  $\sim 1$  s. Error bars indicate propagated uncertainties ( $\pm 1\sigma$ ) on non-negligible (net) HONO production rates.



**Figure 38.** A plausible chemical pathway, (M13), for the origin of acetal impurities in commercial methanol. From: Guella et al. (2007).

As an extension to the NO<sub>2</sub> uptake experiments on *ortho*-nitrophenols, the possibility of analysing the WWFT effluent for NO<sub>2</sub><sup>-</sup> was examined by chromatographic analysis of a 100-μL injection of a derivatized sample (50% v/v SA/NED working solution) containing the selected 2-NP solution (50% v/v 5 mg L<sup>-1</sup> in 5% MeOH) using the optimized HPLC method for detection of HONO. The first injection did not reveal any undesirable chromatographic interferences, however, after subsequent injections, several interfering peaks appeared in the chromatogram (see **Figure 39**) indicative of impurities in the 2-NP solution that remained retained on the column. Subsequent injections of purified water were used to flush in an atte-



**Figure 39.** Chromatogram (10 min.) of subsequent (after initial) injection of derivatized sample containing (50% v/v) SA/NED working solution + (50% v/v) 2-NP solution (5 mg L<sup>-1</sup> in 5% MeOH). Several interfering peaks from the 2-NP (absorption maxima: 230, 276 nm (refer to Table 12)) are seen. Eluent: 23% acetonitrile/77% 15 mM hydrochloric acid.

mpt to flush the large number of contaminants in the 2-NP solution off of the reversed-phase column, however were unsuccessful. Examination of the acquired chromatograms revealed that the separation of the 2-NP impurities required greater than 60 minutes elution time. Further efforts to remove the contaminants from the column included flushing the column with 100% MeOH and 100% acetonitrile (ACN), respectively, for several 24-hr intervals, at the maximum pump flow rate of 5 mL min<sup>-1</sup>, which, unfortunately, too were unsuccessful.

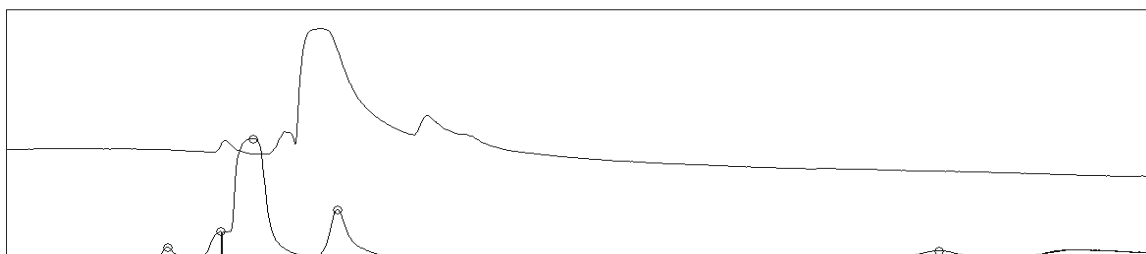
A more rigorous cleaning/regeneration procedure (in order of increasing solvent strength) for the contaminated reversed-phase column as recommended by Majors (2003) as outlined was used: 100% methanol (MeOH); 100% acetonitrile (ACN); 75% v/v ACN, 25% v/v isopropanol; 100% methylene chloride; and 100% hexane. A minimum of 10 column volumes of each solvent was passed at 2 mL min<sup>-1</sup>. In order to return to the original mobile phase (23% v/v ACN, 77% v/v HCl (15-mM), 100% isopropanol was used as an intermediate solvent after flushing the column with hexane, followed by 100% ACN, and finally the original mobile phase, as advised by Majors (2003).

Several injections of purified water revealed that the rigorous cleanup procedure, unfortunately, was unsuccessful, as well as the possibility of using the current chromatographic method (without modification) to measure the aqueous-phase nitrite during *ortho*-nitrophenol uptake experiments diminished. An isocratic ion pair HPLC method with UV-VIS detection (at 290 nm) with chromatographic separation on a C<sub>18</sub> column (at 1.0 mL min<sup>-1</sup>) with a mobile phase consisting of methanol-0.01 M citrate buffer pH 6.2 (47:53 v/v) containing 0.03 M tetrabutylammoniumbromide (TBAB) would need to be developed in-house in order to accomplish such measurements (Almási et al., 2011).

Due to the deterioration of the reversed-phase column in use, the contamination of the stationary phase was unfortunately detrimental, and accordingly, a new reversed-phase column (5 μm, 4.6×100 mm analytical column, Waters) was installed, providing the following chromatographic advantages (see **Figure 40**): significantly better resolution between the SA and internal standard peaks (peaks #3 and #4); considerably less peak tailing; less peak asymmetry, and a faster elution time. Increasing the organic content of eluent by 2% (from 23% v/v ACN to 25% v/v ACN), reduced the run-time to approximately 7 minutes for the remaining experiments, yielding sufficient resolution between the SA and KHP peaks.



**Figure 40.** Comparison of old and new reversed-phase column chromatography (7.5 min. length): (top) old column; (bottom) new column. Injected sample: 50% v/v SA/NED working solution + 50% v/v phosphate buffer (0.5 mM KHP, pH 7). The offset in the retention times is due to different HPLC pump flow rates: (a) old column: 1.5 mL/min; (b) new column: 2.5 mL/min. Peaks #1 and #2 are solvent peaks; peak #5 is the nitrite peak. Eluent: 23% acetonitrile/77% 15 mM hydrochloric acid.



#### 4.4 POTASSIUM HYDROGEN PHTHALATE (KHP)

Very recently, the  $\text{NO}_2$  uptake on water has been shown to be *significantly* enhanced by cationic surfactants ( $\gamma_{\text{max}} > 10^3$  larger than that in neat water), weakly inhibited by anionic surfactants, and unaffected by 1-octanol (Kinugawa et al., 2011) under extreme  $\text{NO}_2$  conditions (ppmv levels) and surfactants [i.e., sodium bromide, 1-octanol, tetrabutylammonium bromide ( $\text{TBA}^+\text{Br}^-$ ), tetradecyltrimethylammonium bromide ( $\text{TDTMA}^+\text{Br}^-$ ), and potassium perfluorooctanesulfonate ( $\text{PFOS}^- \text{K}^+$ )] in the **1-3 mM** concentrations range.

Kinugawa et al. (2011) have found that such surfactants modulate interfacial anion coverage via electrostatic interactions with charged headgroups. They propose the following mechanism (M14) to account for their observations

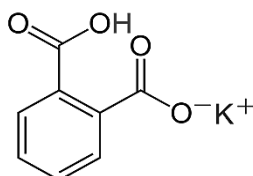


in which  $\text{NO}_2(\text{g})$  disproportionates in two steps, (R41) and (R42), via persistent, interfacial intermediary  $\text{X-NO}_2^{\bullet-}$  radical anions. Kinuwaga et al. (2011) show that according to their proposed mechanism, (M14), the overall rate of the hydrolytic disproportionation of gas-phase  $\text{NO}_2$  on water's surface (aq.) is limited by the slow uptake of  $\text{NO}_2$  via (R41), followed by the subsequent rapid uptake of a second  $\text{NO}_2$  molecule via (R42) (having a significantly higher reaction probability). Thus, the proposed  $\text{NO}_2(\text{g})$  uptake enhancement, is a case of general base catalysis (Anslyn and Dougherty, 2006), with the catalytic role of anions in (R41) and (R42) clearly shown in similar experiments (Yabushita et al., 2009).

The special grade KHP used in the uptake experiments (immediately following) investigating the possibility of utilizing the internal standard (*recall*, during gas-phase HONO sampling) to correct for variations in evaporation of the WWFT film, contains metallic impurities displayed in **Table 15** in the concentration range of  $\sim 0.30 - 44 \mu\text{g g}^{-1}$  as found by Shibata et al. (1992). The chemical structure of the internal standard is shown in **Figure 41**. As KHP is unreactive itself (internal standard), and highly stable in (acidic) solution, it is plausible to assume that the metallic impurities must be driving the increase (i.e., acting as **catalysts**) in the observed HONO production rates, up to  $\sim 135 \text{ pptv s}^{-1}$  for simulated typical urban and extreme  $\text{NO}_2$  conditions (see **Table 16**) over that of the purified solvent. However, catalysis by reactive species, such as transition metals (Nash, 1970), has been previously found to have minimal impact on the hydrolytic disproportionation of gaseous  $\text{NO}_2$  on water's surface (M10) (Lee and Schwartz, 1981), making this explanation unlikely. Interest in a plausible HONO production mechanism for this film, motivated the experiment under extreme (i.e., unrealistic)  $\text{NO}_2$  conditions (**Table 16 (b)**).

Element	NEB-ICP-MS (n = 5)	ETV-ICP-MS (n = 3)	Ion exchange- ETV-ICP-MS (n = 3)
Li	ND	$0.014 \pm 0.002$	- <sup>c</sup>
Na	$(44 \pm 1)$	$73 \pm 5$	- <sup>c</sup>
Mg	$0.59 \pm 0.07$	- <sup>a</sup>	$(18 \pm 0.1)$ <sup>d</sup>
Al	$2.3 \pm 0.1$	$(4.1 \pm 0.4)$ <sup>a</sup>	- <sup>d</sup>
Ca	- <sup>a</sup>	- <sup>a</sup>	$< 20 \pm 1$
Sc	- <sup>a</sup>	- <sup>a</sup>	$< 0.48 \pm 0.05$
Mn	ND	$0.19 \pm 0.03$	$0.33 \pm 0.01$
Fe	- <sup>a</sup>	$14 \pm 1$	$< 17 \pm 6$
Co	- <sup>b</sup>	$0.27 \pm 0.01$	$0.30 \pm 0.01$
Zn	$0.31 \pm 0.08$	ND	$0.54 \pm 0.03$
Rb	$12 \pm 1$	$10 \pm 1$	- <sup>c</sup>
Cd	ND	- <sup>b</sup>	$< 0.10 \pm 0.01$
Ba	$23 \pm 3$	- <sup>b</sup>	$20 \pm 1$
Pb	$0.56 \pm 0.08$	$0.64 \pm 0.09$	$0.49 \pm 0.01$

**Table 15 (above).** Analytical results for potassium hydrogen phthalate (KHP), sample R1 (commercial reagent, JIS special grade) ( $\mu\text{g g}^{-1}$ ) obtain via three different techniques: NEB-ICP-MS or conventional nebulization inductively-coupled plasma mass spectrometry; ETV-ICP-MS or electrothermal vaporization-ICP-MS; and Ion exchange-ETV-ICP-MS. <sup>a</sup> Spectral interferences. <sup>b</sup> Uncertainty of blank value. <sup>c</sup> Excluded by ion-exchange separation. <sup>d</sup> Contamination in concentration procedure. <sup>e</sup> Values in parentheses are values not certainly determined. From: Shibata et al. (1992).



**Figure 41.** Structure of the internal standard potassium hydrogen phthalate (KHP). The word ‘hydrogen’ is referring to the acidic hydrogen.

It is highly plausible that the aforementioned mechanism, (M14) (of general base catalysis) explains the non-negligible HONO production observed for the studied potassium hydrogen phthalate (KHP) film (0.5 mM, 5% MeOH as solvent, pH 2), which is of similar concentration to those surfactants investigated by Kinuwaga et al. (2011) (1-3 mM). Drawing on the results of Kinuwaga et al. (2011), it can be concluded that it is very likely that the surfactant  $\text{K}^+$  counterion draws the phthalate ion closer to the surface, thus enhancing the  $\text{NO}_2$  uptake on water (5% MeOH) via (R41) and (R42). Furthermore, the data here suggests that the results of Kinuwaga et al. (2011) under extreme  $\text{NO}_2$  conditions need to be extrapolated to atmospheric levels in order to accurately assess the importance of (M14) for the production of tropospheric HONO. It is also interesting to note that the magnitude of HONO production for the tested KHP film (0.5 mM, 5% MeOH as solvent, pH 2) is nearly identical to that seen for the studied *ortho*-nitrophenol films (5 mg  $\text{L}^{-1}$  in 5% MeOH, pH 2) suggesting that the reaction kinetics are equally favorable under extreme  $\text{NO}_2$  conditions ( $t_{\text{reac}}$  of 1 s, 4 lamps) for the tested conditions only. Finally, the slight (non-negligible) HONO production rate ( $2.8 \pm 28$  pptv  $\text{s}^{-1}$ , 95% confidence interval computed for 2 *d.o.f.*) that was observed for the KHP film under environmentally realistic  $\text{NO}_2$  conditions (72 ppbv), likely eliminates the possibility of utilizing the internal standard to correct for changes in evaporation in the liquid film.

(a)

72 ppbv NO <sub>2</sub>	Blank film	KHP film
P(HONO) (pptv/s)	<b>117.1</b>	<b>119.9</b>
± 1σ	11.0	12.5
RSD(%)	9.4	10.5
no. of data pts., <i>n</i>	3	3

$$\Delta P(\text{HONO})_{0.5 \text{ mM KHP}, 72 \text{ ppbv NO}_2} = 2.8 (\pm 17) \text{ pptv s}^{-1}$$

(b)

~ 1.0 ppmv NO <sub>2</sub>	Blank film	KHP film
P(HONO) (pptv/s)	<b>642.4</b>	<b>778.0</b>
± 1σ	20.0	42.8
RSD(%)	3.1	5.5
no. of data pts., <i>n</i>	3	4

$$\Delta P(\text{HONO})_{0.5 \text{ mM KHP}, \sim 1 \text{ ppmv NO}_2} = 135.6 (\pm 47.2) \text{ pptv s}^{-1}$$

**Table 16.** HONO yields for the photochemistry (4 lamps) of the studied KHP film (0.5 mM in 5% MeOH, pH 2) and the corresponding reference (blank) film (5 % MeOH, pH 2) for simulated: (a) environmentally relevant NO<sub>2</sub> conditions (72 ppbv) and (b) extreme NO<sub>2</sub> conditions (~ 1.0 ppmv) using the WWFT method and a  $t_{\text{reac}}$  of ~ 1 s. Net HONO production rates,  $\Delta P(\text{HONO})_{0.5 \text{ mM KHP}}$  (pptv s<sup>-1</sup>) are also given, along with propagated uncertainties.

## 5 EXPERIMENTS ON HUMIC ACIDS (HA)

*In this second results chapter, the focus of the thesis shifts to the kinetics of the  $\text{NO}_2$  uptake on acidified commercial humic acid films using the WWFT photoreactor for typical operating conditions ( $t_{\text{reac}} \sim 1$  s,  $85.7$   $\text{W}/\text{m}^2$ ). The experimentally determined reaction rate with respect to  $[\text{NO}_2]$  is given in **Section 5.1** using the WWFT photoreactor (at  $\text{pH } 2$  &  $1$   $\text{g}/\text{L} = [\text{HA}]_{\text{sol'n}}$ ). Neglecting gas-phase diffusion, an estimate of the uptake coefficient,  $\gamma_{\text{expt}}$  is computed and compared with the data of Stemmler et al. (2006) for considerably less acidic conditions. The section is concluded with a corresponding discussion of whether a surface layer reaction is expected based on this data, in combination with experimental HONO production data obtained by varying the film thickness. **Section 5.2** begins with a display of pH drift plots, corresponding to the time-dependent measurable pH drift of the commercial HA solution observed over the duration of the uptake experiments. Best-fit values of averaged reaction probabilities and the corresponding values of precision are presented for a large film pH interval ( $\sim 1.5$  to  $4.3$ ). As well, model-predicted parameters are tabulated for the reader. Next, various parameterizations are presented in this section which may be useful for describing the complex  $\text{pH}_{\text{treat}}$ -dependent  $\gamma_{\text{best-fit}}$  behavior observed in this study. Lastly, the data is qualitatively compared with that of Stemmler et al. (2006) on more basic solid commercial HA films. For film  $\text{pH } 3$  ( $[\text{HA}]_{\text{sol'n}} = 0.84$   $\text{g}/\text{L}$ ), the experimentally determined  $k_{\text{rxn}}$  is given in **Section 5.3**. The relatively simple analytic expression for  $\gamma_{\text{rxn}}$  is presented and is used to determine the fraction that both  $\gamma_{\text{rxn}}$  and  $\gamma_{\text{diffusion}}$  contribute to the total uptake (under the valid assumption that  $\gamma_{\text{rxn}}$  is rate limiting). **Section 5.4** continues with the observed exponential correlation of  $\gamma_{\text{best-fit}}$  vs. (photoreactor) irradiance (film  $\text{pH } 3$ ,  $[\text{HA}]_{\text{sol'n}} = 0.84$   $\text{g}/\text{L}$ ,  $0 - 85.7$   $\text{W}/\text{m}^2$ ). Experimental data and model-predicted parameters are once again tabulated for the reader. A photochemical  $\text{NO}_2$  reduction mechanism is postulated based on the exponential dependence between reaction probability and irradiance. A discussion concerning the generation of HONO from the photoexcitation of HA concludes the section. In the final section (5.5) of this second results chapter, the variation in the averaged best-fit reaction*

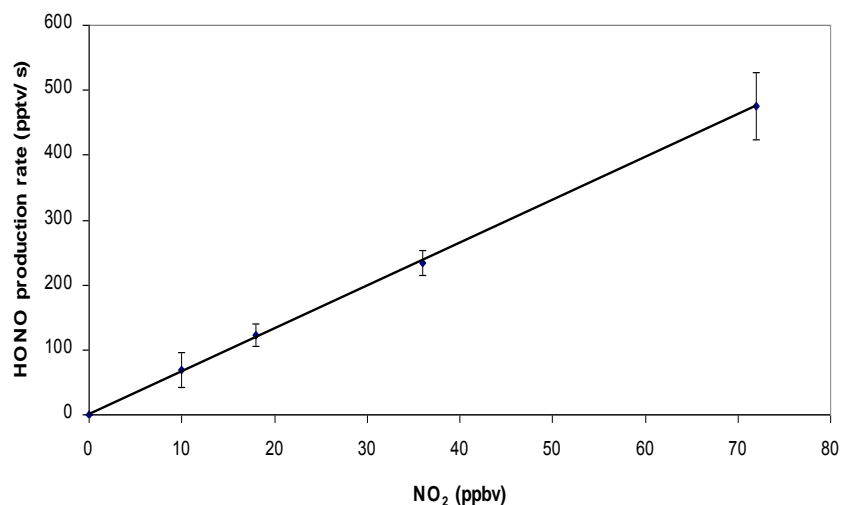
*probability with HA standard (Commercial, Pahokee Peat, Leonardite, and Elliott Soil) is given (in tabulated and bar chart form) and discussed in limited context, with respect to the available elemental composition data for the examined HA standards (also tabulated). Finally, this modest environmentally diverse kinetic dataset is compared with that of Stemmler et al. (2006) (again, under less acidic conditions), and conclusive comments reconnect to the proposed photochemical NO<sub>2</sub> reduction mechanism (stated in Section 5.4).*

### 5.1 DEPENDENCE OF HONO YIELD ON NO<sub>2</sub> CONCENTRATION

Prior to conducting experiments with the lights on in the WWFT, a dark experiment was performed with 72 ppbv NO<sub>2</sub>, in order to rule out the possibility of HONO formation resulting from aromatic moieties and high phenolic functionalities of humic acids, which can act as electron donors and even show (dark) reactivity towards NO<sub>2</sub> (Ammann et al., 2005). No HONO formation, however, was observed as a result of the dark experiment with the concentrated (1 g L<sup>-1</sup>) acidic (pH 2) HA film, suggesting that this dark reactivity is not environmentally important only under these conditions. This is inconsistent with the study of Stemmler et al. (2006; and 2007), who observed HONO formation centred near the detection limit of their measurement method (LOPAP) in the dark (i.e.,  $\gamma < 10^{-7}$ ) from the interaction of solid HA films ( $[HA]_{\text{film}} = 8 \mu\text{g cm}^{-2}$ ) and HA aerosols (unrealistically concentrated), respectively, both at pH 4.4, with gaseous NO<sub>2</sub> (20 ppb). This is not unexpected, as at the higher operating pH, more phenolic functionalities in the commercial HA standard showing dark reactivity towards NO<sub>2</sub> would be dissociated.

The dependence of the HONO formation on the acidic (pH 2) concentrated (1 g L<sup>-1</sup>) humic acid films on the NO<sub>2</sub> concentration (10 – 72 ppb) is shown in **Figure 42** for a  $t_{\text{reac}}$  of 1 s. Average values of  $\Delta\text{P}(\text{HONO})$  along with statistical parameters given in **Table 17**. Unlike in the studies of photosensitized reduction of NO<sub>2</sub> on solid humic acid films and humic acid aerosols, completed by Stemmler et al. (2006) and Stemmler et al. (2007), a saturation of HONO yields at higher NO<sub>2</sub> concentrations (> 50 ppbv), is not observed. Instead, a highly linear correlation ( $R^2 = 0.9997$ ) over the entire range examined is seen. Note that the  $\Delta\text{P}(\text{HONO})$  value for the photoenhanced uptake of 10 ppbv NO<sub>2</sub> on the concentrated (1 g L<sup>-1</sup>) acidic (pH 2) commercial HA film has a significantly larger experimental error ( $\pm 40\%$ ) due to integration of

HONO peaks with areas near the detection limit of the HONO detector. The reference film, 2 mM NaOH adjusted to pH 2, yielded negligible HONO production for all tested NO<sub>2</sub> levels. No comparable reactivity was observed ( $n = 5$ ,  $N = 1$ ) for the Aldrich HA film photolysis ( $[\text{NO}_2]_0 = 0$  ppbv).



**Figure 42.** Correlation plot of tested NO<sub>2</sub> concentration (ppbv) against measured  $\Delta P(\text{HONO})$  values. HONO yields obtained for the photoenhanced uptake of NO<sub>2</sub> on the acidic (pH 2) concentrated (1 g L<sup>-1</sup>) commercial HA film using the WWFT photoreactor (4 lamps) and a  $t_{\text{reac}}$  of  $\sim 1$  s. Tested concentrations of NO<sub>2</sub> include: 10, 18, 36 and 72 ppbv, mixing ratios typical of rural and urban cities in Ontario, Canada (Arain et al. (2007)).

[NO <sub>2</sub> ] (ppbv)	$\Delta P(\text{HONO}) \pm 1 \sigma$ (pptv/s)	RSD,% ( $n$ )	$R_{\text{HA}}$ ,% ( $N$ )
10	68.4 ( $\pm 27.1$ )	39.5 (6)	55.3 (2)
18	122.5 ( $\pm 16.5$ )	13.5 (8)	22.5 (2)
36	242.2 ( $\pm 12.6$ )	6.6 (7)	5.2 (2)
72	475.7 ( $\pm 51.5$ )	10.8 (10)	16.7 (3)

**Table 17.** HONO yields for the photoenhanced uptake of NO<sub>2</sub> on the acidic (pH 2) concentrated (1 g L<sup>-1</sup>) commercial HA film using the WWFT photoreactor (4 lamps) and a  $t_{\text{reac}}$  of  $\sim 1$  s. Concentrations of NO<sub>2</sub> are varied from 10 to 72 ppbv.

An elementary photochemical mechanism, (M15) – activation of reductive centres ( $A^{\text{red}}$ ) within the organic film by light, (R43), the corresponding deactivation process, (R44), and the reaction of  $A^{\text{red}}$  with adsorbed  $\text{NO}_2$ , (R45) proposed by Stemmler et al. (2006) – predicts such a saturation:



Compounds X introduced in (R43) and (R44) suggest that the reactions may involve a photo-induced intra- or inter-molecular electron transfer and its back- reaction, and thus, must be regarded as oxidants. Alternative explanations, including a Langmuir adsorption of  $\text{NO}_2$  coupled to a surface reaction, which is often referred to in heterogeneous chemistry (Ammann et al., 2003; Arens et al., 2001; and Pöschl et al., 2001), and saturation of the adsorption sites by  $\text{NO}_2$  (Stemmler et al., 2006) may, too, justify their observed saturation curves.

At firsthand, the experimentally determined uptake coefficient,  $\gamma_{\text{expt}}$  for such a slow liquid-phase reaction can be easily estimated as (*recall*)

$$\gamma_{\text{expt}} = \frac{2rk_1}{w} \quad (\text{E2}),$$

(Fickert et al., 1998), if gas-phase diffusion is simply neglected. In (E2):  $r$  is the radius of the tube (0.6 cm);  $w$  is the average molecular velocity of the gas,  $w = 37000 \text{ cm s}^{-1}$  for  $\text{NO}_2$  (g) at 298 K; and  $k_1$  is the first-order rate coefficient for the reaction,  $k_1 = 6.7 \times 10^{-3} \text{ s}^{-1}$  only under the tested conditions. Hence, using (E2), the calculated uptake coefficient (neglecting gas-phase diffusion) for the uptake of  $\text{NO}_2$  (0 -72 ppbv) on a concentrated ( $1 \text{ g L}^{-1}$ ) acidic (pH 2) commercial HA film ( $6.91 \mu\text{g cm}^{-2}$ ) is  $\gamma_{\text{expt}} = 2.2 \times 10^{-7}$  for the usual gas-liquid reaction time of 1 s in the WWFT photoreactor. This is approximately an order of magnitude below the maximum reported uptake coefficient of  $\text{NO}_2$  on humic acid aerosol (pH 4.4, RH = 26%) of  $\gamma = 1.8 \times 10^{-6}$  (Stemmler et al., 2007) for a maximum actinic flux of  $1.0 \times 10^{17} \text{ photons cm}^{-2} \text{ s}^{-1}$  (7 lamps,  $\lambda = 400 - 750 \text{ nm}$ ) and an aerosol surface concentration of  $\sim 0.151 \text{ m}^2 \text{ m}^{-3}$ . As previously mentioned, however, the aerosol conditions employed by Stemmler et al. (2007) were environmentally unrealistic, and, additionally, the generated aerosol consisted entirely of humic acid. Rural and urban continental aerosol is composed only of 20 to 30% by mass of organic matter (Hueglin et al., 2005), and



the photoreactivity of these airborne organic materials towards  $\text{NO}_2$  has yet been demonstrated – accordingly the uptake coefficient reported by Stemmler et al. (2007) must be considered as an upper limit. The higher reactivity observed by Stemmler et al. (2007) is also not unanticipated since a larger fraction of the Aldrich-HA carboxylic acid groups will be dissociated under the less acidic conditions (pH 4.4 vs. pH 2). By comparison, the uptake coefficients derived from the solid humic acid films ( $8 \mu\text{g cm}^{-2}$ , pH 4.4) are approximately a factor of 3 higher than those observed on the aerosol under comparable humidity and light conditions (and thus, 3 orders of magnitude greater than the derived  $\gamma_{\text{expt}}$  at pH 2 for the WWFT photoreactor study herein), with the difference likely due to uncertainties in the quantification of the HA surface areas (Stemmler et al., 2006).

The experimentally determined first-order reaction rate with respect to  $[\text{NO}_2]$  for the pH 2 commercial HA film using the WWFT photoreactor, suggests that saturation of the adsorption sites by  $\text{NO}_2$  does not occur within the system. This is conceptually consistent with a continuously renewed surface ( $t_{\text{renewal}}$  of 1.94 minutes) layer reaction, and with the surface process proposed for the photolytic HONO formation by  $\text{NO}_2$  reactions in the presence of phenolic compounds (George et al., 2005; Stemmler et al., 2005; and Stemmler et al., 2006).

From a theoretical standpoint, as seen from (E41) (in **Chapter 3**), increasing the film thickness significantly reduces the depth to which the  $\text{NO}_2^-$  particles on average can diffuse. However, if the reaction is occurring in the surface layer, as suspected, the  $\text{NO}_2^-$  particles should only diffuse throughout the depth of the surface layer, regardless of any variation in film thickness – that is, the observed HONO yield should be independent of film thickness.

To support this argument, the  $\text{NO}_2$  uptake was investigated on HA films of two thicknesses,  $f$ : the usual  $f$  of 0.032 cm, and a film thickness 1.59 times this, namely, 0.051 cm. The computed flow dynamics (with parameters previously defined) for the corresponding tested liquid flow rates,  $F_l$ , are given in **Table 18** for the reader's reference. Computations were completed based on the following physical properties of a solution of phenol at 293 K:  $\eta = 1.22 \times 10^{-2} \text{ g cm}^{-1} \text{ s}^{-1}$ , and  $\rho = 1.078 \text{ g cm}^{-3}$ . For both tested values of  $F_l$ , the liquid flow is laminar, as verified by  $N_{\text{RE}}'s \ll 250$ , where turbulent transport is favoured. **Table 18** summarizes the results of the  $\text{NO}_2$  (36 ppbv) photoenhanced (4 lamps) uptake experiments on concentrated ( $1 \text{ g L}^{-1}$ ) commercial acidic (pH 2.5) HA films for the tested film thicknesses. The percentage difference in the HONO efficiency rates,  $E_{\text{HONO}}$  ( $\text{pptv HONO/ppbv NO}_2/\text{s}$ ) is approximately 1%, which is less

than the individual precisions on the individual efficiency rates. Accordingly, it can be stated with confidence that the measured HONO efficiency rates are statistically equal within experimental error over a four-fold increase in film flow rate (a 160% increase in film thickness). Thus, the observed independence of  $E_{\text{HONO}}$  on film thickness,  $f$ , does indeed imply that the reaction is occurring only in the surface layer.

FLOW DYNAMICS PARAMETERS				EXPERIMENTAL OUTPUTS		
$F_l$ (mL min <sup>-1</sup> )	$v_{\text{max}}$ (cm s <sup>-1</sup> )	$N_{\text{Re}}$	$f$ (cm)	$E_{\text{HONO}} \pm 1\sigma$ (pptv HONO/ppbv NO <sub>2</sub> /s)	RSD(%) ( $n$ )	$N$
a) 0.24	0.48	~ 0.1	$3.32 \times 10^{-2}$	$16.2 \pm 1.0$	6.4 (11)	2
b) 0.96	1.21	~ 0.4	$5.28 \times 10^{-2}$	$16.4 \pm 1.6$	9.7 (6)	2

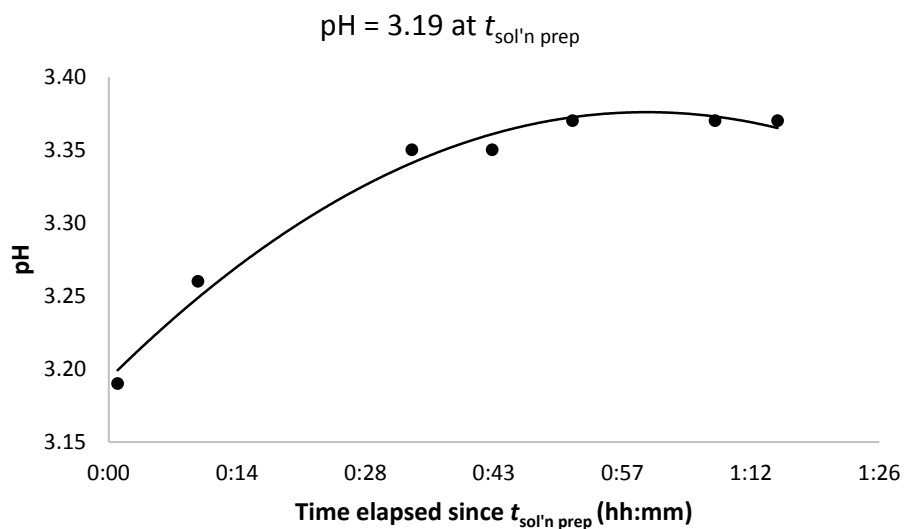
**Table 18.** HONO efficiency rate data,  $E_{\text{HONO}}$  (pptv HONO/ppbv NO<sub>2</sub>/s) for the photoenhanced uptake of NO<sub>2</sub> (36 ppbv) on concentrated (1 g L<sup>-1</sup>) commercial acidic (pH 2.5) HA films of varying film thickness,  $f$ , using the WWFT photoreactor (4 lamps) and a  $t_{\text{reac}}$  of ~ 1 s. Calculated values of  $t_{\text{delay}}$ , the time delay between subsequent injections during uptake experiments are: a) 1.94; and b) 0.77 min., respectively.

## 5.2 PH-DEPENDENT REACTION KINETICS STUDY

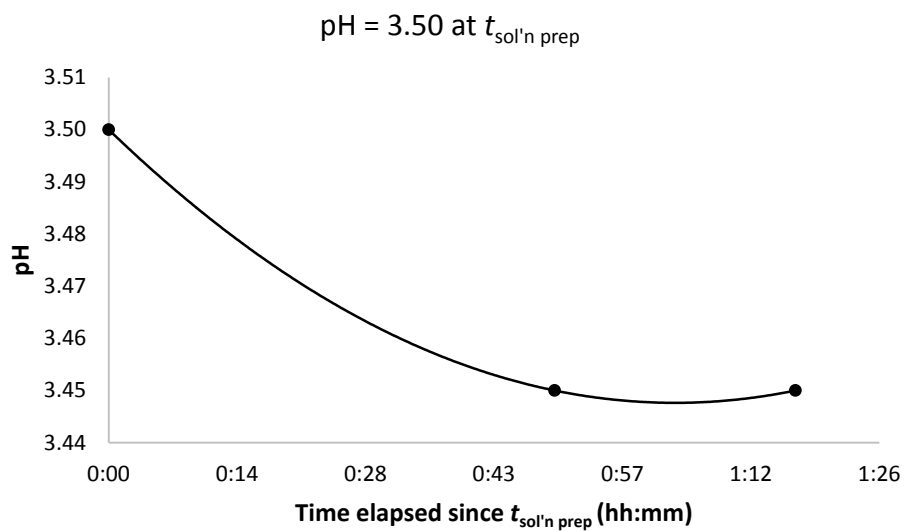
Issues with stability of the commercial HA solution (0.84 g L<sup>-1</sup>) were observed for solutions of pH > 3 over the duration of the NO<sub>2</sub> photochemistry experiments, approximately 1.0 to 2.5 hrs., in the form of pH drift (> 1 hr.). Specifically, at around roughly HA solution pH of 3.1, measurable pH drift began to occur within tens of seconds of the solution preparation time ( $t_{\text{sol'n prep}}$ ). For each tested film pH above approximately 3.1, the HA solution pH was recorded at random time intervals (elapsed from  $t_{\text{sol'n prep}}$ ) both before and during the uptake experiments. Plotting this pH data as a function of elapsed time produces the corresponding **pH drift plot**, with all plots displayed in **Figure 43** for the tested acidities. *Quadratic* correlations were then fitted to each pH drift plot (with  $R^2 > 0.96$ , as seen in **Figure 43**) for each tested HA solution pH above 3.1 in order to extrapolate the initial solution pH,  $\text{pH}_{\text{sol'n}}$  (necessary model input parameter), at the time of the individual gas-phase HONO measurement during the respective NO<sub>2</sub> uptake experiments.

The increasing pH drift observed in **Figure 43(a) – (f)**, for the sets of initial film pHs of (3.19; and 3.85,4.14), suggests a slow absorption of protons in the respective HA solution, speeding up equilibrium, that is, pH approaching  $pK_{a,n}$  for the appropriate  $n$  ( $n = 1, 2$  respectively for the discussed pH sets). As a point of reference, Paxéus and Wedborg (1985) found that the first three groups of commercial HA with  $pK_a$  values of 3.39, 4.78 and 6.06 are due to carboxylic groups measured as individual inflection points in their potentiometric titration. On the contrary, the (overall) decreasing pH drift observed for the initial film pHs of 3.50 and 3.59 (**Figure 43 (b)**) indicates a slow release of protons in the solution that slows down in reaching the respective point of equilibrium ( $pK_{a,1}$ ). Finally, the pH drift curve at pH = 3.55 at  $t_{sol'n prep}$  (**Figure 43 (c)**) indicates a rapidly established equilibrium with essentially no pH drift observed over the elapsed time interval measured. This negligible, or much slower than expected drift is easily explained, since the film pH is within  $\sim 0.15$  pH units of  $pK_{a,1}$ . At all initial (acidic) film pHs under consideration, the intensity of the pH instability due to the hysteresis effect (Paxéus and Wedborg, 1985) for the (concentr-

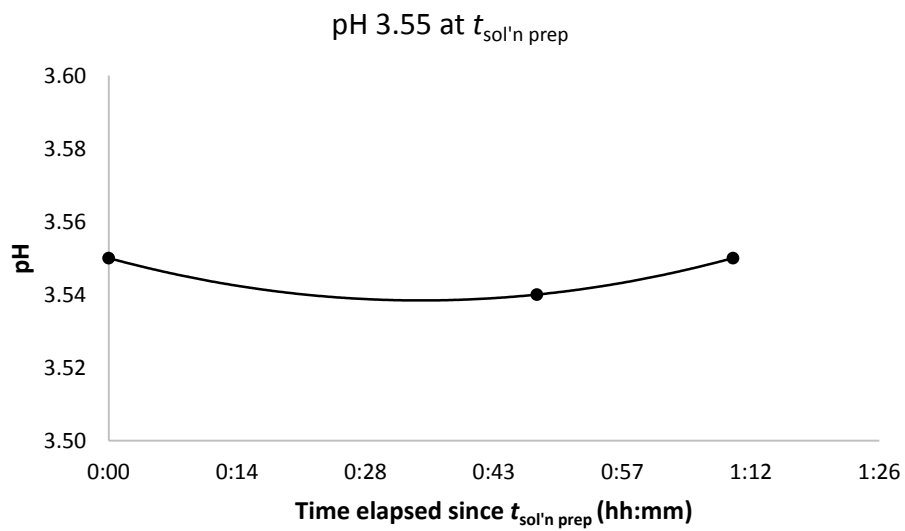
(a)



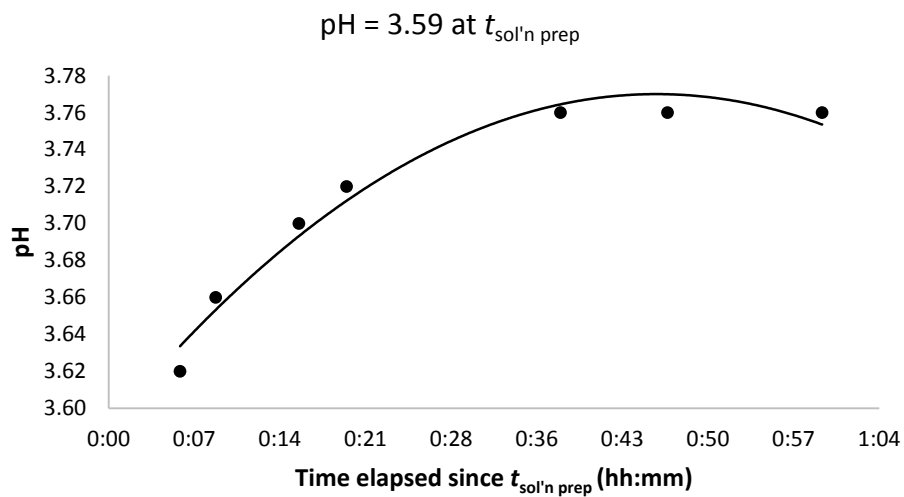
(b)



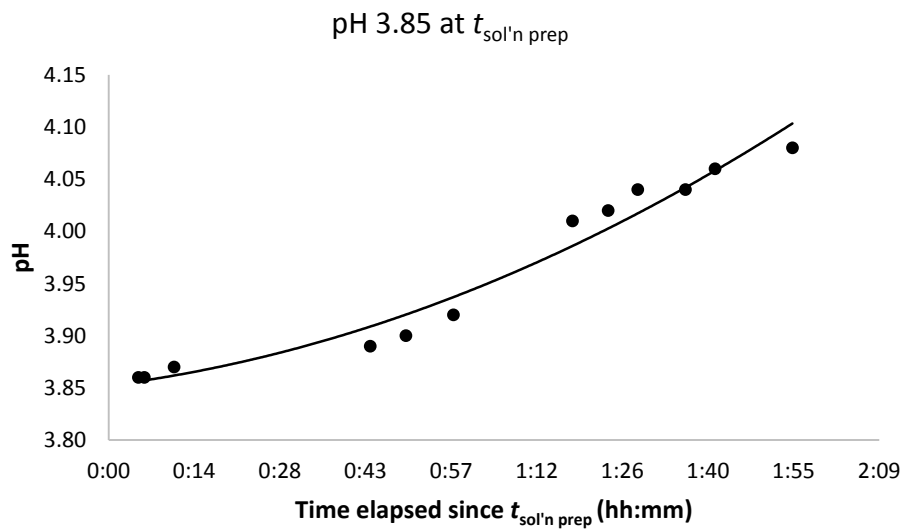
(c)



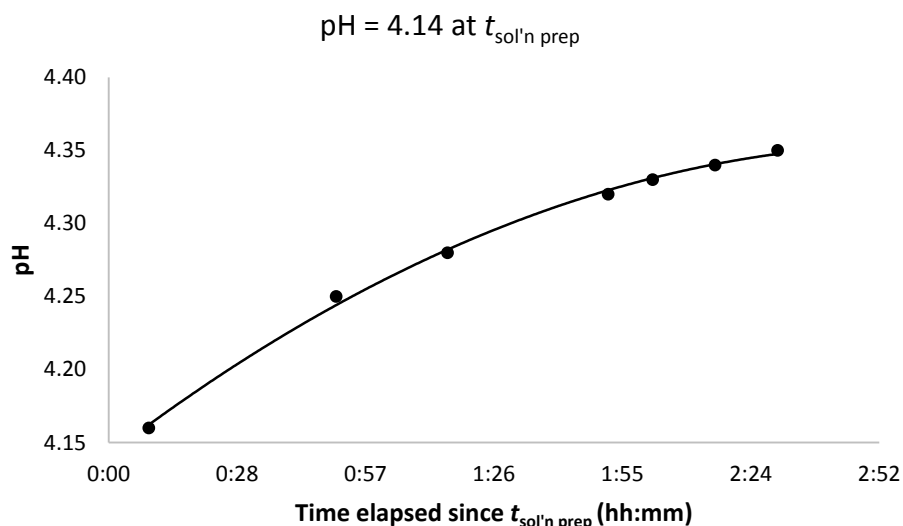
(d)



(e)



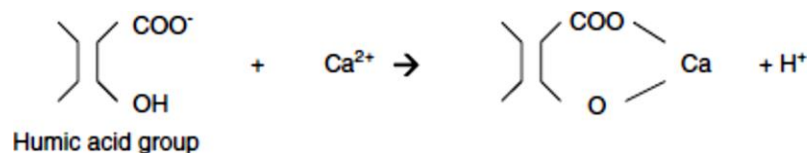
(f)



**Figure 43.** Experimentally determined pH drift plots (pH data as a function of elapsed time since  $t_{\text{sol'n prep}}$ ) for  $[\text{HA}]_{\text{solution}} = 0.84 \text{ g L}^{-1}$  and the following corresponding  $\text{pH}_{\text{sol'n}}$  studied for the  $\text{NO}_2$  uptake data to follow (pH at  $t_{\text{sol'n prep}}$  also given on respective plots): (a) pH 3.35; (b) pH 3.45; (c) pH 3.55; (d) pH 3.75; (e) pH 4.00; (f) pH 4.30 range. HA solution pH data was obtained by recording solution pH at random time intervals before and during the individual uptake experiments.

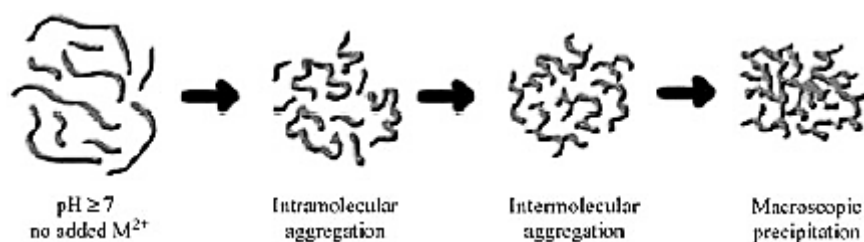
ated) commercial HA ( $[\text{HA}]_{\text{solution}} = 0.84 \text{ g L}^{-1}$ ) was less than about 0.4 pH units, in excellent agreement with recent pH drift (hysteresis effect) data over a comparable timescale for an HA extracted from an Irish peat *Sphagnum* with main chemical characteristics: pH = 4.8; ash = 4.5%; total organic C = 52.3%; total N = 0.72% (Montecchio et al., 2001).

The latter plausible reason for the observed pH drift, which may have resulted from binding with the available carboxyl groups of the HA molecule with several of its metallic ions as found as impurities (including aluminum, chromium and iron) in solution under acidic conditions, must be rejected since it has been recently reported that at pHs higher than 4.5, the disaggregation rate of a (peat) humic acid increases by more than three orders of magnitude per pH unit increase. Refer to **Figure 44** for a proposed chelation mechanism, (M16). Hence, under the experimental conditions in this pH study, the aggregation property predominates, and a very low probability of metal-binding sites exists (Marcelo and Wilkinson, 2002).



**Figure 44.** Reaction mechanism, (M16) for humic-Ca<sup>2+</sup>-H<sup>+</sup> system for a typical humic acid group. The two weakly acidic groups, the carboxylate (-COOH) or phenolic hydroxyl (-OH) group, help bind to the metal cation, Ca<sup>2+</sup>, forming a chelate. Protonation of the carboxylate ion (COO<sup>-</sup>), followed by H<sup>+</sup> ion abstraction from the adjacent phenolic hydroxyl group binds the humics together with Ca<sup>2+</sup> (Tipping et al., 1988). Chelation is observed to be predominant at lower and near neutral pH. From: Parida and Ng (2012).

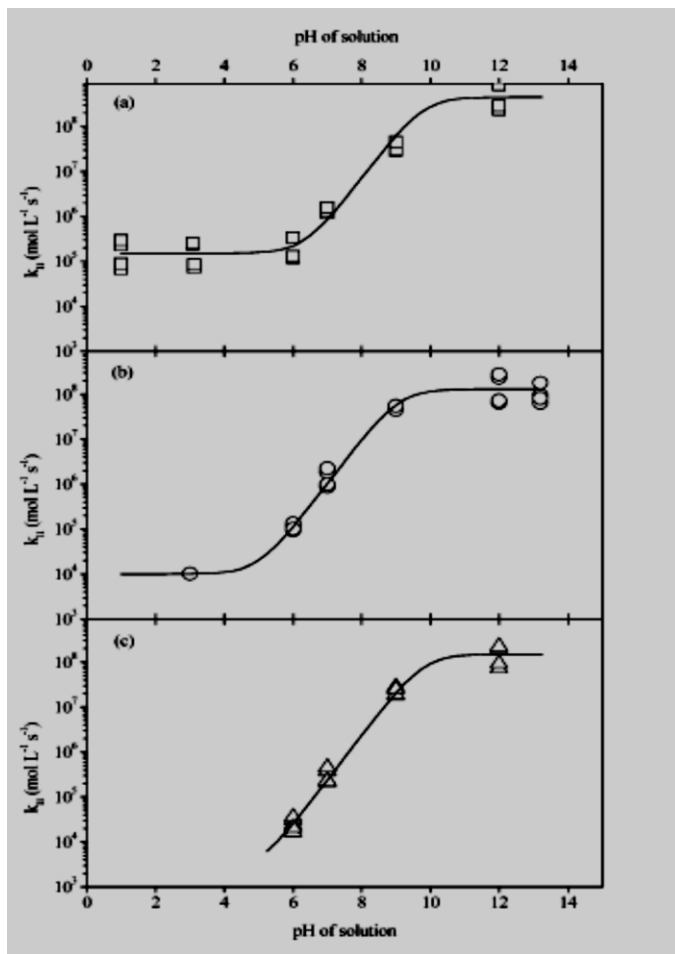
It is important to note that lowering the pH of aqueous HA solutions has an effect similar to adding metal salts (see **Figure 45**), however, in a less distinct manner (Engebretson et al., 1996) – increasing the [H<sup>+</sup>] causes protonation of the humic acid carboxy groups, typically beginning at around pH 3-2 and reaching completion at near pH 1. This continuous process, commencing at the intramolecular level, progresses through intermolecular aggregation, enhancing the detergent character of HAs via the establishment of hydrophobic domains, eventually producing a precipitate (von Wandruszka, 2000). Accordingly, frequent agitation of the acidic HA solutions under study (pH 1.5 to 4.3) used to generate the films was needed (and was accomplished using a stir-plate) in order to reduce sedimentation/precipitation during the course of the NO<sub>2</sub> uptake experiments. No sedimentation was observed for all acidities under consideration.



**Figure 45.** Visualization of HA aggregation through continued addition of a metal ion, M<sup>2+</sup> for an aqueous HA solution of pH ≥ 7. From: von Wandruszka (2000).

An obvious factor strongly affecting the uptake coefficient is the pH of the tested film solution (Ammann et al., 2005). Higher uptake coefficients have been previously reported for other compounds with

increasing pH (see **Figure 46**) due to the increasing fraction of the more reactive deprotonated species at higher pH (Ammann et al., 2005). The correlation between the average values for  $\gamma_{\text{best-fit}}$  and the average

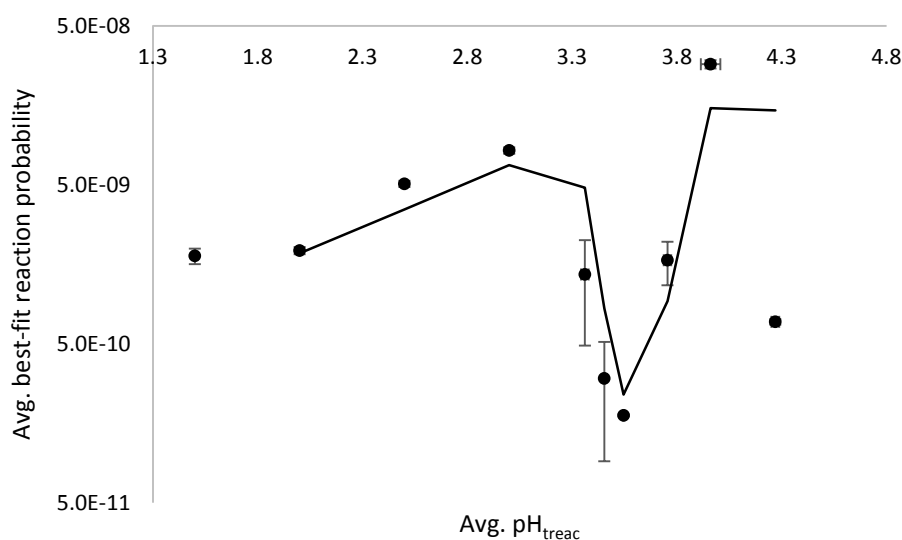


**Figure 46.** Overall aqueous-phase second-order rate constant of  $\text{NO}_2$  with ArOH solution ( $k_{\text{X}}^{\text{II}}$ ), plotted as a function of pH. Squares, circles, triangles refer to syringol, catechol, guaiacol, respectively.  $k_{\text{X}}^{\text{II}}$  values obtained from the measured uptake coefficients. For details, refer to the original text: Ammann et al. (2005).

film pH at the end of the gas-liquid reaction time ( $\text{pH}_{\text{treac}}$ ) is displayed graphically in **Figure 47**, fitted using the individual  $\text{P}(\text{HONO})$  data from the photoenhanced uptake of  $\text{NO}_2$  (36 ppbv) on commercial acidic concentrated ( $0.84 \text{ g L}^{-1}$ ) HA films of varying initial film pH (1.5 to about 4.29) experiments using the WWFT photoreactor (4 lamps). The corresponding numerical values are tabulated in **Table 19**, along with the individual experimental and corresponding model-predicted parameters given in **Table 20** for the reader's reference. Note that  $\gamma_{\text{best-fit}}$  was fitted such that the accumulated  $\text{P}_{\text{HONO,predict}}$  minimized the percentage difference between that of the observed ( $[\text{HONO}]_{\text{treac}}$ ) and the predicted HONO concentration ( $[\text{HONO}]_{\text{treac,predict}}$ ) at  $1 \text{ s}$  ( $= t_{\text{reac}}$ ). A *moving average* trendline was fitted to the data (in **Figure 47**), with



average  $\gamma_{\text{best-fit}}$  ranging from a minimum value of  $1.77 \times 10^{-11}$  ( $\pm 2.66 \times 10^{-12}$ ) at  $\text{pH}_{\text{treac}}$  of 3.55 ( $\pm 3.62 \times 10^{-3}$ ) to a maximum of  $2.87 \times 10^{-8}$  ( $\pm 1.73 \times 10^{-9}$ ) at  $\text{pH}_{\text{treac}}$  of 3.96 ( $\pm 4.65 \times 10^{-2}$ ). The decrease in the photoenhanced  $\text{NO}_2$  reduction reaction's kinetic favourability ( $\gamma_{\text{best-fit}}$ ) begins at approximately  $\text{pK}_{\text{a}(\text{HONO})}$ , the physical reasoning for which is unclear at this point in time. The averaged computed values for  $\gamma_{\text{best-fit}}$  span about three orders of magnitude in range (see **Table 19**), with precisions (RSD) less than 30% for all acidities tested, excluding the values determined for  $\text{pH}_{\text{treac}}$  of 3.36 ( $\pm 1.82 \times 10^{-2}$ ) and 3.45 ( $\pm 4.07 \times 10^{-3}$ ), respectively, which had significantly larger precisions near 70%. The high instability in the average (minimum) values of  $\gamma_{\text{best-fit}}$  at these values of  $\text{pH}_{\text{treac}}$  (3.36, 3.45) is not unexpected, as the values of  $\text{pH}_{\text{treac}}$  are within 0.06 pH units of  $\text{pK}_{\text{a}(\text{HONO})}$  and  $\text{pK}_{\text{a}1,\text{carboxylic}(\text{HA})}$ , respectively. The percentage decrease



**Figure 47.** Correlation between average  $\text{pH}_{\text{treac}}$  and average  $\gamma_{\text{best-fit}}$  for the photoenhanced uptake of  $\text{NO}_2$  (36 ppbv) on commercial acidic (pH 1.5 to 4.27) concentrated HA films ( $[\text{HA}]_{\text{solution}} = 0.84 \text{ g L}^{-1}$ ) using the WWFT photoreactor (4 lamps). Moving average trendline shown. Error bars represent  $\pm 1\sigma$ .

in pH due  $\text{HNO}_2$  dissociation at the end of the 1 s reaction time (% decrease from  $\text{pH}_{\text{sol'n}}$ ) was only found to be a minor issue for the dataset, that is, with the only non-negligible decreases in HA solution pH of 0.24 – 0.30% corresponding to the  $\text{pH}_{\text{sol'n}}$  range of 3.91 to 4.04 (see **Table 20**). Over the entire analysed  $\text{pH}_{\text{treac}}$  range (excluding  $\text{pH}_{\text{treac}}$  of  $3.96 (\pm 4.65 \times 10^{-2})$ ), < 0.50% loss in the initial  $\text{NO}_2$  mixing ratio (36 ppbv), was observed, smaller than the corresponding values of  $\text{RSD}\gamma_{\text{best-fit}}$  (%) (refer to **Tables 19 & 20**). A maximum  $\text{NO}_2$  loss of  $3.66 (\pm 0.18) \%$  is seen at the  $\text{pH}_{\text{treac}}$  of  $3.96 (\pm 4.65 \times 10^{-2})$ , still less than the precision of 6.03% on the complementary mean  $\gamma_{\text{best-fit}}$ . Thus, the assumption holds true over all acidities studied, that the rapid aqueous film renewal rate of about 2 minutes prevents accumulation of reaction products in the WWFT photoreactor.

$\text{pH}_{\text{treac}}(\pm 1\sigma)$	$\gamma_{\text{best-fit}}(\pm 1\sigma)$	$\text{RSD}\gamma_{\text{best-fit}}(\%)$
1.50 ( $\pm 5.03 \times 10^{-9}$ )	$1.79 \times 10^{-9}$ ( $\pm 1.99 \times 10^{-10}$ )	11.2
2.00 ( $\pm 2.47 \times 10^{-8}$ )	$1.93 \times 10^{-9}$ ( $\pm 1.01 \times 10^{-10}$ )	5.24
2.50 ( $\pm 5.16 \times 10^{-7}$ )	$5.08 \times 10^{-9}$ ( $\pm 2.33 \times 10^{-10}$ )	4.60
3.00 ( $\pm 6.58 \times 10^{-6}$ )	$8.23 \times 10^{-9}$ ( $\pm 3.86 \times 10^{-10}$ )	4.69
3.36 ( $\pm 1.82 \times 10^{-2}$ )	$1.37 \times 10^{-9}$ ( $\pm 8.79 \times 10^{-10}$ )	64.3
3.45 ( $\pm 4.07 \times 10^{-3}$ )	$3.02 \times 10^{-10}$ ( $\pm 2.11 \times 10^{-10}$ )	69.9
3.55 ( $\pm 3.62 \times 10^{-3}$ )	$1.77 \times 10^{-10}$ ( $\pm 2.66 \times 10^{-12}$ )	1.50
3.75 ( $\pm 1.80 \times 10^{-2}$ )	$1.68 \times 10^{-9}$ ( $\pm 5.12 \times 10^{-10}$ )	30.4
3.96 ( $\pm 4.65 \times 10^{-2}$ )	$2.87 \times 10^{-8}$ ( $\pm 1.73 \times 10^{-9}$ )	6.03
4.27 ( $\pm 1.89 \times 10^{-2}$ )	$6.87 \times 10^{-10}$ ( $\pm 2.71 \times 10^{-11}$ )	3.94

**Table 19.** Model-predicted values of mean  $\gamma_{\text{best-fit}} (\pm 1\sigma)$ , as well as precision,  $\text{RSD}\gamma_{\text{best-fit}} (\%)$ , obtained based on averaging of individual data in the corresponding film pH interval (pH 1.5 to 4.27 ( $\pm 1\sigma$ )) from the photoenhanced uptake of  $\text{NO}_2$  (36 ppbv) on commercial concentrated ( $[\text{HA}]_{\text{solution}} = 0.84 \text{ g L}^{-1}$ ) HA films experiments using the WWFT photoreactor (4 lamps).

EXPERIMENTAL PARAMETERS	MODEL-PREDICTED PARAMETERS				
	$\text{pH}_{\text{sol'n}}$	Best-fit reaction probability ( $\gamma_{\text{best-fit}}$ )	$\text{pH}_{\text{treac}}$ (% decrease from $\text{pH}_{\text{sol'n}}$ ) <sup>a</sup>	$[\text{HONO}]_{\text{treac,predict}}$ (pptv) (% difference from $[\text{HONO}]_{\text{treac}}$ ) <sup>a</sup>	% $\text{NO}_2$ remaining at $t_{\text{reac}} = 1 \text{ s}$
	1.50	$1.57 \times 10^{-9}$	1.50	79.35	99.98
	1.50	$1.66 \times 10^{-9}$	1.50	83.76	99.98
	1.50	$1.98 \times 10^{-9}$	1.50	100.02	99.98
	1.50	$1.93 \times 10^{-9}$	1.50	97.14	99.98

EXPERIMENTAL PARAMETERS	MODEL-PREDICTED PARAMETERS			
	pH <sub>sol'n</sub>	Best-fit reaction probability ( $\gamma_{\text{best-fit}}$ )	pH <sub>treac</sub> (% decrease from pH <sub>sol'n</sub> ) <sup>a</sup>	[HONO] <sub>treac,predict.</sub> (pptv) (% difference from [HONO] <sub>treac</sub> ) <sup>a</sup>
2.00	1.81×10 <sup>-9</sup>	2.00	88.43	99.97
2.00	2.00×10 <sup>-9</sup>	2.00	97.47	99.97
2.00	1.89×10 <sup>-9</sup>	2.00	92.12	99.97
2.00	1.88 <sub>g</sub> ×10 <sup>-9</sup>	2.00	92.13	99.97
2.00	2.07×10 <sup>-9</sup>	2.00	100.89	99.97
2.50	5.26×10 <sup>-9</sup>	2.50	232.59	99.85
2.50	4.82×10 <sup>-9</sup>	2.50	213.31	99.86
2.50	4.92×10 <sup>-9</sup>	2.50	217.60	99.86
2.50	5.18×10 <sup>-9</sup>	2.50	229.01	99.85
2.50	5.14×10 <sup>-9</sup>	2.50	227.15	99.85
2.50	4.80×10 <sup>-9</sup>	2.50	212.10	99.86
2.50	5.41×10 <sup>-9</sup>	2.50	239.31	99.85
3.00	8.31×10 <sup>-9</sup>	3.00	283.29	99.52
3.00	7.52×10 <sup>-9</sup>	3.00	256.40	99.57
3.00	8.54×10 <sup>-9</sup>	3.00	290.94	99.51
3.00	8.10×10 <sup>-9</sup>	3.00	276.02	99.54
3.00	8.38×10 <sup>-9</sup>	3.00	285.64	99.52
3.00	8.55×10 <sup>-9</sup>	3.00	291.51	99.51
3.34	2.64×10 <sup>-9</sup>	3.34	64.84	99.78
3.36	1.23×10 <sup>-9</sup>	3.36	29.48	99.89
3.37	9.12×10 <sup>-10</sup>	3.37	21.43	99.92
3.38	6.79×10 <sup>-10</sup>	3.38	15.89	99.94
3.45	7.93×10 <sup>-11</sup>	3.45	1.69	99.99
3.46	5.39×10 <sup>-10</sup>	3.46	11.31	99.95
3.45 <sub>26</sub>	1.77×10 <sup>-10</sup>	3.45 <sub>26</sub>	3.75	99.98
3.45 <sub>31</sub>	4.14×10 <sup>-10</sup>	3.45 <sub>31</sub>	8.76	99.96

EXPERIMENTAL PARAMETERS	MODEL-PREDICTED PARAMETERS			
	$\text{pH}_{\text{sol'n}}$	Best-fit reaction probability ( $\gamma_{\text{best-fit}}$ )	$\text{pH}_{\text{treac}}$ (% decrease from $\text{pH}_{\text{sol'n}}$ ) <sup>a</sup>	$[\text{HONO}]_{\text{treac,predict}}$ (pptv) (% difference from $[\text{HONO}]_{\text{treac}}$ ) <sup>a</sup>
3.54	$1.79 \times 10^{-10}$	3.54	3.34	99.98
3.55	$1.75 \times 10^{-10}$	3.55	3.24	99.98
3.76	$2.43 \times 10^{-9}$	3.76	31.81	99.71
3.77	$1.57 \times 10^{-9}$	3.77	20.43	99.81
3.76	$1.31 \times 10^{-9}$	3.76	17.38	99.85
3.73	$1.40 \times 10^{-9}$	3.73	19.51	99.84
3.91	$2.91 \times 10^{-8}$	3.90 (0.24)	290.99	96.37
3.93	$2.96 \times 10^{-8}$	3.92 (0.26)	285.41	96.27
3.96	$3.15 \times 10^{-8}$	3.94 (0.29)	290.32	96.01
3.98	$2.79 \times 10^{-8}$	3.97 (0.28)	246.01 ( $4.08 \times 10^{-3}$ )	96.42
4.01	$2.78 \times 10^{-8}$	4.00 (0.29)	232.14	96.40
4.04	$2.65 \times 10^{-8}$	4.03 (0.30)	208.70	96.54
4.24 <sub>73</sub>	$7.06 \times 10^{-10}$	4.24 <sub>68</sub> (0.013)	3.67	99.90
4.26 <sub>32</sub>	$7.14 \times 10^{-10}$	4.26 <sub>26</sub> (0.014)	3.59	99.90
4.28 <sub>79</sub>	$6.58 \times 10^{-10}$	4.27 <sub>73</sub> (0.013)	3.21	99.91
4.29 <sub>12</sub>	$6.71 \times 10^{-10}$	4.29 <sub>06</sub> (0.014)	3.18	99.90

**Table 20.** Model-predicted parameters, including  $\gamma_{\text{best-fit}}$ ,  $[\text{HONO}]_{\text{treac,predict}}$ ,  $\text{pH}_{\text{treac}}$ , and the reactive  $\text{NO}_2$  loss percentage at  $t_{\text{treac}}$  of 1 s determined by means of the model developed herein (including diffusion), based on the individual data input parameters ( $[\text{HONO}]_{\text{treac}}$ ) obtained from the photoenhanced uptake of  $\text{NO}_2$  (36 ppbv) on the commercial acidic concentrated ( $[\text{HA}]_{\text{solution}} = 0.84 \text{ g L}^{-1}$ ) HA films of varying pH (1.5 to 4.29) using the WWFT photoreactor. <sup>a</sup> Shown only if it is non-negligible.

Knowing the values of  $pK_{a_{\text{carboxylic},n}}$  for the carboxylic acids present in the commercial HA over the studied pH range of interest (i.e.,  $pK_{a_{\text{carboxylic},1}}$  and  $pK_{a_{\text{carboxylic},2}}$ ), the relative amount,  $\Theta_n$  of the singly dissociated species at a certain  $pH_{\text{treac}}$  can be easily calculated using the Henderson-Hasselbalch formula (Albert and Serjeant, 1984):

$$\Theta_n = \frac{1}{1 + 10^{(pK_{a_{\text{carboxylic},n}} - pH_{\text{treac}})}} \quad (\text{E66}).$$

Note that (E66) is valid since the approach used by Paxéus and Wedborg (1985) considers the commercial HA as a mixture of monoprotic acids, with  $pK_{a_{\text{carboxylic},1}} = 3.39$  and  $pK_{a_{\text{carboxylic},2}} = 4.78$  (no precisions given). As seen in **Table 21**, the computed values of  $\Theta_{\text{carboxylic},1}$  or the relative amount of singly dissociated carboxylic species with  $pK_{a_{\text{carboxylic},1}} = 3.39$  range almost over two orders of magnitude from  $\Theta_{\text{carboxylic},1} = 0.0127 (\pm 4.27 \times 10^{-11})$  at (average)  $pH_{\text{treac}}$  of 1.50 to  $\Theta_{\text{carboxylic},1} = 0.483 (\pm 2.62 \times 10^{-3})$  for a mean  $pH_{\text{treac}}$  of 3.36. The relative amount of singly dissociated carboxylic species with  $pK_{a_{\text{carboxylic},2}} = 4.78$ , or calculated values of  $\Theta_{\text{carboxylic},2}$ , on the other hand, only differ by nearly a factor of 2.50 from  $\Theta_{\text{carboxylic},2} = 0.0724 (\pm 1.35 \times 10^{-3})$  at (average)  $pH_{\text{treac}}$  of 3.50 to  $\Theta_{\text{carboxylic},2} = 0.164 \pm (7.24 \times 10^{-4})$  for mean  $pH_{\text{treac}}$  of 4.27.

The following excellent correlations (E67) (*quadratic*; see **Figure 48**) and (E68) (*exponential*; see **Figure 49**), both with  $R^2 \geq 0.994$ , are obtained when  $\Theta_{\text{carboxylic},n}$  ( $n = 1, 2$ , respectively) is plotted against the mean  $\chi_{\text{best-fit}}$  for the respective (average)  $pH_{\text{treac}}$  data subsets cited below:

$$(1) \chi_{\text{quadratic}} = - (1.34 \times 10^{-7} \Theta_{\text{carboxylic},1}^2) + (6.93 \times 10^{-8} \Theta_{\text{carboxylic},1}) - 7.61 \times 10^{-10} \quad (\text{E67})$$

For  $\Theta_{\text{carboxylic},1}$  between 0.0391 - 0.483 (pH = 2.00 – 3.36);

$$(2) \chi_{\text{exponential}} = 1.53 \times 10^{-14} e^{1.32 \times 10^2 \Theta_{\text{carboxylic},2}} \quad (\text{E68})$$

For  $\Theta_{\text{carboxylic},2}$  between 0.0724 – 0.109 (pH = 3.50 – 3.96).

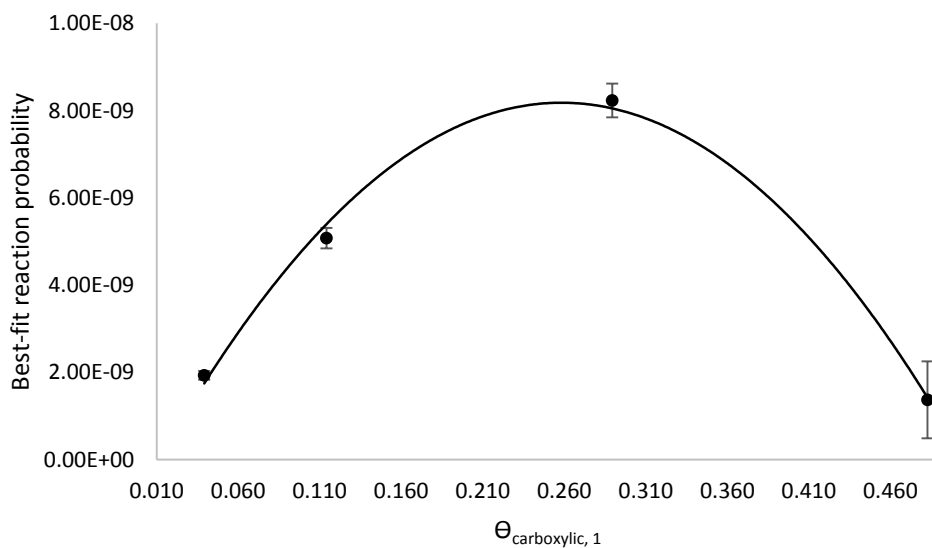
Note that in (E68), the mean values of  $\chi_{\text{best-fit}}$  at  $pH_{\text{treac}}$  of 3.45 and 3.55 were averaged to obtain the data point at 3.50 since their corresponding average values of  $\Theta_{\text{carboxylic},2}$  (0.0699 and 0.0752, respectively) differed by only 7%, excluding propagated uncertainties. The exceptions to the excellent correlations

$\text{pH}_{\text{treac}}$	$\Theta_{\text{carboxylic},1}$	$\sigma\Theta_{\text{carboxylic},1}$	$\frac{\sigma\Theta_{\text{carboxylic},1}}{\Theta_{\text{carboxylic},1}} (\%)$	$\chi_{\text{best-fit}}$	$\text{RSD}\chi_{\text{best-fit}} (\%)$
1.50	0.0127	$4.27 \times 10^{-11}$	$3.35 \times 10^{-7}$	$1.79 \times 10^{-9}$	11.2
2.00	0.0391	$4.83 \times 10^{-10}$	$1.23 \times 10^{-6}$	$1.93 \times 10^{-9}$	5.24
2.50	0.114	$2.36 \times 10^{-8}$	$2.06 \times 10^{-5}$	$5.08 \times 10^{-9}$	4.60
3.00	0.289	$6.35 \times 10^{-7}$	$2.19 \times 10^{-4}$	$8.23 \times 10^{-9}$	4.69
3.36	0.483	$2.62 \times 10^{-3}$	0.54	$1.37 \times 10^{-9}$	64.3
3.50	0.0724	$1.35 \times 10^{-3}$	1.86	$2.40 \times 10^{-10}$	36.9
3.75	0.0889	$4.27 \times 10^{-4}$	0.48	$1.68 \times 10^{-9}$	30.4
3.96	0.109	$1.28 \times 10^{-3}$	1.17	$2.87 \times 10^{-8}$	6.03

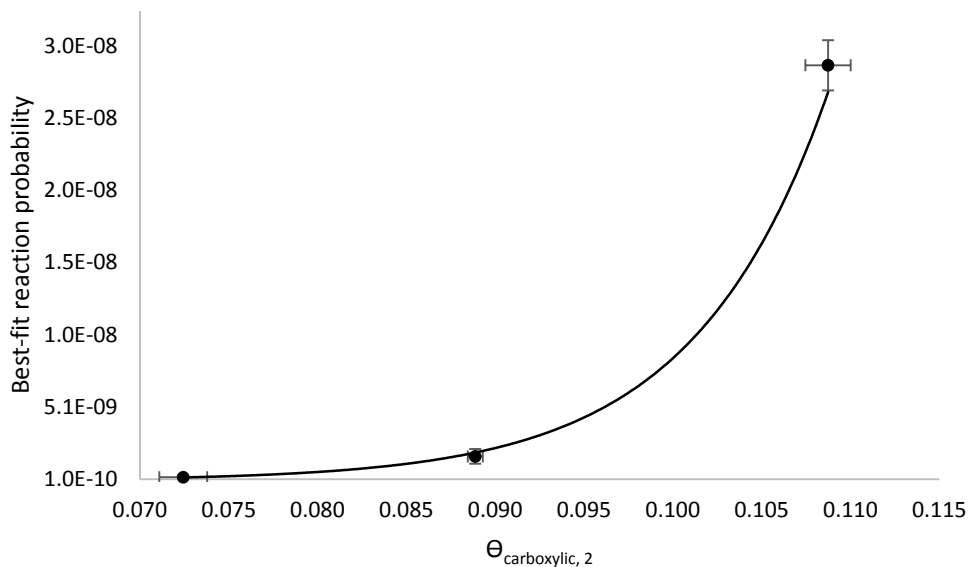
**Table 21.** Computed values of  $\Theta_{\text{carboxylic},1}$  for mean values of  $\text{pH}_{\text{treac}}$  ranging from 1.50 to 3.96 for the commercial HA standard. The propagated uncertainty on  $\Theta_{\text{carboxylic},1}$  denoted  $\sigma\Theta_{\text{carboxylic},1}$  is also given, along with the corresponding relative uncertainty,  $\sigma\Theta_{\text{carboxylic},1}/\Theta_{\text{carboxylic},1}$  (%). Mean values of  $\chi_{\text{best-fit}}$  and corresponding precisions ( $\text{RSD}\chi_{\text{best-fit}}$  (%)) are also shown for the  $\text{pH}_{\text{treac}}$  interval (data originally presented in Table 19 for identical operating conditions).

(E67) and (E68), along with plausible explanations are as follows:

- (1) The (average)  $\chi_{\text{best-fit}}$  for the most acidic film ( $\text{pH}_{\text{treac}} = 1.50$ ), appears to be overestimated (refer back to **Figure 47**; moving average trendline), and hence, was removed from the observed quadratic correlation in (E67). The most likely reason for such a discrepancy is the occurrence of secondary reactions of HONO decomposition into NO and  $\text{NO}_2$  under the highly acidic conditions. However, it is expected that this would result in an underestimation of  $\chi_{\text{best-fit}}$ , and hence, the HA film may have been contaminated.
- (2) The mean  $\chi_{\text{best-fit}}$  obtained at the maximum value of  $\Theta_{\text{carboxylic},2}$  ( $= 0.164$ ) for the least acidic film,  $\text{pH} = 4.27$ , appears to be significantly underestimated (i.e., is an outlier; refer again to **Figure 47**), and hence, was excluded from (E68). This was not unexpected, as a very low HONO production rate at  $\text{pH}_{\text{treac}}$  values greater than 1.00 pH unit away from  $\text{pK}_{\text{a(HONO)}}$  was anticipated to be observed – in fact,  $[\text{NO}_2^-]$  is estimated to be roughly three orders of magnitude greater than  $[\text{HONO}_{(\text{aq})}]$  using the derived model and observed  $P_{\text{HONO}}$  at this film acidity. This does not exclude the possibility that the least acidic HA film could also have been contaminated.



**Figure 48.** Quadratic (second-order polynomial) relationship between  $\Theta_{\text{carboxylic},1}$  ( $\text{pK}_{\text{a}_{\text{carboxylic},1}} = 3.39$ ) and the mean  $\gamma_{\text{best-fit}}$  data for the commercial HA standard and the (average)  $\text{pH}_{\text{treac}}$  data subset of 2.00 – 3.36 (i.e., 1.36 pH unit subset). Average values of  $\gamma_{\text{best-fit}}$  and  $\text{pH}_{\text{treac}}$  originally presented in Table 19 for identical operating conditions.



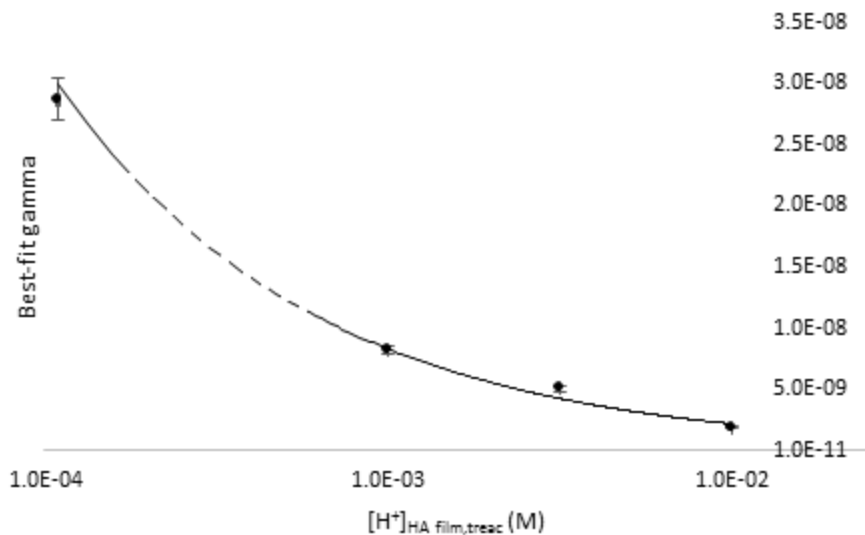
**Figure 49.** Exponential relationship between  $\Theta_{\text{carboxylic},2}$  ( $\text{pK}_{\text{a}_{\text{carboxylic},2}} = 4.78$ ) and the mean  $\gamma_{\text{best-fit}}$  data for the commercial HA standard and the (average)  $\text{pH}_{\text{treac}}$  data subset of 3.50 – 3.96 (i.e.,  $\sim 0.50$  pH unit subset). Average values of  $\gamma_{\text{best-fit}}$  and  $\text{pH}_{\text{treac}}$  originally presented in Table 19 for identical operating conditions.

Both the observed increase in mean  $\gamma_{\text{best-fit}}$  by a factor of about 4 from  $\text{pH}_{\text{treac}}$  2.00 to 3.00 and the subsequent detected decrease in the average  $\gamma_{\text{best-fit}}$  by approximately a factor of six from  $\text{pH}_{\text{treac}}$  3.00 to

pH 3.36, are described by the exceptional *quadratic* correlation in (E67). The *exponential* correlation (E68) obtained for the relationship between  $\Theta_{\text{carboxylic},2}$  and the mean best-fit reaction probability ( $\gamma_{\text{best-fit}}$ ) for the  $\sim 0.50$  pH<sub>tr<sub>reac</sub></sub> unit subset (factor of 2.50 range in  $\Theta_{\text{carboxylic},2}$ ) is indicative of the high-sensitivity of the NO<sub>2</sub> reduction to the fraction of available or dissociated carboxyl groups in solution with pK<sub>a</sub><sub>carboxylic,2</sub> of 4.78. This kinetically preferential reaction probability behavior, most likely due to increases in deprotonation, is necessary to maintain the noteworthy *power* correlation ( $R^2 > 0.985$ ) of mean  $\gamma_{\text{best-fit}}$  with (average) hydronium ion concentration of the HA film observed at the end of the gas-liquid reaction time ( $[\text{H}^+]_{\text{HA film,treac}}$  (M)) over the pH<sub>tr<sub>reac</sub></sub> range of 1.5 to 4.0 (see **Figure 50**):

$$\gamma_{\text{power}} = 2 \times 10^{-10} [\text{H}^+]_{\text{HA film,treac}} (\text{M})^{-0.579}; \text{ for pH 1.5 to 4.0 (excl. pHs 3.36 to 3.75)} \quad (\text{E69}).$$

Of course, this correlation excludes values of pH<sub>tr<sub>reac</sub></sub> between 3.36 and 3.75, where complex pH<sub>tr<sub>reac</sub></sub>-dependent  $\gamma_{\text{best-fit}}$  behavior was seen.

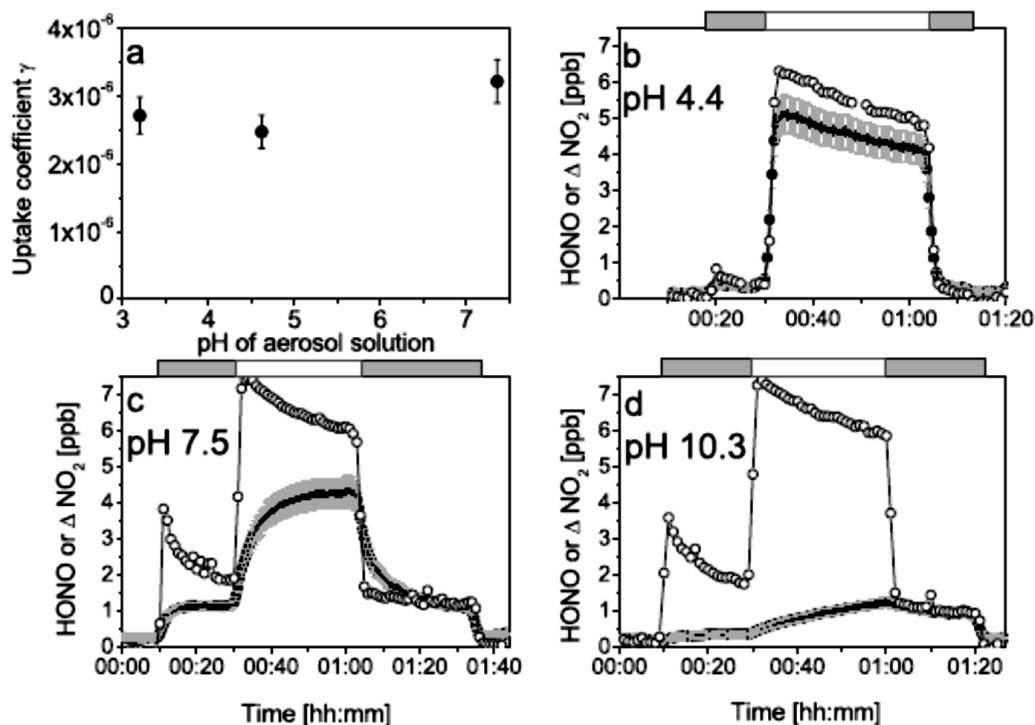


**Figure 50.** Power relationship between the (average) value of  $[\text{H}^+]_{\text{HA film,treac}}$  (M) and the corresponding mean value of  $\gamma_{\text{best-fit}}$  for the commercial humic acid standard over the pH<sub>tr<sub>reac</sub></sub> range of 1.5 to 4.0. The film pH range (at t<sub>reac</sub>) from 3.36 to 3.75 (drawn in dashes - - -), is excluded from the trend, as complex pH<sub>tr<sub>reac</sub></sub>-dependent  $\gamma_{\text{best-fit}}$  behavior was observed in this range. Error bars represent  $\pm 1\sigma$ .

Although the various parameterizations presented may be useful for describing the complex pH<sub>tr<sub>reac</sub></sub>-dependent  $\gamma_{\text{best-fit}}$  behavior observed in this pH study, the reader must note that given the data available at hand, no physical meaning can yet be attributed for the functional forms given.



It is important to note, that deprotonation, will additionally affect the conformation and the surface structure of HA, so that, the observed changes cannot be explicitly related to the direct effects of the deprotonation (Ammann et al., 2005). For comparison, Stemmler et al. (2006) found that the photoenhanced (and dark) reaction of  $\text{NO}_2$  ( $[\text{NO}_2]_0 = 20$  ppb) with the concentrated ( $[\text{HA}]_{\text{solution}} = 1 \text{ g L}^{-1}$  or  $[\text{HA}]_{\text{film}} = 8 \mu\text{g cm}^{-2}$ ) environmentally unrealistic *solid* humic acid coating increases with pH, leading to an enhanced formation of HONO, with a pronounced effect observed between pH 4.4, and 7.5, but no further increase between pH 7.5 and 10.3 was detected (see **Figure 51 (b) – (d)**). Ammann et al. (2005) suggest that this is likely due to drastic increases in reactivity in the reaction between  $\text{NO}_2$  with the abundant phenolic groups or aromatic amines (within the HA) with deprotonation. The results are qualitatively consistent with those of Stemmler et al. (2006), however concentrate on more realistic pH conditions of anaerobic humic soils. Increases in the photoenhanced HONO formation with pH were observed, but for highly to moderately acidic conditions, specifically, between pH 1.5 and 4.3, due to



**Figure 51.** Formation of HONO as a function of acidity of the: (a) humic acid aerosol ( $\text{NO}_2$  uptake coefficient); and (b) – (d) humic acid coatings (HONO-formation ( $\bullet$ ), and  $\text{NO}_2$ -loss ( $\circ$ )). In the case of the solid HA films, the ratio of the film volume to the reactor volume is much higher, leading to increased partitioning of HONO to the condensed phase under the same pH conditions. Also, at similar HONO concentrations, it takes significantly longer for HONO to titrate the basic capacity of the film. The exchange of HONO between gas and condensed phase also leads to the delayed response observed at high pH. From: Stemmler et al. (2007).

increases in reactivity in the reaction with NO<sub>2</sub> with the several carboxyl groups (pK<sub>a,1</sub> = 3.39; pK<sub>a,2</sub> = 4.78) within the commercial HA with deprotonation. It is important to note, however, that this observation, precludes the values of pH<sub>treac</sub> between 3.36 and 3.75 where complex pH<sub>treac</sub>-dependent  $\gamma_{\text{best-fit}}$  behaviour was seen, as pH<sub>treac</sub> was centred near both pK<sub>a</sub>(HONO) and pK<sub>a1,carboxylic(HA)</sub>, respectively. This is contrary to the study of Stemmler et al. (2007) concerning the photoenhanced reduction of NO<sub>2</sub> ([NO<sub>2</sub>]<sub>0</sub> = 25 ppbv) on HA aerosols of unenvironmentally genuine concentrations (20 g L<sup>-1</sup>), who observed no significant change in the yields of gaseous HONO for moderate acidic to neutral aerosols (pH 3.2, 4.6, and 7.4; see **Figure 51 (a)**), indicative that nitrite salts are sufficiently rapidly desorbing as HONO to not affect the HONO yields of the experiments with aerosols of varying acidities.

### 5.3 DETERMINATION OF $k_{\text{rxn}}$

**Figure 52** shows a plot of the (average) net HONO production rate,  $\Delta P(\text{HONO})(\text{ppbv s}^{-1})$  versus the corresponding tested (average) commercial HA film concentration, denoted  $[\text{HA}]_{\text{film}}$  (ppbv) for HA solution concentrations ( $[\text{HA}]_{\text{solution}}$ ) ranging from 0.50 g – 0.84 g L<sup>-1</sup>. The corresponding numerical data is given in **Table 22** for the reader's reference. Note that the HA film concentrations ( $[\text{HA}]_{\text{film}}$ ) given in units of ppbv (or  $\mu\text{g L}^{-1}$ ) were computed as:

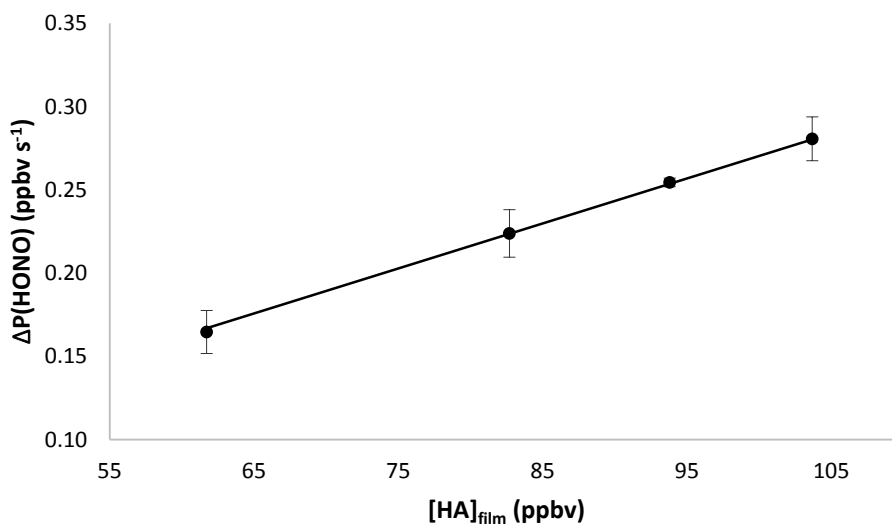
$$[\text{HA}]_{\text{film}} = [\text{HA}]_{\text{solution}} \left( \text{g L}^{-1} \right) \times \frac{V_{\text{film,diff}}}{V_{\text{solution}}} \quad (\text{E70})$$

where the HA film volume (incorporating diffusion),  $V_{\text{film,diff}}$  and the (HA) solution volume,  $V_{\text{solution}}$  are both in units of L, and have been previously defined.

The HONO production data exhibits a highly linear dependence ( $R^2 = 0.999$ ) with a zero intercept for the following tested  $[\text{HA}]_{\text{film}}$  range with an experimentally determined value of  $k_{\text{rxn}}$  of

$$k_{\text{rxn}} = 2.70 \times 10^{-3} \text{ s}^{-1} \text{ at } [\text{NO}_2]_0 = 36 \text{ ppbv for } [\text{HA}]_{\text{film}} (\text{pH } 3) \text{ ranging from } 62 \text{ to } 104 \text{ ppbv (E71).}$$

This shows that the uptake is effectively and exclusively driven by the reaction of NO<sub>2</sub> with the tested aromatic commercial HA, i.e., there is no competition with the hydrolysis reaction discussed previously.



**Figure 52.** Correlation plot of  $[HA]_{\text{film}}$  (ppbv or  $\mu\text{g L}^{-1}$ ) against the corresponding average value of the net HONO production rate  $\Delta P(\text{HONO})$  (ppbv  $\text{HNO}_2 \text{ s}^{-1}$ ) for the photoenhanced uptake of  $\text{NO}_2$  (36 ppbv) on commercial acidic (pH 3) HA films of varying concentration ( $[HA]_{\text{solution}} = 62 - 104$  ppbv) using the WWFT photoreactor (4 lamps) and a  $t_{\text{reac}}$  of  $\sim 1$  s.

$[HA]_{\text{solution}}$ ( $\text{g L}^{-1}$ )	$[HA]_{\text{film}}$ (ppbv)	$\Delta P(\text{HONO})$ ( $\pm 1\sigma$ ) (pptv $\text{HONO s}^{-1}$ )	RSD (%)	$n$	$N$
0.50	61.71	164.64 ( $\pm 12.91$ )	7.84	8	3
0.67	82.69	223.79 ( $\pm 14.27$ )	6.38	8	2
0.76	93.80	254.43 ( $\pm 2.57$ )	1.01	5	1
0.84	103.68	280.63 ( $\pm 13.16$ )	4.69	6	2
1.00	123.42	718.29 ( $\pm 36.07$ )	5.02	8	2

**Table 22.** (Average) net HONO production rate data,  $\Delta P(\text{HONO})$  (pptv  $\text{HNO}_2 \text{ s}^{-1}$ ) for the photoenhanced uptake of  $\text{NO}_2$  (36 ppbv) on commercial acidic (pH 3) HA films of varying concentration ( $[HA]_{\text{solution}} = 0.50 - 1.00 \text{ g L}^{-1}$ ) using the WWFT photoreactor (4 lamps) and a  $t_{\text{reac}}$  of  $\sim 1$  s.

The exception to the linear correlation, the  $\Delta P(\text{HONO})$  data corresponding to the HA film concentration of about 123 ppbv, appears to be overestimated, and is likely due to the fact that this HA solution concentration is at the lower limit of the critical micelle concentration (CMC) of  $1 - 10 \text{ g L}^{-1}$  (for HAs of different natures) (Engbretson and von Wandruszka, 1994), at which increased product yield due to the enhanced detergent character of the HA through the establishment of hydrophobic domains (von Wandruszka, 2000) is expected.

Under the conditions chosen in this study, uptake into the liquid was expected to be limited by the combined effects of reaction and diffusion in the liquid-phase (HA) – it was assumed that the mass accommodation coefficient ( $\alpha$ ) was much larger than the uptake coefficient,  $\gamma_{\text{expt}}$ . Under the assumption that the reaction of  $\text{NO}_2$  with HA in solution (in excess concentration) becomes rate-limiting for the experimental uptake, then computation of the reaction probability,  $\gamma_{\text{rxn}}$ , is achieved via the relatively simple analytic expression (Kolb et al., 1994):

$$\gamma_{\text{rxn}} = \frac{4H_{\text{NO}_2}RT\sqrt{k_{\text{rxn}}D_{\text{NO}_2}}}{\langle c \rangle} \quad (\text{E72}).$$

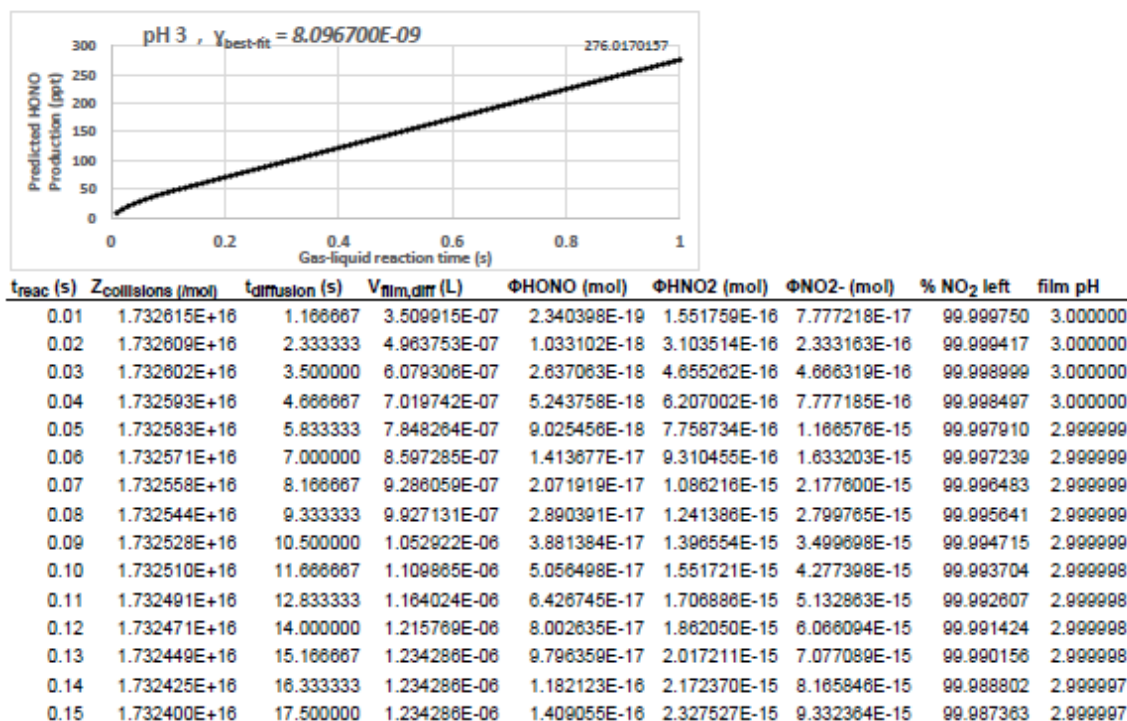
Using the correct equation parameters given in **Table 23**, (E72) yields a value of  $\gamma_{\text{rxn}}$  of  $6.68 \times 10^{-9}$  for the HA film pH of 3 ( $[\text{NO}_2]_0 = 36$  ppbv,  $[\text{HA}]_{\text{film}} = 62 - 104$  ppbv). This accounts for the majority,  $81.17 (\pm 0.29)\%$  of the model-predicted best-fit  $\gamma_{\text{best-fit}}$  of  $8.23 \times 10^{-9} (\pm 3.86 \times 10^{-10})$  (under the same experimental conditions for  $[\text{HA}]_{\text{film}}$  of 104 ppbv), suggesting that the uptake due to diffusion,  $\gamma_{\text{diffusion}}$  should correspond to the remaining  $18.83 (\pm 0.29)\%$  of the overall uptake ( $\gamma_{\text{best-fit}}$ ), or  $\gamma_{\text{diffusion}} = 1.55 \times 10^{-9} (\pm 3.86 \times 10^{-10})$ . In fact, the model developed herein reveals that diffusion is only important for 14 s of the  $\sim 116$  s, nearly

Parameter	Value	Units	Reference
$H_{\text{NO}_2}$	0.014	$\text{M atm}^{-1}$	Cheung et al., 2000
$D_{\text{NO}_2}$	$1.23 \times 10^{-5}$	$\text{cm}^2 \text{s}^{-1}$	Cheung et al., 2000
T	295	K	-
$k_{\text{rxn}}$	$2.70 \times 10^{-3}$	$\text{s}^{-1}$	(E71) herein

**Table 23.** Parameters for computation of  $\gamma_{\text{rxn}}$  using (E72). Note that  $H_{\text{NO}_2}$  denotes the Henry's law constant and the aqueous-phase diffusion coefficient for  $\text{NO}_2$ , respectively; T is the film temperature; and  $k_{\text{rxn}}$  is the experimentally determined pseudo-first order rate constant at pH 3 for  $[\text{HA}]_{\text{film}}$  ranging from 62 to 104 ppb ( $t_{\text{reac}}$  of 1 s; 4 lamps).

12% of the total reaction time scale, as seen by a deviation in the linearity in the predicted time-dependent HONO concentration profile. This is illustrated in **Figure 53**, for the HA film discussed above (recall:  $[\text{HA}]_{\text{solution}}$  of  $0.84 \text{ g L}^{-1}$ ; pH 3;  $[\text{NO}_2]_0 = 36$  ppb,  $t_{\text{reac}}$  of 1 s). In excellent agreement with the fraction of total uptake calculated due to diffusion ( $18.83 (\pm 0.29)\%$ ) for this film under the tested conditions only,

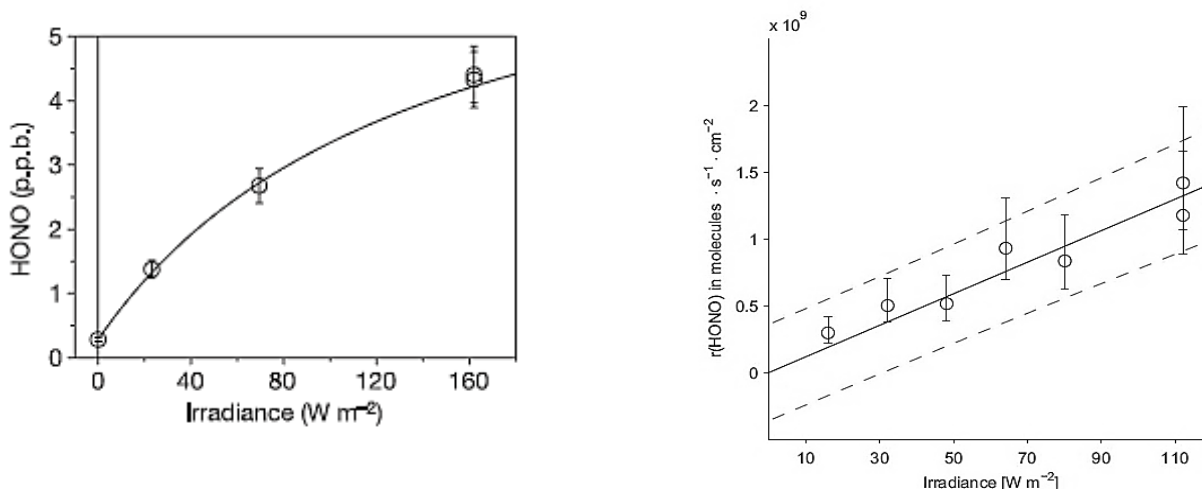
the model derived herein finds that  $18.51 (\pm 1.24 \times 10^{-3})$  % of the total (average) HONO yield ( $280.63 \pm 13.15$  pptv) is accumulated in this diffusion-dependent time interval (or  $51.96 \pm 0.12$  pptv).



**Figure 53.** Portion of data output file (given in **Appendix C**) displaying computations (shown to excess significant figures) of selected model output parameters, including the model-predicted best-fit reaction probability,  $\gamma_{\text{best-fit}}$  (seen on profile) fitted for the previously shown individual data point ( $[\text{HONO}]_{\text{t}_{\text{reac}}} = 276.02$  pptv  $\text{s}^{-1}$ ) obtained from the photoenhanced uptake of NO<sub>2</sub> (36 ppbv) on commercial acidic concentrated ( $0.84 \text{ g L}^{-1}$ ) HA films at pH 3 using the WWFT photoreactor (4 lamps)). The predicted time-dependent HONO concentration profile is also given over the entire gas-liquid reaction time.

#### 5.4 DEPENDENCE OF $\gamma_{\text{best-fit}}$ ON IRRADIANCE

A linear dependency of the production rate on the irradiance up to  $195 \text{ W m}^{-2}$  and  $80 \text{ W m}^{-2}$  has been found in the preliminary studies of photoenhanced NO<sub>2</sub> → HONO conversion on humic acid aerosol and pure solid humic acid films (see **Figure 54 (left)**), respectively, as conducted by Stemmler et al. (2006, 2007). Saturation of the observed HONO production was seen by Stemmler et al. (2006, 2007) at higher irradiation intensities in both studies, which they explained with a deactivation mechanism of the photochemically produced transient species (**sensitizer\***) (recall):



**Figure 54.** The dependence of the HONO formation on the light intensity ( $\lambda = 400 - 700$  nm) for the conversion of  $\text{NO}_2 \rightarrow \text{HONO}$  on commercial humic acid: (left)  $8 \mu\text{g cm}^{-2}$  - solid HA layers (pH 4.4),  $[\text{NO}_2]_0 = 20$  ppb. Error bars represent  $\pm 2\sigma$ . From Stemmler et al. (2006). (Right)  $0.3 \mu\text{g cm}^{-2}$  - HA embedded in an ice matrix (pH 5), with the error bars denoting standard errors introduced by normalization of experimental results to 41 ppb  $\text{NO}_2$ . The solid line gives the best linear fit through the data, and the dashed line denotes 95% C.I. From: Bartels-Rausch et al. (2010).

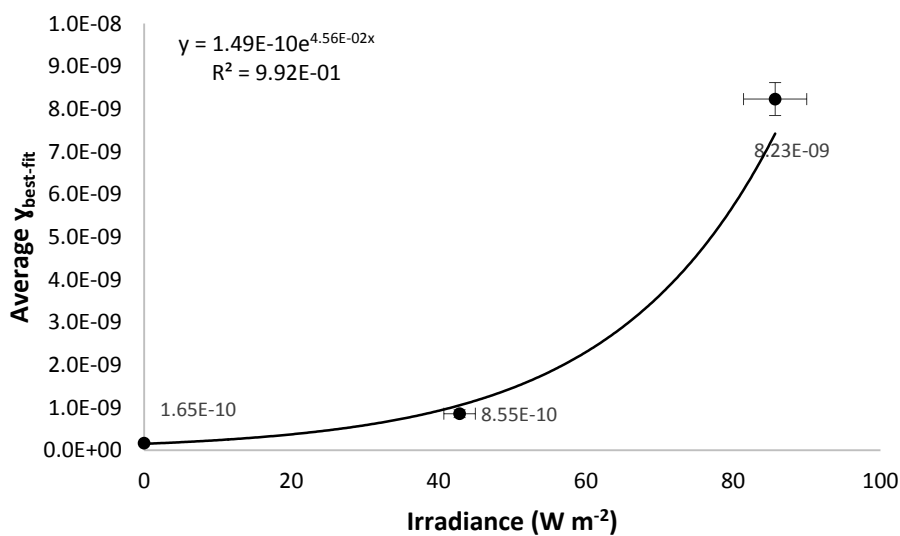
Contrary to the results of Stemmler et al. (2006, 2007), and, in spite of the lower concentration of HA (sensitizer) tested,  $0.3$  vs.  $8 \mu\text{g cm}^{-2}$ , Bartels-Rausch et al. (2010) did **not** observe such a saturation (see **Figure 54 (right)**) for HA doped in an ice matrix. In comparison to the pure humic acid substrates (Stemmler et al., 2006, 2007), Bartels-Rausch et al. (2010) suspect that the ice matrix, in which the commercial HA was embedded, likely led to a decrease in the rate of the deactivation process of the reduced sensitizer radical via (R10) in competition to their reaction with  $\text{NO}_2$ ,



(this generates nitrite or HONO, depending on the acidity (R9)).

Consistent with the results of Bartels-Rausch et al. (2010), a saturation in HONO production at higher irradiation intensities ( $\sim 86 \text{ W m}^{-2}$  or 4 lamps;  $\lambda = 300 - 420$  nm) for the photoenhanced uptake of  $\text{NO}_2$  on acidic commercial HA films ( $[\text{NO}_2]_0 = 36$  ppbv,  $[\text{HA}]_{\text{sol'n}}$  (pH 3) =  $0.84 \text{ g L}^{-1}$  or  $[\text{HA}]_{\text{film}}$  (pH 3) =  $5.81 \mu\text{g cm}^{-2}$ ; and  $t_{\text{reac}}$  of 1 s) using the WWFT photoreactor was not observed. Instead, an *exponential* dependence of the model-predicted best-fit reaction probability on irradiance was obtained (see **Figure 55**), with the

individual experimental and corresponding model-predicted parameters given in **Table 24**. Note that the irradiance at the reactor surface under irradiation conditions (2 and 4 lamps) was estimated based on scaling the measured value of  $150 \text{ W m}^{-2}$  (for 7 lamps) in a similar arrangement used by George et al. (2005) and Stemmler et al. (2006), which has been detailed previously in **Section 2.1**. A maximum



**Figure 55.** Correlation plot of average  $Y_{\text{best-fit}}$  (values shown as data labels) against the corresponding tested irradiation intensity based on fitting the individual data obtained from photoenhanced uptake experiments of  $\text{NO}_2$  (36 ppbv) on commercial acidic (pH 3) concentrated ( $0.84 \text{ g L}^{-1}$ ) HA films using the WWFT photoreactor (0, 2, and 4 lamps, respectively) and a  $t_{\text{reac}}$  of  $\sim 1 \text{ s}$ . Error bars on average  $Y_{\text{best-fit}}$  represent  $\pm 1\sigma$ .

uncertainty in the corresponding estimates of  $\pm 5\%$  is assigned. The highest reaction probability observed for 4 lamps,  $(8.23 \pm 0.39) \times 10^{-9}$ , was about 50 times greater than (the non-negligible)  $Y_{\text{best-fit}}$  for 0 lamps, of  $(1.65 \pm 0.16) \times 10^{-10}$ , resulting from aromatic moieties and high phenolic functionalities of the (commercial) HA acting as electron donors towards  $\text{NO}_2$  in the dark. Note that a maximum  $\text{NO}_2$  loss of 0.49 % is seen for the dataset collected at an irradiance of  $85.7 \text{ W m}^{-2}$  (4 lamps), still less than the determined RSD of 4.69% on the corresponding average  $Y_{\text{best-fit}}$ , and, thus the assumption holds true over all irradiation intensities studied (at film pH 3) that the rapid aqueous film renewal rate of about 2 minutes prevents accumulation of reaction products during uptake experiments. Although the tested

EXPERIMENTAL PARAMETERS	MODEL-PREDICTED PARAMETERS			
No. of lamps	Best-fit reaction probability ( $\gamma_{\text{best-fit}}$ )	pH <sub>treac</sub> (% decrease from pH <sub>sol'n</sub> ) <sup>a</sup>	[HONO] <sub>treac,predict.</sub> (pptv) (% difference from [HONO] <sub>treac</sub> ) <sup>a</sup>	% NO <sub>2</sub> remaining at t <sub>reac</sub> = 1 s
0	1.80×10 <sup>-10</sup>	3.00	6.15	99.99
	1.39×10 <sup>-10</sup>	3.00	4.76	99.99
	1.73×10 <sup>-10</sup>	3.00	5.91	99.99
	1.74×10 <sup>-10</sup>	3.00	5.95	99.99
	1.48×10 <sup>-10</sup>	3.00	5.07	99.99
	1.77×10 <sup>-10</sup>	3.00	6.06	99.99
	1.65×10 <sup>-10</sup>	3.00	5.65	99.99
2	7.61×10 <sup>-10</sup>	3.00	25.97	99.96
	9.18 <sub>5</sub> ×10 <sup>-10</sup>	3.00	31.35	99.95
	8.81×10 <sup>-10</sup>	3.00	30.08	99.95
	9.44×10 <sup>-10</sup>	3.00	32.22	99.95
	9.32×10 <sup>-10</sup>	3.00	31.83	99.95
	8.48×10 <sup>-10</sup>	3.00	28.95	99.95
	7.00×10 <sup>-10</sup>	3.00	23.91	99.95
4	8.31×10 <sup>-9</sup>	3.00	283.29	99.52
	7.52×10 <sup>-9</sup>	3.00	256.40	99.57
	8.54×10 <sup>-9</sup>	3.00	290.94	99.51
	8.10×10 <sup>-9</sup>	3.00	276.02	99.54
	8.38×10 <sup>-9</sup>	3.00	285.64	99.52
	8.55×10 <sup>-9</sup>	3.00	291.51	99.51

**Table 24.** Model-predicted parameters, including  $\gamma_{\text{best-fit}}$ , [HONO]<sub>treac,predict.</sub>, pH<sub>treac</sub>, and the reactive NO<sub>2</sub> loss percentage at t<sub>reac</sub> of 1 s determined by means of the model developed herein (including diffusion), based on the individual data input parameters ([HONO]<sub>treac</sub>) obtained from the photoenhanced uptake of NO<sub>2</sub> (36 ppbv) on the commercial acidic (pH<sub>sol'n</sub> = 3) concentrated (0.84 g L<sup>-1</sup>) HA films using the WWFT photoreactor and varying the no. of lamps (0, 2, and 4 lamps, respectively). <sup>a</sup> Shown only if value is non-negligible.



aqueous commercial HA film concentration ( $6.91 \mu\text{g cm}^{-2}$ ) is of similar magnitude to the solid substrate ( $8 \mu\text{g cm}^{-2}$ ) tested by Stemmler et al. (2006), it is clear that for the aqueous (renewable) film studied here, the rate of the deactivation process of the reduced sensitizer radical (via (R10)) is likely kinetically too slow to be of any importance to the overall proposed mechanism (M1). The exponential dependence of  $\gamma_{\text{best-fit}}$  on irradiation intensity may, in fact, imply numerous chromophoric sensitizers, capable of reducing  $\text{NO}_2$  to HONO, probably generated by photodegradation of the HA molecule itself. This is supported by the fact that humic (and fulvic) acid absorb solar irradiance, notably in the UV portion of the spectrum (Leifer, 1988; Kirk 1994a,b), with photolytic degradation of individual proteinaceous and humic (plant polyphenols) compounds by UV radiation well-known (see Allard et al., 1994).

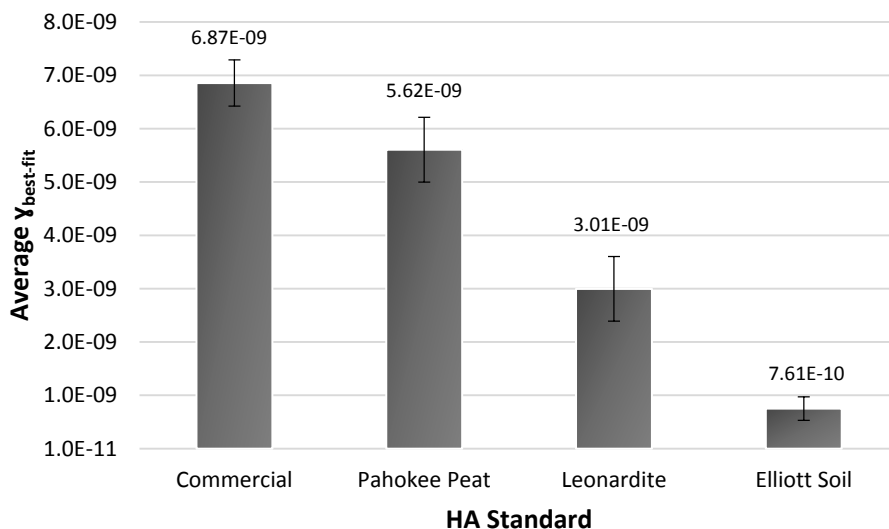
In fact, Wetzel et al. (1995) observed significant bacterial production rates of around  $5 - 10 \mu\text{g L}^{-1} \text{h}^{-1}$  when HA fractions isolated from decomposing littoral aquatic plants were exposed to simulated natural UV irradiance of known spectral range (287 – 320 nm), with < 3% reduction in total DOC ( $15 \text{ mg C L}^{-1}$ ) over time attributed to this photodegradation. In the very short UV exposure time of 1 s ( $t_{\text{reac}}$ ), however, the expected bacterial production rates in-situ are likely too slow to be of any significance for the highly refractive (Francioso et al., 2006), lignite-derived commercial sample. Still, the bacteria generated from the earlier, substantial humification likely function as multicellular aggregates on the acidic HA substrate, in essence, producing a 'biofilm'. This biofilm is defined as an 'assemblage of surface-associated microbial cells that is enclosed in an extracellular polymeric substance matrix' (in Donlan, 2002). It is this 'extracellular polymeric substance matrix' that is expected to contain many possible chromophoric sensitizer units, capable of photochemically reducing  $\text{NO}_2$  to HONO, justifying the observed exponential dependence of HONO yield vs. irradiation intensity under the tested conditions ( $[\text{HA}]_{\text{sol'n}} = 0.84 \text{ g L}^{-1}$  or  $[\text{HA}]_{\text{film}} (\text{pH } 3) = 5.81 \mu\text{g cm}^{-2}$ ;  $[\text{NO}_2]_0 = 36 \text{ ppbv}$ ;  $t_{\text{reac}}$  of 1 s; 4 lamps). Note, that this is a highly speculative mechanism that requires further experimental verification.

In a similar manner, the photoexcited HA molecules can act as precursors ('sensitizers') for the production of reactive intermediates, including singlet oxygen ( $^1\text{O}_2$ ), peroxy radicals (ROO), hydrogen peroxide ( $\text{H}_2\text{O}_2$ ), solvated electrons, superoxide anions ( $\text{O}_2^-$ ), and humic structures excited to the triplet state (Vidali et al., NTUA), however, it is not expected that these extremely reactive, short lived species (Polewski et al., 2005) will play a significant role as intermediate photoproducts in the production of HONO overnight, since the estimated photoexcited half-life ( $t_{1/2}$ ) of HA (in particular,  $20 \text{ mg L}^{-1}$  IHSS Pahokee Peat standard solution) is about 12 days (Vidali et al., NTUA). It follows that the generation of

HONO from the photoexcitation of HA remains to be resolved with ambient measurements exhibiting that HONO accumulates overnight in the absence of UV irradiation.

### 5.5 DEPENDENCE OF $\gamma_{\text{best-fit}}$ ON HA STANDARD

It is important to note, that the commercial humic acid compound (Aldrich) used in this photochemical  $\text{NO}_2$  reduction study may have a higher photoreactivity than environmentally-isolated HAs, and, accordingly, the reported uptake coefficients herein should be deemed as upper limits. The variation in the (average)  $\gamma_{\text{best-fit}}$  with HA standard for the photoenhanced uptake of  $\text{NO}_2$  ( $[\text{NO}_2]_0 = 36$  ppbv) on the acidic (pH 3) concentrated ( $[\text{HA}]_{\text{solution}} = 0.76 \text{ g L}^{-1}$ ) HA films (Commercial, Pahokee Peat, Leonardite, and Elliott Soil) using the WWFT photoreactor (4 lamps) is given in **Figure 56**. The individual experimental and corresponding model-predicted parameters are given in **Table 25**. About a nine-fold increase is seen in the average reaction probability for the commercial HA standard (Aldrich) over that of the Elliottsoil standard (IHSS).



**Figure 56.** Average  $\gamma_{\text{best-fit}}$  (data labels also given), fitted based on the photoenhanced uptake of  $\text{NO}_2$  on acidic (pH 3) HA films ( $[\text{HA}]_{\text{solution}} = 0.76 \text{ g L}^{-1}$ ) experiments ( $[\text{NO}_2]_0 = 36$  ppbv) using the WWFT photoreactor (4 lamps) and a  $t_{\text{reac}}$  of  $\sim 1$  s for varying HA standards (Commercial, Elliot Soil, Leonardite, and Pahokee Peat). Error bars represent  $\pm 1\sigma$ .

Given in **Table 26 (a)** is the available elemental composition data for the examined HA standards. In particular, the phosphorous content of HA samples can provide the reader with a picture of the unique environment of the sample source (McKnight et al., 1985). For instance, an HA sample with a significantly higher phosphorous content implies a greater content of organic phosphate esters or possibly inositol phosphates, with the latter, being key phosphorous products arising from the either breakdown of plant material or from microbial activity (McKnight et al., 1985). However, since this elemental composition

EXPERIMENTAL PARAMETERS	MODEL-PREDICTED PARAMETERS			
HA Standard	Best-fit reaction probability ( $\gamma_{\text{best-fit}}$ )	pH <sub>treac</sub> (% decrease from pH <sub>sol'n</sub> ) <sup>a</sup>	[HONO] <sub>treac,predict.</sub> (pptv) (% difference from [HONO] <sub>treac</sub> ) <sup>a</sup>	% NO <sub>2</sub> remaining at t <sub>treac</sub> = 1 s
Commercial	6.60×10 <sup>-9</sup>	3.00	225.10	99.62
	7.46×10 <sup>-9</sup>	3.00	254.39	99.57
	6.50×10 <sup>-9</sup>	3.00	221.75	99.63
	6.86×10 <sup>-9</sup>	3.00	233.93 <sub>5</sub>	99.61
	6.54×10 <sup>-9</sup>	3.00	222.90	99.63
	6.60×10 <sup>-9</sup>	3.00	225.14	99.62
	7.49×10 <sup>-9</sup>	3.00	255.48	99.57
Pahokee Peat	6.22×10 <sup>-9</sup>	3.00	212.19	99.64
	5.84×10 <sup>-9</sup>	3.00	199.05	99.67
	6.10×10 <sup>-9</sup>	3.00	208.05	99.65
	6.06×10 <sup>-9</sup>	3.00	206.70	99.65
	4.96×10 <sup>-9</sup>	3.00	169.18	99.72
	5.47×10 <sup>-9</sup>	3.00	186.52	99.69
	4.67×10 <sup>-9</sup>	3.00	159.02	99.73
Leonardite	3.19×10 <sup>-9</sup>	3.00	108.80 <sub>5</sub>	99.82
	2.78×10 <sup>-9</sup>	3.00	94.72	99.84
	2.32×10 <sup>-9</sup>	3.00	79.06	99.87
	3.74×10 <sup>-9</sup>	3.00	127.63	99.79

EXPERIMENTAL PARAMETERS	MODEL-PREDICTED PARAMETERS			
HA Standard	Best-fit reaction probability ( $\gamma_{\text{best-fit}}$ )	$\text{pH}_{\text{treac}}$ (% decrease from $\text{pH}_{\text{sol'n}}$ ) <sup>a</sup>	$[\text{HONO}]_{\text{treac,predict.}}$ (pptv) (% difference from $[\text{HONO}]_{\text{treac}}$ ) <sup>a</sup>	% $\text{NO}_2$ remaining at $t_{\text{reac}} = 1 \text{ s}$
Elliott Soil	$9.18 \times 10^{-10}$	3.00	31.32	99.95
	$5.26 \times 10^{-10}$	3.00	17.95	99.97
	$5.33 \times 10^{-10}$	3.00	18.19	99.97
	$5.72 \times 10^{-10}$	3.00	19.54	99.97
	$7.71 \times 10^{-10}$	3.00	26.32	99.96
	$1.06 \times 10^{-9}$	3.00	36.18	99.94
	$9.49 \times 10^{-10}$	3.00	32.41	99.95

**Table 25.** Model-predicted parameters, including  $\gamma_{\text{best-fit}}$ ,  $[\text{HONO}]_{\text{treac,predict.}}$ ,  $\text{pH}_{\text{treac}}$ , and the reactive  $\text{NO}_2$  loss percentage at  $t_{\text{reac}}$  of 1 s determined by means of the model developed herein (including diffusion), based on the individual data input parameters ( $[\text{HONO}]_{\text{treac}}$ ) obtained from the photoenhanced uptake of  $\text{NO}_2$  (36 ppbv) on the commercial acidic ( $\text{pH}_{\text{sol'n}} = 3$ ) concentrated ( $0.76 \text{ g L}^{-1}$ ) HA films using the WWFT photoreactor and varying the HA standard (Commercial, Elliott Soil, Leonardite, and Pahokee Peat, respectively). <sup>a</sup> Shown only if value is non-negligible.

(a)

HA Sample	C	H	O	N	S	P
Commercial <sup>a</sup>	54.7	4.3	36.8	0.7	3.5	–
Elliott Soil <sup>b</sup>	58.13	3.68	34.08	4.14	0.44	0.24
Pahokee Peat <sup>b</sup>	56.37	3.82	37.34	3.69	0.71	0.03
Leonardite <sup>b</sup>	63.81	3.70	31.27	1.23	0.76	<0.01

(b)

HA Sample	C=O	COOH	Arom.	Acetal	Carbohy.	Aliph.
Commercial <sup>a</sup>	1	13	65	–	< 1/2	19
Elliott Soil <sup>c</sup>	6	18	50	4	6	16
Pahokee Peat <sup>c</sup>	5	20	47	4	5	19
Leonardite <sup>c</sup>	8	15	58	4	1	14

(c)

HA Sample	pK <sub>a2, carboxylic</sub>
Commercial <sup>d</sup>	4.78
Elliott Soil <sup>e</sup>	4.36
Pahokee Peat <sup>e</sup>	4.33
Leonardite <sup>e</sup>	4.59

(d)

HA Sample	MW <sub>N</sub> (×10 <sup>3</sup> )	Conditions for analysis
Elliott Soil <sup>f</sup>	19	280 nm detection, in: 0.05 M phosphate buffer solution (pH 7.5), 0.03 M NaCl, and ACN (30%)
Pahokee Peat <sup>f</sup>	8.5	same as entry above
Commercial <sup>g</sup>	2.25	254 nm detection, in 0.1 M NaCl solution

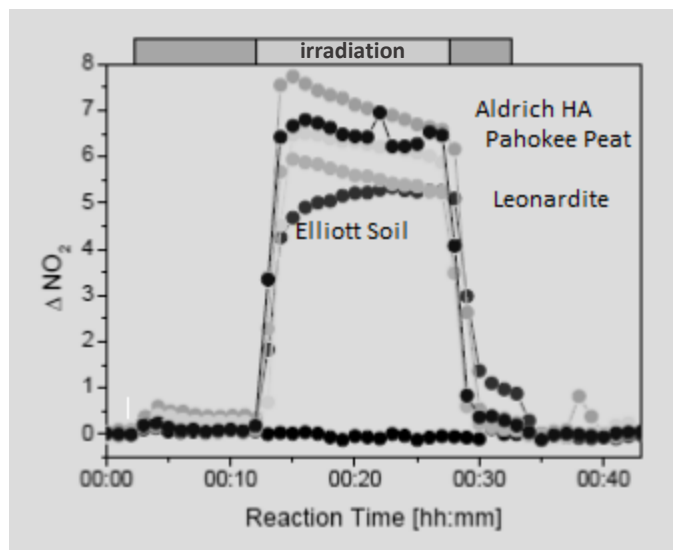
**Table 26.** (a) Elemental compositions of the selected HA samples in %(w/w) of a dry, ash-free sample. (b) Solution state <sup>13</sup>C NMR estimates of carbon distribution for a neutral solution (electronically integrated peak area percentages for selected ranges of chemical shift). (c) pK<sub>a2</sub> data for HA samples of interest. (d) Number averaged molecular weights (Da) for selected HA samples (when available). <sup>a</sup> From: Albers et al. (2008). <sup>b</sup> From: [www.humicsubstances.org/elements.html](http://www.humicsubstances.org/elements.html) <sup>c</sup> From: Thorn et al. (1989). <sup>d</sup> From: Paxéus and Wedburg (1985). <sup>e</sup> From: Ritchie and Perdue (2002). <sup>f</sup> From Shinozuka et al. (2004). <sup>g</sup> From: Hur and Schlautman (2003).

data, applies to dry, ash-free samples only, preliminary deductions to the limited representative dataset on selected HA films cannot be made from such information. Likewise, the available solution state <sup>13</sup>C NMR carbon distribution data (given in **Table 26 (b)**), and the qualitative structural information it can provide, is not useful for interpreting the rather restricted environmental dataset under the operating pH (3) < pK<sub>a2, carboxylic</sub> (see **Table 26 (c)** for reported values), since the state of aggregation of the HA molecule in solution is expected to differ significantly over four pH units. Note that this data, does however, illustrate that these are suitable environmentally representative HA standards of varying composition.

On this point, it is possible to perform a final interpretation of the collected (best-fit) reaction probability data utilizing the number averaged molecular weights (MW<sub>N</sub>), defined as the total weight of the molecules present divided by the total number of molecules, since a contributing factor to the range of molecular weights of soil HAs is the formation of molecular aggregates in solution (Wershaw and Pickney, 1971). However, any correlations drawn will only be applicable to the limited environmental HA samples tested herein. Although the molecular weight values for the tested HA standards (when available, see **Table 26 (d)**) were obtained via the same analytical technique, (High Performance Size Exclusion

Chromatography (HPSEC), the conventional method for the measurement of MWs; Shinozuka et al., 2004), the analytical conditions of the measurements differ considerably (**Table 26 (d)**). Given that the extent of aggregation, including the shape of the molecule in solution is easily influenced by the analytical conditions of the measurement method, this data can only be used qualitatively to arrive at any conclusions. It is evident from the reaction probability dataset (and the available  $MW_N$  data) that the photoenhanced  $\text{NO}_2$  uptake reaction is most kinetically favourable on acidic films (pH 3) of the tested HA standards (Commercial, Elliott Soil, Leonardite, Pahokee Peat) having *lower* values of  $MW_N$  under the tested conditions only ( $[\text{NO}_2]_0 = 36$  ppbv;  $[\text{HA}]_{\text{solution}} = 0.76 \text{ g L}^{-1}$  or  $[\text{HA}]_{\text{film}} = 5.25 \mu\text{g cm}^{-2}$ ;  $\lambda = 300 - 420$  nm, 4 lamps;  $t_{\text{reac}}$  of 1 s).

In fact, in a previous study (Stemmler et al., 2006), acidic (pH 4.8) solid commercial HA ( $8 \mu\text{g cm}^{-2}$ ) films showed a similar photoreactivity towards  $\text{NO}_2$  as the identical environmentally-isolated IHSS humic acids from soil (Elliott Soil HA), brown coal (Leonardite HA) or peat (Pahokee Peat HA) (see **Figure 57**). Stemmler et al. (2006), also observed a maximum reaction probability (under the selected operating conditions) for the more refractive (Francioso et al., 2006), lignite-derived commercial sample, closest in reactivity to the selected IHSS peat sample. For both the data of Stemmler et al. (2006) and the results presented here using the renewable HA films, the least kinetically favourable reaction probabilities were observed for the remaining IHSS HA standards (Leonardite and Elliott Soil), with the smallest HONO yield obtained for the *fine* Elliott Soil. Although the dataset of Stemmler et al. (2006) suggests that the humic acid model compound (commercial HA) used in their photochemical  $\text{NO}_2$  reduction study on environmentally *unrealistic* solid films does not have a much higher photoreactivity than the ecologically-isolated IHSS HAs, with only less than a factor of two difference, the data obtained under considerably more acidic conditions on renewable films using the same IHSS HA standards in this study, implies otherwise. The data collected on renewable acidic HA films suggests that the HA model compound has a significantly higher photoreactivity, by about an order of magnitude than the selected IHSS HAs representative of environmental samples. This is most likely inherently due to the fact that the elucidated photochemical mechanism is most efficient for the HA standard which is the most 'bioactive' prior to exposure to the UV irradiation in the WWFT under typical operating conditions, that is, contains the highest bacterial population upon photodegradation. This is, indeed consistent with the lignite-derived commercial sample, which has undergone a relatively large extent of diagenetic changes and humification (Francioso et al., 2006), the lowest  $MW_N$  aggregate (Hur and Schlautman, 2003).



**Figure 57.** Photoreactivity of different humic acids towards  $\text{NO}_2$  ( $[\text{NO}_2]_0 = 30 \text{ ppb}$ ;  $\text{RH} = 28\%$ ; residence time =  $0.6 \text{ s}$ ;  $8 \mu\text{g cm}^{-2}$  of the selected humic acid;  $\lambda = 400 - 700 \text{ nm}$  range; irradiance =  $162 \text{ W m}^{-2}$  at reactor surface, 7 lamps). The baseline circles represent a reference experiment on an uncoated glass surface under the same experimental conditions. Modified from: Stemmler et al. (2006).

## 6 CONCLUSIONS

The research project was, indeed, a success. The NO<sub>2</sub> uptake kinetics on several phenolic-containing organic films was successfully studied using the WWFT photoreactor specifically designed for this project. Accordingly, several sets of conclusions can be reached, regarding the: **experimental data** (see **Appendix B** for summary of raw experimental data), for the tested non-humic and humic compounds, respectively; and finally **atmospheric implications**, where they apply.

With regards to the plethora of experimental results, the conclusions of the tested non-humic (water, DOPAC, selected *ortho*-nitrophenols, and KHP) and humic compounds (humic acid) will be examined separately.

### Non-humic compounds

In the dark and under irradiation, the uptake of NO<sub>2</sub> on a purified **water** film (pH's 2 and 6; for [NO<sub>2</sub>]<sub>0</sub> = 14, 42, and 71 ppbv; t<sub>reac</sub> of 1 s; 4 lamps when irradiated) in the WWFT photoreactor due to the hydrolytic disproportionation of NO<sub>2</sub> on the borosilicate column and/or an electron transfer reaction of NO<sub>2</sub> with an organic impurity (in the ultrapure water) was found to be unimportant under the tested conditions. The exceedingly low probability of (R29), hydrolytic disproportionation on the glass surface observed (upper limit for model-predicted best-fit  $\gamma_{\text{pH}=2}$  of  $1.26 \times 10^{-10}$ ) was consistent with molecular dynamics (MD) calculations illustrating that the hydrophobic free radical NO<sub>2</sub> has a strong propensity for the surface of neutral clusters NO<sub>2</sub>(H<sub>2</sub>O)<sub>n</sub> (Bezrukov et al., 2004; and Yabushita et al., 2009).

George et al. (2005), observed a 6 % (no precision given) reactive loss of NO<sub>2</sub> ([NO<sub>2</sub>]<sub>0</sub> = 20 ppbv, RH = 20 %) for a 1 mg mL<sup>-1</sup>-DOPAC solid film in the dark, with no significant photoenhancement under the tested irradiation conditions. Under the typical experimental conditions (used in this study), an 11 (± 0.07) % reactive loss of NO<sub>2</sub> ([NO<sub>2</sub>]<sub>0</sub> = 75 ppbv), with a slight photoenhancement (12 ± 0.1 % reactive loss of NO<sub>2</sub>) was observed using the WWFT photoreactor (λ<sub>max</sub> = 354 nm) for a fresh unbuffered 1.4 mg L<sup>-1</sup> DOPAC solution (pH 5) and a t<sub>reac</sub> of 1 s, in good accord with the result of George et al. (2005), thus providing confidence in the tested method. Since DOPAC is scarcely absorbing under the tested light conditions, the negligible HONO production observed was rather unexpected, and may be related to impurities present in the ≥ 96% purity standard used or on the reactor wall, or even possibly to absorbing species



generated during the exposure of the compounds to the NO<sub>2</sub>/zero-air mixture in the reactor (George et al., 2005).

While *no* HONO production ( $n = 4$ ) was observed as a result of photolysis (4 lamps,  $\lambda = 354$  nm,  $t_{\text{reac}}$  of 1 s) of the acidic (pH 2) *ortho*-nitrophenol (2-NP and 4M2NP) films at an environmentally relevant concentration (5 mg L<sup>-1</sup>), aqueous 2-NP photolysis particulate product yield was detected via the generation of red-orange/copper particulate on the walls of the WWFT (identical  $t_{\text{reac}}$  and no. of lamps) for a significantly more concentrated (100 mg L<sup>-1</sup> in 100% MeOH) and basic film (pH 11), likely attributed to nitrohydroquinone production (Bing et al., 2005). Although these photolysis experiments, which are the first to be performed under acidic conditions (pH 2) at environmentally realistic *ortho*-nitrophenol levels, *alluded* that the phototransformation of such compounds is not a significant source of atmospheric nitrous acid, however, this was *not* conclusive, as further studies with *ortho*-nitrophenol surfaces with different acidic properties (multi-pH study) and at other environmentally relevant concentrations would be necessary to justify this claim, as well as to better understand the occurring photochemistry. In addition, other *ortho*-nitrophenol species would need to be included in these future studies.

The dependence of HONO production rate on [NO<sub>2</sub>]<sub>0</sub> produced using data from NO<sub>2</sub> photochemistry experiments on acidic (pH 2, 5 mg L<sup>-1</sup> in 5% MeOH) *ortho*-nitrophenol (2-NP and 4M2NP) films obtained over the entire tested [NO<sub>2</sub>]<sub>0</sub> concentration array (0, 72 and 1000 ppbv) were found to be non-linear for both *ortho*-nitrophenol species. Although the small (net) HONO production rates (centred around the detection limit for the HONO detector) obtained for typical urban NO<sub>2</sub> levels, *suggested* that the uptake processes on the tested *ortho*-nitrophenols are unimportant as sources as HONO, further experiments using films with different acidic properties and at different environmentally relevant concentrations (as well as for other *ortho*-nitrophenol species) would need to be performed in order to confirm this conclusion. Additionally, the considerably more significant HONO production rate observed for the reference (blank) film, 5% MeOH, ranging from about 100 to 600 pptv s<sup>-1</sup> for environmentally relevant to extreme NO<sub>2</sub> conditions, indicated that the uptake of NO<sub>2</sub> on the organic impurities in the HPLC grade MeOH including acetone, and dimethyl acetals of simple alkyl ketones (such as propanone, butanone, and pentanone in the range of 10 to 100 ppm), with a plausible chemical pathway of origin as proposed by Guella et al. (2007), was kinetically *more favourable* than that on the selected *ortho*-nitrophenol films (for the tested conditions).

It was concluded that the aforementioned mechanism, (M14) of general base catalysis, conceivably explained the non-negligible HONO production observed for the potassium hydrogen phthalate (KHP) film (0.5 mM in 5% MeOH, pH 2), of similar concentration to those surfactants investigated by Kinuwaga et al. (2011) (1-3 mM). Drawing on the results of Kinuwaga et al. (2011), it is very likely that the surfactant  $K^+$  counterion draws the phthalate ion closer to the surface, thus enhancing the  $NO_2$  uptake on water (5% MeOH) via (R41) and (R42). Furthermore, the data obtained for the acidified KHP film suggests that the results of Kinuwaga et al. (2011) under extreme  $NO_2$  conditions need to be extrapolated to atmospheric levels in order to accurately assess the importance of (M14) for the production of tropospheric HONO. It was also interesting to note that the magnitude of HONO production observed for the tested KHP film (0.5 mM, 5% MeOH as solvent, pH 2) was nearly identical to that seen for the studied *ortho*-nitrophenol films (5 mg  $L^{-1}$  in 5% MeOH, pH 2), suggesting that the reaction kinetics are equally favorable under extreme  $NO_2$  conditions ( $t_{\text{reac}}$  of 1 s, 4 lamps).

## Humic compounds

Complementary to the studies of photosensitized reduction of  $NO_2$  on solid humic acid films and humic acid aerosols, completed by Stemmler et al. (2006) and Stemmler et al. (2007), a saturation of HONO yields at higher  $NO_2$  concentrations ( $> 50$  ppbv) ( $[NO_2]_0 = 10 - 72$  ppbv;  $[HA]_{\text{film}} (\text{pH } 2) = 6.91 \mu\text{g cm}^{-2}$ ; 4 lamps ( $\lambda_{\text{max}} = 354$  nm);  $t_{\text{reac}} \sim 1$  s) was not observed. Instead, a highly *linear* correlation over the entire range examined ( $k_1 = 6.7 \times 10^{-3} \text{ s}^{-1}$ ), with negligible reactivity for Aldrich HA film photolysis ( $[NO_2]_0 = 0$  ppbv) was seen. The linear dependence of HONO production rate on  $[NO_2]_0$  obtained using the tested WWFT photoreactor suggested that saturation of the adsorption sites by  $NO_2$  previously proposed by Stemmler et al. (2006) (as a plausible explanation for saturation of HONO yields at higher  $NO_2$  concentrations), did not occur within the examined system. This was conceptually coherent with the  $NO_2^-$  particles only diffusing throughout the depth of the surface layer, regardless of any variation in film thickness, consistent with the independence of observed HONO yield on  $f$  ( $f = 3.32 \times 10^{-2}$  cm (usual) and  $5.28 \times 10^{-2}$  cm;  $[NO_2]_0 = 36$  ppbv;  $[HA]_{\text{film}} (\text{pH } 2.5) = 6.91 \mu\text{g cm}^{-2}$ ; 4 lamps;  $t_{\text{reac}} \sim 1$  s). Neglecting gas-phase diffusion, a corresponding uptake coefficient,  $\gamma_{\text{expt}} = 2.2 \times 10^{-7}$  was estimated, approximately an order of magnitude below the maximum reported uptake coefficient of  $NO_2$  on humic acid aerosol (pH 4.4, RH = 26%) of  $\gamma = 1.8 \times 10^{-6}$  (Stemmler et al., 2007) for a maximum actinic flux ( $1.0 \times 10^{17}$  photons  $\text{cm}^{-2} \text{ s}^{-1}$ , 7 lamps,  $\lambda = 400 - 750$  nm) and an environmentally unrealistic aerosol surface concentration of  $\sim 0.151 \text{ m}^2$

$\text{m}^{-3}$ . The higher reactivity observed by Stemmler et al. (2007) was also not surprising as a larger fraction of the Aldrich-HA carboxylic acid groups was dissociated under the less acidic conditions (pH 4.4 vs. pH 2).

An exceptional *quadratic* correlation (E67) was found to describe both: (i) the observed increase in  $\gamma_{\text{best-fit}}$  by a factor of about 4 from pH 2.00 to pH 3.00 ( $\gamma_{\text{best-fit}} = 1.93 \times 10^{-9}$  to  $8.23 \times 10^{-9}$ ); and (ii) the subsequent detected decrease in  $\gamma_{\text{best-fit}}$  from pH 3.00 to pH 3.36 ( $\gamma_{\text{best-fit}} = 8.23 \times 10^{-9}$  to  $1.37 \times 10^{-9}$ ) by approximately a factor of six (tested conditions:  $[\text{NO}_2]_0 = 36$  ppbv;  $[\text{HA}]_{\text{film}} = 5.81 \mu\text{g cm}^{-2}$ ; 4 lamps;  $t_{\text{reac}}$  of 1 s). The *exponential* correlation (E68) obtained for the relationship between  $\Theta_{\text{carboxylic},2}$  and  $\gamma_{\text{best-fit}}$  for the  $\sim 0.50$  pH unit subset (pH 3.50 – pH 3.96) was indicative of the high-sensitivity  $\text{NO}_2$  reduction to the fraction of available (dissociated) carboxyl groups in solution with  $\text{pK}_{\text{a,carboxylic},2}$  of 4.78. This kinetically favoured reaction probability behavior, was most plausibly a result of increases in deprotonation — essential to maintain the important *power* correlation (E69) of  $\gamma_{\text{best-fit}}$  with  $[\text{H}^+]_{\text{HA film,treac}}$  (M) observed over the pH range of 1.5 to 4.0 ( $\gamma_{\text{best-fit}} = 1.79 \times 10^{-9}$  to  $\gamma_{\text{best-fit}} = 2.87 \times 10^{-8}$ ). Of course, this excluded data at pHs 3.36 to 3.75 ( $\gamma_{\text{best-fit}} = 1.68 \times 10^{-9}$ ), where complex pH-dependent  $\gamma_{\text{best-fit}}$  behavior was observed, since the individual tested film pHs were centred near both  $\text{pK}_{\text{a}(\text{HONO})}$  and  $\text{pK}_{\text{a},1,\text{carboxylic}(\text{HA})}$ , respectively in this pH range. Although the various parameterizations presented in the pH study may be useful for describing the complex  $\text{pH}_{\text{treac}}$ -dependent  $\gamma_{\text{best-fit}}$  behavior observed, the reader must note that given the data available at hand, no physical meaning can yet be attributed for the functional forms given. Overall, the pH-dependent results presented were qualitatively coherent with those of Stemmler et al. (2006), however centred on more authentic pH conditions of anaerobic humic soils: increases in the photoenhanced HONO formation with pH were monitored, too, but for highly to moderately acidic conditions (specifically, between pH 1.5 and 4.3), owing to increases in reactivity in the reaction with  $\text{NO}_2$  with the several carboxyl groups ( $\text{pK}_{\text{a},1} = 3.39$ ;  $\text{pK}_{\text{a},2} = 4.78$ ) within the commercial HA with deprotonation.

The HONO production exhibited an excellent *linear* dependence on HA solution concentration (with a zero intercept) for  $[\text{HA}]_{\text{solution}}$  ranging from 0.50 g – 0.84 g  $\text{L}^{-1}$ . An experimentally determined value of  $k_{\text{rxn}} = 2.70 \times 10^{-3} \text{ s}^{-1}$  at pH 3 ( $[\text{NO}_2]_0 = 36$  ppbv; 4 lamps;  $t_{\text{reac}}$  of 1 s) was obtained, indicative that there was no competition with the hydrolysis reaction. It was rationalized that the outlier data corresponding to the renewable film generated from the most concentrated HA solution (1 g  $\text{L}^{-1}$ ), was overestimated, owing to the fact that  $[\text{HA}]_{\text{solution}}$  was at the reported lower limit of the CMC of environmental HAs (Engebretson and von Wandruszka, 1994; and Guetzloff and Rice, 1994) at which increased product yield due to the enhanced detergent nature of the HA (von Wandruszka, 2000) was expected. Under the assumption that

the reaction of  $\text{NO}_2$  with HA in solution (in excess concentration) became rate-limiting for the experimental uptake, a corresponding value of  $6.68 \times 10^{-9}$  for  $\gamma_{\text{rxn}}$  was computed. This accounted for the majority, (about 81%) of the model-predicted best-fit  $\gamma_{\text{expt}}$  of under the same experimental conditions (with  $[\text{HA}]_{\text{solution}} = 0.84 \text{ g L}^{-1}$ ) suggesting that the uptake due to diffusion,  $\gamma_{\text{diffusion}}$  should correspond to the remaining  $\sim 19\%$  of the overall measured uptake. This was, in fact, consistent with the developed model results which predicted nearly 19% of the total HONO yield accumulated in the diffusion-dependent time interval (12% of the corresponding reaction time scale).

In contrast to the studies conducted by Stemmler et al. (2006, 2007) on solid HA films and HA aerosols, respectively, a saturation in HONO production at higher irradiation intensities was not observed, but, instead an *exponential* dependence of the model-predicted best-fit reaction probability on irradiance ( $\gamma_{\text{best-fit}} = 1.65 \times 10^{-10}$  to  $8.23 \times 10^{-9}$ ) was discovered for the photoenhanced uptake of  $\text{NO}_2$  on acidic commercial HA films ( $[\text{NO}_2]_0 = 36 \text{ ppbv}$ ,  $[\text{HA}]_{\text{film}} (\text{pH } 3) = 5.81 \text{ } \mu\text{g cm}^{-2}$ ;  $0 - 85.7 \text{ W m}^{-2}$  irradiance; and  $t_{\text{reac}}$  of 1 s). While the tested aqueous commercial HA film concentration ( $5.81 \text{ } \mu\text{g cm}^{-2}$ ) was of similar magnitude to the solid substrate ( $8 \text{ } \mu\text{g cm}^{-2}$ ) tested by Stemmler et al. (2006), it was clear that for the aqueous (renewable) film, the rate of the deactivation process of the reduced sensitizer radical (via (R10)) was likely kinetically too slow to be of any importance to the overall proposed mechanism (M1). It was speculated that the exponential dependence of  $\gamma_{\text{best-fit}}$  on irradiation intensity likely implied numerous chromophoric sensitizers (capable of reducing  $\text{NO}_2$  to HONO), probably generated by photodegradation of the HA molecule itself. The conclusion was drawn that the humification-generated bacteria (prior to UV exposure in the WWFT) likely functioned as multicellular aggregates on the acidic HA substrate, in essence, producing a biofilm expected to contain numerous feasible chromophoric sensitizer units capable of photochemically reducing  $\text{NO}_2$  to HONO, thus, defending the observed exponential dependence of HONO yield vs. irradiation intensity under the tested conditions.

Compared to the dataset of Stemmler et al. (2006) which suggested that the humic acid model compound (commercial HA) used in their photochemical  $\text{NO}_2$  reduction study on solid films (environmentally *unrealistic*) did not have a much higher photoreactivity than the environmentally-isolated IHSS HAs (less than a factor of two difference), the data at hand, obtained on renewable HA films (of identical IHSS HA standards) under considerably more acidic conditions (operating conditions:  $[\text{NO}_2]_0 = 36 \text{ ppbv}$ ;  $[\text{HA}]_{\text{film}}$  of  $5.25 \text{ } \mu\text{g cm}^{-2}$ ; 4 lamps), implied otherwise. Using the tested method (WWFT photoreactor), it was observed that the HA model compound did, indeed, have significantly higher

photoreactivity ( $\gamma_{\text{best-fit}} = 6.87 \times 10^{-9}$ ) than the selected IHSS HAs representative of environmental samples (about an order of magnitude difference in  $\gamma_{\text{best-fit}}$ ), closest in reactivity to the selected Pahokee Peat sample ( $\gamma_{\text{best-fit}} = 5.61 \times 10^{-9}$ ). The smallest HONO yield was obtained for the *fine* Elliott Soil ( $\gamma_{\text{best-fit}} = 7.61 \times 10^{-10}$ ). This was most likely owing to the fact that the deduced photochemical mechanism was most effective for the HA standard which had peak levels of ‘bioactivity’ preceding UV irradiation exposure in the WWFT under the typical operating conditions. This, undeniably, is coherent with the more refractive, lignite-derived commercial sample, the lowest  $\text{MW}_N$  aggregate.

### Atmospheric Implications

The kinetic datasets presented herein for the photoenhanced reaction of  $\text{NO}_2$  on acidic (commercial) humic acid films provided a rather complete kinetic ‘picture’ of such a potentially important surface reaction ( $\gamma_{\text{best-fit,max}}$  of  $10^{-8}$  at pH 4;  $[\text{HA}]_{\text{film}} = 5.81 \mu\text{g cm}^{-2}$ ; 36 ppbv  $[\text{NO}_2]_0$ ; 4 lamps;  $\tau_{\text{reac}}$  of 1 s). It is important to note, that the data may depend on uncontrolled variables, including temperature, and irradiation wavelength. It is expected that the latter parameter will have a greater effect on the reaction kinetics in light of the possible wavelength dependency of HONO production. This is supported by the fact that Stemmler et al. (2006) observed a decrease in the overall quantum yield for the photochemical  $\text{NO}_2 \rightarrow \text{HONO}$  conversion on solid HA films of around 2.8, when switching from UVA irradiation (300 – 420 nm) to visible irradiation (400 – 700 nm) at light intensities of  $162 \text{ W m}^{-2}$ , 20 ppb  $[\text{NO}_2]_0$  and 20% RH. However, considerable effort is still required to scale up the kinetic results of the small-scale (WWFT) photoreactor to that of a regional scale, such a saturated wetland or forested soil area (i.e., in the case of an urban geographic scale).

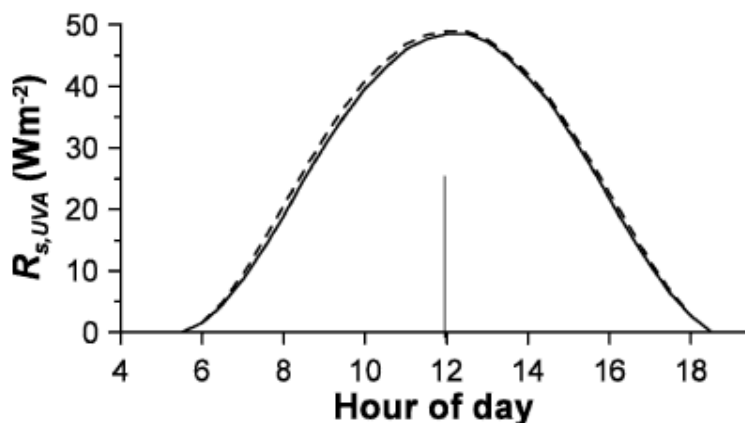
Regional areas, either for rural or urban regions are required in order to reliably estimate atmospheric HONO production rates ( $\text{pptv s}^{-1}$ ) based upon the (small-scale) reaction probabilities presented herein. Note that, ideally, this computation would be achieved using wetland areas for rural locales, as opposed to forested areas, as boreal forests are considerably less humic (and acidic) than wetlands (Tipping and Woof, 1990). In particular, wetlands developed on Precambrian Shield rocks, commonly made up of ponds surrounded by oligotrophic bogs of Fibrisol peats, are representative of such acidic high humic conditions (Moore et al., 2003) (Moore et al., 2003) — a corresponding range of HA concentrations ( $\text{mg C L}^{-1}$ ), for which, would be a requisite parameter.

Of course, scaling up to an urban location of interest, such as Toronto, appears to be more complex due to the scarce amount of data available concerning the coverage of (thin,  $\mu\text{g cm}^{-2}$  for the generated films), acidic humic acid-rich films in such a setting. As such humic acid-rich films are likely not associated with mineral-rich soils, the studied photoenhanced  $\text{NO}_2$  reduction on  $\text{HA}_{(\text{aq})}$  reaction studied herein is important *in-situ*, that is, under acidic conditions, and we expect **impervious** urban surfaces (defined as surfaces through which water cannot infiltrate) to be important reaction substrates. Additional information regarding impervious surface moisture availability (%), which would vary seasonally, of course (and could be averaged), and the number of months of the year (in Toronto, for example) that there is significant moisture at the impervious surface are two necessary parameters for the calculation. While this data is readily available for soils, no such information is easily found for impervious surfaces within an urban locale — perhaps, it may be simplest to assume that, within an urban setting, the impervious surfaces form acidic films half of the time (on average) for the non-winter ( $7/12$ ) months (i.e., in Toronto), therefore, corresponding to around 106 days  $\text{yr}^{-1}$ . Additionally, an estimate of urban HA concentrations on impervious surface films is compulsory to fully appreciate the atmospheric implications of the studied reaction on a urban scale — despite the lack of relevant figures available, it is expected that this range of HA concentrations ( $\text{mg C L}^{-1}$ ) will be considerably lower than that of wetland soils (Molot, personal communication). The final mandatory parameter for the assessment using the reaction probability data is the impervious surface area for the city of interest, which would not be very difficult to obtain.

To further complicate the matter, the scaling up assessments for both rural and urban regions need to be performed at several environmentally relevant acidities corresponding to the complex pH-dependent kinetic behaviour observed for the photoenhanced  $\text{NO}_2 \rightarrow \text{HONO}$  reduction reaction on (acidic)  $\text{HA}_{(\text{aq})}$  studied herein, in order to obtain a clear picture of the HONO yield with surfaces (simulated wetland soils or impervious urban surfaces) under the appropriate  $\text{NO}_2$  atmospheric conditions for the geographic scale. These assessments would be compositionally limited, in that, they could only be carried out using the kinetic data obtained for the commercial (model) HA compound and the tested IHSS HA standards herein. Preferentially, the data for the HA standard which has the closest degree of humification would need to be utilized, and could be visually established via soil colour (i.e., using Munsell soil colour charts), since humus increases in its (dark) brown colour due to an accumulation of organic C (Weber, University of Wroclaw). Lastly, the total estimated photochemical HONO production for both urban and rural geographic scales (assessed separately), would need to be scaled for the lamp intensities used in the small-

scale photoreactor. This parameter will have a significant effect on the scaled-up interpretations due to the exponential dependence of  $\gamma_{\text{best-fit}}$  on irradiance observed. For instance, in order to extrapolate the presented kinetic data under the typical irradiance ( $85.7 \text{ W m}^{-2}$ ), to a mid-morning/afternoon simulation (under clear skies), about  $42.5 \text{ W m}^{-2}$  irradiance (for a North American site) (see **Figure 58**), would ensue a reduction in the small-scale HONO reaction probability of approximately an order of magnitude.

It is evident that the scaling up assessments of the kinetic results of the photoenhanced reduction reaction of  $\text{NO}_2 \rightarrow \text{HONO}_{(\text{aq})}$  under acidic conditions (studied herein) of the small-scale (WWFT) photoreactor to that of both urban and rural scales require considerable effort, however, are possible, despite some limited figure availability required for such computations. It is highly recommended that such evaluations are completed within the near future, for the data in this text, which suggests on the reactor-scale that it is a potentially important reaction for ubiquitously- present environmental substrates ( $\text{HA}_{(\text{aq})}$ ). Furthermore, it is suggested that Stemmler et al. (2006), too, complete such scaling up assessments, of their kinetic results concerning the photoenhanced reduction reaction of  $\text{NO}_2 \rightarrow \text{HONO}_{(\text{s})}$  for that of both urban and rural scales for their similarly-dimensioned photoreactor.



**Figure 58.** Diurnal pattern of UVA irradiance,  $R_{s,UVA}$  on 5 Sep 2000 at a North American site (California, USA) for a generally clear-sky day. Hour 12 indicates noon. From: Grant and Slusser (2005).

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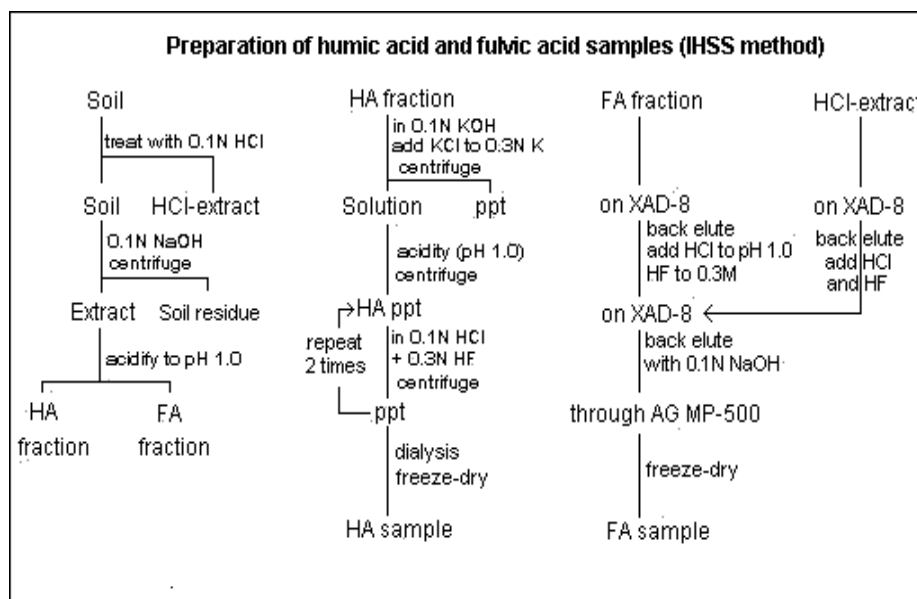
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APPENDIX A:

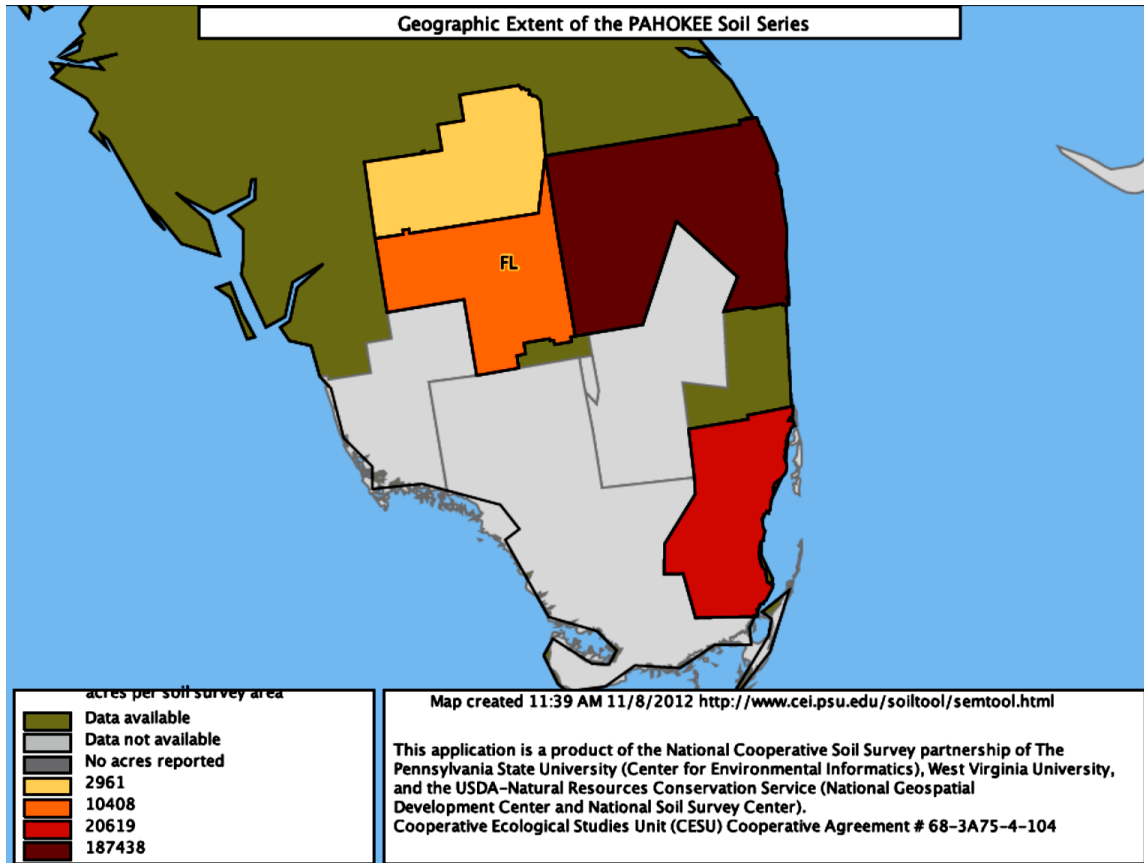
SUPPLEMENTARY INFORMATION ON IHSS HA STANDARDS

APPENDIX A1: FLOWCHART OUTLINING EXTRACTION PROCEDURES FOR THE PREPARATION OF HA AND FA SAMPLES FROM A SOIL SAMPLE<sup>a</sup>



<sup>a</sup>The amberlite XAD-8 resin has been the most frequently used method for the isolation and subsequent purification of HS (Janos, 2003). All organic acids are fully protonated, non-ionic and can adsorb onto the resin surface under acidic conditions. Using an alkaline solution, the organic acids are then desorbed from the resin and are referred to as HS or hydrophobic acids (McDonald et al., 2004 and references therein). Ag MP-500 refers to the H<sup>+</sup>- saturated cation exchange resin (Bio-Rad AG-MP-5) ([www.humicsubstances.org](http://www.humicsubstances.org)). From: <http://karnet.up.wroc.pl/~weber/ekstrak2.htm>

## APPENDIX A2: GEOGRAPHIC EXTENT MAPS OF SELECTED IHSS HA STANDARDS



### LOCATION PAHOKEE FL

Established Series  
Rev. SHM: GWH/GRB  
09/2011

### PAHOKEE SERIES

The Pahokee series consists of deep, very poorly drained, rapidly permeable soils in fresh water marshes. They formed in 36 to 51 inches of well decomposed, hydrophytic, herbaceous plant remains overlying limestone bedrock. Near the type location, the mean annual precipitation is about 61 inches and the mean annual temperature is about 75 degrees F. Slopes are 0 to 1 percent.

**TAXONOMIC CLASS:** Euic, hyperthermic Lithic Haplosaprists

**TYPICAL PEDON:** Pahokee muck--cultivated.

**Oap**--0 to 10 inches; black (N 2/) muck; moderate coarse subangular blocky structure parting to moderate fine and medium granular; very friable; less than 5 percent fiber, unrubbed; about 10 percent estimated mineral content; sodium pyrophosphate extract is brown (10YR 4/3) slightly acid; clear smooth boundary.

**Oa1**--10 to 28 inches; black (5YR 2/1) muck; massive; friable; about 65 percent fiber, unrubbed and 10 percent rubbed; about 10 percent estimated mineral content; sodium phosphate extract is pale brown (10YR 6/3); slightly acid; gradual smooth boundary.

**Oa2**--28 to 42 inches; dark reddish brown (5YR 2/2) muck; massive; friable; about 10 percent rubbed fiber and 40 percent unrubbed; about 10 percent estimated mineral content; sodium phosphate extract is pale brown (10YR 6/3); slightly acid; abrupt wavy boundary. (Combined thickness of the Oa horizon ranges from 26 to 51 inches).

**R**--42 inches; soft to hard but rippable limestone bedrock.

**TYPE LOCATION:** Palm Beach County, Florida. About 200 feet N. of S.R. 827 and 1/2 mile west of S.R. 827A; NE1/4, SE1/4, NW1/4, Sec. 30, T. 44 S., R. 37 E.

**RANGE IN CHARACTERISTICS:** Thickness of the organic material ranges from 26 to 51 inches and depth to hard limestone ranges from 36 to 51 inches. Calcium chloride reaction ranges from strongly acid to neutral and reaction in water ranges from moderately acid to slightly alkaline. Mineral content ranges from 5 to 25 percent.

The Oap horizon, where present, has hue of 5YR to 10YR, value of 2 or 3 and chroma of 3 or less; or it is neutral with value of 2 or 3. Texture is muck with an unrubbed fiber content of 15 to 30 percent and less than 10 percent rubbed.

The Oa horizon has hue of 5YR to 10YR, value of 2 to 4, and chroma of 3 or less. Texture is muck with an unrubbed fiber content of 30 to 60 percent and a rubbed fiber content of less than 16 percent.

Some pedons have a thin Oe horizon of mucky peat less than 4 inches thick. Where present, the Oe horizon has hue 5YR to 10YR, value of 3 or 4, and chroma of 2 to 4. Fiber content ranges from 50 to 75 percent unrubbed, and more than 16 percent rubbed.

Some pedons have Cg horizons less than 10 inches thick. Where present, the Cg horizon has hue of 10YR to 5Y, value of 2 to 7, and chroma of 2 or less. Textures are dominantly fine sand, sand, loamy fine sand, or loamy sand, or their mucky analogs. Some pedons may have textures of sandy loam, loam, silt loam, or their mucky analogs.

The 2R horizon is soft to hard but rippable limestone.

**COMPETING SERIES:** These are the Lauderhill and Tamiami series along with the closely related Dania series. Dania soils are shallow to limestone bedrock. Lauderhill soils have limestone within 36 inches of the surface. Tamiami soils are moderately deep and deep to limestone bedrock and have Cg horizons within the control section but having a combined thickness of less than one-half of the control section.

**GEOGRAPHIC SETTING:** Pahokee soils are in freshwater marshes within peninsular Florida. They formed in 36 to 51 inches of well decomposed, hydrophytic, herbaceous plant remains overlying limestone bedrock. Slopes are less than 1 percent. Precipitation averages 59 inches and air temperature averages 75 degrees F.

**GEOGRAPHICALLY ASSOCIATED SOILS:** These include the competing Dania and Lauderhill soils along with the Terra Ceia and Torry soils. All of the associated soils are on similar positions. Terra Ceia and Torry soils are more than 50 inches deep to limestone bedrock. In addition, Torry soils have 40 percent or more mineral content.

**DRAINAGE AND PERMEABILITY:** Very poorly drained; rapid permeability. In natural areas the water table is at or above the surface for much of the year; in other areas the water table is controlled by man.

**USE AND VEGETATION:** Pahokee soils are used for growing sugarcane, corn, truck crops, sod, and improved pasture. The natural vegetation consists of sawgrass, sedges, lilies, willow, spikerush, elderberry, and cypress.

**DISTRIBUTION AND EXTENT:** Interior of Southern Peninsular Florida. The series is of large extent (about 220,000 acres).

**MLRA SOIL SURVEY REGIONAL OFFICE (MO) RESPONSIBLE:** Auburn, Alabama.

**SERIES ESTABLISHED:** Palm Beach County, Florida; 1975.

**REMARKS:** Diagnostic horizons and features recognized in this pedon:

Sapric soil materials - the zone from the surface to a depth of 42 inches (Oap, Oa1 and Oa2 horizons).

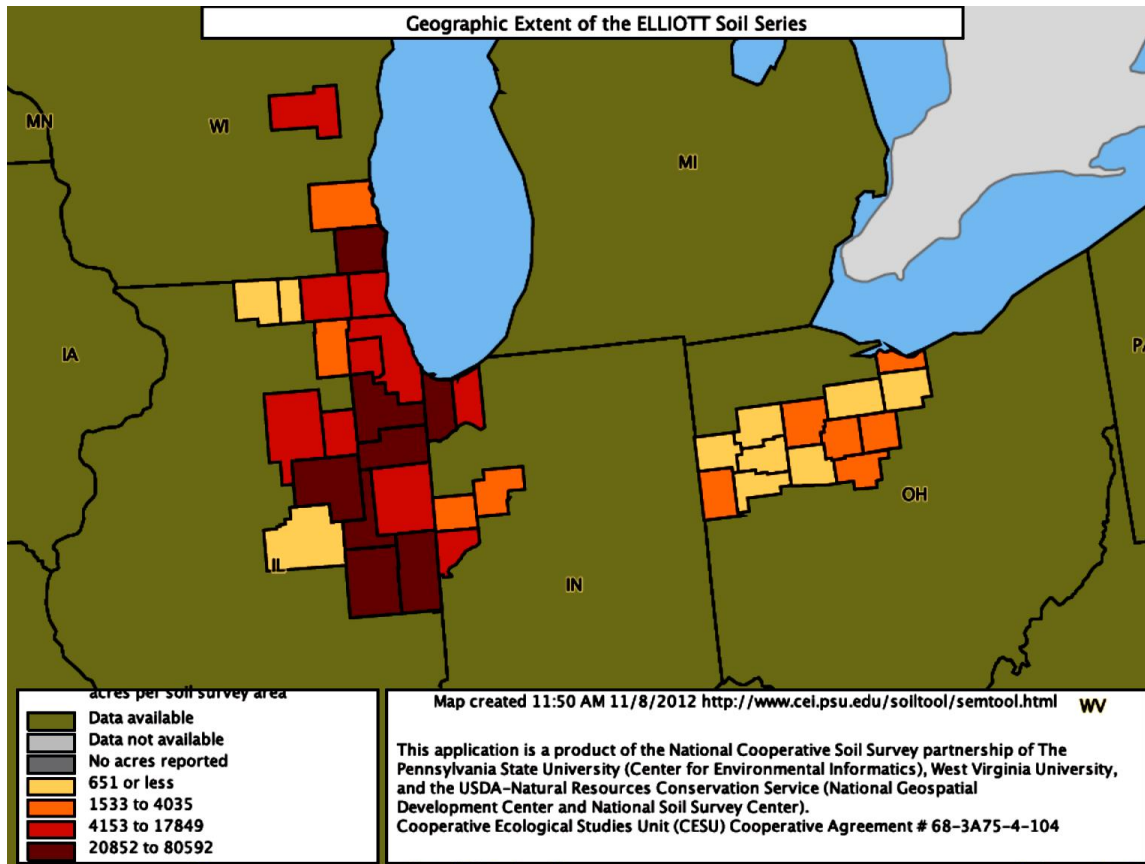
Lithic contact - at a depth of 42 inches (2R horizon).

**ADDITIONAL DATA:** Laboratory characterization data from the University of Florida (IFAS) Characterization Laboratory is available for the typical pedon, S50-008 (1-4).

Pahokee soils are in MLRAs 155, 156A and 156B.

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National Cooperative Soil Survey  
U.S.A.



LOCATION ELLIOTT IL+IN OH WI

Established Series  
 Rev. JBF-JWS-EJE-DEC  
 05/2011

### ELLIOTT SERIES

The Elliott series consists of very deep, somewhat poorly drained soils on till plains. They formed in up to 51 cm (20 inches) of loess or other silty material and in the underlying silty clay loam till. Slope ranges from 0 to 7 percent. Mean annual precipitation is about 914 mm (36 inches), and mean annual air temperature is about 10 degrees C (50 degrees F).

**TAXONOMIC CLASS:** Fine, illitic, mesic Aquic Argiudolls

**TYPICAL PEDON:** Elliott silt loam - on a west-facing slope with less than a 1 percent gradient in a cultivated field at an elevation of 704 feet (215 meters) above mean sea level. (Colors are for moist soil unless otherwise stated.)

**Ap**--0 to 15 cm (0 to 6 inches); black (10YR 2/1) silt loam, dark gray (10YR 4/1) dry; moderate fine granular structure; friable; common fine roots; moderately acid; abrupt smooth boundary.

**A**--15 to 28 cm (6 to 11 inches); black (10YR 2/1) silty clay loam, dark gray (10YR 4/1) dry; moderate fine granular structure; friable; common fine roots; slightly acid; clear smooth boundary. [Combined thickness of the A horizon is 25 to 51 cm (10 to 20 inches).]

**Bt1**--28 to 41 cm (11 to 16 inches); light olive brown (2.5Y 5/4) silty clay; moderate fine subangular blocky structure; friable; common fine roots; few distinct black (10YR 2/1) organic coatings on faces of peds; many distinct dark grayish brown (2.5Y 4/2) clay films on faces of peds; neutral; clear smooth boundary. [0 to 25 cm (0 to 10 inches) thick]

**2Bt2**--41 to 58 cm (16 to 23 inches); light olive brown (2.5Y 5/4) silty clay loam; moderate fine prismatic structure parting to moderate fine angular blocky; friable; few fine roots; common distinct dark grayish brown (2.5Y 4/2) clay films on faces of peds; few fine distinct yellowish brown (10YR 5/6) masses of oxidized iron in the matrix; few fine distinct grayish brown (2.5Y 5/2) iron depletions in the matrix; 1 percent gravel; neutral; clear smooth boundary.

**2Bt3**--58 to 71 cm (23 to 28 inches); grayish brown (2.5Y 5/2) silty clay loam; moderate fine prismatic structure parting to moderate fine angular blocky; friable; few fine roots; common distinct dark grayish brown (2.5Y 4/2) clay films on faces of peds; common fine prominent yellowish brown (10YR 5/6) masses of oxidized iron in the matrix; 1 percent gravel; neutral; clear smooth boundary.

**2Bt4**--71 to 89 cm (28 to 35 inches); olive brown (2.5Y 4/4) silty clay loam; moderate fine prismatic structure parting to moderate fine angular blocky; firm; few fine roots; many distinct dark grayish brown (2.5Y 4/2) clay films on faces of peds; few fine black (7.5YR 2.5/1) very weakly cemented iron-manganese concretions throughout; few medium white (10YR 8/1) moderately cemented calcium carbonate concretions throughout; few fine distinct yellowish brown (10YR 5/6) masses of oxidized iron in the matrix; 1 percent Gravel; slightly effervescent; slightly alkaline; clear smooth boundary.

**2Bt5**--89 to 104 cm (35 to 41 inches); olive brown (2.5Y 4/4) silty clay loam; weak fine prismatic structure parting to moderate medium angular blocky; firm; few fine roots; common distinct gray (5Y 6/1) clay films on faces of peds; few fine distinct yellowish brown (10YR 5/6) masses of oxidized iron in the matrix; 2 percent gravel; strongly effervescent; slightly alkaline; clear smooth boundary. [Combined thickness of the 2Bt horizon is 25 to 104 cm (10 to 28 inches).]

**2Cd**--104 to 152 cm (41 to 60 inches); olive brown (2.5Y 4/4) silty clay loam; massive; very firm; common fine prominent gray (5Y 5/1) iron depletions in the matrix; 3 percent gravel; strongly effervescent; moderately alkaline.

**TYPE LOCATION:** Livingston County, Illinois; about 2 miles (3.2 kilometers) east of Emmington; 690 feet (210 meters) south and 2,436 feet (742 meters) west of the center of sec. 21, T. 29 N., R. 8 E.; USGS Cullom topographic quadrangle; lat. 40 degrees 58 minutes 12 seconds N. and long. 88 degrees 19 minutes 19 seconds W., NAD 83; UTM Zone 16, 388762 easting and 4536262 northing, NAD 83.

**RANGE IN CHARACTERISTICS:**

Thickness of the mollic epipedon: 25 to 51 cm (10 to 20 inches)

Depth to the base of soil development: 51 to 114 cm (20 to 45 inches)

Depth to carbonates: 43 to 102 cm (17 to 40 inches)

Particle-size control section: averages between 35 and 45 percent clay

Ap, A, and/or AB horizons:

Hue: 10YR

Value: 2 or 3 (4 or 5 dry)

Chroma: 1 to 3

Texture: silt loam, silty clay loam or loam

Rock fragment content: 0 to 5 percent

Reaction: moderately acid to neutral

BA, Bt, 2Bt, and/or 2Btg horizons:

Hue: 10YR or 2.5Y

Value: 4 to 6

Chroma: 2 to 4

Texture: silty clay loam or silty clay, and less commonly clay and clay loam  
Clay content: 35 to 50 percent  
Sand content: 4 to 25 percent  
Rock fragment content: 0 to 10 percent  
Reaction: typically moderately acid to neutral but is slightly alkaline in the lower part in some pedons.  
Redox features: Redoximorphic features have chroma of 1 to 8.

2BC, 2BCg, 2Cd, and/or 2Cdg horizons:  
Hue: 10YR, 2.5Y or 5Y  
Value: 4 to 6  
Chroma: 1 to 6  
Texture: silty clay loam or clay loam  
Clay content: 27 to 40 percent  
Sand content: 5 to 30 percent  
Rock fragment content: 1 to 15 percent  
Reaction: slightly alkaline or moderately alkaline  
Redox features: Redoximorphic features are commonly present  
Bulk density of the 2Cd or 2Cdg horizons: 1.7 to 1.9 gm/cc.

**COMPETING SERIES:** These are the Chenoa, Clarence, Martinton, and Strole series. Chenoa soils average less than 8 percent fine sand and coarser in the upper part of the particle-size control section. Clarence and Strole soils average more than 45 percent clay in the particle-size control section. Martinton soils average less than 27 percent clay in some subhorizon in the lower part of the series control section. In addition, the sand fraction of the Martinton soil is predominantly fine or very fine.

**GEOGRAPHIC SETTING:** Elliott soils are on relatively undissected parts of till plains of Wisconsinan Age. Slope gradients range from 0 to 7 percent. The soils typically formed in silty clay loam till with a surface mantle of loess or other silty material ranging from 0 to 51 cm (0 to 20 inches) thick. Mean annual air temperature ranges from 7 to 11 degrees C (45 to 52 degrees F), mean annual precipitation ranges from 711 to 1016 mm (28 to 40 inches), frost-free period ranges from 140 to 180 days, and elevation ranges from 165 to 311 meters (541 to 1020 feet) above mean sea level.

**GEOGRAPHICALLY ASSOCIATED SOILS:** These are the Ashkum, Beecher, Blount, and Varna soils. The moderately well drained Varna soils and the poorly drained Ashkum soils form a hydro-sequence with Elliott soils. Ashkum soils are on lower landform positions and Varna soils are on higher landform positions. The somewhat poorly drained Beecher and Blount soils form a biosequence with Elliott soils and are on similar parts of landforms. Blount soils have a light colored surface layer, and Beecher soils lack the required surface layer thickness for a mollic epipedon.

**DRAINAGE AND SATURATED HYDRAULIC CONDUCTIVITY:** Somewhat poorly drained. The potential for surface runoff is low to high. Saturated hydraulic conductivity is moderately low or moderately high (0.42 to 1.41 micrometers/s). Permeability is slow. An intermittent perched seasonal high water table is at a depth of 31 to 61 cm (1.0 to 2.0 feet) at some time between January and May in most years.

**USE AND VEGETATION:** Most areas are cultivated. Corn, soybeans, small grain, and meadow are the principal crops. Native vegetation is prairie grasses.

**DISTRIBUTION AND EXTENT:** Northeastern Illinois, southeastern Wisconsin, northern Indiana, and Ohio. The series is of large extent in MLRA's 95B, 108A, 110, 111B, and 111C. More than 300,000 acres (121,408 hectares) have been correlated in the four states named.

**MLRA SOIL SURVEY REGIONAL OFFICE (MO) RESPONSIBLE:** Indianapolis, Indiana.

**SERIES ESTABLISHED:** Ford County, Illinois, 1929.



**REMARKS:** A bedrock substratum phase is recognized with limestone bedrock at depths of 60 to 80 inches (152 to 203 cm). This phase will need to be evaluated during future MLRA update activities.

Diagnostic horizons and features recognized in this pedon are: mollic epipedon - the zone from the surface of the soil to a depth of 28 cm (11 inches) (Ap and A horizons); argillic horizon - the zone from approximately 28 to 104 cm (11 to 41 inches) (Bt1, 2Bt2, 2Bt3, 2Bt4, and 2Bt5 horizons); udic moisture regime.

**ADDITIONAL DATA:** Refer to pedon number 85IL105034 from the University of Illinois Pedology Laboratory. This data is on file at the Illinois NRCS State Office and Indianapolis MLRA Region 11 Office.

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National Cooperative Soil Survey  
U.S.A.

APPENDIX B:  
EXPERIMENTAL DATA

APPENDIX B1:  
SIMPLE ORGANIC COMPOUNDS

## APPENDIX B1-1: DOPAC

(1.4 mg L<sup>-1</sup> in H<sub>2</sub>O, pH 5; **(a)** 0 & **(b)** 4 lamps, respectively; t<sub>reac</sub> of 1s)

**(a)** 0 lamps

<i>Organic Film</i> : 1.4 mg L <sup>-1</sup> 3,4-dihydroxyphenylacetic acid (DOPAC) in H <sub>2</sub> O, pH 5					
N	Dark Experiment		N	Dark Experiment	
1	Effluent NO <sub>2</sub> Signal	Effluent NO <sub>2</sub> (ppbv)	2	Effluent NO <sub>2</sub> Signal	Effluent NO <sub>2</sub> (ppbv)
	90.95	67.35		91.03	67.40
	91.44	67.68		91.28	67.57
	90.63	67.13		91.77	67.91
	91.29	67.58		91.32	67.60
	90.68	67.16		91.26	67.56
	91.39	67.65		91.83	67.95
	90.88	67.30		91.32	67.60
	91.12	67.46		91.28	67.57
	90.83	67.26		91.86	67.97
	90.48	67.02		91.47	67.70
	90.69	67.17		91.59	67.79
	91.28	67.57		91.39	67.65
	90.38	66.95		91.20	67.52
	90.39	66.96		91.50	67.72
	90.60	67.10		91.79	67.92
	90.74	67.20		91.18	67.50
	91.18	67.50		91.19	67.51
	90.74	67.20		91.86	67.97
	91.33	67.61		91.29	67.58
	90.97	67.36		91.24	67.55
	90.58	67.09		91.78	67.92
	91.09	67.44		91.68	67.85
	91.28	67.57		91.17	67.50
	90.87	67.29		91.85	67.97
	91.08	67.44		91.08	67.44

(b) 4 lamps

<i>Organic Film: 1.4 mg L<sup>-1</sup> 3,4-dihydroxyphenylacetic acid (DOPAC) in H<sub>2</sub>O, pH 5</i>					
<i>N</i>	<b>Light Experiment</b>		<i>N</i>	<b>Light Experiment</b>	
1	Effluent NO <sub>2</sub> Signal	Effluent NO <sub>2</sub> (ppbv)	2	Effluent NO <sub>2</sub> Signal	Effluent NO <sub>2</sub> (ppbv)
	90.46	67.01		89.05	66.04
	90.47	67.02		89.28	66.20
	90.33	66.92		89.33	66.23
	90.59	67.10		89.70	66.49
	90.65	67.14		89.26	66.18
	90.59	67.10		88.90	65.93
	89.86	66.60		89.49	66.34
	90.03	66.71		89.89	66.62
	89.99	66.68		89.46	66.32
	90.83	67.26		89.30	66.21
	90.95	67.35		89.09	66.07
	90.16	66.80		89.77	66.53
	90.92	67.32		89.09	66.07
	90.65	67.14		89.88	66.61
	90.48	67.02		89.35	66.24
	90.22	66.84		89.94	66.65
	90.63	67.13		89.68	66.47
	90.79	67.24		89.44	66.31
	91.35	67.62		89.28	66.20
	90.68	67.16		89.87	66.60
	91.52	67.74		89.14	66.10
	90.89	67.30		89.60	66.42
	91.38	67.64		89.89	66.62
	90.60	67.10		89.22	66.15
	91.44	67.68		89.83	66.57

## APPENDIX B1-2: 2-NP

(pH 2, 5 mg L<sup>-1</sup>, [NO<sub>2</sub>]<sub>0</sub> = 72, 1000 ppbv; 4 lamps; t<sub>reac</sub> of 1 s)

<i>Blank Film: pH 2 5% MeOH</i>					<i>Organic Film: pH 2 5 mg L<sup>-1</sup> 2-NP in 5% MeOH</i>			
NO <sub>2</sub> (ppbv)	Injections	Area of HONO Peak	HONO (μM)	P(HONO) (pptv s <sup>-1</sup> )	Injections	Area of HONO Peak	HONO (μM)	P(HONO) (pptv s <sup>-1</sup> )
72	1	3.724	0.007168	17.48	1	5.441	0.01047	25.55
	2	7.026	0.01352	32.99	2	4.348	0.008370	20.41
	3	5.191	0.009991	24.37	3	5.406	0.01041	25.38
					4	7.311	0.01407	34.32
1000	1	134.3	0.2586	630.6	1	144.5	0.2782	678.5
	2	132.1	0.2543	620.3	2	147.1	0.2832	690.7
	3	131.5	0.2531	617.3	3	176.2	0.3392	827.2

### APPENDIX B1-3: 4M2NP

(pH 2, 5 mg L<sup>-1</sup>, [NO<sub>2</sub>]<sub>0</sub> = 72, 1000 ppbv; 4 lamps; t<sub>reac</sub> of 1 s)

<i>Blank Film: pH 2 5% MeOH</i>					<i>Organic Film: pH 2 5 mg L<sup>-1</sup> 4M2NP in 5% MeOH</i>			
NO <sub>2</sub> (ppbv)	Injections	Area of HONO Peak	HONO (μM)	P(HONO) (pptv s <sup>-1</sup> )	Injections	Area of HONO Peak	HONO (μM)	P(HONO) (pptv s <sup>-1</sup> )
72	1	6.676	0.01285	31.34	1	7.016	0.1350	32.94
	2	2.340	0.004505	10.99	2	5.654	0.01088	26.54
	3	5.016	0.009654	23.55	3	3.994	0.007688	18.75
	4	2.208	0.004250	10.37	4	1.372	0.002641	6.44
1000	1	137.4	0.2644	644.9	1	157.7	0.3036	740.5
	2	135.6	0.2610	636.6	2	157.5	0.3031	739.4
					3	149.0	0.2867	699.3
					4	174.8	0.3365	820.8

## APPENDIX B1-4: KHP

(pH 2, 0.5 mM,  $[\text{NO}_2]_0 = 72, 1000$  ppbv; 4 lamps;  $t_{\text{reac}}$  of 1 s)

<i>Blank Film: pH 2 5% MeOH</i>					<i>Organic Film: pH 2 0.5 mM KHP in 5% MeOH</i>			
NO <sub>2</sub> (ppbv)	Injections	Area of HONO Peak	HONO (μM)	P(HONO) (pptv s <sup>-1</sup> )	Injections	Area of HONO Peak	HONO (μM)	P(HONO) (pptv s <sup>-1</sup> )
72	1	26.40	0.05081	123.9	1	28.29	0.05446	132.8
	2	26.19	0.05040	122.9	2	22.96	0.04419	107.8
	3	22.25	0.04282	104.4	3	25.38	0.04886	119.2
1000	1	141.6	0.2726	664.9	1	166.5	0.3205	781.7
	2	135.3	0.2604	635.2	2	175.1	0.3371	822.1
	3	133.6	0.2571	627.0	3	168.0	0.3233	788.6
					4	153.3	0.2950	719.5



APPENDIX B2:  
HUMIC ACIDS (HA)

## APPENDIX B2-1: DEPENDENCE OF HONO YIELD ON NO<sub>2</sub> CONCENTRATION

([HA]<sub>solution</sub> = 1 g L<sup>-1</sup>; 4 lamps; t<sub>reac</sub> of 1 s)

10 ppbv NO <sub>2</sub>			
	Area of HONO Peak	[HONO] (μM)	ΔP(HONO) (pptv s <sup>-1</sup> )
N = 1, n =			
1	15.6559	0.030135	73.50077
2	12.0043	0.023107	56.35737
3	23.4332	0.045105	110.0134
	Area of HONO Peak	[HONO] (μM)	ΔP(HONO) (pptv s <sup>-1</sup> )
N = 2, n =			
4	16.9164	0.0325616	79.41853
5	6.0442	0.0116342	28.3761
6	13.3728	0.0257407	62.78216

18 ppbv NO <sub>2</sub>			
	Area of HONO Peak	[HONO] (μM)	ΔP(HONO) (pptv s <sup>-1</sup> )
N = 1, n =			
1	26.04	0.050123	122.2517
2	20.609	0.039669	96.75441
3	30.6409	0.058979	143.8518
	Area of HONO Peak	[HONO] (μM)	ΔP(HONO) (pptv s <sup>-1</sup> )
N = 2, n =			
4	25.8389	0.049736103	121.3076
5	24.776	0.047690176	116.3175
6	27.2936	0.052536187	128.137
7	30.7832	0.059253157	144.5199
8	22.7925	0.043872228	107.0054

36 ppbv NO <sub>2</sub>			
	Area of HONO Peak	[HONO] (μM)	ΔP(HONO) (pptv s <sup>-1</sup> )
N = 1, n =			
1	50.1766	0.096582615	235.5674
2	48.4975	0.093350593	227.6844
3	48.0722	0.092531953	225.6877
	Area of HONO Peak	[HONO] (μM)	ΔP(HONO) (pptv s <sup>-1</sup> )
N = 2, n =			
4	55.3056	0.106455189	259.6468
5	52.2743	0.10062038	245.4156
6	52.277	0.100625577	245.4282
7	57.2486	0.11019518	268.7687

72 ppbv			
	Area of HONO Peak	[HONO] (μM)	ΔP(HONO) (pptv s <sup>-1</sup> )
N = 1, n =			
1	103.8642	0.199923	487.618
2	94.5702	0.182034	443.9849
3	100.8682	0.194157	473.5525
	Area of HONO Peak	[HONO] (μM)	ΔP(HONO) (pptv s <sup>-1</sup> )
N = 2, n =			
4	88.4427	0.170239259	415.2177
5	95.1534	0.183156375	446.7229
6	87.909	0.169211965	412.7121
7	110.9056	0.213477056	520.6757
	Area of HONO Peak	[HONO] (μM)	ΔP(HONO) (pptv s <sup>-1</sup> )
N = 3, n =			
8	96.6157	0.185971089	453.588
9	120.0979	0.231170889	563.8314
10	114.7175	0.220814406	538.5717

## APPENDIX B2-2: pH-DEPENDENT REACTION KINETICS STUDY

( $[\text{HA}]_{\text{solution}} = 0.84 \text{ g L}^{-1}$ ;  $[\text{NO}_2]_0 = 32 \text{ ppbv}$ ; 4 lamps;  $t_{\text{reac}}$  of 1 s)

pH 1.5			
	Area of HONO Peak	[HONO] (nM)	$\Delta\text{P}(\text{HONO})$ (pptv s <sup>-1</sup> )
N = 1, n =			
1	16.83931907	32.4132258	79.34652267
2	17.77635776	34.2168882	83.76182957
	Area of HONO Peak	[HONO] (nM)	$\Delta\text{P}(\text{HONO})$ (pptv s <sup>-1</sup> )
N = 2, n =			
3	21.22695206	40.85877744	100.0209584
4	20.61485119	39.68057281	97.13675182
pH 2			
	Area of HONO Peak	[HONO] (nM)	$\Delta\text{P}(\text{HONO})$ (pptv s <sup>-1</sup> )
N = 1, n =			
1	18.76643073	36.12263383	88.42703291
2	20.68471581	39.81505199	97.46595248
	Area of HONO Peak	[HONO] (nM)	$\Delta\text{P}(\text{HONO})$ (pptv s <sup>-1</sup> )
N = 2, n =			
3	19.55098651	37.63278895	92.12384351
4	19.55199633	37.6347327	92.12860176
5	21.41141262	41.21383703	100.8901328
pH 2.5			
	Area of HONO Peak	[HONO] (nM)	$\Delta\text{P}(\text{HONO})$ (pptv s <sup>-1</sup> )
N = 1, n =			
1	49.36096463	95.01263596	232.587843
2	45.26928387	87.13674906	213.307928
3	46.18107705	88.89181754	217.6042786
	Area of HONO Peak	[HONO] (nM)	$\Delta\text{P}(\text{HONO})$ (pptv s <sup>-1</sup> )
N = 2, n =			
4	48.60083155	93.54949097	229.0061116
5	48.20771214	92.79279361	227.1537411
6	45.01177963	86.64109106	212.0945733
7	50.78679388	97.75714868	239.3063209

pH 3				
	Area of HONO Peak		[HONO] (nM)	$\Delta P(\text{HONO})$ (pptv s <sup>-1</sup> )
N = 1, n =				
1	60.12127605		115.7246613	283.2902075
2	54.41436859		104.7396993	256.3993778
3	61.74574075		118.8515182	290.9446515
	Area of HONO Peak		[HONO] (nM)	$\Delta P(\text{HONO})$ (pptv s <sup>-1</sup> )
N = 2, n =				
4	58.5775596		112.753233	276.0162476
5	60.6191924		116.6830775	285.636379
6	61.86628341		119.0835452	291.512646

pH 3.3 range						
	Area of HONO Peak (3 integrations, N =1)			[HONO] ( $\mu\text{M}$ )	$\Delta P(\text{HONO})$ (pptv s <sup>-1</sup> )	
Interpolated pH						
3.335648	13.8106	15.2652	13.1247	0.026583385	64.83752357	
3.359060	6.2801	6.7971	6.5499	0.012088274	29.48359461	
3.372422	4.248	5.1846	4.2602	0.008785546	21.42816008	
3.375736	4.1018	2.9256	3.1226	0.006512422	15.88395542	

pH 3.4 range						
	Area of HONO Peak (3 integrations, N =1)			[HONO] ( $\mu\text{M}$ )	$\Delta P(\text{HONO})$ (pptv s <sup>-1</sup> )	
Interpolated pH						
3.458934	2.4523	2.3479	2.4294	0.00463864	11.31375804	
3.452570	1.2713	1.1258	0	0.00153802	3.751273846	
3.449063	0	1.0774	0	0.00069128	1.686046657	
3.453089	2.113	1.2468	2.2392	0.00359242	8.76199669	

pH 3.5 range					
	Area of HONO Peak (3 integrations, N =1)			[HONO] ( $\mu\text{M}$ )	$\Delta\text{P}(\text{HONO})$ (pptv $\text{s}^{-1}$ )
Interpolated pH					
3.542984	1.0748	1.0588	0	0.00136896	3.338916974
3.548098	1.0215	1.0516	0	0.00133014	3.24423921

pH 3.7 range					
	Area of HONO Peak (3 integrations, N =1)			[HONO] ( $\mu\text{M}$ )	$\Delta\text{P}(\text{HONO})$ (pptv $\text{s}^{-1}$ )
Interpolated pH					
3.764389	6.8148	7.2895	6.2207	0.01304088	31.80703388
3.769611	4.3613	4.3336	4.3623	0.00837773	20.43349583
3.757843	3.5477	3.5664	3.9908	0.0071251	17.37829917
3.729085	3.9019	3.8976	4.6698	0.00800053	19.51347836

pH 4.0 range					
	Area of HONO Peak (3 integrations, N =1)			[HONO] ( $\mu\text{M}$ )	$\Delta\text{P}(\text{HONO})$ (pptv $\text{s}^{-1}$ )
Interpolated pH					
3.912455	61.9819	63.4271	66.1226	0.11930609	290.990464
3.932638	60.7937	60.6118	60.4979	0.11701898	285.412144
3.955359	61.8385	61.8506	61.944	0.11903007	290.3172347
3.980618	52.3998	53.7089	52.6252	0.10086195	246.0047549
4.008415	49.4461	48.6795	50.483	0.09517651	232.137827
4.038749	44.4534	41.6137	44.315	0.08556629	208.6982731

pH 4.3 range					
	Area of HONO Peak (3 integrations, N =1)			[HONO] ( $\mu\text{M}$ )	$\Delta\text{P}(\text{HONO})$ (pptv $\text{s}^{-1}$ )
Interpolated pH					
4.247327	1.2562	1.0904	0	0.001505621	3.6722453
4.263235	0	1.259	1.0368	0.001473026	3.592747276
4.277860	1.0221	1.0308	0	0.001317177	3.212627792
4.291202	1.0218	1.0122	0	0.001305051	3.183050771

### APPENDIX B2-3: DETERMINATION OF $k_{rxn}$

( $[HA]_{\text{solution}} = 0.5 - 1.0 \text{ g L}^{-1}$ ; pH 3 film;  $[NO_2]_0 = 36 \text{ ppbv}$ ; 4 lamps;  $t_{\text{reac}}$  of 1 s)

0.5 g/L			
	Area of HONO Peak	[HONO] ( $\mu\text{M}$ )	$\Delta P(\text{HONO})$ (pptv $\text{s}^{-1}$ )
N = 1, n =			
1	35.9629	0.069223	168.8373696
2	34.4587	0.066328	161.7755038
	Area of HONO Peak	[HONO] ( $\mu\text{M}$ )	$\Delta P(\text{HONO})$ (pptv $\text{s}^{-1}$ )
N = 2, n =			
3	40.7879	0.078510741	191.4896114
4	36.6051	0.070459463	171.8523478
5	33.0568	0.063629504	155.1939126
	Area of HONO Peak	[HONO] ( $\mu\text{M}$ )	$\Delta P(\text{HONO})$ (pptv $\text{s}^{-1}$ )
N = 3, n =			
6	32.7378	0.063015476	153.6962825
7	32.489	0.062536572	152.5282249
8	34.3173	0.066055782	161.1116641

0.67 g/L			
	Area of HONO Peak	[HONO] ( $\mu\text{M}$ )	$\Delta P(\text{HONO})$ (pptv $\text{s}^{-1}$ )
N = 1, n =			
1	45.2495	0.087099	212.4357756
2	46.0595	0.088658	216.2385354
3	51.242	0.098633	240.5691558
4	50.9251	0.098023	239.0813847
5	43.6524	0.084024	204.9377662
6	46.2641	0.089052	217.1990843
	Area of HONO Peak	[HONO] ( $\mu\text{M}$ )	$\Delta P(\text{HONO})$ (pptv $\text{s}^{-1}$ )
N = 2, n =			
7	45.3867	0.087362758	213.0798974
8	50.8238	0.09782838	238.605805

0.76 g/L			
	Area of HONO Peak	[HONO] ( $\mu\text{M}$ )	$\Delta\text{P}(\text{HONO})$ (pptv $\text{s}^{-1}$ )
N = 1, n =			
1	54.9882	0.105844241	258.156685
2	53.6357	0.103240876	251.8070151
3	54.1849	0.104298006	254.3853801
4	53.7439	0.103449145	252.3149887
5	54.4173	0.104745342	255.4764435

0.84 g/L			
	Area of HONO Peak	[HONO] (nM)	$\Delta\text{P}(\text{HONO})$ (pptv $\text{s}^{-1}$ )
N = 1, n =			
1	60.12127605	115.7246613	283.2902075
2	54.41436859	104.7396993	256.3993778
3	61.74574075	118.8515182	290.9446515
	Area of HONO Peak	[HONO] (nM)	$\Delta\text{P}(\text{HONO})$ (pptv $\text{s}^{-1}$ )
N = 2, n =			
4	58.5775596	112.753233	276.0162476
5	60.6191924	116.6830775	285.636379
6	61.86628341	119.0835452	291.512646

1.00 g/L			
	Area of HONO Peak	[HONO] ( $\mu\text{M}$ )	$\Delta\text{P}(\text{HONO})$ (pptv $\text{s}^{-1}$ )
N = 1, n =			
1	155.8266	0.299943409	731.5693
2	138.7703	0.267112527	651.494
3	146.2179	0.281448067	686.4587
4	159.297	0.306623422	747.862
	Area of HONO Peak	[HONO] ( $\mu\text{M}$ )	$\Delta\text{P}(\text{HONO})$ (pptv $\text{s}^{-1}$ )
N = 2, n =			
5	156.6046	0.30144095	735.2218
6	162.0801	0.31198048	760.928
7	155.8692	0.30002541	731.7693
8	149.3273	0.28743321	701.0566



## APPENDIX B2-4: DEPENDENCE OF $y_{\text{best-fit}}$ ON IRRADIANCE

( $[\text{HA}]_{\text{solution}}$  (pH 3) = 0.84 g L<sup>-1</sup>;  $[\text{NO}_2]_0$  = 36 ppbv; 0 to 4 lamps;  $t_{\text{reac}}$  of 1 s)

0 lamps			
	Area of HONO Peak	[HONO] ( $\mu\text{M}$ )	$\Delta\text{P}(\text{HONO})$ (pptv s <sup>-1</sup> )
N = 1, n =			
1	1.3092	0.002520018	6.146386533
2	1.0134	0.001950647	4.757675002
3	1.258	0.002421466	5.906014558
	Area of HONO Peak	[HONO] ( $\mu\text{M}$ )	$\Delta\text{P}(\text{HONO})$ (pptv s <sup>-1</sup> )
N = 2, n =			
4	1.268	0.002440715	5.952962209
5	1.0794	0.002077687	5.067529502
6	1.2898	0.002482676	6.055308089
7	1.2032	0.002315984	5.648741427

2 lamps			
	Area of HONO Peak	[HONO] ( $\mu\text{M}$ )	$\Delta\text{P}(\text{HONO})$ (pptv s <sup>-1</sup> )
N = 1, n =			
1	5.5322	0.010648676	25.97237976
2	6.678	0.012854173	31.35164167
3	6.4062	0.012330998	30.0756045
	Area of HONO Peak	[HONO] ( $\mu\text{M}$ )	$\Delta\text{P}(\text{HONO})$ (pptv s <sup>-1</sup> )
N = 2, n =			
4	6.8627	0.013209694	32.21876479
5	6.7792	0.013048968	31.8267519
6	6.1674	0.011871343	28.95449458
7	5.0921	0.009801548	23.90621362

4 lamps			
	Area of HONO Peak	[HONO] (nM)	$\Delta P(\text{HONO})$ (pptv s <sup>-1</sup> )
N = 1, n =			
1	60.12127605	115.7246613	283.2902075
2	54.41436859	104.7396993	256.3993778
3	61.74574075	118.8515182	290.9446515
	Area of HONO Peak	[HONO] (nM)	$\Delta P(\text{HONO})$ (pptv s <sup>-1</sup> )
N = 2, n =			
4	58.5775596	112.753233	276.0162476
5	60.6191924	116.6830775	285.636379
6	61.86628341	119.0835452	291.512646

## APPENDIX B2-5: DEPENDENCE OF $y_{\text{best-fit}}$ ON HA STANDARD

( $[\text{HA}]_{\text{solution}}$  (pH 3) = 0.76 g L<sup>-1</sup>;  $[\text{NO}_2]_0$  = 36 ppbv; 4 lamps;  $t_{\text{reac}}$  of 1 s)

Commercial HA			
	Area of HONO Peak	[HONO] ( $\mu\text{M}$ )	$\Delta\text{P}(\text{HONO})$ (pptv s <sup>-1</sup> )
N = 1, n =			
1	47.9476	0.0923	225.1027215
2	49.2079	0.0947	254.3853801
3	47.2337	0.0909	221.7511286
4	49.8289	0.0959	233.9349831
5	47.8184	0.0920	255.4764435
	Area of HONO Peak	[HONO] ( $\mu\text{M}$ )	$\Delta\text{P}(\text{HONO})$ (pptv s <sup>-1</sup> )
N = 2, n =			
6	47.4780	0.0914	222.8980597
7	47.9556	0.0923	225.1402796

Pahoee Peat HA			
	Area of HONO Peak	[HONO] ( $\mu\text{M}$ )	$\Delta\text{P}(\text{HONO})$ (pptv s <sup>-1</sup> )
N = 1, n =			
1	45.1980	0.0870	212.1939952
2	42.3974	0.0816	199.0458359
3	44.3159	0.0853	208.0527429
4	44.0284	0.0847	206.7029979
	Area of HONO Peak	[HONO] ( $\mu\text{M}$ )	$\Delta\text{P}(\text{HONO})$ (pptv s <sup>-1</sup> )
N = 2, n =			
5	36.0356	0.0694	169.178679
6	39.7300	0.0765	186.5230194
7	33.8713	0.0652	159.0177988

Leonardite HA			
	Area of HONO Peak	[HONO] ( $\mu\text{M}$ )	$\Delta\text{P}(\text{HONO})$ (pptv $\text{s}^{-1}$ )
N = 1, n =			
1	23.1758	0.0446	108.8049381
2	20.176	0.0388	94.72158165
3	16.8406	0.0324	79.06266197
4	27.1853	0.0523	127.628599
Elliot Soil HA			
	Area of HONO Peak	[HONO] ( $\mu\text{M}$ )	$\Delta\text{P}(\text{HONO})$ (pptv $\text{s}^{-1}$ )
N = 1, n =			
1	6.6718	0.0128	31.32253412
2	3.8243	0.0074	17.95419036
3	3.8736	0.0075	18.18564228
	Area of HONO Peak	[HONO] ( $\mu\text{M}$ )	$\Delta\text{P}(\text{HONO})$ (pptv $\text{s}^{-1}$ )
N = 2, n =			
4	4.1623	0.0080	19.54102098
5	5.6064	0.0108	26.32073133
6	7.7061	0.0148	36.17832972
7	6.9031	0.0133	32.4084333

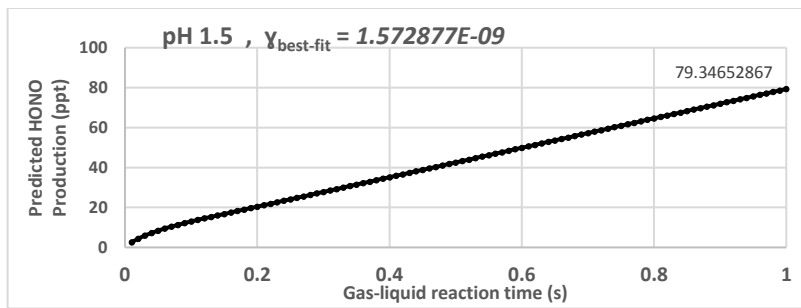
APPENDIX C:  
MODEL OUTPUT DATA

APPENDIX C1:

HUMIC ACIDS

## APPENDIX C1-1: pH-DEPENDENT REACTION KINETICS STUDY

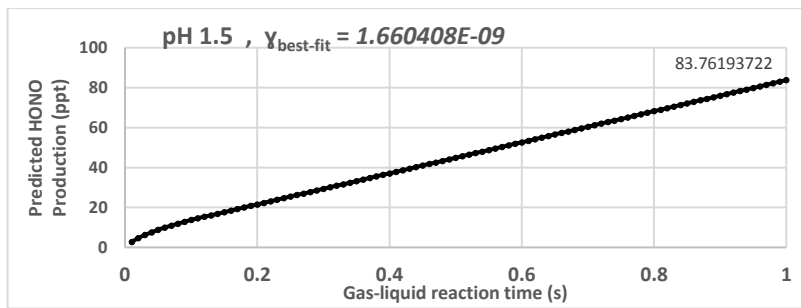
( $[\text{HA}]_{\text{solution}} = 0.84 \text{ g L}^{-1}$ ;  $[\text{NO}_2]_0 = 32 \text{ ppbv}$ ; 4 lamps;  $t_{\text{reac}}$  of 1 s)



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO2}}$ (mol)	$\Phi_{\text{NO2}}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732618E+16	1.166667	3.509922E-07	6.718649E-20	4.454691E-17	7.060209E-19	99.999951	1.500000
0.02	1.732617E+16	2.333333	4.963777E-07	2.965755E-19	8.909379E-17	2.118062E-18	99.999902	1.500000
0.03	1.732617E+16	3.500000	6.079357E-07	7.570295E-19	1.336406E-16	4.236124E-18	99.999852	1.500000
0.04	1.732616E+16	4.666667	7.019834E-07	1.505341E-18	1.781875E-16	7.060205E-18	99.999800	1.500000
0.05	1.732615E+16	5.833333	7.848408E-07	2.590964E-18	2.227343E-16	1.059031E-17	99.999747	1.500000
0.06	1.732614E+16	7.000000	8.597496E-07	4.058284E-18	2.672811E-16	1.482643E-17	99.999694	1.500000
0.07	1.732613E+16	8.166667	9.286352E-07	5.947917E-18	3.118279E-16	1.976856E-17	99.999639	1.500000
0.08	1.732612E+16	9.333333	9.927522E-07	8.297529E-18	3.563746E-16	2.541672E-17	99.999582	1.500000
0.09	1.732611E+16	10.500000	1.052972E-06	1.114240E-17	4.009213E-16	3.177090E-17	99.999525	1.500000
0.10	1.732610E+16	11.666667	1.109929E-06	1.451583E-17	4.454680E-16	3.883109E-17	99.999466	1.500000
0.11	1.732609E+16	12.833333	1.164103E-06	1.844944E-17	4.900147E-16	4.659730E-17	99.999406	1.500000
0.12	1.732608E+16	14.000000	1.215865E-06	2.297339E-17	5.345613E-16	5.506952E-17	99.999344	1.500000
0.13	1.732607E+16	15.166667	1.234286E-06	2.812271E-17	5.791079E-16	6.424776E-17	99.999281	1.500000
0.14	1.732606E+16	16.333333	1.234286E-06	3.393561E-17	6.236545E-16	7.413202E-17	99.999216	1.500000
0.15	1.732604E+16	17.500000	1.234286E-06	4.045030E-17	6.682010E-16	8.472229E-17	99.999150	1.500000
0.16	1.732603E+16	18.666667	1.234286E-06	4.770499E-17	7.127476E-16	9.601858E-17	99.999083	1.500000
0.17	1.732602E+16	19.833333	1.234286E-06	5.573789E-17	7.572940E-16	1.080209E-16	99.999014	1.500000
0.18	1.732601E+16	21.000000	1.234286E-06	6.458722E-17	8.018405E-16	1.207292E-16	99.998943	1.500000
0.19	1.732600E+16	22.166667	1.234286E-06	7.429118E-17	8.463869E-16	1.341435E-16	99.998870	1.500000
0.20	1.732598E+16	23.333333	1.234286E-06	8.488798E-17	8.909333E-16	1.482639E-16	99.998796	1.500000
0.21	1.732597E+16	24.500000	1.234286E-06	9.641584E-17	9.354797E-16	1.630902E-16	99.998720	1.500000
0.22	1.732596E+16	25.666667	1.234286E-06	1.089130E-16	9.800260E-16	1.786226E-16	99.998643	1.500000
0.23	1.732594E+16	26.833333	1.234286E-06	1.224176E-16	1.024572E-15	1.948610E-16	99.998563	1.500000
0.24	1.732593E+16	28.000000	1.234286E-06	1.369679E-16	1.069119E-15	2.118053E-16	99.998482	1.500000
0.25	1.732591E+16	29.166667	1.234286E-06	1.526021E-16	1.113665E-15	2.294557E-16	99.998398	1.500000
0.26	1.732590E+16	30.333333	1.234286E-06	1.693584E-16	1.158211E-15	2.478122E-16	99.998313	1.500000
0.27	1.732588E+16	31.500000	1.234286E-06	1.872750E-16	1.202757E-15	2.668746E-16	99.998226	1.500000
0.28	1.732587E+16	32.666667	1.234286E-06	2.063901E-16	1.247303E-15	2.866430E-16	99.998136	1.500000
0.29	1.732585E+16	33.833333	1.234286E-06	2.267420E-16	1.291849E-15	3.071174E-16	99.998045	1.500000
0.30	1.732584E+16	35.000000	1.234286E-06	2.483688E-16	1.336395E-15	3.282979E-16	99.997951	1.500000
0.31	1.732582E+16	36.166667	1.234286E-06	2.713088E-16	1.380941E-15	3.501843E-16	99.997856	1.500000
0.32	1.732580E+16	37.333333	1.234286E-06	2.956002E-16	1.425487E-15	3.727767E-16	99.997758	1.500000
0.33	1.732579E+16	38.500000	1.234286E-06	3.212812E-16	1.470033E-15	3.960752E-16	99.997658	1.500000
0.34	1.732577E+16	39.666667	1.234286E-06	3.483899E-16	1.514579E-15	4.200797E-16	99.997555	1.500000
0.35	1.732575E+16	40.833333	1.234286E-06	3.769646E-16	1.559125E-15	4.447901E-16	99.997450	1.500000
0.36	1.732573E+16	42.000000	1.234286E-06	4.070436E-16	1.603670E-15	4.702066E-16	99.997343	1.500000
0.37	1.732571E+16	43.166667	1.234286E-06	4.386649E-16	1.648216E-15	4.963290E-16	99.997234	1.500000
0.38	1.732569E+16	44.333333	1.234286E-06	4.718669E-16	1.692762E-15	5.231575E-16	99.997122	1.500000
0.39	1.732567E+16	45.500000	1.234286E-06	5.066878E-16	1.737307E-15	5.506920E-16	99.997007	1.500000
0.40	1.732565E+16	46.666667	1.234286E-06	5.431657E-16	1.781853E-15	5.789324E-16	99.996890	1.500000
0.41	1.732563E+16	47.833333	1.234286E-06	5.813388E-16	1.826398E-15	6.078789E-16	99.996771	1.500000
0.42	1.732561E+16	49.000000	1.234286E-06	6.212454E-16	1.870944E-15	6.375314E-16	99.996648	1.500000
0.43	1.732559E+16	50.166667	1.234286E-06	6.629237E-16	1.915489E-15	6.678898E-16	99.996524	1.500000
0.44	1.732557E+16	51.333333	1.234286E-06	7.064118E-16	1.960034E-15	6.989543E-16	99.996396	1.500000
0.45	1.732554E+16	52.500000	1.234286E-06	7.517481E-16	2.004580E-15	7.307247E-16	99.996266	1.500000

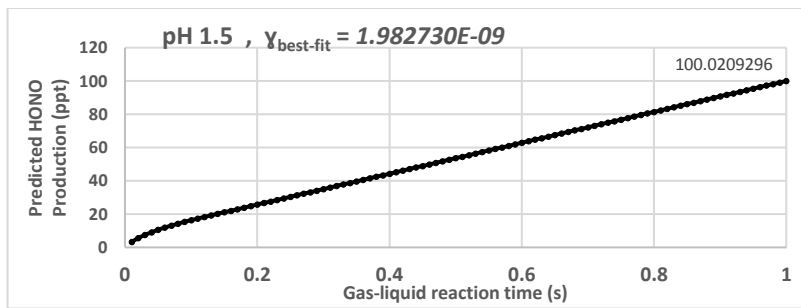


0.46	1.732552E+16	53.666667	1.234286E-06	7.989707E-16	2.049125E-15	7.632012E-16	99.996133	1.500000
0.47	1.732550E+16	54.833333	1.234286E-06	8.481177E-16	2.093670E-15	7.963836E-16	99.995997	1.500000
0.48	1.732547E+16	56.000000	1.234286E-06	8.992275E-16	2.138215E-15	8.302720E-16	99.995858	1.500000
0.49	1.732545E+16	57.166667	1.234286E-06	9.523382E-16	2.182760E-15	8.648664E-16	99.995717	1.500000
0.50	1.732542E+16	58.333333	1.234286E-06	1.007488E-15	2.227305E-15	9.001668E-16	99.995572	1.500000
0.51	1.732540E+16	59.500000	1.234286E-06	1.064715E-15	2.271850E-15	9.361732E-16	99.995424	1.500000
0.52	1.732537E+16	60.666667	1.234286E-06	1.124058E-15	2.316395E-15	9.728856E-16	99.995274	1.500000
0.53	1.732535E+16	61.833333	1.234286E-06	1.185555E-15	2.360940E-15	1.010304E-15	99.995120	1.500000
0.54	1.732532E+16	63.000000	1.234286E-06	1.249243E-15	2.405484E-15	1.048428E-15	99.994963	1.500000
0.55	1.732529E+16	64.166667	1.234286E-06	1.315162E-15	2.450029E-15	1.087259E-15	99.994804	1.500000
0.56	1.732526E+16	65.333333	1.234286E-06	1.383349E-15	2.494573E-15	1.126795E-15	99.994641	1.500000
0.57	1.732523E+16	66.500000	1.234286E-06	1.453842E-15	2.539118E-15	1.167037E-15	99.994474	1.500000
0.58	1.732520E+16	67.666667	1.234286E-06	1.526681E-15	2.583662E-15	1.207986E-15	99.994305	1.500000
0.59	1.732517E+16	68.833333	1.234286E-06	1.601902E-15	2.628207E-15	1.249640E-15	99.994132	1.500000
0.60	1.732514E+16	70.000000	1.234286E-06	1.679545E-15	2.672751E-15	1.292000E-15	99.993956	1.500000
0.61	1.732511E+16	71.166667	1.234286E-06	1.759647E-15	2.717295E-15	1.335066E-15	99.993776	1.500000
0.62	1.732508E+16	72.333333	1.234286E-06	1.842247E-15	2.761839E-15	1.378839E-15	99.993593	1.500000
0.63	1.732505E+16	73.500000	1.234286E-06	1.927382E-15	2.806383E-15	1.423317E-15	99.993407	1.500000
0.64	1.732502E+16	74.666667	1.234286E-06	2.015092E-15	2.850927E-15	1.468501E-15	99.993217	1.500000
0.65	1.732498E+16	75.833333	1.234286E-06	2.105414E-15	2.895471E-15	1.514391E-15	99.993023	1.500000
0.66	1.732495E+16	77.000000	1.234286E-06	2.198386E-15	2.940015E-15	1.560987E-15	99.992826	1.500000
0.67	1.732491E+16	78.166667	1.234286E-06	2.294047E-15	2.984558E-15	1.608289E-15	99.992625	1.500000
0.68	1.732488E+16	79.333333	1.234286E-06	2.392435E-15	3.029102E-15	1.656297E-15	99.992421	1.500000
0.69	1.732484E+16	80.500000	1.234286E-06	2.493588E-15	3.073645E-15	1.705011E-15	99.992212	1.500000
0.70	1.732481E+16	81.666667	1.234286E-06	2.597544E-15	3.118189E-15	1.754431E-15	99.992000	1.500000
0.71	1.732477E+16	82.833333	1.234286E-06	2.704342E-15	3.162732E-15	1.804557E-15	99.991785	1.500000
0.72	1.732473E+16	84.000000	1.234286E-06	2.814019E-15	3.207275E-15	1.855389E-15	99.991565	1.500000
0.73	1.732469E+16	85.166667	1.234286E-06	2.926614E-15	3.251818E-15	1.906927E-15	99.991342	1.500000
0.74	1.732465E+16	86.333333	1.234286E-06	3.042166E-15	3.296361E-15	1.959171E-15	99.991114	1.500000
0.75	1.732461E+16	87.500000	1.234286E-06	3.160711E-15	3.340904E-15	2.012120E-15	99.990883	1.500000
0.76	1.732457E+16	88.666667	1.234286E-06	3.282290E-15	3.385447E-15	2.065776E-15	99.990647	1.500000
0.77	1.732453E+16	89.833333	1.234286E-06	3.406938E-15	3.429989E-15	2.120138E-15	99.990408	1.500000
0.78	1.732449E+16	91.000000	1.234286E-06	3.534696E-15	3.474532E-15	2.175205E-15	99.990165	1.500000
0.79	1.732444E+16	92.166667	1.234286E-06	3.665601E-15	3.519074E-15	2.230979E-15	99.989917	1.500000
0.80	1.732440E+16	93.333333	1.234286E-06	3.799691E-15	3.563617E-15	2.287458E-15	99.989665	1.500000
0.81	1.732436E+16	94.500000	1.234286E-06	3.937005E-15	3.608159E-15	2.344644E-15	99.989409	1.500000
0.82	1.732431E+16	95.666667	1.234286E-06	4.077581E-15	3.652701E-15	2.402535E-15	99.989149	1.500000
0.83	1.732427E+16	96.833333	1.234286E-06	4.221456E-15	3.697243E-15	2.461133E-15	99.988884	1.500000
0.84	1.732422E+16	98.000000	1.234286E-06	4.368670E-15	3.741785E-15	2.520436E-15	99.988616	1.500000
0.85	1.732417E+16	99.166667	1.234286E-06	4.519260E-15	3.786326E-15	2.580445E-15	99.988342	1.500000
0.86	1.732412E+16	100.333333	1.234286E-06	4.673264E-15	3.830868E-15	2.641160E-15	99.988065	1.500000
0.87	1.732407E+16	101.500000	1.234286E-06	4.830721E-15	3.875410E-15	2.702581E-15	99.987783	1.500000
0.88	1.732402E+16	102.666667	1.234286E-06	4.991670E-15	3.919951E-15	2.764708E-15	99.987496	1.500000
0.89	1.732397E+16	103.833333	1.234286E-06	5.156147E-15	3.964492E-15	2.827541E-15	99.987205	1.500000
0.90	1.732392E+16	105.000000	1.234286E-06	5.324192E-15	4.009033E-15	2.891080E-15	99.986909	1.500000
0.91	1.732387E+16	106.166667	1.234286E-06	5.495842E-15	4.053574E-15	2.955325E-15	99.986609	1.500000
0.92	1.732382E+16	107.333333	1.234286E-06	5.671136E-15	4.098115E-15	3.020276E-15	99.986304	1.500000
0.93	1.732376E+16	108.500000	1.234286E-06	5.850112E-15	4.142656E-15	3.085932E-15	99.985994	1.500000
0.94	1.732371E+16	109.666667	1.234286E-06	6.032808E-15	4.187196E-15	3.152295E-15	99.985680	1.500000
0.95	1.732365E+16	110.833333	1.234286E-06	6.219262E-15	4.231737E-15	3.219364E-15	99.985361	1.500000
0.96	1.732360E+16	112.000000	1.234286E-06	6.409513E-15	4.276277E-15	3.287138E-15	99.985037	1.500000
0.97	1.732354E+16	113.166667	1.234286E-06	6.603599E-15	4.320817E-15	3.355618E-15	99.984708	1.500000
0.98	1.732348E+16	114.333333	1.234286E-06	6.801558E-15	4.365357E-15	3.424804E-15	99.984374	1.500000
0.99	1.732343E+16	115.500000	1.234286E-06	7.003428E-15	4.409897E-15	3.494697E-15	99.984035	1.500000
1.00	1.732337E+16	116.666667	1.234286E-06	7.209247E-15	4.454436E-15	3.565295E-15	99.983692	1.500000



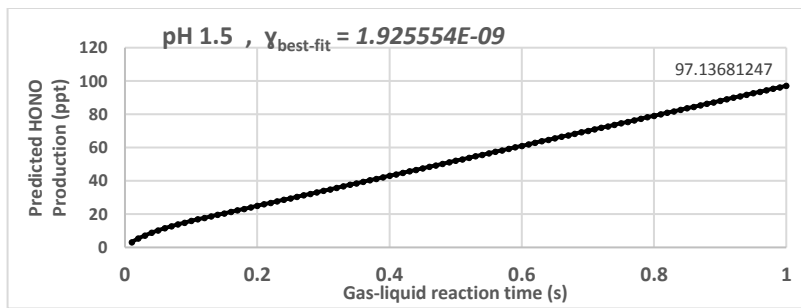
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732618E+16	1.166667	3.509922E-07	7.092544E-20	4.702595E-17	7.453111E-19	99.999949	1.500000
0.02	1.732617E+16	2.333333	4.963777E-07	3.130800E-19	9.405188E-17	2.235933E-18	99.999897	1.500000
0.03	1.732616E+16	3.500000	6.079357E-07	7.991584E-19	1.410778E-16	4.471865E-18	99.999843	1.500000
0.04	1.732615E+16	4.666667	7.019833E-07	1.589114E-18	1.881037E-16	7.453107E-18	99.999789	1.500000
0.05	1.732614E+16	5.833333	7.848407E-07	2.735152E-18	2.351295E-16	1.117966E-17	99.999733	1.500000
0.06	1.732614E+16	7.000000	8.597495E-07	4.284129E-18	2.821553E-16	1.565152E-17	99.999676	1.500000
0.07	1.732613E+16	8.166667	9.286350E-07	6.278920E-18	3.291811E-16	2.086869E-17	99.999618	1.500000
0.08	1.732611E+16	9.333333	9.927520E-07	8.759289E-18	3.762069E-16	2.683117E-17	99.999559	1.500000
0.09	1.732610E+16	10.500000	1.052972E-06	1.176248E-17	4.232326E-16	3.353895E-17	99.999498	1.500000
0.10	1.732609E+16	11.666667	1.109929E-06	1.532364E-17	4.702583E-16	4.099204E-17	99.999436	1.500000
0.11	1.732608E+16	12.833333	1.164103E-06	1.947616E-17	5.172840E-16	4.919044E-17	99.999373	1.500000
0.12	1.732607E+16	14.000000	1.215865E-06	2.425187E-17	5.643097E-16	5.813415E-17	99.999307	1.500000
0.13	1.732606E+16	15.166667	1.234286E-06	2.968775E-17	6.113353E-16	6.782316E-17	99.999241	1.500000
0.14	1.732605E+16	16.333333	1.234286E-06	3.582413E-17	6.583609E-16	7.825748E-17	99.999173	1.500000
0.15	1.732604E+16	17.500000	1.234286E-06	4.270137E-17	7.053864E-16	8.943710E-17	99.999103	1.500000
0.16	1.732602E+16	18.666667	1.234286E-06	5.035978E-17	7.524120E-16	1.013620E-16	99.999032	1.500000
0.17	1.732601E+16	19.833333	1.234286E-06	5.883972E-17	7.994374E-16	1.140323E-16	99.998959	1.500000
0.18	1.732600E+16	21.000000	1.234286E-06	6.818151E-17	8.464629E-16	1.274478E-16	99.998884	1.500000
0.19	1.732598E+16	22.166667	1.234286E-06	7.842550E-17	8.934883E-16	1.416086E-16	99.998808	1.500000
0.20	1.732597E+16	23.333333	1.234286E-06	8.961201E-17	9.405137E-16	1.565148E-16	99.998729	1.500000
0.21	1.732596E+16	24.500000	1.234286E-06	1.017814E-16	9.875390E-16	1.721662E-16	99.998649	1.500000
0.22	1.732594E+16	25.666667	1.234286E-06	1.149740E-16	1.034564E-15	1.885629E-16	99.998567	1.500000
0.23	1.732593E+16	26.833333	1.234286E-06	1.292301E-16	1.081590E-15	2.057050E-16	99.998483	1.500000
0.24	1.732591E+16	28.000000	1.234286E-06	1.445901E-16	1.128615E-15	2.235923E-16	99.998397	1.500000
0.25	1.732590E+16	29.166667	1.234286E-06	1.610944E-16	1.175640E-15	2.422250E-16	99.998309	1.500000
0.26	1.732588E+16	30.333333	1.234286E-06	1.787832E-16	1.222665E-15	2.616029E-16	99.998219	1.500000
0.27	1.732587E+16	31.500000	1.234286E-06	1.976968E-16	1.269690E-15	2.817261E-16	99.998127	1.500000
0.28	1.732585E+16	32.666667	1.234286E-06	2.178758E-16	1.316715E-15	3.025947E-16	99.998033	1.500000
0.29	1.732583E+16	33.833333	1.234286E-06	2.393602E-16	1.363740E-15	3.242085E-16	99.997936	1.500000
0.30	1.732582E+16	35.000000	1.234286E-06	2.621906E-16	1.410765E-15	3.465676E-16	99.997837	1.500000
0.31	1.732580E+16	36.166667	1.234286E-06	2.864072E-16	1.457790E-15	3.696720E-16	99.997736	1.500000
0.32	1.732578E+16	37.333333	1.234286E-06	3.120504E-16	1.504815E-15	3.935217E-16	99.997633	1.500000
0.33	1.732576E+16	38.500000	1.234286E-06	3.391605E-16	1.551840E-15	4.181167E-16	99.997527	1.500000
0.34	1.732574E+16	39.666667	1.234286E-06	3.677778E-16	1.598865E-15	4.434570E-16	99.997419	1.500000
0.35	1.732572E+16	40.833333	1.234286E-06	3.979427E-16	1.645889E-15	4.695426E-16	99.997308	1.500000
0.36	1.732571E+16	42.000000	1.234286E-06	4.296955E-16	1.692914E-15	4.963735E-16	99.997195	1.500000
0.37	1.732569E+16	43.166667	1.234286E-06	4.630766E-16	1.739939E-15	5.239497E-16	99.997080	1.500000
0.38	1.732566E+16	44.333333	1.234286E-06	4.981263E-16	1.786963E-15	5.522711E-16	99.996962	1.500000
0.39	1.732564E+16	45.500000	1.234286E-06	5.348849E-16	1.833988E-15	5.813379E-16	99.996841	1.500000
0.40	1.732562E+16	46.666667	1.234286E-06	5.733928E-16	1.881012E-15	6.111499E-16	99.996717	1.500000
0.41	1.732560E+16	47.833333	1.234286E-06	6.136902E-16	1.928036E-15	6.417072E-16	99.996591	1.500000
0.42	1.732558E+16	49.000000	1.234286E-06	6.558176E-16	1.975061E-15	6.730098E-16	99.996462	1.500000
0.43	1.732556E+16	50.166667	1.234286E-06	6.998153E-16	2.022085E-15	7.050577E-16	99.996330	1.500000
0.44	1.732553E+16	51.333333	1.234286E-06	7.457235E-16	2.069109E-15	7.378509E-16	99.996196	1.500000
0.45	1.732551E+16	52.500000	1.234286E-06	7.935827E-16	2.116133E-15	7.713893E-16	99.996058	1.500000

0.46	1.732548E+16	53.666667	1.234286E-06	8.434332E-16	2.163157E-15	8.056730E-16	99.995918	1.500000
0.47	1.732546E+16	54.833333	1.234286E-06	8.953153E-16	2.210181E-15	8.407021E-16	99.995774	1.500000
0.48	1.732543E+16	56.000000	1.234286E-06	9.492693E-16	2.257205E-15	8.764764E-16	99.995628	1.500000
0.49	1.732541E+16	57.166667	1.234286E-06	1.005336E-15	2.304229E-15	9.129959E-16	99.995478	1.500000
0.50	1.732538E+16	58.333333	1.234286E-06	1.063555E-15	2.351253E-15	9.502608E-16	99.995326	1.500000
0.51	1.732535E+16	59.500000	1.234286E-06	1.123966E-15	2.398277E-15	9.882709E-16	99.995170	1.500000
0.52	1.732533E+16	60.666667	1.234286E-06	1.186612E-15	2.445300E-15	1.027026E-15	99.995011	1.500000
0.53	1.732530E+16	61.833333	1.234286E-06	1.251530E-15	2.492324E-15	1.066527E-15	99.994849	1.500000
0.54	1.732527E+16	63.000000	1.234286E-06	1.318763E-15	2.539347E-15	1.106773E-15	99.994683	1.500000
0.55	1.732524E+16	64.166667	1.234286E-06	1.388350E-15	2.586371E-15	1.147764E-15	99.994514	1.500000
0.56	1.732521E+16	65.333333	1.234286E-06	1.460332E-15	2.633394E-15	1.189501E-15	99.994342	1.500000
0.57	1.732518E+16	66.500000	1.234286E-06	1.534748E-15	2.680417E-15	1.231982E-15	99.994167	1.500000
0.58	1.732515E+16	67.666667	1.234286E-06	1.611640E-15	2.727440E-15	1.275209E-15	99.993988	1.500000
0.59	1.732512E+16	68.833333	1.234286E-06	1.691047E-15	2.774463E-15	1.319182E-15	99.993805	1.500000
0.60	1.732509E+16	70.000000	1.234286E-06	1.773011E-15	2.821486E-15	1.363899E-15	99.993619	1.500000
0.61	1.732505E+16	71.166667	1.234286E-06	1.857571E-15	2.868509E-15	1.409362E-15	99.993430	1.500000
0.62	1.732502E+16	72.333333	1.234286E-06	1.944767E-15	2.915532E-15	1.455570E-15	99.993236	1.500000
0.63	1.732499E+16	73.500000	1.234286E-06	2.034640E-15	2.962555E-15	1.502523E-15	99.993040	1.500000
0.64	1.732495E+16	74.666667	1.234286E-06	2.127231E-15	3.009577E-15	1.550222E-15	99.992839	1.500000
0.65	1.732492E+16	75.833333	1.234286E-06	2.222579E-15	3.056600E-15	1.598666E-15	99.992635	1.500000
0.66	1.732488E+16	77.000000	1.234286E-06	2.320725E-15	3.103622E-15	1.647855E-15	99.992427	1.500000
0.67	1.732484E+16	78.166667	1.234286E-06	2.421709E-15	3.150645E-15	1.697789E-15	99.992215	1.500000
0.68	1.732480E+16	79.333333	1.234286E-06	2.525572E-15	3.197667E-15	1.748469E-15	99.991999	1.500000
0.69	1.732477E+16	80.500000	1.234286E-06	2.632354E-15	3.244689E-15	1.799894E-15	99.991779	1.500000
0.70	1.732473E+16	81.666667	1.234286E-06	2.742095E-15	3.291711E-15	1.852064E-15	99.991555	1.500000
0.71	1.732469E+16	82.833333	1.234286E-06	2.854836E-15	3.338733E-15	1.904979E-15	99.991327	1.500000
0.72	1.732465E+16	84.000000	1.234286E-06	2.970617E-15	3.385755E-15	1.958640E-15	99.991096	1.500000
0.73	1.732461E+16	85.166667	1.234286E-06	3.089478E-15	3.432776E-15	2.013046E-15	99.990860	1.500000
0.74	1.732457E+16	86.333333	1.234286E-06	3.211460E-15	3.479798E-15	2.068197E-15	99.990620	1.500000
0.75	1.732452E+16	87.500000	1.234286E-06	3.336602E-15	3.526819E-15	2.124093E-15	99.990375	1.500000
0.76	1.732448E+16	88.666667	1.234286E-06	3.464946E-15	3.573841E-15	2.180734E-15	99.990127	1.500000
0.77	1.732444E+16	89.833333	1.234286E-06	3.596531E-15	3.620862E-15	2.238121E-15	99.989874	1.500000
0.78	1.732439E+16	91.000000	1.234286E-06	3.731399E-15	3.667883E-15	2.296253E-15	99.989617	1.500000
0.79	1.732435E+16	92.166667	1.234286E-06	3.869588E-15	3.714904E-15	2.355131E-15	99.989356	1.500000
0.80	1.732430E+16	93.333333	1.234286E-06	4.011140E-15	3.761925E-15	2.414753E-15	99.989090	1.500000
0.81	1.732425E+16	94.500000	1.234286E-06	4.156095E-15	3.808945E-15	2.475121E-15	99.988820	1.500000
0.82	1.732421E+16	95.666667	1.234286E-06	4.304494E-15	3.855966E-15	2.536234E-15	99.988545	1.500000
0.83	1.732416E+16	96.833333	1.234286E-06	4.456376E-15	3.902986E-15	2.598092E-15	99.988266	1.500000
0.84	1.732411E+16	98.000000	1.234286E-06	4.611781E-15	3.950007E-15	2.660695E-15	99.987982	1.500000
0.85	1.732406E+16	99.166667	1.234286E-06	4.770751E-15	3.997027E-15	2.724044E-15	99.987694	1.500000
0.86	1.732401E+16	100.333333	1.234286E-06	4.933326E-15	4.044047E-15	2.788138E-15	99.987401	1.500000
0.87	1.732396E+16	101.500000	1.234286E-06	5.099545E-15	4.091067E-15	2.852977E-15	99.987103	1.500000
0.88	1.732390E+16	102.666667	1.234286E-06	5.269450E-15	4.138087E-15	2.918561E-15	99.986800	1.500000
0.89	1.732385E+16	103.833333	1.234286E-06	5.443080E-15	4.185106E-15	2.984890E-15	99.986493	1.500000
0.90	1.732380E+16	105.000000	1.234286E-06	5.620476E-15	4.232126E-15	3.051965E-15	99.986181	1.500000
0.91	1.732374E+16	106.166667	1.234286E-06	5.801678E-15	4.279145E-15	3.119785E-15	99.985864	1.500000
0.92	1.732369E+16	107.333333	1.234286E-06	5.986727E-15	4.326164E-15	3.188350E-15	99.985542	1.500000
0.93	1.732363E+16	108.500000	1.234286E-06	6.175662E-15	4.373183E-15	3.257660E-15	99.985215	1.500000
0.94	1.732357E+16	109.666667	1.234286E-06	6.368525E-15	4.420202E-15	3.327716E-15	99.984883	1.500000
0.95	1.732351E+16	110.833333	1.234286E-06	6.565355E-15	4.467221E-15	3.398516E-15	99.984546	1.500000
0.96	1.732345E+16	112.000000	1.234286E-06	6.766193E-15	4.514239E-15	3.470062E-15	99.984204	1.500000
0.97	1.732339E+16	113.166667	1.234286E-06	6.971079E-15	4.561258E-15	3.542353E-15	99.983857	1.500000
0.98	1.732333E+16	114.333333	1.234286E-06	7.180054E-15	4.608276E-15	3.615390E-15	99.983505	1.500000
0.99	1.732327E+16	115.500000	1.234286E-06	7.393157E-15	4.655294E-15	3.689171E-15	99.983147	1.500000
1.00	1.732321E+16	116.666667	1.234286E-06	7.610429E-15	4.702312E-15	3.763698E-15	99.982784	1.500000



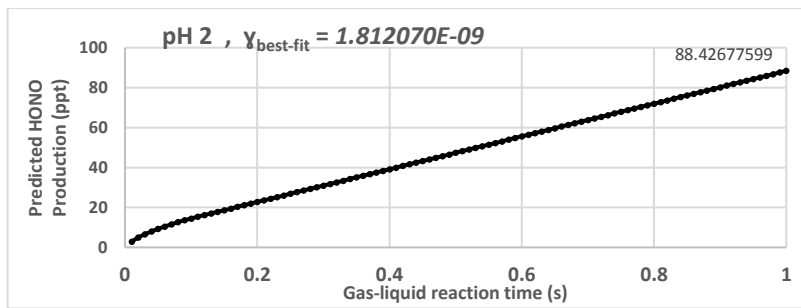
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732618E+16	1.166667	3.509922E-07	8.469366E-20	5.615474E-17	8.899927E-19	99.999939	1.500000
0.02	1.732617E+16	2.333333	4.963776E-07	3.738559E-19	1.123094E-16	2.669978E-18	99.999876	1.500000
0.03	1.732616E+16	3.500000	6.079355E-07	9.542930E-19	1.684641E-16	5.339954E-18	99.999813	1.500000
0.04	1.732615E+16	4.666667	7.019830E-07	1.897596E-18	2.246188E-16	8.899921E-18	99.999748	1.500000
0.05	1.732614E+16	5.833333	7.848403E-07	3.266107E-18	2.807734E-16	1.334988E-17	99.999682	1.500000
0.06	1.732612E+16	7.000000	8.597489E-07	5.115775E-18	3.369279E-16	1.868983E-17	99.999614	1.500000
0.07	1.732611E+16	8.166667	9.286343E-07	7.497800E-18	3.930824E-16	2.491976E-17	99.999544	1.500000
0.08	1.732610E+16	9.333333	9.927512E-07	1.045966E-17	4.492369E-16	3.203969E-17	99.999473	1.500000
0.09	1.732609E+16	10.500000	1.052971E-06	1.404584E-17	5.053914E-16	4.004960E-17	99.999401	1.500000
0.10	1.732607E+16	11.666667	1.109928E-06	1.829831E-17	5.615458E-16	4.894950E-17	99.999327	1.500000
0.11	1.732606E+16	12.833333	1.164101E-06	2.325692E-17	6.177001E-16	5.873939E-17	99.999251	1.500000
0.12	1.732605E+16	14.000000	1.215863E-06	2.895970E-17	6.738544E-16	6.941926E-17	99.999173	1.500000
0.13	1.732603E+16	15.166667	1.234286E-06	3.545081E-17	7.300087E-16	8.098912E-17	99.999094	1.500000
0.14	1.732602E+16	16.333333	1.234286E-06	4.277840E-17	7.861629E-16	9.344896E-17	99.999012	1.500000
0.15	1.732601E+16	17.500000	1.234286E-06	5.099066E-17	8.423171E-16	1.067988E-16	99.998929	1.500000
0.16	1.732599E+16	18.666667	1.234286E-06	6.013574E-17	8.984712E-16	1.210386E-16	99.998844	1.500000
0.17	1.732598E+16	19.833333	1.234286E-06	7.026182E-17	9.546253E-16	1.361684E-16	99.998757	1.500000
0.18	1.732596E+16	21.000000	1.234286E-06	8.141706E-17	1.010779E-15	1.521882E-16	99.998667	1.500000
0.19	1.732594E+16	22.166667	1.234286E-06	9.364963E-17	1.066933E-15	1.690979E-16	99.998576	1.500000
0.20	1.732593E+16	23.333333	1.234286E-06	1.070077E-16	1.123087E-15	1.868976E-16	99.998483	1.500000
0.21	1.732591E+16	24.500000	1.234286E-06	1.215394E-16	1.179241E-15	2.055874E-16	99.998387	1.500000
0.22	1.732589E+16	25.666667	1.234286E-06	1.372930E-16	1.235395E-15	2.251670E-16	99.998289	1.500000
0.23	1.732588E+16	26.833333	1.234286E-06	1.543166E-16	1.291549E-15	2.456367E-16	99.998189	1.500000
0.24	1.732586E+16	28.000000	1.234286E-06	1.726583E-16	1.347702E-15	2.669964E-16	99.998086	1.500000
0.25	1.732584E+16	29.166667	1.234286E-06	1.923663E-16	1.403856E-15	2.892460E-16	99.997981	1.500000
0.26	1.732582E+16	30.333333	1.234286E-06	2.134889E-16	1.460010E-15	3.123856E-16	99.997873	1.500000
0.27	1.732580E+16	31.500000	1.234286E-06	2.360741E-16	1.516163E-15	3.364151E-16	99.997763	1.500000
0.28	1.732578E+16	32.666667	1.234286E-06	2.601702E-16	1.572317E-15	3.613347E-16	99.997651	1.500000
0.29	1.732576E+16	33.833333	1.234286E-06	2.858252E-16	1.628470E-15	3.871442E-16	99.997535	1.500000
0.30	1.732574E+16	35.000000	1.234286E-06	3.130875E-16	1.684623E-15	4.138437E-16	99.997418	1.500000
0.31	1.732572E+16	36.166667	1.234286E-06	3.420050E-16	1.740777E-15	4.414331E-16	99.997297	1.500000
0.32	1.732570E+16	37.333333	1.234286E-06	3.726261E-16	1.796930E-15	4.699125E-16	99.997173	1.500000
0.33	1.732568E+16	38.500000	1.234286E-06	4.049988E-16	1.853083E-15	4.992819E-16	99.997047	1.500000
0.34	1.732566E+16	39.666667	1.234286E-06	4.391713E-16	1.909236E-15	5.295413E-16	99.996918	1.500000
0.35	1.732563E+16	40.833333	1.234286E-06	4.751919E-16	1.965389E-15	5.606906E-16	99.996786	1.500000
0.36	1.732561E+16	42.000000	1.234286E-06	5.131086E-16	2.021542E-15	5.927299E-16	99.996651	1.500000
0.37	1.732559E+16	43.166667	1.234286E-06	5.529696E-16	2.077695E-15	6.256591E-16	99.996513	1.500000
0.38	1.732556E+16	44.333333	1.234286E-06	5.948231E-16	2.133847E-15	6.594783E-16	99.996372	1.500000
0.39	1.732554E+16	45.500000	1.234286E-06	6.387173E-16	2.190000E-15	6.941875E-16	99.996227	1.500000
0.40	1.732551E+16	46.666667	1.234286E-06	6.847003E-16	2.246153E-15	7.297866E-16	99.996080	1.500000
0.41	1.732549E+16	47.833333	1.234286E-06	7.328203E-16	2.302305E-15	7.662756E-16	99.995929	1.500000
0.42	1.732546E+16	49.000000	1.234286E-06	7.831254E-16	2.358457E-15	8.036547E-16	99.995775	1.500000
0.43	1.732543E+16	50.166667	1.234286E-06	8.356639E-16	2.414610E-15	8.419237E-16	99.995618	1.500000
0.44	1.732540E+16	51.333333	1.234286E-06	8.904839E-16	2.470762E-15	8.810826E-16	99.995457	1.500000
0.45	1.732538E+16	52.500000	1.234286E-06	9.476335E-16	2.526914E-15	9.211315E-16	99.995293	1.500000

0.46	1.732535E+16	53.666667	1.234286E-06	1.007161E-15	2.583066E-15	9.620703E-16	99.995125	1.500000
0.47	1.732532E+16	54.833333	1.234286E-06	1.069114E-15	2.639218E-15	1.003899E-15	99.994954	1.500000
0.48	1.732529E+16	56.000000	1.234286E-06	1.133542E-15	2.695370E-15	1.046618E-15	99.994779	1.500000
0.49	1.732526E+16	57.166667	1.234286E-06	1.200492E-15	2.751522E-15	1.090227E-15	99.994600	1.500000
0.50	1.732522E+16	58.333333	1.234286E-06	1.270012E-15	2.807673E-15	1.134725E-15	99.994418	1.500000
0.51	1.732519E+16	59.500000	1.234286E-06	1.342151E-15	2.863825E-15	1.180114E-15	99.994232	1.500000
0.52	1.732516E+16	60.666667	1.234286E-06	1.416957E-15	2.919976E-15	1.226392E-15	99.994042	1.500000
0.53	1.732513E+16	61.833333	1.234286E-06	1.494477E-15	2.976128E-15	1.273561E-15	99.993849	1.500000
0.54	1.732509E+16	63.000000	1.234286E-06	1.574761E-15	3.032279E-15	1.321619E-15	99.993651	1.500000
0.55	1.732506E+16	64.166667	1.234286E-06	1.657856E-15	3.088430E-15	1.370567E-15	99.993450	1.500000
0.56	1.732502E+16	65.333333	1.234286E-06	1.743811E-15	3.144581E-15	1.420406E-15	99.993244	1.500000
0.57	1.732498E+16	66.500000	1.234286E-06	1.832673E-15	3.200732E-15	1.471134E-15	99.993034	1.500000
0.58	1.732495E+16	67.666667	1.234286E-06	1.924491E-15	3.256883E-15	1.522752E-15	99.992821	1.500000
0.59	1.732491E+16	68.833333	1.234286E-06	2.019313E-15	3.313033E-15	1.575260E-15	99.992603	1.500000
0.60	1.732487E+16	70.000000	1.234286E-06	2.117186E-15	3.369184E-15	1.628658E-15	99.992381	1.500000
0.61	1.732483E+16	71.166667	1.234286E-06	2.218161E-15	3.425334E-15	1.682946E-15	99.992154	1.500000
0.62	1.732479E+16	72.333333	1.234286E-06	2.322283E-15	3.481484E-15	1.738124E-15	99.991924	1.500000
0.63	1.732475E+16	73.500000	1.234286E-06	2.429602E-15	3.537634E-15	1.794191E-15	99.991688	1.500000
0.64	1.732471E+16	74.666667	1.234286E-06	2.540166E-15	3.593784E-15	1.851149E-15	99.991449	1.500000
0.65	1.732467E+16	75.833333	1.234286E-06	2.654023E-15	3.649934E-15	1.908996E-15	99.991205	1.500000
0.66	1.732462E+16	77.000000	1.234286E-06	2.771221E-15	3.706084E-15	1.967734E-15	99.990956	1.500000
0.67	1.732458E+16	78.166667	1.234286E-06	2.891808E-15	3.762233E-15	2.027361E-15	99.990703	1.500000
0.68	1.732454E+16	79.333333	1.234286E-06	3.015833E-15	3.818383E-15	2.087879E-15	99.990446	1.500000
0.69	1.732449E+16	80.500000	1.234286E-06	3.143343E-15	3.874532E-15	2.149286E-15	99.990183	1.500000
0.70	1.732444E+16	81.666667	1.234286E-06	3.274386E-15	3.930681E-15	2.211583E-15	99.989916	1.500000
0.71	1.732440E+16	82.833333	1.234286E-06	3.409012E-15	3.986830E-15	2.274770E-15	99.989644	1.500000
0.72	1.732435E+16	84.000000	1.234286E-06	3.547268E-15	4.042979E-15	2.338847E-15	99.989367	1.500000
0.73	1.732430E+16	85.166667	1.234286E-06	3.689201E-15	4.099128E-15	2.403814E-15	99.989085	1.500000
0.74	1.732425E+16	86.333333	1.234286E-06	3.834861E-15	4.155276E-15	2.469670E-15	99.988799	1.500000
0.75	1.732420E+16	87.500000	1.234286E-06	3.984296E-15	4.211424E-15	2.536417E-15	99.988507	1.500000
0.76	1.732415E+16	88.666667	1.234286E-06	4.137553E-15	4.267573E-15	2.604053E-15	99.988211	1.500000
0.77	1.732410E+16	89.833333	1.234286E-06	4.294681E-15	4.323721E-15	2.672580E-15	99.987909	1.500000
0.78	1.732404E+16	91.000000	1.234286E-06	4.455728E-15	4.379868E-15	2.741996E-15	99.987602	1.500000
0.79	1.732399E+16	92.166667	1.234286E-06	4.620742E-15	4.436016E-15	2.812302E-15	99.987290	1.500000
0.80	1.732393E+16	93.333333	1.234286E-06	4.789772E-15	4.492164E-15	2.883498E-15	99.986972	1.500000
0.81	1.732388E+16	94.500000	1.234286E-06	4.962865E-15	4.548311E-15	2.955584E-15	99.986650	1.500000
0.82	1.732382E+16	95.666667	1.234286E-06	5.140069E-15	4.604458E-15	3.028560E-15	99.986322	1.500000
0.83	1.732376E+16	96.833333	1.234286E-06	5.321433E-15	4.660605E-15	3.102425E-15	99.985988	1.500000
0.84	1.732370E+16	98.000000	1.234286E-06	5.507005E-15	4.716752E-15	3.177181E-15	99.985649	1.500000
0.85	1.732365E+16	99.166667	1.234286E-06	5.696833E-15	4.772898E-15	3.252826E-15	99.985305	1.500000
0.86	1.732358E+16	100.333333	1.234286E-06	5.890966E-15	4.829044E-15	3.329361E-15	99.984955	1.500000
0.87	1.732352E+16	101.500000	1.234286E-06	6.089450E-15	4.885191E-15	3.406786E-15	99.984599	1.500000
0.88	1.732346E+16	102.666667	1.234286E-06	6.292335E-15	4.941336E-15	3.485101E-15	99.984238	1.500000
0.89	1.732340E+16	103.833333	1.234286E-06	6.499669E-15	4.997482E-15	3.564306E-15	99.983871	1.500000
0.90	1.732333E+16	105.000000	1.234286E-06	6.711500E-15	5.053628E-15	3.644400E-15	99.983498	1.500000
0.91	1.732327E+16	106.166667	1.234286E-06	6.927876E-15	5.109773E-15	3.725385E-15	99.983120	1.500000
0.92	1.732320E+16	107.333333	1.234286E-06	7.148844E-15	5.165918E-15	3.807259E-15	99.982735	1.500000
0.93	1.732313E+16	108.500000	1.234286E-06	7.374454E-15	5.222063E-15	3.890023E-15	99.982345	1.500000
0.94	1.732306E+16	109.666667	1.234286E-06	7.604754E-15	5.278208E-15	3.973677E-15	99.981949	1.500000
0.95	1.732299E+16	110.833333	1.234286E-06	7.839791E-15	5.334352E-15	4.058221E-15	99.981546	1.500000
0.96	1.732292E+16	112.000000	1.234286E-06	8.079614E-15	5.390496E-15	4.143655E-15	99.981138	1.500000
0.97	1.732285E+16	113.166667	1.234286E-06	8.324270E-15	5.446640E-15	4.229978E-15	99.980723	1.500000
0.98	1.732278E+16	114.333333	1.234286E-06	8.573809E-15	5.502784E-15	4.317191E-15	99.980303	1.500000
0.99	1.732270E+16	115.500000	1.234286E-06	8.828278E-15	5.558927E-15	4.405294E-15	99.979876	1.500000
1.00	1.732263E+16	116.666667	1.234286E-06	9.087725E-15	5.615071E-15	4.494287E-15	99.979442	1.500000



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO2}}$ (mol)	$\Phi_{\text{NO2}}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732618E+16	1.166667	3.509922E-07	8.225135E-20	5.453541E-17	8.643280E-19	99.999941	1.500000
0.02	1.732617E+16	2.333333	4.963776E-07	3.630750E-19	1.090708E-16	2.592983E-18	99.999880	1.500000
0.03	1.732616E+16	3.500000	6.079355E-07	9.267741E-19	1.636061E-16	5.185966E-18	99.999818	1.500000
0.04	1.732615E+16	4.666667	7.019830E-07	1.842875E-18	2.181414E-16	8.643274E-18	99.999755	1.500000
0.05	1.732614E+16	5.833333	7.848404E-07	3.171922E-18	2.726767E-16	1.296491E-17	99.999691	1.500000
0.06	1.732613E+16	7.000000	8.597490E-07	4.968251E-18	3.272119E-16	1.815087E-17	99.999625	1.500000
0.07	1.732611E+16	8.166667	9.286345E-07	7.281586E-18	3.817471E-16	2.420115E-17	99.999557	1.500000
0.08	1.732610E+16	9.333333	9.927513E-07	1.015804E-17	4.362823E-16	3.111576E-17	99.999489	1.500000
0.09	1.732609E+16	10.500000	1.052971E-06	1.364080E-17	4.908174E-16	3.889469E-17	99.999418	1.500000
0.10	1.732608E+16	11.666667	1.109928E-06	1.777064E-17	5.453525E-16	4.753795E-17	99.999346	1.500000
0.11	1.732607E+16	12.833333	1.164102E-06	2.258626E-17	5.998876E-16	5.704553E-17	99.999272	1.500000
0.12	1.732605E+16	14.000000	1.215864E-06	2.812459E-17	6.544226E-16	6.741742E-17	99.999197	1.500000
0.13	1.732604E+16	15.166667	1.234286E-06	3.442851E-17	7.089575E-16	7.865364E-17	99.999120	1.500000
0.14	1.732602E+16	16.333333	1.234286E-06	4.154480E-17	7.634924E-16	9.075418E-17	99.999041	1.500000
0.15	1.732601E+16	17.500000	1.234286E-06	4.952024E-17	8.180273E-16	1.037190E-16	99.998960	1.500000
0.16	1.732600E+16	18.666667	1.234286E-06	5.840161E-17	8.725621E-16	1.175482E-16	99.998877	1.500000
0.17	1.732598E+16	19.833333	1.234286E-06	6.823568E-17	9.270969E-16	1.322417E-16	99.998793	1.500000
0.18	1.732597E+16	21.000000	1.234286E-06	7.906924E-17	9.816317E-16	1.477995E-16	99.998706	1.500000
0.19	1.732595E+16	22.166667	1.234286E-06	9.094906E-17	1.036166E-15	1.642217E-16	99.998617	1.500000
0.20	1.732594E+16	23.333333	1.234286E-06	1.039219E-16	1.090701E-15	1.815081E-16	99.998526	1.500000
0.21	1.732592E+16	24.500000	1.234286E-06	1.180346E-16	1.145236E-15	1.996589E-16	99.998433	1.500000
0.22	1.732590E+16	25.666667	1.234286E-06	1.333339E-16	1.199770E-15	2.186739E-16	99.998338	1.500000
0.23	1.732589E+16	26.833333	1.234286E-06	1.498665E-16	1.254305E-15	2.385533E-16	99.998241	1.500000
0.24	1.732587E+16	28.000000	1.234286E-06	1.676793E-16	1.308839E-15	2.592970E-16	99.998141	1.500000
0.25	1.732585E+16	29.166667	1.234286E-06	1.868191E-16	1.363373E-15	2.809050E-16	99.998039	1.500000
0.26	1.732583E+16	30.333333	1.234286E-06	2.073325E-16	1.417908E-15	3.033774E-16	99.997935	1.500000
0.27	1.732581E+16	31.500000	1.234286E-06	2.292665E-16	1.472442E-15	3.267140E-16	99.997828	1.500000
0.28	1.732580E+16	32.666667	1.234286E-06	2.526677E-16	1.526976E-15	3.509149E-16	99.997718	1.500000
0.29	1.732578E+16	33.833333	1.234286E-06	2.775829E-16	1.581510E-15	3.759802E-16	99.997607	1.500000
0.30	1.732576E+16	35.000000	1.234286E-06	3.040590E-16	1.636044E-15	4.019097E-16	99.997492	1.500000
0.31	1.732574E+16	36.166667	1.234286E-06	3.321427E-16	1.690578E-15	4.287036E-16	99.997375	1.500000
0.32	1.732572E+16	37.333333	1.234286E-06	3.618807E-16	1.745112E-15	4.563618E-16	99.997255	1.500000
0.33	1.732569E+16	38.500000	1.234286E-06	3.933199E-16	1.799646E-15	4.848842E-16	99.997132	1.500000
0.34	1.732567E+16	39.666667	1.234286E-06	4.265070E-16	1.854180E-15	5.142710E-16	99.997007	1.500000
0.35	1.732565E+16	40.833333	1.234286E-06	4.614888E-16	1.908714E-15	5.445221E-16	99.996879	1.500000
0.36	1.732563E+16	42.000000	1.234286E-06	4.983121E-16	1.963247E-15	5.756375E-16	99.996748	1.500000
0.37	1.732560E+16	43.166667	1.234286E-06	5.370237E-16	2.017781E-15	6.076171E-16	99.996613	1.500000
0.38	1.732558E+16	44.333333	1.234286E-06	5.776703E-16	2.072315E-15	6.404611E-16	99.996476	1.500000
0.39	1.732556E+16	45.500000	1.234286E-06	6.202987E-16	2.126848E-15	6.741694E-16	99.996336	1.500000
0.40	1.732553E+16	46.666667	1.234286E-06	6.649558E-16	2.181381E-15	7.087419E-16	99.996193	1.500000
0.41	1.732551E+16	47.833333	1.234286E-06	7.116881E-16	2.235915E-15	7.441788E-16	99.996047	1.500000
0.42	1.732548E+16	49.000000	1.234286E-06	7.605426E-16	2.290448E-15	7.804799E-16	99.995897	1.500000
0.43	1.732545E+16	50.166667	1.234286E-06	8.115661E-16	2.344981E-15	8.176454E-16	99.995744	1.500000
0.44	1.732543E+16	51.333333	1.234286E-06	8.648052E-16	2.399514E-15	8.556751E-16	99.995588	1.500000
0.45	1.732540E+16	52.500000	1.234286E-06	9.203068E-16	2.454047E-15	8.945691E-16	99.995429	1.500000

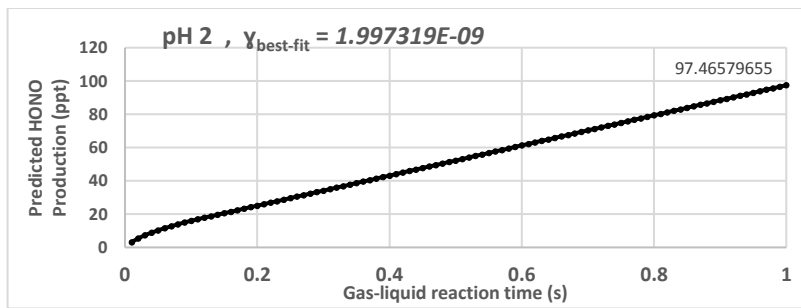
0.46	1.732537E+16	53.666667	1.234286E-06	9.781177E-16	2.508580E-15	9.343274E-16	99.995266	1.500000
0.47	1.732534E+16	54.833333	1.234286E-06	1.038285E-15	2.563113E-15	9.749500E-16	99.995099	1.500000
0.48	1.732531E+16	56.000000	1.234286E-06	1.100854E-15	2.617645E-15	1.016437E-15	99.994929	1.500000
0.49	1.732528E+16	57.166667	1.234286E-06	1.165873E-15	2.672178E-15	1.058788E-15	99.994756	1.500000
0.50	1.732525E+16	58.333333	1.234286E-06	1.233389E-15	2.726710E-15	1.102004E-15	99.994579	1.500000
0.51	1.732522E+16	59.500000	1.234286E-06	1.303448E-15	2.781243E-15	1.146083E-15	99.994398	1.500000
0.52	1.732519E+16	60.666667	1.234286E-06	1.376096E-15	2.835775E-15	1.191027E-15	99.994214	1.500000
0.53	1.732516E+16	61.833333	1.234286E-06	1.451382E-15	2.890307E-15	1.236836E-15	99.994026	1.500000
0.54	1.732512E+16	63.000000	1.234286E-06	1.529350E-15	2.944839E-15	1.283508E-15	99.993834	1.500000
0.55	1.732509E+16	64.166667	1.234286E-06	1.610049E-15	2.999371E-15	1.331045E-15	99.993638	1.500000
0.56	1.732505E+16	65.333333	1.234286E-06	1.693525E-15	3.053903E-15	1.379446E-15	99.993439	1.500000
0.57	1.732502E+16	66.500000	1.234286E-06	1.779825E-15	3.108435E-15	1.428711E-15	99.993235	1.500000
0.58	1.732498E+16	67.666667	1.234286E-06	1.868995E-15	3.162966E-15	1.478841E-15	99.993028	1.500000
0.59	1.732495E+16	68.833333	1.234286E-06	1.961083E-15	3.217498E-15	1.529835E-15	99.992816	1.500000
0.60	1.732491E+16	70.000000	1.234286E-06	2.056134E-15	3.272029E-15	1.581693E-15	99.992600	1.500000
0.61	1.732487E+16	71.166667	1.234286E-06	2.154197E-15	3.326561E-15	1.634416E-15	99.992381	1.500000
0.62	1.732483E+16	72.333333	1.234286E-06	2.255317E-15	3.381092E-15	1.688002E-15	99.992156	1.500000
0.63	1.732479E+16	73.500000	1.234286E-06	2.359541E-15	3.435623E-15	1.742453E-15	99.991928	1.500000
0.64	1.732475E+16	74.666667	1.234286E-06	2.466917E-15	3.490154E-15	1.797768E-15	99.991696	1.500000
0.65	1.732471E+16	75.833333	1.234286E-06	2.577491E-15	3.544685E-15	1.853948E-15	99.991459	1.500000
0.66	1.732467E+16	77.000000	1.234286E-06	2.691309E-15	3.599215E-15	1.910992E-15	99.991217	1.500000
0.67	1.732463E+16	78.166667	1.234286E-06	2.808419E-15	3.653746E-15	1.968900E-15	99.990971	1.500000
0.68	1.732458E+16	79.333333	1.234286E-06	2.928867E-15	3.708276E-15	2.027672E-15	99.990721	1.500000
0.69	1.732454E+16	80.500000	1.234286E-06	3.052700E-15	3.762806E-15	2.087308E-15	99.990466	1.500000
0.70	1.732449E+16	81.666667	1.234286E-06	3.179965E-15	3.817336E-15	2.147809E-15	99.990207	1.500000
0.71	1.732445E+16	82.833333	1.234286E-06	3.310708E-15	3.871866E-15	2.209174E-15	99.989943	1.500000
0.72	1.732440E+16	84.000000	1.234286E-06	3.444977E-15	3.926396E-15	2.271403E-15	99.989674	1.500000
0.73	1.732435E+16	85.166667	1.234286E-06	3.582818E-15	3.980926E-15	2.334496E-15	99.989400	1.500000
0.74	1.732431E+16	86.333333	1.234286E-06	3.724278E-15	4.035455E-15	2.398454E-15	99.989122	1.500000
0.75	1.732426E+16	87.500000	1.234286E-06	3.869404E-15	4.089985E-15	2.463276E-15	99.988839	1.500000
0.76	1.732421E+16	88.666667	1.234286E-06	4.018242E-15	4.144514E-15	2.528962E-15	99.988550	1.500000
0.77	1.732416E+16	89.833333	1.234286E-06	4.170839E-15	4.199043E-15	2.595512E-15	99.988257	1.500000
0.78	1.732410E+16	91.000000	1.234286E-06	4.327242E-15	4.253572E-15	2.662927E-15	99.987959	1.500000
0.79	1.732405E+16	92.166667	1.234286E-06	4.487498E-15	4.308101E-15	2.731206E-15	99.987656	1.500000
0.80	1.732400E+16	93.333333	1.234286E-06	4.651653E-15	4.362629E-15	2.800349E-15	99.987348	1.500000
0.81	1.732394E+16	94.500000	1.234286E-06	4.819754E-15	4.417157E-15	2.870356E-15	99.987035	1.500000
0.82	1.732389E+16	95.666667	1.234286E-06	4.991849E-15	4.471686E-15	2.941227E-15	99.986716	1.500000
0.83	1.732383E+16	96.833333	1.234286E-06	5.167983E-15	4.526214E-15	3.012963E-15	99.986392	1.500000
0.84	1.732378E+16	98.000000	1.234286E-06	5.348204E-15	4.580742E-15	3.085563E-15	99.986063	1.500000
0.85	1.732372E+16	99.166667	1.234286E-06	5.532559E-15	4.635269E-15	3.159027E-15	99.985729	1.500000
0.86	1.732366E+16	100.333333	1.234286E-06	5.721093E-15	4.689797E-15	3.233355E-15	99.985389	1.500000
0.87	1.732360E+16	101.500000	1.234286E-06	5.913854E-15	4.744324E-15	3.308548E-15	99.985043	1.500000
0.88	1.732354E+16	102.666667	1.234286E-06	6.110889E-15	4.798851E-15	3.384604E-15	99.984693	1.500000
0.89	1.732348E+16	103.833333	1.234286E-06	6.312244E-15	4.853378E-15	3.461525E-15	99.984336	1.500000
0.90	1.732341E+16	105.000000	1.234286E-06	6.517967E-15	4.907905E-15	3.539310E-15	99.983974	1.500000
0.91	1.732335E+16	106.166667	1.234286E-06	6.728103E-15	4.962431E-15	3.617960E-15	99.983606	1.500000
0.92	1.732329E+16	107.333333	1.234286E-06	6.942700E-15	5.016957E-15	3.697473E-15	99.983233	1.500000
0.93	1.732322E+16	108.500000	1.234286E-06	7.161805E-15	5.071484E-15	3.777851E-15	99.982854	1.500000
0.94	1.732315E+16	109.666667	1.234286E-06	7.385463E-15	5.126009E-15	3.859092E-15	99.982469	1.500000
0.95	1.732309E+16	110.833333	1.234286E-06	7.613723E-15	5.180535E-15	3.941198E-15	99.982078	1.500000
0.96	1.732302E+16	112.000000	1.234286E-06	7.846630E-15	5.235061E-15	4.024168E-15	99.981682	1.500000
0.97	1.732295E+16	113.166667	1.234286E-06	8.084232E-15	5.289586E-15	4.108003E-15	99.981279	1.500000
0.98	1.732288E+16	114.333333	1.234286E-06	8.326575E-15	5.344111E-15	4.192701E-15	99.980871	1.500000
0.99	1.732280E+16	115.500000	1.234286E-06	8.573706E-15	5.398636E-15	4.278264E-15	99.980456	1.500000
1.00	1.732273E+16	116.666667	1.234286E-06	8.825672E-15	5.453160E-15	4.364690E-15	99.980035	1.500000



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO2}}$ (mol)	$\Phi_{\text{NO2}}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732618E+16	1.166667	3.509922E-07	7.487779E-20	4.964649E-17	2.488219E-18	99.999944	2.000000
0.02	1.732617E+16	2.333333	4.963776E-07	3.305266E-19	9.929296E-17	7.464655E-18	99.999885	2.000000
0.03	1.732616E+16	3.500000	6.079356E-07	8.436919E-19	1.489394E-16	1.492931E-17	99.999824	2.000000
0.04	1.732615E+16	4.666667	7.019831E-07	1.677668E-18	1.985858E-16	2.488217E-17	99.999759	2.000000
0.05	1.732614E+16	5.833333	7.848404E-07	2.887570E-18	2.482322E-16	3.732325E-17	99.999691	2.000000
0.06	1.732613E+16	7.000000	8.597490E-07	4.522864E-18	2.978785E-16	5.225254E-17	99.999620	2.000000
0.07	1.732611E+16	8.166667	9.286343E-07	6.628816E-18	3.475248E-16	6.967004E-17	99.999546	2.000000
0.08	1.732610E+16	9.333333	9.927511E-07	9.247404E-18	3.971710E-16	8.957575E-17	99.999469	2.000000
0.09	1.732609E+16	10.500000	1.052971E-06	1.241795E-17	4.468173E-16	1.119697E-16	99.999388	2.000000
0.10	1.732607E+16	11.666667	1.109928E-06	1.617756E-17	4.964634E-16	1.368518E-16	99.999304	2.000000
0.11	1.732606E+16	12.833333	1.164101E-06	2.056148E-17	5.461096E-16	1.642221E-16	99.999217	2.000000
0.12	1.732604E+16	14.000000	1.215863E-06	2.560331E-17	5.957557E-16	1.940806E-16	99.999127	2.000000
0.13	1.732602E+16	15.166667	1.234286E-06	3.134211E-17	6.454017E-16	2.264273E-16	99.999033	2.000000
0.14	1.732601E+16	16.333333	1.234286E-06	3.782045E-17	6.950477E-16	2.612622E-16	99.998935	2.000000
0.15	1.732599E+16	17.500000	1.234286E-06	4.508092E-17	7.446936E-16	2.985853E-16	99.998835	2.000000
0.16	1.732597E+16	18.666667	1.234286E-06	5.316610E-17	7.943395E-16	3.383966E-16	99.998730	2.000000
0.17	1.732595E+16	19.833333	1.234286E-06	6.211858E-17	8.439854E-16	3.806961E-16	99.998622	2.000000
0.18	1.732593E+16	21.000000	1.234286E-06	7.198094E-17	8.936311E-16	4.254837E-16	99.998510	2.000000
0.19	1.732591E+16	22.166667	1.234286E-06	8.279577E-17	9.432769E-16	4.727595E-16	99.998395	2.000000
0.20	1.732589E+16	23.333333	1.234286E-06	9.460565E-17	9.929225E-16	5.225235E-16	99.998276	2.000000
0.21	1.732587E+16	24.500000	1.234286E-06	1.074532E-16	1.042568E-15	5.747757E-16	99.998153	2.000000
0.22	1.732585E+16	25.666667	1.234286E-06	1.213809E-16	1.092214E-15	6.295161E-16	99.998026	2.000000
0.23	1.732583E+16	26.833333	1.234286E-06	1.364315E-16	1.141859E-15	6.867446E-16	99.997896	2.000000
0.24	1.732580E+16	28.000000	1.234286E-06	1.526474E-16	1.191505E-15	7.464613E-16	99.997761	2.000000
0.25	1.732578E+16	29.166667	1.234286E-06	1.700713E-16	1.241150E-15	8.086661E-16	99.997623	2.000000
0.26	1.732575E+16	30.333333	1.234286E-06	1.887458E-16	1.290795E-15	8.733591E-16	99.997480	2.000000
0.27	1.732573E+16	31.500000	1.234286E-06	2.087134E-16	1.340440E-15	9.405403E-16	99.997334	2.000000
0.28	1.732570E+16	32.666667	1.234286E-06	2.300167E-16	1.390086E-15	1.010210E-15	99.997183	2.000000
0.29	1.732568E+16	33.833333	1.234286E-06	2.526984E-16	1.439731E-15	1.082367E-15	99.997029	2.000000
0.30	1.732565E+16	35.000000	1.234286E-06	2.768009E-16	1.489376E-15	1.157013E-15	99.996870	2.000000
0.31	1.732562E+16	36.166667	1.234286E-06	3.023669E-16	1.539020E-15	1.234146E-15	99.996706	2.000000
0.32	1.732559E+16	37.333333	1.234286E-06	3.294390E-16	1.588665E-15	1.313768E-15	99.996539	2.000000
0.33	1.732556E+16	38.500000	1.234286E-06	3.580597E-16	1.638310E-15	1.395878E-15	99.996367	2.000000
0.34	1.732553E+16	39.666667	1.234286E-06	3.882717E-16	1.687955E-15	1.480476E-15	99.996191	2.000000
0.35	1.732550E+16	40.833333	1.234286E-06	4.201174E-16	1.737599E-15	1.567563E-15	99.996011	2.000000
0.36	1.732547E+16	42.000000	1.234286E-06	4.536396E-16	1.787244E-15	1.657137E-15	99.995826	2.000000
0.37	1.732544E+16	43.166667	1.234286E-06	4.888807E-16	1.836888E-15	1.749199E-15	99.995636	2.000000
0.38	1.732540E+16	44.333333	1.234286E-06	5.258833E-16	1.886532E-15	1.843750E-15	99.995442	2.000000
0.39	1.732537E+16	45.500000	1.234286E-06	5.646902E-16	1.936176E-15	1.940789E-15	99.995244	2.000000
0.40	1.732533E+16	46.666667	1.234286E-06	6.053437E-16	1.985820E-15	2.040315E-15	99.995040	2.000000
0.41	1.732530E+16	47.833333	1.234286E-06	6.478865E-16	2.035464E-15	2.142330E-15	99.994832	2.000000
0.42	1.732526E+16	49.000000	1.234286E-06	6.923613E-16	2.085108E-15	2.246833E-15	99.994620	2.000000
0.43	1.732522E+16	50.166667	1.234286E-06	7.388104E-16	2.134752E-15	2.353824E-15	99.994402	2.000000
0.44	1.732518E+16	51.333333	1.234286E-06	7.872767E-16	2.184396E-15	2.463303E-15	99.994180	2.000000
0.45	1.732514E+16	52.500000	1.234286E-06	8.378025E-16	2.234039E-15	2.575270E-15	99.993953	2.000000

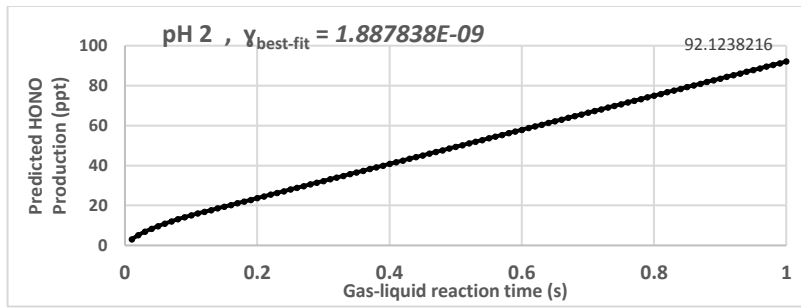


0.46	1.732510E+16	53.666667	1.234286E-06	8.904306E-16	2.283682E-15	2.689726E-15	99.993721	2.000000
0.47	1.732506E+16	54.833333	1.234286E-06	9.452035E-16	2.333326E-15	2.806669E-15	99.993484	2.000000
0.48	1.732502E+16	56.000000	1.234286E-06	1.002164E-15	2.382969E-15	2.926100E-15	99.993241	2.000000
0.49	1.732498E+16	57.166667	1.234286E-06	1.061354E-15	2.432612E-15	3.048020E-15	99.992994	2.000000
0.50	1.732493E+16	58.333333	1.234286E-06	1.122817E-15	2.482255E-15	3.172427E-15	99.992742	2.000000
0.51	1.732489E+16	59.500000	1.234286E-06	1.186594E-15	2.531898E-15	3.299323E-15	99.992485	2.000000
0.52	1.732484E+16	60.666667	1.234286E-06	1.252730E-15	2.581540E-15	3.428706E-15	99.992222	2.000000
0.53	1.732480E+16	61.833333	1.234286E-06	1.321266E-15	2.631183E-15	3.560578E-15	99.991954	2.000000
0.54	1.732475E+16	63.000000	1.234286E-06	1.392244E-15	2.680825E-15	3.694937E-15	99.991681	2.000000
0.55	1.732470E+16	64.166667	1.234286E-06	1.465708E-15	2.730468E-15	3.831785E-15	99.991403	2.000000
0.56	1.732465E+16	65.333333	1.234286E-06	1.541700E-15	2.780110E-15	3.971120E-15	99.991119	2.000000
0.57	1.732460E+16	66.500000	1.234286E-06	1.620263E-15	2.829752E-15	4.112944E-15	99.990830	2.000000
0.58	1.732455E+16	67.666667	1.234286E-06	1.701439E-15	2.879393E-15	4.257255E-15	99.990535	2.000000
0.59	1.732450E+16	68.833333	1.234286E-06	1.785271E-15	2.929035E-15	4.404054E-15	99.990235	2.000000
0.60	1.732445E+16	70.000000	1.234286E-06	1.871800E-15	2.978677E-15	4.553342E-15	99.989930	2.000000
0.61	1.732439E+16	71.166667	1.234286E-06	1.961071E-15	3.028318E-15	4.705117E-15	99.989618	2.000000
0.62	1.732434E+16	72.333333	1.234286E-06	2.053125E-15	3.077959E-15	4.859381E-15	99.989301	2.000000
0.63	1.732428E+16	73.500000	1.234286E-06	2.148006E-15	3.127600E-15	5.016132E-15	99.988979	2.000000
0.64	1.732422E+16	74.666667	1.234286E-06	2.245755E-15	3.177241E-15	5.175371E-15	99.988650	2.000000
0.65	1.732417E+16	75.833333	1.234286E-06	2.346415E-15	3.226882E-15	5.337098E-15	99.988316	2.000000
0.66	1.732411E+16	77.000000	1.234286E-06	2.450029E-15	3.276522E-15	5.501313E-15	99.987976	2.000000
0.67	1.732405E+16	78.166667	1.234286E-06	2.556639E-15	3.326163E-15	5.668016E-15	99.987630	2.000000
0.68	1.732399E+16	79.333333	1.234286E-06	2.666288E-15	3.375803E-15	5.837207E-15	99.987279	2.000000
0.69	1.732393E+16	80.500000	1.234286E-06	2.779019E-15	3.425443E-15	6.008886E-15	99.986921	2.000000
0.70	1.732386E+16	81.666667	1.234286E-06	2.894874E-15	3.475083E-15	6.183052E-15	99.986557	2.000000
0.71	1.732380E+16	82.833333	1.234286E-06	3.013895E-15	3.524723E-15	6.359707E-15	99.986187	2.000000
0.72	1.732373E+16	84.000000	1.234286E-06	3.136126E-15	3.574362E-15	6.538849E-15	99.985812	2.000000
0.73	1.732367E+16	85.166667	1.234286E-06	3.261608E-15	3.624001E-15	6.720479E-15	99.985430	2.000000
0.74	1.732360E+16	86.333333	1.234286E-06	3.390385E-15	3.673640E-15	6.904598E-15	99.985041	2.000000
0.75	1.732353E+16	87.500000	1.234286E-06	3.522499E-15	3.723279E-15	7.091203E-15	99.984647	2.000000
0.76	1.732346E+16	88.666667	1.234286E-06	3.657992E-15	3.772918E-15	7.280297E-15	99.984246	2.000000
0.77	1.732339E+16	89.833333	1.234286E-06	3.796908E-15	3.822557E-15	7.471879E-15	99.983839	2.000000
0.78	1.732332E+16	91.000000	1.234286E-06	3.939288E-15	3.872195E-15	7.665948E-15	99.983426	2.000000
0.79	1.732325E+16	92.166667	1.234286E-06	4.085175E-15	3.921833E-15	7.862505E-15	99.983006	2.000000
0.80	1.732317E+16	93.333333	1.234286E-06	4.234612E-15	3.971471E-15	8.061550E-15	99.982579	2.000000
0.81	1.732310E+16	94.500000	1.234286E-06	4.387642E-15	4.021108E-15	8.263083E-15	99.982147	2.000000
0.82	1.732302E+16	95.666667	1.234286E-06	4.544307E-15	4.070746E-15	8.467103E-15	99.981707	2.000000
0.83	1.732294E+16	96.833333	1.234286E-06	4.704649E-15	4.120383E-15	8.673611E-15	99.981261	2.000000
0.84	1.732287E+16	98.000000	1.234286E-06	4.868711E-15	4.170020E-15	8.882607E-15	99.980808	2.000000
0.85	1.732279E+16	99.166667	1.234286E-06	5.036535E-15	4.219657E-15	9.094091E-15	99.980349	2.000000
0.86	1.732271E+16	100.333333	1.234286E-06	5.208165E-15	4.269293E-15	9.308062E-15	99.979883	2.000000
0.87	1.732262E+16	101.500000	1.234286E-06	5.383643E-15	4.318930E-15	9.524521E-15	99.979410	2.000000
0.88	1.732254E+16	102.666667	1.234286E-06	5.563011E-15	4.368566E-15	9.743468E-15	99.978930	2.000000
0.89	1.732246E+16	103.833333	1.234286E-06	5.746313E-15	4.418202E-15	9.964903E-15	99.978444	2.000000
0.90	1.732237E+16	105.000000	1.234286E-06	5.933589E-15	4.467837E-15	1.018882E-14	99.977950	2.000000
0.91	1.732228E+16	106.166667	1.234286E-06	6.124884E-15	4.517472E-15	1.041523E-14	99.977450	2.000000
0.92	1.732220E+16	107.333333	1.234286E-06	6.320239E-15	4.567108E-15	1.064413E-14	99.976942	2.000000
0.93	1.732211E+16	108.500000	1.234286E-06	6.519698E-15	4.616742E-15	1.087552E-14	99.976428	2.000000
0.94	1.732202E+16	109.666667	1.234286E-06	6.723302E-15	4.666377E-15	1.110939E-14	99.975906	2.000000
0.95	1.732193E+16	110.833333	1.234286E-06	6.931095E-15	4.716011E-15	1.134575E-14	99.975377	2.000000
0.96	1.732183E+16	112.000000	1.234286E-06	7.143118E-15	4.765645E-15	1.158460E-14	99.974842	2.000000
0.97	1.732174E+16	113.166667	1.234286E-06	7.359415E-15	4.815279E-15	1.182593E-14	99.974298	2.000000
0.98	1.732164E+16	114.333333	1.234286E-06	7.580028E-15	4.864913E-15	1.206976E-14	99.973748	2.000000
0.99	1.732155E+16	115.500000	1.234286E-06	7.805000E-15	4.914546E-15	1.231607E-14	99.973190	2.000000
1.00	1.732145E+16	116.666667	1.234286E-06	8.034372E-15	4.964179E-15	1.256486E-14	99.972625	2.000000



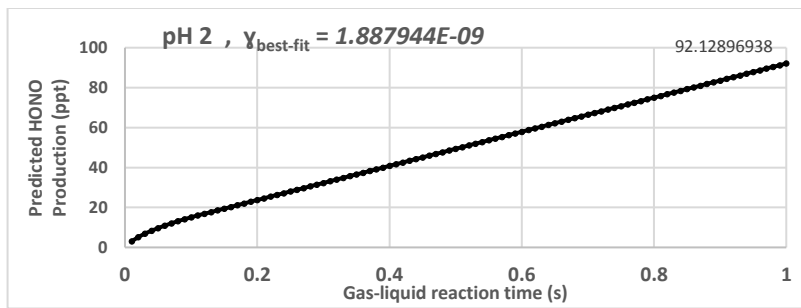
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732618E+16	1.166667	3.509922E-07	8.253257E-20	5.472187E-17	2.742590E-18	99.999938	2.000000
0.02	1.732617E+16	2.333333	4.963776E-07	3.643164E-19	1.094437E-16	8.227769E-18	99.999874	2.000000
0.03	1.732616E+16	3.500000	6.079355E-07	9.299428E-19	1.641655E-16	1.645553E-17	99.999806	2.000000
0.04	1.732615E+16	4.666667	7.019829E-07	1.849176E-18	2.188872E-16	2.742588E-17	99.999734	2.000000
0.05	1.732613E+16	5.833333	7.848402E-07	3.182767E-18	2.736090E-16	4.113881E-17	99.999660	2.000000
0.06	1.732612E+16	7.000000	8.597486E-07	4.985238E-18	3.283306E-16	5.759433E-17	99.999581	2.000000
0.07	1.732610E+16	8.166667	9.286339E-07	7.306482E-18	3.830523E-16	7.679242E-17	99.999500	2.000000
0.08	1.732609E+16	9.333333	9.927506E-07	1.019277E-17	4.377738E-16	9.873308E-17	99.999415	2.000000
0.09	1.732607E+16	10.500000	1.052970E-06	1.368744E-17	4.924954E-16	1.234163E-16	99.999326	2.000000
0.10	1.732606E+16	11.666667	1.109927E-06	1.783140E-17	5.472169E-16	1.508421E-16	99.999233	2.000000
0.11	1.732604E+16	12.833333	1.164100E-06	2.266348E-17	6.019383E-16	1.810105E-16	99.999137	2.000000
0.12	1.732602E+16	14.000000	1.215862E-06	2.822075E-17	6.566597E-16	2.139215E-16	99.999037	2.000000
0.13	1.732601E+16	15.166667	1.234286E-06	3.454622E-17	7.113810E-16	2.495750E-16	99.998934	2.000000
0.14	1.732599E+16	16.333333	1.234286E-06	4.168684E-17	7.661022E-16	2.879710E-16	99.998827	2.000000
0.15	1.732597E+16	17.500000	1.234286E-06	4.968955E-17	8.208234E-16	3.291096E-16	99.998715	2.000000
0.16	1.732595E+16	18.666667	1.234286E-06	5.860128E-17	8.755446E-16	3.729908E-16	99.998600	2.000000
0.17	1.732593E+16	19.833333	1.234286E-06	6.846897E-17	9.302656E-16	4.196145E-16	99.998481	2.000000
0.18	1.732591E+16	21.000000	1.234286E-06	7.933956E-17	9.849866E-16	4.689808E-16	99.998358	2.000000
0.19	1.732588E+16	22.166667	1.234286E-06	9.125999E-17	1.039708E-15	5.210896E-16	99.998231	2.000000
0.20	1.732586E+16	23.333333	1.234286E-06	1.042772E-16	1.094428E-15	5.759410E-16	99.998100	2.000000
0.21	1.732584E+16	24.500000	1.234286E-06	1.184381E-16	1.149149E-15	6.335349E-16	99.997964	2.000000
0.22	1.732581E+16	25.666667	1.234286E-06	1.337897E-16	1.203870E-15	6.938713E-16	99.997824	2.000000
0.23	1.732579E+16	26.833333	1.234286E-06	1.503788E-16	1.258591E-15	7.569502E-16	99.997681	2.000000
0.24	1.732576E+16	28.000000	1.234286E-06	1.682525E-16	1.313311E-15	8.227717E-16	99.997532	2.000000
0.25	1.732574E+16	29.166667	1.234286E-06	1.874577E-16	1.368032E-15	8.913357E-16	99.997380	2.000000
0.26	1.732571E+16	30.333333	1.234286E-06	2.080412E-16	1.422752E-15	9.626422E-16	99.997223	2.000000
0.27	1.732568E+16	31.500000	1.234286E-06	2.300501E-16	1.477472E-15	1.036691E-15	99.997061	2.000000
0.28	1.732565E+16	32.666667	1.234286E-06	2.535313E-16	1.532192E-15	1.113483E-15	99.996895	2.000000
0.29	1.732562E+16	33.833333	1.234286E-06	2.785317E-16	1.586913E-15	1.193017E-15	99.996725	2.000000
0.30	1.732559E+16	35.000000	1.234286E-06	3.050982E-16	1.641633E-15	1.275293E-15	99.996550	2.000000
0.31	1.732556E+16	36.166667	1.234286E-06	3.332778E-16	1.696353E-15	1.360312E-15	99.996370	2.000000
0.32	1.732553E+16	37.333333	1.234286E-06	3.631174E-16	1.751072E-15	1.448074E-15	99.996185	2.000000
0.33	1.732550E+16	38.500000	1.234286E-06	3.946640E-16	1.805792E-15	1.538578E-15	99.995996	2.000000
0.34	1.732546E+16	39.666667	1.234286E-06	4.279645E-16	1.860512E-15	1.631824E-15	99.995802	2.000000
0.35	1.732543E+16	40.833333	1.234286E-06	4.630658E-16	1.915231E-15	1.727813E-15	99.995603	2.000000
0.36	1.732539E+16	42.000000	1.234286E-06	5.000149E-16	1.969951E-15	1.826545E-15	99.995399	2.000000
0.37	1.732536E+16	43.166667	1.234286E-06	5.388586E-16	2.024670E-15	1.928018E-15	99.995190	2.000000
0.38	1.732532E+16	44.333333	1.234286E-06	5.796441E-16	2.079389E-15	2.032235E-15	99.994976	2.000000
0.39	1.732528E+16	45.500000	1.234286E-06	6.224180E-16	2.134108E-15	2.139193E-15	99.994757	2.000000
0.40	1.732524E+16	46.666667	1.234286E-06	6.672275E-16	2.188827E-15	2.248895E-15	99.994533	2.000000
0.41	1.732520E+16	47.833333	1.234286E-06	7.141194E-16	2.243546E-15	2.361338E-15	99.994304	2.000000
0.42	1.732516E+16	49.000000	1.234286E-06	7.631407E-16	2.298264E-15	2.476524E-15	99.994070	2.000000
0.43	1.732512E+16	50.166667	1.234286E-06	8.143384E-16	2.352983E-15	2.594453E-15	99.993830	2.000000
0.44	1.732508E+16	51.333333	1.234286E-06	8.677592E-16	2.407701E-15	2.715124E-15	99.993585	2.000000
0.45	1.732504E+16	52.500000	1.234286E-06	9.234502E-16	2.462419E-15	2.838537E-15	99.993334	2.000000

0.46	1.732499E+16	53.666667	1.234286E-06	9.814584E-16	2.517138E-15	2.964693E-15	99.993079	2.000000
0.47	1.732495E+16	54.833333	1.234286E-06	1.041831E-15	2.571856E-15	3.093591E-15	99.992817	2.000000
0.48	1.732490E+16	56.000000	1.234286E-06	1.104614E-15	2.626573E-15	3.225231E-15	99.992551	2.000000
0.49	1.732485E+16	57.166667	1.234286E-06	1.169855E-15	2.681291E-15	3.359614E-15	99.992278	2.000000
0.50	1.732481E+16	58.333333	1.234286E-06	1.237601E-15	2.736009E-15	3.496739E-15	99.992000	2.000000
0.51	1.732476E+16	59.500000	1.234286E-06	1.307898E-15	2.790726E-15	3.636607E-15	99.991717	2.000000
0.52	1.732471E+16	60.666667	1.234286E-06	1.380795E-15	2.845443E-15	3.779217E-15	99.991427	2.000000
0.53	1.732465E+16	61.833333	1.234286E-06	1.456337E-15	2.900160E-15	3.924569E-15	99.991132	2.000000
0.54	1.732460E+16	63.000000	1.234286E-06	1.534571E-15	2.954877E-15	4.072664E-15	99.990831	2.000000
0.55	1.732455E+16	64.166667	1.234286E-06	1.615545E-15	3.009594E-15	4.223501E-15	99.990524	2.000000
0.56	1.732450E+16	65.333333	1.234286E-06	1.699306E-15	3.064310E-15	4.377080E-15	99.990211	2.000000
0.57	1.732444E+16	66.500000	1.234286E-06	1.785900E-15	3.119027E-15	4.533402E-15	99.989893	2.000000
0.58	1.732438E+16	67.666667	1.234286E-06	1.875374E-15	3.173743E-15	4.692465E-15	99.989568	2.000000
0.59	1.732433E+16	68.833333	1.234286E-06	1.967775E-15	3.228459E-15	4.854272E-15	99.989237	2.000000
0.60	1.732427E+16	70.000000	1.234286E-06	2.063151E-15	3.283175E-15	5.018820E-15	99.988900	2.000000
0.61	1.732421E+16	71.166667	1.234286E-06	2.161547E-15	3.337890E-15	5.186111E-15	99.988557	2.000000
0.62	1.732415E+16	72.333333	1.234286E-06	2.263012E-15	3.392606E-15	5.356144E-15	99.988208	2.000000
0.63	1.732409E+16	73.500000	1.234286E-06	2.367592E-15	3.447321E-15	5.528919E-15	99.987852	2.000000
0.64	1.732402E+16	74.666667	1.234286E-06	2.475333E-15	3.502036E-15	5.704437E-15	99.987490	2.000000
0.65	1.732396E+16	75.833333	1.234286E-06	2.586283E-15	3.556751E-15	5.882696E-15	99.987122	2.000000
0.66	1.732389E+16	77.000000	1.234286E-06	2.700489E-15	3.611466E-15	6.063698E-15	99.986747	2.000000
0.67	1.732383E+16	78.166667	1.234286E-06	2.817998E-15	3.666180E-15	6.247442E-15	99.986366	2.000000
0.68	1.732376E+16	79.333333	1.234286E-06	2.938856E-15	3.720894E-15	6.433929E-15	99.985978	2.000000
0.69	1.732369E+16	80.500000	1.234286E-06	3.063111E-15	3.775608E-15	6.623157E-15	99.985584	2.000000
0.70	1.732362E+16	81.666667	1.234286E-06	3.190809E-15	3.830322E-15	6.815128E-15	99.985183	2.000000
0.71	1.732355E+16	82.833333	1.234286E-06	3.321997E-15	3.885036E-15	7.009841E-15	99.984775	2.000000
0.72	1.732348E+16	84.000000	1.234286E-06	3.456723E-15	3.939749E-15	7.207296E-15	99.984361	2.000000
0.73	1.732341E+16	85.166667	1.234286E-06	3.595033E-15	3.994462E-15	7.407493E-15	99.983940	2.000000
0.74	1.732333E+16	86.333333	1.234286E-06	3.736974E-15	4.049175E-15	7.610433E-15	99.983512	2.000000
0.75	1.732326E+16	87.500000	1.234286E-06	3.882593E-15	4.103888E-15	7.816114E-15	99.983077	2.000000
0.76	1.732318E+16	88.666667	1.234286E-06	4.031937E-15	4.158600E-15	8.024538E-15	99.982636	2.000000
0.77	1.732310E+16	89.833333	1.234286E-06	4.185053E-15	4.213312E-15	8.235703E-15	99.982187	2.000000
0.78	1.732303E+16	91.000000	1.234286E-06	4.341988E-15	4.268024E-15	8.449611E-15	99.981731	2.000000
0.79	1.732295E+16	92.166667	1.234286E-06	4.502788E-15	4.322736E-15	8.666261E-15	99.981268	2.000000
0.80	1.732286E+16	93.333333	1.234286E-06	4.667502E-15	4.377447E-15	8.885653E-15	99.980799	2.000000
0.81	1.732278E+16	94.500000	1.234286E-06	4.836174E-15	4.432158E-15	9.107787E-15	99.980321	2.000000
0.82	1.732270E+16	95.666667	1.234286E-06	5.008854E-15	4.486869E-15	9.332663E-15	99.979837	2.000000
0.83	1.732261E+16	96.833333	1.234286E-06	5.185586E-15	4.541580E-15	9.560281E-15	99.979346	2.000000
0.84	1.732253E+16	98.000000	1.234286E-06	5.366420E-15	4.596290E-15	9.790641E-15	99.978847	2.000000
0.85	1.732244E+16	99.166667	1.234286E-06	5.551400E-15	4.651000E-15	1.002374E-14	99.978340	2.000000
0.86	1.732235E+16	100.333333	1.234286E-06	5.740574E-15	4.705710E-15	1.025959E-14	99.977827	2.000000
0.87	1.732226E+16	101.500000	1.234286E-06	5.933990E-15	4.760419E-15	1.049817E-14	99.977305	2.000000
0.88	1.732217E+16	102.666667	1.234286E-06	6.131694E-15	4.815129E-15	1.073950E-14	99.976777	2.000000
0.89	1.732207E+16	103.833333	1.234286E-06	6.333732E-15	4.869838E-15	1.098357E-14	99.976240	2.000000
0.90	1.732198E+16	105.000000	1.234286E-06	6.540153E-15	4.924546E-15	1.123038E-14	99.975696	2.000000
0.91	1.732188E+16	106.166667	1.234286E-06	6.751002E-15	4.979254E-15	1.147994E-14	99.975145	2.000000
0.92	1.732179E+16	107.333333	1.234286E-06	6.966327E-15	5.033962E-15	1.173223E-14	99.974585	2.000000
0.93	1.732169E+16	108.500000	1.234286E-06	7.186174E-15	5.088670E-15	1.198727E-14	99.974018	2.000000
0.94	1.732159E+16	109.666667	1.234286E-06	7.410591E-15	5.143378E-15	1.224505E-14	99.973443	2.000000
0.95	1.732149E+16	110.833333	1.234286E-06	7.639625E-15	5.198085E-15	1.250557E-14	99.972860	2.000000
0.96	1.732139E+16	112.000000	1.234286E-06	7.873322E-15	5.252791E-15	1.276883E-14	99.972270	2.000000
0.97	1.732128E+16	113.166667	1.234286E-06	8.111729E-15	5.307498E-15	1.303484E-14	99.971671	2.000000
0.98	1.732118E+16	114.333333	1.234286E-06	8.354893E-15	5.362204E-15	1.330358E-14	99.971064	2.000000
0.99	1.732107E+16	115.500000	1.234286E-06	8.602861E-15	5.416910E-15	1.357507E-14	99.970449	2.000000
1.00	1.732096E+16	116.666667	1.234286E-06	8.855681E-15	5.471615E-15	1.384930E-14	99.969826	2.000000



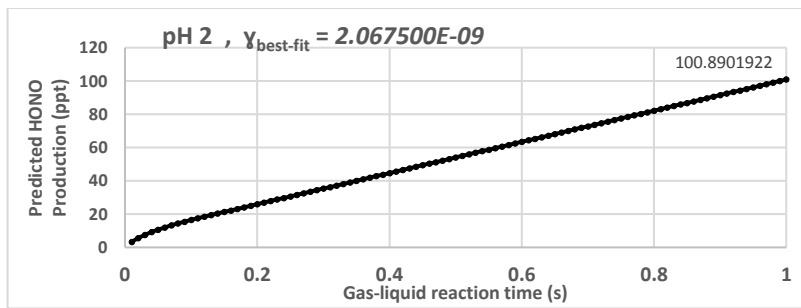
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732618E+16	1.166667	3.509922E-07	7.800865E-20	5.172236E-17	2.592259E-18	99.999942	2.000000
0.02	1.732617E+16	2.333333	4.963776E-07	3.443469E-19	1.034447E-16	7.776774E-18	99.999881	2.000000
0.03	1.732616E+16	3.500000	6.079355E-07	8.789691E-19	1.551670E-16	1.555355E-17	99.999816	2.000000
0.04	1.732615E+16	4.666667	7.019830E-07	1.747816E-18	2.068892E-16	2.592257E-17	99.999749	2.000000
0.05	1.732614E+16	5.833333	7.848403E-07	3.008308E-18	2.586115E-16	3.888385E-17	99.999678	2.000000
0.06	1.732612E+16	7.000000	8.597488E-07	4.711979E-18	3.103336E-16	5.443737E-17	99.999604	2.000000
0.07	1.732611E+16	8.166667	9.286342E-07	6.905986E-18	3.620558E-16	7.258315E-17	99.999527	2.000000
0.08	1.732610E+16	9.333333	9.927509E-07	9.634066E-18	4.137779E-16	9.332117E-17	99.999447	2.000000
0.09	1.732608E+16	10.500000	1.052970E-06	1.293718E-17	4.655000E-16	1.166514E-16	99.999363	2.000000
0.10	1.732607E+16	11.666667	1.109927E-06	1.685399E-17	5.172220E-16	1.425739E-16	99.999275	2.000000
0.11	1.732605E+16	12.833333	1.164101E-06	2.142121E-17	5.689439E-16	1.710887E-16	99.999185	2.000000
0.12	1.732603E+16	14.000000	1.215862E-06	2.667386E-17	6.206659E-16	2.021957E-16	99.999090	2.000000
0.13	1.732602E+16	15.166667	1.234286E-06	3.265262E-17	6.723877E-16	2.358949E-16	99.998992	2.000000
0.14	1.732600E+16	16.333333	1.234286E-06	3.940183E-17	7.241095E-16	2.721863E-16	99.998891	2.000000
0.15	1.732598E+16	17.500000	1.234286E-06	4.696588E-17	7.758313E-16	3.110700E-16	99.998786	2.000000
0.16	1.732596E+16	18.666667	1.234286E-06	5.538913E-17	8.275530E-16	3.525459E-16	99.998677	2.000000
0.17	1.732594E+16	19.833333	1.234286E-06	6.471593E-17	8.792746E-16	3.966140E-16	99.998564	2.000000
0.18	1.732592E+16	21.000000	1.234286E-06	7.499067E-17	9.309962E-16	4.432743E-16	99.998448	2.000000
0.19	1.732590E+16	22.166667	1.234286E-06	8.625770E-17	9.827178E-16	4.925269E-16	99.998328	2.000000
0.20	1.732588E+16	23.333333	1.234286E-06	9.856138E-17	1.034439E-15	5.443717E-16	99.998204	2.000000
0.21	1.732586E+16	24.500000	1.234286E-06	1.119461E-16	1.086161E-15	5.988087E-16	99.998076	2.000000
0.22	1.732583E+16	25.666667	1.234286E-06	1.264562E-16	1.137882E-15	6.558378E-16	99.997944	2.000000
0.23	1.732581E+16	26.833333	1.234286E-06	1.421360E-16	1.189603E-15	7.154592E-16	99.997808	2.000000
0.24	1.732579E+16	28.000000	1.234286E-06	1.590300E-16	1.241324E-15	7.776728E-16	99.997668	2.000000
0.25	1.732576E+16	29.166667	1.234286E-06	1.771825E-16	1.293045E-15	8.424786E-16	99.997523	2.000000
0.26	1.732574E+16	30.333333	1.234286E-06	1.966378E-16	1.344767E-15	9.098766E-16	99.997375	2.000000
0.27	1.732571E+16	31.500000	1.234286E-06	2.174403E-16	1.396487E-15	9.798667E-16	99.997222	2.000000
0.28	1.732568E+16	32.666667	1.234286E-06	2.396344E-16	1.448208E-15	1.052449E-15	99.997065	2.000000
0.29	1.732565E+16	33.833333	1.234286E-06	2.632644E-16	1.499929E-15	1.127624E-15	99.996904	2.000000
0.30	1.732563E+16	35.000000	1.234286E-06	2.883747E-16	1.551650E-15	1.205390E-15	99.996739	2.000000
0.31	1.732560E+16	36.166667	1.234286E-06	3.150097E-16	1.603370E-15	1.285749E-15	99.996569	2.000000
0.32	1.732557E+16	37.333333	1.234286E-06	3.432137E-16	1.655091E-15	1.368700E-15	99.996394	2.000000
0.33	1.732554E+16	38.500000	1.234286E-06	3.730311E-16	1.706811E-15	1.454243E-15	99.996215	2.000000
0.34	1.732550E+16	39.666667	1.234286E-06	4.045063E-16	1.758532E-15	1.542379E-15	99.996032	2.000000
0.35	1.732547E+16	40.833333	1.234286E-06	4.376836E-16	1.810252E-15	1.633106E-15	99.995844	2.000000
0.36	1.732544E+16	42.000000	1.234286E-06	4.726074E-16	1.861972E-15	1.726426E-15	99.995651	2.000000
0.37	1.732540E+16	43.166667	1.234286E-06	5.093220E-16	1.913692E-15	1.822338E-15	99.995454	2.000000
0.38	1.732537E+16	44.333333	1.234286E-06	5.478719E-16	1.965412E-15	1.920842E-15	99.995252	2.000000
0.39	1.732533E+16	45.500000	1.234286E-06	5.883013E-16	2.017132E-15	2.021938E-15	99.995045	2.000000
0.40	1.732530E+16	46.666667	1.234286E-06	6.306546E-16	2.068852E-15	2.125626E-15	99.994833	2.000000
0.41	1.732526E+16	47.833333	1.234286E-06	6.749763E-16	2.120571E-15	2.231906E-15	99.994616	2.000000
0.42	1.732522E+16	49.000000	1.234286E-06	7.213106E-16	2.172291E-15	2.340779E-15	99.994395	2.000000
0.43	1.732518E+16	50.166667	1.234286E-06	7.697019E-16	2.224010E-15	2.452243E-15	99.994168	2.000000
0.44	1.732514E+16	51.333333	1.234286E-06	8.201946E-16	2.275729E-15	2.566300E-15	99.993936	2.000000
0.45	1.732510E+16	52.500000	1.234286E-06	8.728331E-16	2.327448E-15	2.682949E-15	99.993700	2.000000

0.46	1.732506E+16	53.666667	1.234286E-06	9.276617E-16	2.379167E-15	2.802189E-15	99.993458	2.000000
0.47	1.732501E+16	54.833333	1.234286E-06	9.847247E-16	2.430886E-15	2.924022E-15	99.993211	2.000000
0.48	1.732497E+16	56.000000	1.234286E-06	1.044067E-15	2.482605E-15	3.048447E-15	99.992959	2.000000
0.49	1.732493E+16	57.166667	1.234286E-06	1.105732E-15	2.534324E-15	3.175464E-15	99.992701	2.000000
0.50	1.732488E+16	58.333333	1.234286E-06	1.169764E-15	2.586042E-15	3.305073E-15	99.992439	2.000000
0.51	1.732483E+16	59.500000	1.234286E-06	1.236209E-15	2.637761E-15	3.437274E-15	99.992171	2.000000
0.52	1.732479E+16	60.666667	1.234286E-06	1.305109E-15	2.689479E-15	3.572068E-15	99.991897	2.000000
0.53	1.732474E+16	61.833333	1.234286E-06	1.376511E-15	2.741197E-15	3.709453E-15	99.991618	2.000000
0.54	1.732469E+16	63.000000	1.234286E-06	1.450457E-15	2.792915E-15	3.849430E-15	99.991334	2.000000
0.55	1.732464E+16	64.166667	1.234286E-06	1.526993E-15	2.844632E-15	3.991999E-15	99.991044	2.000000
0.56	1.732459E+16	65.333333	1.234286E-06	1.606162E-15	2.896350E-15	4.137161E-15	99.990748	2.000000
0.57	1.732454E+16	66.500000	1.234286E-06	1.688010E-15	2.948068E-15	4.284914E-15	99.990447	2.000000
0.58	1.732448E+16	67.666667	1.234286E-06	1.772580E-15	2.999785E-15	4.435259E-15	99.990140	2.000000
0.59	1.732443E+16	68.833333	1.234286E-06	1.859916E-15	3.051502E-15	4.588197E-15	99.989827	2.000000
0.60	1.732437E+16	70.000000	1.234286E-06	1.950064E-15	3.103219E-15	4.743726E-15	99.989509	2.000000
0.61	1.732432E+16	71.166667	1.234286E-06	2.043068E-15	3.154936E-15	4.901847E-15	99.989184	2.000000
0.62	1.732426E+16	72.333333	1.234286E-06	2.138971E-15	3.206652E-15	5.062561E-15	99.988854	2.000000
0.63	1.732420E+16	73.500000	1.234286E-06	2.237818E-15	3.258369E-15	5.225866E-15	99.988518	2.000000
0.64	1.732414E+16	74.666667	1.234286E-06	2.339654E-15	3.310085E-15	5.391763E-15	99.988176	2.000000
0.65	1.732408E+16	75.833333	1.234286E-06	2.444523E-15	3.361801E-15	5.560252E-15	99.987828	2.000000
0.66	1.732402E+16	77.000000	1.234286E-06	2.552469E-15	3.413517E-15	5.731333E-15	99.987474	2.000000
0.67	1.732396E+16	78.166667	1.234286E-06	2.663537E-15	3.465233E-15	5.905006E-15	99.987113	2.000000
0.68	1.732389E+16	79.333333	1.234286E-06	2.777771E-15	3.516948E-15	6.081271E-15	99.986747	2.000000
0.69	1.732383E+16	80.500000	1.234286E-06	2.895215E-15	3.568664E-15	6.260128E-15	99.986374	2.000000
0.70	1.732376E+16	81.666667	1.234286E-06	3.015914E-15	3.620379E-15	6.441576E-15	99.985995	2.000000
0.71	1.732370E+16	82.833333	1.234286E-06	3.139911E-15	3.672094E-15	6.625617E-15	99.985610	2.000000
0.72	1.732363E+16	84.000000	1.234286E-06	3.267253E-15	3.723808E-15	6.812249E-15	99.985218	2.000000
0.73	1.732356E+16	85.166667	1.234286E-06	3.397982E-15	3.775523E-15	7.001474E-15	99.984820	2.000000
0.74	1.732349E+16	86.333333	1.234286E-06	3.532143E-15	3.827237E-15	7.193290E-15	99.984416	2.000000
0.75	1.732342E+16	87.500000	1.234286E-06	3.669780E-15	3.878951E-15	7.387698E-15	99.984005	2.000000
0.76	1.732335E+16	88.666667	1.234286E-06	3.810939E-15	3.930665E-15	7.584698E-15	99.983587	2.000000
0.77	1.732327E+16	89.833333	1.234286E-06	3.955662E-15	3.982379E-15	7.784289E-15	99.983163	2.000000
0.78	1.732320E+16	91.000000	1.234286E-06	4.103996E-15	4.034093E-15	7.986473E-15	99.982733	2.000000
0.79	1.732312E+16	92.166667	1.234286E-06	4.255983E-15	4.085806E-15	8.191248E-15	99.982295	2.000000
0.80	1.732305E+16	93.333333	1.234286E-06	4.411668E-15	4.137519E-15	8.398615E-15	99.981851	2.000000
0.81	1.732297E+16	94.500000	1.234286E-06	4.571095E-15	4.189232E-15	8.608574E-15	99.981400	2.000000
0.82	1.732289E+16	95.666667	1.234286E-06	4.734310E-15	4.240944E-15	8.821124E-15	99.980942	2.000000
0.83	1.732281E+16	96.833333	1.234286E-06	4.901356E-15	4.292656E-15	9.036267E-15	99.980478	2.000000
0.84	1.732273E+16	98.000000	1.234286E-06	5.072278E-15	4.344368E-15	9.254001E-15	99.980006	2.000000
0.85	1.732264E+16	99.166667	1.234286E-06	5.247119E-15	4.396080E-15	9.474326E-15	99.979527	2.000000
0.86	1.732256E+16	100.333333	1.234286E-06	5.425925E-15	4.447792E-15	9.697244E-15	99.979042	2.000000
0.87	1.732247E+16	101.500000	1.234286E-06	5.608740E-15	4.499503E-15	9.922753E-15	99.978549	2.000000
0.88	1.732239E+16	102.666667	1.234286E-06	5.795607E-15	4.551214E-15	1.015085E-14	99.978050	2.000000
0.89	1.732230E+16	103.833333	1.234286E-06	5.986572E-15	4.602925E-15	1.038155E-14	99.977543	2.000000
0.90	1.732221E+16	105.000000	1.234286E-06	6.181679E-15	4.654635E-15	1.061483E-14	99.977028	2.000000
0.91	1.732212E+16	106.166667	1.234286E-06	6.380971E-15	4.706346E-15	1.085071E-14	99.976507	2.000000
0.92	1.732203E+16	107.333333	1.234286E-06	6.584494E-15	4.758056E-15	1.108917E-14	99.975978	2.000000
0.93	1.732194E+16	108.500000	1.234286E-06	6.792292E-15	4.809765E-15	1.133023E-14	99.975442	2.000000
0.94	1.732184E+16	109.666667	1.234286E-06	7.004409E-15	4.861475E-15	1.157388E-14	99.974899	2.000000
0.95	1.732175E+16	110.833333	1.234286E-06	7.220889E-15	4.913184E-15	1.182013E-14	99.974348	2.000000
0.96	1.732165E+16	112.000000	1.234286E-06	7.441778E-15	4.964893E-15	1.206896E-14	99.973790	2.000000
0.97	1.732155E+16	113.166667	1.234286E-06	7.667118E-15	5.016601E-15	1.232039E-14	99.973224	2.000000
0.98	1.732145E+16	114.333333	1.234286E-06	7.896954E-15	5.068309E-15	1.257440E-14	99.972650	2.000000
0.99	1.732135E+16	115.500000	1.234286E-06	8.131332E-15	5.120017E-15	1.283101E-14	99.972069	2.000000
1.00	1.732125E+16	116.666667	1.234286E-06	8.370294E-15	5.171725E-15	1.309021E-14	99.971480	2.000000



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732618E+16	1.166667	3.509922E-07	7.801301E-20	5.172525E-17	2.592403E-18	99.999942	2.000000
0.02	1.732617E+16	2.333333	4.963776E-07	3.443661E-19	1.034505E-16	7.777209E-18	99.999881	2.000000
0.03	1.732616E+16	3.500000	6.079355E-07	8.790182E-19	1.551757E-16	1.555441E-17	99.999816	2.000000
0.04	1.732615E+16	4.666667	7.019830E-07	1.747914E-18	2.069008E-16	2.592402E-17	99.999749	2.000000
0.05	1.732614E+16	5.833333	7.848403E-07	3.008476E-18	2.586259E-16	3.888602E-17	99.999678	2.000000
0.06	1.732612E+16	7.000000	8.597488E-07	4.712242E-18	3.103510E-16	5.444041E-17	99.999604	2.000000
0.07	1.732611E+16	8.166667	9.286342E-07	6.906372E-18	3.620760E-16	7.258720E-17	99.999527	2.000000
0.08	1.732610E+16	9.333333	9.927509E-07	9.634604E-18	4.138010E-16	9.332638E-17	99.999447	2.000000
0.09	1.732608E+16	10.500000	1.052970E-06	1.293790E-17	4.655260E-16	1.166579E-16	99.999363	2.000000
0.10	1.732607E+16	11.666667	1.109927E-06	1.685494E-17	5.172509E-16	1.425819E-16	99.999275	2.000000
0.11	1.732605E+16	12.833333	1.164101E-06	2.142241E-17	5.689757E-16	1.710982E-16	99.999185	2.000000
0.12	1.732603E+16	14.000000	1.215862E-06	2.667536E-17	6.207005E-16	2.022070E-16	99.999090	2.000000
0.13	1.732602E+16	15.166667	1.234286E-06	3.265444E-17	6.724253E-16	2.359081E-16	99.998992	2.000000
0.14	1.732600E+16	16.333333	1.234286E-06	3.940403E-17	7.241500E-16	2.722015E-16	99.998891	2.000000
0.15	1.732598E+16	17.500000	1.234286E-06	4.696851E-17	7.758747E-16	3.110874E-16	99.998786	2.000000
0.16	1.732596E+16	18.666667	1.234286E-06	5.539222E-17	8.275992E-16	3.525656E-16	99.998677	2.000000
0.17	1.732594E+16	19.833333	1.234286E-06	6.471955E-17	8.793238E-16	3.966362E-16	99.998564	2.000000
0.18	1.732592E+16	21.000000	1.234286E-06	7.499486E-17	9.310483E-16	4.432991E-16	99.998448	2.000000
0.19	1.732590E+16	22.166667	1.234286E-06	8.626252E-17	9.827727E-16	4.925544E-16	99.998328	2.000000
0.20	1.732588E+16	23.333333	1.234286E-06	9.856689E-17	1.034497E-15	5.444021E-16	99.998204	2.000000
0.21	1.732586E+16	24.500000	1.234286E-06	1.119523E-16	1.086221E-15	5.988421E-16	99.998076	2.000000
0.22	1.732583E+16	25.666667	1.234286E-06	1.264633E-16	1.137946E-15	6.558745E-16	99.997944	2.000000
0.23	1.732581E+16	26.833333	1.234286E-06	1.421440E-16	1.189670E-15	7.154992E-16	99.997808	2.000000
0.24	1.732579E+16	28.000000	1.234286E-06	1.590389E-16	1.241394E-15	7.777163E-16	99.997667	2.000000
0.25	1.732576E+16	29.166667	1.234286E-06	1.771924E-16	1.293118E-15	8.425257E-16	99.997523	2.000000
0.26	1.732574E+16	30.333333	1.234286E-06	1.966487E-16	1.344842E-15	9.099274E-16	99.997375	2.000000
0.27	1.732571E+16	31.500000	1.234286E-06	2.174524E-16	1.396566E-15	9.799215E-16	99.997222	2.000000
0.28	1.732568E+16	32.666667	1.234286E-06	2.396477E-16	1.448289E-15	1.052508E-15	99.997065	2.000000
0.29	1.732565E+16	33.833333	1.234286E-06	2.632791E-16	1.500013E-15	1.127687E-15	99.996904	2.000000
0.30	1.732563E+16	35.000000	1.234286E-06	2.883908E-16	1.551737E-15	1.205458E-15	99.996739	2.000000
0.31	1.732560E+16	36.166667	1.234286E-06	3.150273E-16	1.603460E-15	1.285821E-15	99.996569	2.000000
0.32	1.732557E+16	37.333333	1.234286E-06	3.432329E-16	1.655183E-15	1.368777E-15	99.996394	2.000000
0.33	1.732554E+16	38.500000	1.234286E-06	3.730520E-16	1.706907E-15	1.454325E-15	99.996215	2.000000
0.34	1.732550E+16	39.666667	1.234286E-06	4.045289E-16	1.758630E-15	1.542465E-15	99.996032	2.000000
0.35	1.732547E+16	40.833333	1.234286E-06	4.377081E-16	1.810353E-15	1.633198E-15	99.995844	2.000000
0.36	1.732544E+16	42.000000	1.234286E-06	4.726338E-16	1.862076E-15	1.726522E-15	99.995651	2.000000
0.37	1.732540E+16	43.166667	1.234286E-06	5.093505E-16	1.913799E-15	1.822440E-15	99.995453	2.000000
0.38	1.732537E+16	44.333333	1.234286E-06	5.479025E-16	1.965522E-15	1.920949E-15	99.995251	2.000000
0.39	1.732533E+16	45.500000	1.234286E-06	5.883342E-16	2.017245E-15	2.022051E-15	99.995044	2.000000
0.40	1.732530E+16	46.666667	1.234286E-06	6.306899E-16	2.068967E-15	2.125745E-15	99.994833	2.000000
0.41	1.732526E+16	47.833333	1.234286E-06	6.750140E-16	2.120690E-15	2.232031E-15	99.994616	2.000000
0.42	1.732522E+16	49.000000	1.234286E-06	7.213509E-16	2.172412E-15	2.340909E-15	99.994394	2.000000
0.43	1.732518E+16	50.166667	1.234286E-06	7.697449E-16	2.224134E-15	2.452380E-15	99.994168	2.000000
0.44	1.732514E+16	51.333333	1.234286E-06	8.202405E-16	2.275857E-15	2.566443E-15	99.993936	2.000000
0.45	1.732510E+16	52.500000	1.234286E-06	8.728819E-16	2.327579E-15	2.683098E-15	99.993699	2.000000

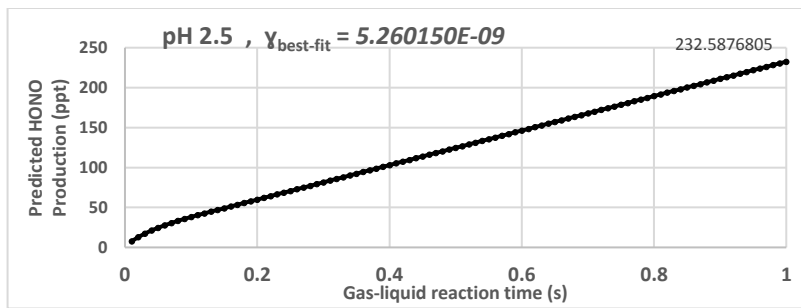
0.46	1.732506E+16	53.666667	1.234286E-06	9.277135E-16	2.379300E-15	2.802346E-15	99.993458	2.000000
0.47	1.732501E+16	54.833333	1.234286E-06	9.847797E-16	2.431022E-15	2.924186E-15	99.993211	2.000000
0.48	1.732497E+16	56.000000	1.234286E-06	1.044125E-15	2.482744E-15	3.048618E-15	99.992958	2.000000
0.49	1.732493E+16	57.166667	1.234286E-06	1.105793E-15	2.534465E-15	3.175642E-15	99.992701	2.000000
0.50	1.732488E+16	58.333333	1.234286E-06	1.169830E-15	2.586187E-15	3.305258E-15	99.992438	2.000000
0.51	1.732483E+16	59.500000	1.234286E-06	1.236278E-15	2.637908E-15	3.437467E-15	99.992170	2.000000
0.52	1.732479E+16	60.666667	1.234286E-06	1.305182E-15	2.689629E-15	3.572267E-15	99.991897	2.000000
0.53	1.732474E+16	61.833333	1.234286E-06	1.376588E-15	2.741350E-15	3.709660E-15	99.991618	2.000000
0.54	1.732469E+16	63.000000	1.234286E-06	1.450538E-15	2.793071E-15	3.849645E-15	99.991333	2.000000
0.55	1.732464E+16	64.166667	1.234286E-06	1.527078E-15	2.844791E-15	3.992223E-15	99.991043	2.000000
0.56	1.732459E+16	65.333333	1.234286E-06	1.606252E-15	2.896512E-15	4.137392E-15	99.990747	2.000000
0.57	1.732454E+16	66.500000	1.234286E-06	1.688104E-15	2.948232E-15	4.285154E-15	99.990446	2.000000
0.58	1.732448E+16	67.666667	1.234286E-06	1.772679E-15	2.999952E-15	4.435507E-15	99.990139	2.000000
0.59	1.732443E+16	68.833333	1.234286E-06	1.860020E-15	3.051672E-15	4.588453E-15	99.989827	2.000000
0.60	1.732437E+16	70.000000	1.234286E-06	1.950173E-15	3.103392E-15	4.743991E-15	99.989508	2.000000
0.61	1.732432E+16	71.166667	1.234286E-06	2.043182E-15	3.155112E-15	4.902121E-15	99.989184	2.000000
0.62	1.732426E+16	72.333333	1.234286E-06	2.139090E-15	3.206832E-15	5.062844E-15	99.988853	2.000000
0.63	1.732420E+16	73.500000	1.234286E-06	2.237943E-15	3.258551E-15	5.226158E-15	99.988517	2.000000
0.64	1.732414E+16	74.666667	1.234286E-06	2.339785E-15	3.310270E-15	5.392064E-15	99.988175	2.000000
0.65	1.732408E+16	75.833333	1.234286E-06	2.444660E-15	3.361989E-15	5.560563E-15	99.987827	2.000000
0.66	1.732402E+16	77.000000	1.234286E-06	2.552612E-15	3.413708E-15	5.731653E-15	99.987473	2.000000
0.67	1.732396E+16	78.166667	1.234286E-06	2.663686E-15	3.465426E-15	5.905336E-15	99.987113	2.000000
0.68	1.732389E+16	79.333333	1.234286E-06	2.777926E-15	3.517145E-15	6.081611E-15	99.986746	2.000000
0.69	1.732383E+16	80.500000	1.234286E-06	2.895377E-15	3.568863E-15	6.260478E-15	99.986373	2.000000
0.70	1.732376E+16	81.666667	1.234286E-06	3.016082E-15	3.620581E-15	6.441936E-15	99.985994	2.000000
0.71	1.732370E+16	82.833333	1.234286E-06	3.140087E-15	3.672299E-15	6.625987E-15	99.985609	2.000000
0.72	1.732363E+16	84.000000	1.234286E-06	3.267435E-15	3.724017E-15	6.812630E-15	99.985218	2.000000
0.73	1.732356E+16	85.166667	1.234286E-06	3.398172E-15	3.775734E-15	7.001865E-15	99.984819	2.000000
0.74	1.732349E+16	86.333333	1.234286E-06	3.532340E-15	3.827451E-15	7.193692E-15	99.984415	2.000000
0.75	1.732342E+16	87.500000	1.234286E-06	3.669986E-15	3.879168E-15	7.388111E-15	99.984004	2.000000
0.76	1.732335E+16	88.666667	1.234286E-06	3.811152E-15	3.930885E-15	7.585121E-15	99.983587	2.000000
0.77	1.732327E+16	89.833333	1.234286E-06	3.955883E-15	3.982602E-15	7.784724E-15	99.983162	2.000000
0.78	1.732320E+16	91.000000	1.234286E-06	4.104225E-15	4.034318E-15	7.986919E-15	99.982732	2.000000
0.79	1.732312E+16	92.166667	1.234286E-06	4.256220E-15	4.086034E-15	8.191706E-15	99.982294	2.000000
0.80	1.732305E+16	93.333333	1.234286E-06	4.411914E-15	4.137750E-15	8.399084E-15	99.981850	2.000000
0.81	1.732297E+16	94.500000	1.234286E-06	4.571351E-15	4.189466E-15	8.609055E-15	99.981399	2.000000
0.82	1.732289E+16	95.666667	1.234286E-06	4.734575E-15	4.241181E-15	8.821617E-15	99.980941	2.000000
0.83	1.732281E+16	96.833333	1.234286E-06	4.901630E-15	4.292896E-15	9.036772E-15	99.980477	2.000000
0.84	1.732273E+16	98.000000	1.234286E-06	5.072561E-15	4.344611E-15	9.254518E-15	99.980005	2.000000
0.85	1.732264E+16	99.166667	1.234286E-06	5.247413E-15	4.396326E-15	9.474856E-15	99.979526	2.000000
0.86	1.732256E+16	100.333333	1.234286E-06	5.426228E-15	4.448040E-15	9.697786E-15	99.979041	2.000000
0.87	1.732247E+16	101.500000	1.234286E-06	5.609053E-15	4.499754E-15	9.923308E-15	99.978548	2.000000
0.88	1.732239E+16	102.666667	1.234286E-06	5.795931E-15	4.551468E-15	1.015142E-14	99.978048	2.000000
0.89	1.732230E+16	103.833333	1.234286E-06	5.986907E-15	4.603182E-15	1.038213E-14	99.977541	2.000000
0.90	1.732221E+16	105.000000	1.234286E-06	6.182024E-15	4.654895E-15	1.061542E-14	99.977027	2.000000
0.91	1.732212E+16	106.166667	1.234286E-06	6.381328E-15	4.706609E-15	1.085131E-14	99.976506	2.000000
0.92	1.732203E+16	107.333333	1.234286E-06	6.584862E-15	4.758321E-15	1.108979E-14	99.975977	2.000000
0.93	1.732194E+16	108.500000	1.234286E-06	6.792672E-15	4.810034E-15	1.133087E-14	99.975441	2.000000
0.94	1.732184E+16	109.666667	1.234286E-06	7.004801E-15	4.861746E-15	1.157453E-14	99.974897	2.000000
0.95	1.732175E+16	110.833333	1.234286E-06	7.221293E-15	4.913458E-15	1.182079E-14	99.974347	2.000000
0.96	1.732165E+16	112.000000	1.234286E-06	7.442193E-15	4.965170E-15	1.206963E-14	99.973788	2.000000
0.97	1.732155E+16	113.166667	1.234286E-06	7.667546E-15	5.016882E-15	1.232107E-14	99.973222	2.000000
0.98	1.732145E+16	114.333333	1.234286E-06	7.897396E-15	5.068593E-15	1.257510E-14	99.972649	2.000000
0.99	1.732135E+16	115.500000	1.234286E-06	8.131786E-15	5.120303E-15	1.283173E-14	99.972067	2.000000
1.00	1.732125E+16	116.666667	1.234286E-06	8.370762E-15	5.172014E-15	1.309094E-14	99.971479	2.000000



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732618E+16	1.166667	3.509922E-07	8.543259E-20	5.664468E-17	2.838959E-18	99.999936	2.000000
0.02	1.732617E+16	2.333333	4.963775E-07	3.771177E-19	1.132893E-16	8.516875E-18	99.999869	2.000000
0.03	1.732616E+16	3.500000	6.079354E-07	9.626190E-19	1.699339E-16	1.703375E-17	99.999799	2.000000
0.04	1.732614E+16	4.666667	7.019828E-07	1.914152E-18	2.265785E-16	2.838957E-17	99.999725	2.000000
0.05	1.732613E+16	5.833333	7.848401E-07	3.294602E-18	2.832230E-16	4.258434E-17	99.999648	2.000000
0.06	1.732612E+16	7.000000	8.597485E-07	5.160409E-18	3.398674E-16	5.961807E-17	99.999567	2.000000
0.07	1.732610E+16	8.166667	9.286338E-07	7.563216E-18	3.965119E-16	7.949073E-17	99.999482	2.000000
0.08	1.732609E+16	9.333333	9.927504E-07	1.055092E-17	4.531562E-16	1.022023E-16	99.999394	2.000000
0.09	1.732607E+16	10.500000	1.052970E-06	1.416839E-17	5.098005E-16	1.277529E-16	99.999302	2.000000
0.10	1.732605E+16	11.666667	1.109927E-06	1.845796E-17	5.664448E-16	1.561424E-16	99.999206	2.000000
0.11	1.732604E+16	12.833333	1.164100E-06	2.345983E-17	6.230890E-16	1.873708E-16	99.999107	2.000000
0.12	1.732602E+16	14.000000	1.215861E-06	2.921237E-17	6.797332E-16	2.214382E-16	99.999004	2.000000
0.13	1.732600E+16	15.166667	1.234286E-06	3.576010E-17	7.363772E-16	2.583445E-16	99.998896	2.000000
0.14	1.732598E+16	16.333333	1.234286E-06	4.315163E-17	7.930213E-16	2.980897E-16	99.998785	2.000000
0.15	1.732596E+16	17.500000	1.234286E-06	5.143553E-17	8.496652E-16	3.406738E-16	99.998670	2.000000
0.16	1.732594E+16	18.666667	1.234286E-06	6.066040E-17	9.063091E-16	3.860969E-16	99.998551	2.000000
0.17	1.732592E+16	19.833333	1.234286E-06	7.087482E-17	9.629529E-16	4.343588E-16	99.998428	2.000000
0.18	1.732590E+16	21.000000	1.234286E-06	8.212738E-17	1.019597E-15	4.854597E-16	99.998300	2.000000
0.19	1.732587E+16	22.166667	1.234286E-06	9.446667E-17	1.076240E-15	5.393995E-16	99.998169	2.000000
0.20	1.732585E+16	23.333333	1.234286E-06	1.079413E-16	1.132884E-15	5.961782E-16	99.998033	2.000000
0.21	1.732583E+16	24.500000	1.234286E-06	1.225998E-16	1.189527E-15	6.557958E-16	99.997893	2.000000
0.22	1.732580E+16	25.666667	1.234286E-06	1.384908E-16	1.246171E-15	7.182523E-16	99.997748	2.000000
0.23	1.732578E+16	26.833333	1.234286E-06	1.556628E-16	1.302814E-15	7.835477E-16	99.997599	2.000000
0.24	1.732575E+16	28.000000	1.234286E-06	1.741645E-16	1.359458E-15	8.516819E-16	99.997446	2.000000
0.25	1.732572E+16	29.166667	1.234286E-06	1.940445E-16	1.416101E-15	9.226551E-16	99.997288	2.000000
0.26	1.732569E+16	30.333333	1.234286E-06	2.153513E-16	1.472744E-15	9.964671E-16	99.997125	2.000000
0.27	1.732566E+16	31.500000	1.234286E-06	2.381336E-16	1.529387E-15	1.073118E-15	99.996958	2.000000
0.28	1.732563E+16	32.666667	1.234286E-06	2.624398E-16	1.586030E-15	1.152608E-15	99.996786	2.000000
0.29	1.732560E+16	33.833333	1.234286E-06	2.883186E-16	1.642672E-15	1.234936E-15	99.996610	2.000000
0.30	1.732557E+16	35.000000	1.234286E-06	3.158186E-16	1.699315E-15	1.320104E-15	99.996428	2.000000
0.31	1.732554E+16	36.166667	1.234286E-06	3.449884E-16	1.755958E-15	1.408110E-15	99.996242	2.000000
0.32	1.732551E+16	37.333333	1.234286E-06	3.758765E-16	1.812600E-15	1.498955E-15	99.996051	2.000000
0.33	1.732547E+16	38.500000	1.234286E-06	4.085316E-16	1.869243E-15	1.592640E-15	99.995855	2.000000
0.34	1.732544E+16	39.666667	1.234286E-06	4.430021E-16	1.925885E-15	1.689162E-15	99.995654	2.000000
0.35	1.732540E+16	40.833333	1.234286E-06	4.793368E-16	1.982527E-15	1.788524E-15	99.995448	2.000000
0.36	1.732537E+16	42.000000	1.234286E-06	5.175842E-16	2.039169E-15	1.890725E-15	99.995237	2.000000
0.37	1.732533E+16	43.166667	1.234286E-06	5.577928E-16	2.095811E-15	1.995764E-15	99.995021	2.000000
0.38	1.732529E+16	44.333333	1.234286E-06	6.000113E-16	2.152453E-15	2.103642E-15	99.994800	2.000000
0.39	1.732525E+16	45.500000	1.234286E-06	6.442882E-16	2.209094E-15	2.214359E-15	99.994573	2.000000
0.40	1.732521E+16	46.666667	1.234286E-06	6.906722E-16	2.265736E-15	2.327915E-15	99.994341	2.000000
0.41	1.732517E+16	47.833333	1.234286E-06	7.392118E-16	2.322377E-15	2.444309E-15	99.994104	2.000000
0.42	1.732513E+16	49.000000	1.234286E-06	7.899556E-16	2.379018E-15	2.563543E-15	99.993861	2.000000
0.43	1.732508E+16	50.166667	1.234286E-06	8.429521E-16	2.435659E-15	2.685615E-15	99.993613	2.000000
0.44	1.732504E+16	51.333333	1.234286E-06	8.982500E-16	2.492300E-15	2.810526E-15	99.993359	2.000000
0.45	1.732500E+16	52.500000	1.234286E-06	9.558978E-16	2.548941E-15	2.938275E-15	99.993100	2.000000

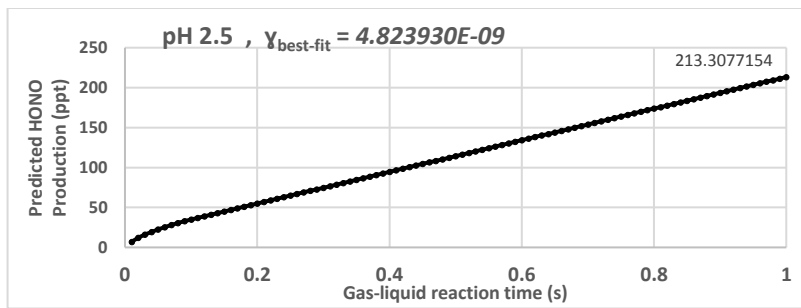


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0.47	1.732490E+16	54.833333	1.234286E-06	1.078438E-15	2.662222E-15	3.202291E-15	99.992565	2.000000
0.48	1.732486E+16	56.000000	1.234286E-06	1.143427E-15	2.718863E-15	3.338557E-15	99.992289	2.000000
0.49	1.732481E+16	57.166667	1.234286E-06	1.210960E-15	2.775503E-15	3.477662E-15	99.992007	2.000000
0.50	1.732476E+16	58.333333	1.234286E-06	1.281087E-15	2.832143E-15	3.619605E-15	99.991719	2.000000
0.51	1.732471E+16	59.500000	1.234286E-06	1.353854E-15	2.888783E-15	3.764387E-15	99.991425	2.000000
0.52	1.732465E+16	60.666667	1.234286E-06	1.429312E-15	2.945422E-15	3.912008E-15	99.991126	2.000000
0.53	1.732460E+16	61.833333	1.234286E-06	1.507508E-15	3.002062E-15	4.062467E-15	99.990820	2.000000
0.54	1.732455E+16	63.000000	1.234286E-06	1.588492E-15	3.058701E-15	4.215765E-15	99.990509	2.000000
0.55	1.732449E+16	64.166667	1.234286E-06	1.672311E-15	3.115340E-15	4.371902E-15	99.990191	2.000000
0.56	1.732444E+16	65.333333	1.234286E-06	1.759015E-15	3.171979E-15	4.530878E-15	99.989868	2.000000
0.57	1.732438E+16	66.500000	1.234286E-06	1.848651E-15	3.228618E-15	4.692692E-15	99.989538	2.000000
0.58	1.732432E+16	67.666667	1.234286E-06	1.941269E-15	3.285257E-15	4.857345E-15	99.989201	2.000000
0.59	1.732426E+16	68.833333	1.234286E-06	2.036917E-15	3.341895E-15	5.024836E-15	99.988859	2.000000
0.60	1.732420E+16	70.000000	1.234286E-06	2.135644E-15	3.398533E-15	5.195166E-15	99.988510	2.000000
0.61	1.732414E+16	71.166667	1.234286E-06	2.237498E-15	3.455171E-15	5.368335E-15	99.988155	2.000000
0.62	1.732408E+16	72.333333	1.234286E-06	2.342528E-15	3.511809E-15	5.544342E-15	99.987793	2.000000
0.63	1.732401E+16	73.500000	1.234286E-06	2.450782E-15	3.568447E-15	5.723188E-15	99.987425	2.000000
0.64	1.732395E+16	74.666667	1.234286E-06	2.562309E-15	3.625084E-15	5.904873E-15	99.987051	2.000000
0.65	1.732388E+16	75.833333	1.234286E-06	2.677157E-15	3.681721E-15	6.089396E-15	99.986669	2.000000
0.66	1.732381E+16	77.000000	1.234286E-06	2.795376E-15	3.738358E-15	6.276757E-15	99.986282	2.000000
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0.68	1.732368E+16	79.333333	1.234286E-06	3.042118E-15	3.851632E-15	6.659996E-15	99.985486	2.000000
0.69	1.732361E+16	80.500000	1.234286E-06	3.170739E-15	3.908268E-15	6.855874E-15	99.985077	2.000000
0.70	1.732353E+16	81.666667	1.234286E-06	3.302924E-15	3.964904E-15	7.054589E-15	99.984662	2.000000
0.71	1.732346E+16	82.833333	1.234286E-06	3.438721E-15	4.021540E-15	7.256144E-15	99.984241	2.000000
0.72	1.732339E+16	84.000000	1.234286E-06	3.578181E-15	4.078175E-15	7.460537E-15	99.983812	2.000000
0.73	1.732331E+16	85.166667	1.234286E-06	3.721350E-15	4.134810E-15	7.667768E-15	99.983376	2.000000
0.74	1.732323E+16	86.333333	1.234286E-06	3.868279E-15	4.191445E-15	7.877838E-15	99.982933	2.000000
0.75	1.732316E+16	87.500000	1.234286E-06	4.019014E-15	4.248080E-15	8.090746E-15	99.982483	2.000000
0.76	1.732308E+16	88.666667	1.234286E-06	4.173606E-15	4.304715E-15	8.306492E-15	99.982026	2.000000
0.77	1.732300E+16	89.833333	1.234286E-06	4.332101E-15	4.361349E-15	8.525078E-15	99.981561	2.000000
0.78	1.732291E+16	91.000000	1.234286E-06	4.494550E-15	4.417983E-15	8.746501E-15	99.981089	2.000000
0.79	1.732283E+16	92.166667	1.234286E-06	4.661001E-15	4.474617E-15	8.970763E-15	99.980610	2.000000
0.80	1.732275E+16	93.333333	1.234286E-06	4.831501E-15	4.531250E-15	9.197863E-15	99.980124	2.000000
0.81	1.732266E+16	94.500000	1.234286E-06	5.006100E-15	4.587883E-15	9.427802E-15	99.979630	2.000000
0.82	1.732257E+16	95.666667	1.234286E-06	5.184847E-15	4.644516E-15	9.660579E-15	99.979129	2.000000
0.83	1.732249E+16	96.833333	1.234286E-06	5.367789E-15	4.701149E-15	9.896194E-15	99.978620	2.000000
0.84	1.732240E+16	98.000000	1.234286E-06	5.554976E-15	4.757781E-15	1.013465E-14	99.978103	2.000000
0.85	1.732231E+16	99.166667	1.234286E-06	5.746456E-15	4.814413E-15	1.037594E-14	99.977579	2.000000
0.86	1.732221E+16	100.333333	1.234286E-06	5.942277E-15	4.871045E-15	1.062007E-14	99.977047	2.000000
0.87	1.732212E+16	101.500000	1.234286E-06	6.142488E-15	4.927676E-15	1.086704E-14	99.976508	2.000000
0.88	1.732203E+16	102.666667	1.234286E-06	6.347138E-15	4.984307E-15	1.111685E-14	99.975961	2.000000
0.89	1.732193E+16	103.833333	1.234286E-06	6.556275E-15	5.040938E-15	1.136949E-14	99.975405	2.000000
0.90	1.732183E+16	105.000000	1.234286E-06	6.769948E-15	5.097569E-15	1.162497E-14	99.974842	2.000000
0.91	1.732173E+16	106.166667	1.234286E-06	6.988206E-15	5.154199E-15	1.188330E-14	99.974271	2.000000
0.92	1.732163E+16	107.333333	1.234286E-06	7.211096E-15	5.210829E-15	1.214446E-14	99.973692	2.000000
0.93	1.732153E+16	108.500000	1.234286E-06	7.438668E-15	5.267458E-15	1.240845E-14	99.973105	2.000000
0.94	1.732143E+16	109.666667	1.234286E-06	7.670970E-15	5.324087E-15	1.267529E-14	99.972510	2.000000
0.95	1.732132E+16	110.833333	1.234286E-06	7.908050E-15	5.380716E-15	1.294496E-14	99.971907	2.000000
0.96	1.732122E+16	112.000000	1.234286E-06	8.149958E-15	5.437345E-15	1.321748E-14	99.971295	2.000000
0.97	1.732111E+16	113.166667	1.234286E-06	8.396741E-15	5.493973E-15	1.349283E-14	99.970676	2.000000
0.98	1.732100E+16	114.333333	1.234286E-06	8.648449E-15	5.550600E-15	1.377102E-14	99.970048	2.000000
0.99	1.732089E+16	115.500000	1.234286E-06	8.905129E-15	5.607228E-15	1.405204E-14	99.969411	2.000000
1.00	1.732078E+16	116.666667	1.234286E-06	9.166831E-15	5.663855E-15	1.433591E-14	99.968766	1.999999



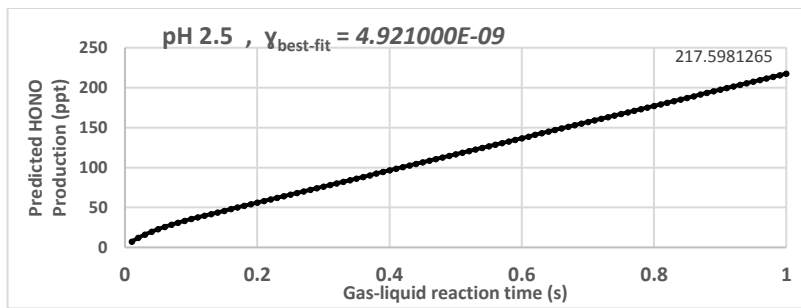
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732616E+16	1.166667	3.509918E-07	1.970256E-19	1.306344E-16	2.070416E-17	99.999838	2.500000
0.02	1.732613E+16	2.333333	4.963765E-07	8.697129E-19	2.612686E-16	6.211244E-17	99.999653	2.500000
0.03	1.732609E+16	3.500000	6.079333E-07	2.220002E-18	3.919025E-16	1.242248E-16	99.999445	2.500000
0.04	1.732605E+16	4.666667	7.019793E-07	4.414439E-18	5.225361E-16	2.070412E-16	99.999214	2.500000
0.05	1.732601E+16	5.833333	7.848347E-07	7.598047E-18	6.531694E-16	3.105616E-16	99.998960	2.500000
0.06	1.732596E+16	7.000000	8.597409E-07	1.190099E-17	7.838023E-16	4.347858E-16	99.998682	2.500000
0.07	1.732591E+16	8.166667	9.286235E-07	1.744237E-17	9.144349E-16	5.797140E-16	99.998381	2.500000
0.08	1.732585E+16	9.333333	9.927371E-07	2.433265E-17	1.045067E-15	7.453459E-16	99.998057	2.500000
0.09	1.732579E+16	10.500000	1.052953E-06	3.267529E-17	1.175699E-15	9.316815E-16	99.997708	2.500000
0.10	1.732573E+16	11.666667	1.109906E-06	4.256794E-17	1.306330E-15	1.138721E-15	99.997336	2.500000
0.11	1.732566E+16	12.833333	1.164074E-06	5.410331E-17	1.436960E-15	1.366464E-15	99.996940	2.500000
0.12	1.732559E+16	14.000000	1.215831E-06	6.736987E-17	1.567591E-15	1.614910E-15	99.996520	2.500000
0.13	1.732551E+16	15.166667	1.234286E-06	8.247031E-17	1.698220E-15	1.884059E-15	99.996076	2.500000
0.14	1.732543E+16	16.333333	1.234286E-06	9.951669E-17	1.828849E-15	2.173912E-15	99.995607	2.500000
0.15	1.732534E+16	17.500000	1.234286E-06	1.186210E-16	1.959477E-15	2.484468E-15	99.995114	2.500000
0.16	1.732525E+16	18.666667	1.234286E-06	1.398954E-16	2.090105E-15	2.815727E-15	99.994597	2.500000
0.17	1.732516E+16	19.833333	1.234286E-06	1.634518E-16	2.220732E-15	3.167689E-15	99.994055	2.500000
0.18	1.732506E+16	21.000000	1.234286E-06	1.894024E-16	2.351358E-15	3.540354E-15	99.993488	2.500000
0.19	1.732496E+16	22.166667	1.234286E-06	2.178591E-16	2.481983E-15	3.933722E-15	99.992896	2.500000
0.20	1.732485E+16	23.333333	1.234286E-06	2.489340E-16	2.612608E-15	4.347792E-15	99.992280	2.500000
0.21	1.732474E+16	24.500000	1.234286E-06	2.827391E-16	2.743232E-15	4.782564E-15	99.991638	2.499999
0.22	1.732463E+16	25.666667	1.234286E-06	3.193865E-16	2.873854E-15	5.238038E-15	99.990971	2.499999
0.23	1.732451E+16	26.833333	1.234286E-06	3.589882E-16	3.004476E-15	5.714215E-15	99.990279	2.499999
0.24	1.732438E+16	28.000000	1.234286E-06	4.016562E-16	3.135097E-15	6.211094E-15	99.989561	2.499999
0.25	1.732425E+16	29.166667	1.234286E-06	4.475027E-16	3.265717E-15	6.728674E-15	99.988818	2.499999
0.26	1.732412E+16	30.333333	1.234286E-06	4.966395E-16	3.396337E-15	7.266956E-15	99.988049	2.499999
0.27	1.732398E+16	31.500000	1.234286E-06	5.491788E-16	3.526955E-15	7.825940E-15	99.987254	2.499999
0.28	1.732384E+16	32.666667	1.234286E-06	6.052325E-16	3.657572E-15	8.405625E-15	99.986434	2.499999
0.29	1.732369E+16	33.833333	1.234286E-06	6.649127E-16	3.788187E-15	9.006011E-15	99.985587	2.499999
0.30	1.732354E+16	35.000000	1.234286E-06	7.283315E-16	3.918802E-15	9.627097E-15	99.984714	2.499999
0.31	1.732339E+16	36.166667	1.234286E-06	7.956008E-16	4.049416E-15	1.026888E-14	99.983815	2.499999
0.32	1.732323E+16	37.333333	1.234286E-06	8.668326E-16	4.180028E-15	1.093137E-14	99.982889	2.499999
0.33	1.732306E+16	38.500000	1.234286E-06	9.421391E-16	4.310639E-15	1.161456E-14	99.981937	2.499999
0.34	1.732289E+16	39.666667	1.234286E-06	1.021632E-15	4.441249E-15	1.231845E-14	99.980958	2.499999
0.35	1.732272E+16	40.833333	1.234286E-06	1.105424E-15	4.571857E-15	1.304304E-14	99.979953	2.499999
0.36	1.732254E+16	42.000000	1.234286E-06	1.193626E-15	4.702465E-15	1.378833E-14	99.978920	2.499998
0.37	1.732236E+16	43.166667	1.234286E-06	1.286351E-15	4.833070E-15	1.455431E-14	99.977861	2.499998
0.38	1.732217E+16	44.333333	1.234286E-06	1.383711E-15	4.963675E-15	1.534100E-14	99.976774	2.499998
0.39	1.732197E+16	45.500000	1.234286E-06	1.485817E-15	5.094278E-15	1.614838E-14	99.975661	2.499998
0.40	1.732178E+16	46.666667	1.234286E-06	1.592782E-15	5.224879E-15	1.697647E-14	99.974519	2.499998
0.41	1.732157E+16	47.833333	1.234286E-06	1.704717E-15	5.355479E-15	1.782525E-14	99.973351	2.499998
0.42	1.732137E+16	49.000000	1.234286E-06	1.821735E-15	5.486077E-15	1.869473E-14	99.972154	2.499998
0.43	1.732115E+16	50.166667	1.234286E-06	1.943948E-15	5.616674E-15	1.958491E-14	99.970930	2.499998
0.44	1.732094E+16	51.333333	1.234286E-06	2.071468E-15	5.747269E-15	2.049578E-14	99.969679	2.499998
0.45	1.732072E+16	52.500000	1.234286E-06	2.204406E-15	5.877863E-15	2.142736E-14	99.968399	2.499998

0.46	1.732049E+16	53.666667	1.234286E-06	2.342875E-15	6.008454E-15	2.237963E-14	99.967091	2.499998
0.47	1.732026E+16	54.833333	1.234286E-06	2.486986E-15	6.139044E-15	2.335260E-14	99.965755	2.499997
0.48	1.732002E+16	56.000000	1.234286E-06	2.636852E-15	6.269633E-15	2.434626E-14	99.964390	2.499997
0.49	1.731978E+16	57.166667	1.234286E-06	2.792584E-15	6.400219E-15	2.536062E-14	99.962998	2.499997
0.50	1.731953E+16	58.333333	1.234286E-06	2.954295E-15	6.530804E-15	2.639567E-14	99.961576	2.499997
0.51	1.731928E+16	59.500000	1.234286E-06	3.122097E-15	6.661386E-15	2.745143E-14	99.960126	2.499997
0.52	1.731903E+16	60.666667	1.234286E-06	3.296101E-15	6.791967E-15	2.852787E-14	99.958647	2.499997
0.53	1.731877E+16	61.833333	1.234286E-06	3.476420E-15	6.922546E-15	2.962501E-14	99.957139	2.499997
0.54	1.731850E+16	63.000000	1.234286E-06	3.663164E-15	7.053123E-15	3.074285E-14	99.955602	2.499997
0.55	1.731823E+16	64.166667	1.234286E-06	3.856448E-15	7.183697E-15	3.188138E-14	99.954036	2.499996
0.56	1.731795E+16	65.333333	1.234286E-06	4.056381E-15	7.314270E-15	3.304060E-14	99.952441	2.499996
0.57	1.731767E+16	66.500000	1.234286E-06	4.263077E-15	7.444841E-15	3.422052E-14	99.950816	2.499996
0.58	1.731738E+16	67.666667	1.234286E-06	4.476647E-15	7.575409E-15	3.542113E-14	99.949162	2.499996
0.59	1.731709E+16	68.833333	1.234286E-06	4.697203E-15	7.705975E-15	3.664243E-14	99.947478	2.499996
0.60	1.731679E+16	70.000000	1.234286E-06	4.924857E-15	7.836539E-15	3.788443E-14	99.945765	2.499996
0.61	1.731649E+16	71.166667	1.234286E-06	5.159722E-15	7.967101E-15	3.914712E-14	99.944021	2.499996
0.62	1.731618E+16	72.333333	1.234286E-06	5.401908E-15	8.097660E-15	4.043050E-14	99.942248	2.499996
0.63	1.731587E+16	73.500000	1.234286E-06	5.651528E-15	8.228217E-15	4.173457E-14	99.940444	2.499995
0.64	1.731555E+16	74.666667	1.234286E-06	5.908694E-15	8.358772E-15	4.305933E-14	99.938610	2.499995
0.65	1.731523E+16	75.833333	1.234286E-06	6.173518E-15	8.489324E-15	4.440478E-14	99.936746	2.499995
0.66	1.731490E+16	77.000000	1.234286E-06	6.446111E-15	8.619874E-15	4.577092E-14	99.934851	2.499995
0.67	1.731457E+16	78.166667	1.234286E-06	6.726586E-15	8.750421E-15	4.715775E-14	99.932926	2.499995
0.68	1.731423E+16	79.333333	1.234286E-06	7.015054E-15	8.880966E-15	4.856528E-14	99.930970	2.499995
0.69	1.731389E+16	80.500000	1.234286E-06	7.311628E-15	9.011508E-15	4.999348E-14	99.928983	2.499994
0.70	1.731354E+16	81.666667	1.234286E-06	7.616419E-15	9.142047E-15	5.144238E-14	99.926965	2.499994
0.71	1.731318E+16	82.833333	1.234286E-06	7.929539E-15	9.272584E-15	5.291197E-14	99.924916	2.499994
0.72	1.731282E+16	84.000000	1.234286E-06	8.251101E-15	9.403118E-15	5.440224E-14	99.922836	2.499994
0.73	1.731246E+16	85.166667	1.234286E-06	8.581215E-15	9.533649E-15	5.591320E-14	99.920725	2.499994
0.74	1.731208E+16	86.333333	1.234286E-06	8.919994E-15	9.664178E-15	5.744485E-14	99.918582	2.499994
0.75	1.731171E+16	87.500000	1.234286E-06	9.267550E-15	9.794704E-15	5.899718E-14	99.916408	2.499993
0.76	1.731133E+16	88.666667	1.234286E-06	9.623994E-15	9.925227E-15	6.057020E-14	99.914202	2.499993
0.77	1.731094E+16	89.833333	1.234286E-06	9.989438E-15	1.005575E-14	6.216390E-14	99.911964	2.499993
0.78	1.731054E+16	91.000000	1.234286E-06	1.036400E-14	1.018626E-14	6.377829E-14	99.909695	2.499993
0.79	1.731015E+16	92.166667	1.234286E-06	1.074778E-14	1.031678E-14	6.541336E-14	99.907393	2.499993
0.80	1.730974E+16	93.333333	1.234286E-06	1.114089E-14	1.044729E-14	6.706912E-14	99.905059	2.499993
0.81	1.730933E+16	94.500000	1.234286E-06	1.154346E-14	1.057780E-14	6.874555E-14	99.902693	2.499992
0.82	1.730892E+16	95.666667	1.234286E-06	1.195558E-14	1.070830E-14	7.044267E-14	99.900294	2.499992
0.83	1.730849E+16	96.833333	1.234286E-06	1.237738E-14	1.083880E-14	7.216048E-14	99.897863	2.499992
0.84	1.730807E+16	98.000000	1.234286E-06	1.280896E-14	1.096930E-14	7.389896E-14	99.895400	2.499992
0.85	1.730764E+16	99.166667	1.234286E-06	1.325043E-14	1.109980E-14	7.565813E-14	99.892903	2.499992
0.86	1.730720E+16	100.333333	1.234286E-06	1.370191E-14	1.123029E-14	7.743797E-14	99.890374	2.499991
0.87	1.730675E+16	101.500000	1.234286E-06	1.416351E-14	1.136078E-14	7.923850E-14	99.887812	2.499991
0.88	1.730630E+16	102.666667	1.234286E-06	1.463534E-14	1.149126E-14	8.105970E-14	99.885217	2.499991
0.89	1.730585E+16	103.833333	1.234286E-06	1.511752E-14	1.162174E-14	8.290158E-14	99.882588	2.499991
0.90	1.730539E+16	105.000000	1.234286E-06	1.561014E-14	1.175222E-14	8.476414E-14	99.879926	2.499991
0.91	1.730492E+16	106.166667	1.234286E-06	1.611334E-14	1.188270E-14	8.664738E-14	99.877231	2.499990
0.92	1.730445E+16	107.333333	1.234286E-06	1.662721E-14	1.201317E-14	8.855130E-14	99.874502	2.499990
0.93	1.730397E+16	108.500000	1.234286E-06	1.715187E-14	1.214363E-14	9.047589E-14	99.871740	2.499990
0.94	1.730348E+16	109.666667	1.234286E-06	1.768743E-14	1.227410E-14	9.242116E-14	99.868943	2.499990
0.95	1.730299E+16	110.833333	1.234286E-06	1.823401E-14	1.240456E-14	9.438710E-14	99.866113	2.499989
0.96	1.730250E+16	112.000000	1.234286E-06	1.879170E-14	1.253501E-14	9.637372E-14	99.863249	2.499989
0.97	1.730200E+16	113.166667	1.234286E-06	1.936064E-14	1.266547E-14	9.838101E-14	99.860350	2.499989
0.98	1.730149E+16	114.333333	1.234286E-06	1.994092E-14	1.279592E-14	1.004090E-13	99.857417	2.499989
0.99	1.730097E+16	115.500000	1.234286E-06	2.053267E-14	1.292636E-14	1.024576E-13	99.854450	2.499989
1.00	1.730045E+16	116.666667	1.234286E-06	2.113598E-14	1.305680E-14	1.045269E-13	99.851448	2.499988



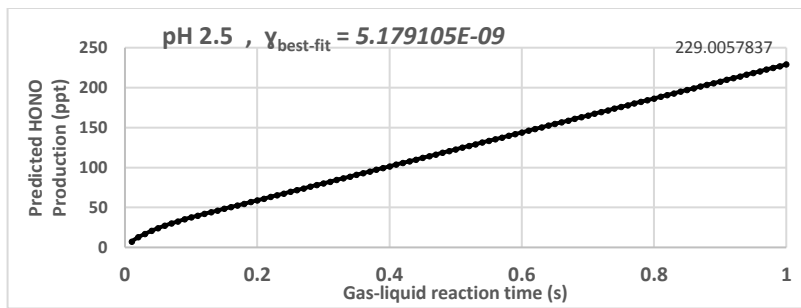
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732617E+16	1.166667	3.509919E-07	1.806864E-19	1.198010E-16	1.898718E-17	99.999851	2.500000
0.02	1.732614E+16	2.333333	4.963766E-07	7.975883E-19	2.396019E-16	5.696152E-17	99.999682	2.500000
0.03	1.732610E+16	3.500000	6.079335E-07	2.035899E-18	3.594025E-16	1.139230E-16	99.999491	2.500000
0.04	1.732607E+16	4.666667	7.019797E-07	4.048353E-18	4.792028E-16	1.898715E-16	99.999279	2.500000
0.05	1.732603E+16	5.833333	7.848353E-07	6.967948E-18	5.990029E-16	2.848070E-16	99.999046	2.500000
0.06	1.732598E+16	7.000000	8.597419E-07	1.091405E-17	7.188027E-16	3.987296E-16	99.998792	2.500000
0.07	1.732593E+16	8.166667	9.286248E-07	1.599589E-17	8.386021E-16	5.316390E-16	99.998516	2.500000
0.08	1.732588E+16	9.333333	9.927387E-07	2.231476E-17	9.584012E-16	6.835353E-16	99.998218	2.500000
0.09	1.732583E+16	10.500000	1.052955E-06	2.996555E-17	1.078200E-15	8.544185E-16	99.997898	2.500000
0.10	1.732577E+16	11.666667	1.109908E-06	3.903781E-17	1.197998E-15	1.044288E-15	99.997557	2.500000
0.11	1.732570E+16	12.833333	1.164077E-06	4.961657E-17	1.317796E-15	1.253145E-15	99.997194	2.500000
0.12	1.732564E+16	14.000000	1.215834E-06	6.178294E-17	1.437593E-15	1.480988E-15	99.996808	2.500000
0.13	1.732557E+16	15.166667	1.234286E-06	7.563112E-17	1.557390E-15	1.727818E-15	99.996401	2.500000
0.14	1.732549E+16	16.333333	1.234286E-06	9.126385E-17	1.677187E-15	1.993634E-15	99.995971	2.500000
0.15	1.732541E+16	17.500000	1.234286E-06	1.087839E-16	1.796983E-15	2.278436E-15	99.995519	2.500000
0.16	1.732533E+16	18.666667	1.234286E-06	1.282940E-16	1.916778E-15	2.582225E-15	99.995045	2.500000
0.17	1.732525E+16	19.833333	1.234286E-06	1.498970E-16	2.036573E-15	2.904999E-15	99.994548	2.500000
0.18	1.732516E+16	21.000000	1.234286E-06	1.736955E-16	2.156367E-15	3.246760E-15	99.994028	2.500000
0.19	1.732506E+16	22.166667	1.234286E-06	1.997923E-16	2.276160E-15	3.607507E-15	99.993485	2.500000
0.20	1.732496E+16	23.333333	1.234286E-06	2.282902E-16	2.395953E-15	3.987239E-15	99.992920	2.500000
0.21	1.732486E+16	24.500000	1.234286E-06	2.592920E-16	2.515745E-15	4.385958E-15	99.992331	2.500000
0.22	1.732476E+16	25.666667	1.234286E-06	2.929003E-16	2.635536E-15	4.803662E-15	99.991720	2.499999
0.23	1.732465E+16	26.833333	1.234286E-06	3.292179E-16	2.755327E-15	5.240351E-15	99.991085	2.499999
0.24	1.732453E+16	28.000000	1.234286E-06	3.683476E-16	2.875116E-15	5.696025E-15	99.990427	2.499999
0.25	1.732441E+16	29.166667	1.234286E-06	4.103921E-16	2.994905E-15	6.170685E-15	99.989745	2.499999
0.26	1.732429E+16	30.333333	1.234286E-06	4.554542E-16	3.114694E-15	6.664330E-15	99.989040	2.499999
0.27	1.732417E+16	31.500000	1.234286E-06	5.036366E-16	3.234481E-15	7.176960E-15	99.988311	2.499999
0.28	1.732404E+16	32.666667	1.234286E-06	5.550420E-16	3.354267E-15	7.708574E-15	99.987559	2.499999
0.29	1.732390E+16	33.833333	1.234286E-06	6.097732E-16	3.474053E-15	8.259173E-15	99.986782	2.499999
0.30	1.732376E+16	35.000000	1.234286E-06	6.679328E-16	3.593837E-15	8.828757E-15	99.985982	2.499999
0.31	1.732362E+16	36.166667	1.234286E-06	7.296238E-16	3.713620E-15	9.417324E-15	99.985157	2.499999
0.32	1.732347E+16	37.333333	1.234286E-06	7.949487E-16	3.833403E-15	1.002488E-14	99.984308	2.499999
0.33	1.732332E+16	38.500000	1.234286E-06	8.640104E-16	3.953184E-15	1.065141E-14	99.983435	2.499999
0.34	1.732317E+16	39.666667	1.234286E-06	9.369115E-16	4.072965E-15	1.129693E-14	99.982537	2.499999
0.35	1.732301E+16	40.833333	1.234286E-06	1.013755E-15	4.192744E-15	1.196143E-14	99.981615	2.499999
0.36	1.732284E+16	42.000000	1.234286E-06	1.094643E-15	4.312522E-15	1.264492E-14	99.980668	2.499999
0.37	1.732267E+16	43.166667	1.234286E-06	1.179679E-15	4.432299E-15	1.334739E-14	99.979697	2.499999
0.38	1.732250E+16	44.333333	1.234286E-06	1.268965E-15	4.552075E-15	1.406884E-14	99.978700	2.499998
0.39	1.732232E+16	45.500000	1.234286E-06	1.362604E-15	4.671849E-15	1.480928E-14	99.977679	2.499998
0.40	1.732214E+16	46.666667	1.234286E-06	1.460699E-15	4.791623E-15	1.556870E-14	99.976632	2.499998
0.41	1.732196E+16	47.833333	1.234286E-06	1.563353E-15	4.911395E-15	1.634710E-14	99.975561	2.499998
0.42	1.732177E+16	49.000000	1.234286E-06	1.670667E-15	5.031165E-15	1.714448E-14	99.974464	2.499998
0.43	1.732157E+16	50.166667	1.234286E-06	1.782746E-15	5.150935E-15	1.796084E-14	99.973341	2.499998
0.44	1.732137E+16	51.333333	1.234286E-06	1.899691E-15	5.270703E-15	1.879619E-14	99.972193	2.499998
0.45	1.732117E+16	52.500000	1.234286E-06	2.021606E-15	5.390469E-15	1.965052E-14	99.971019	2.499998

0.46	1.732096E+16	53.666667	1.234286E-06	2.148593E-15	5.510234E-15	2.052383E-14	99.969820	2.499998
0.47	1.732075E+16	54.833333	1.234286E-06	2.280754E-15	5.629998E-15	2.141612E-14	99.968595	2.499998
0.48	1.732053E+16	56.000000	1.234286E-06	2.418193E-15	5.749760E-15	2.232739E-14	99.967343	2.499998
0.49	1.732031E+16	57.166667	1.234286E-06	2.561012E-15	5.869521E-15	2.325764E-14	99.966066	2.499997
0.50	1.732009E+16	58.333333	1.234286E-06	2.709314E-15	5.989280E-15	2.420687E-14	99.964762	2.499997
0.51	1.731986E+16	59.500000	1.234286E-06	2.863202E-15	6.109037E-15	2.517508E-14	99.963432	2.499997
0.52	1.731962E+16	60.666667	1.234286E-06	3.022777E-15	6.228793E-15	2.616227E-14	99.962076	2.499997
0.53	1.731938E+16	61.833333	1.234286E-06	3.188144E-15	6.348548E-15	2.716844E-14	99.960693	2.499997
0.54	1.731914E+16	63.000000	1.234286E-06	3.359404E-15	6.468300E-15	2.819359E-14	99.959284	2.499997
0.55	1.731889E+16	64.166667	1.234286E-06	3.536661E-15	6.588051E-15	2.923772E-14	99.957848	2.499997
0.56	1.731863E+16	65.333333	1.234286E-06	3.720016E-15	6.707800E-15	3.030082E-14	99.956385	2.499997
0.57	1.731838E+16	66.500000	1.234286E-06	3.909573E-15	6.827547E-15	3.138291E-14	99.954895	2.499997
0.58	1.731811E+16	67.666667	1.234286E-06	4.105435E-15	6.947293E-15	3.248397E-14	99.953378	2.499996
0.59	1.731785E+16	68.833333	1.234286E-06	4.307703E-15	7.067037E-15	3.360401E-14	99.951833	2.499996
0.60	1.731757E+16	70.000000	1.234286E-06	4.516481E-15	7.186778E-15	3.474303E-14	99.950262	2.499996
0.61	1.731730E+16	71.166667	1.234286E-06	4.731871E-15	7.306518E-15	3.590102E-14	99.948663	2.499996
0.62	1.731701E+16	72.333333	1.234286E-06	4.953977E-15	7.426256E-15	3.707799E-14	99.947036	2.499996
0.63	1.731673E+16	73.500000	1.234286E-06	5.182900E-15	7.545992E-15	3.827394E-14	99.945382	2.499996
0.64	1.731644E+16	74.666667	1.234286E-06	5.418743E-15	7.665726E-15	3.948886E-14	99.943700	2.499996
0.65	1.731614E+16	75.833333	1.234286E-06	5.661609E-15	7.785458E-15	4.072276E-14	99.941991	2.499995
0.66	1.731584E+16	77.000000	1.234286E-06	5.911601E-15	7.905188E-15	4.197564E-14	99.940253	2.499995
0.67	1.731553E+16	78.166667	1.234286E-06	6.168821E-15	8.024915E-15	4.324749E-14	99.938488	2.499995
0.68	1.731522E+16	79.333333	1.234286E-06	6.433371E-15	8.144641E-15	4.453831E-14	99.936694	2.499995
0.69	1.731491E+16	80.500000	1.234286E-06	6.705356E-15	8.264364E-15	4.584811E-14	99.934872	2.499995
0.70	1.731459E+16	81.666667	1.234286E-06	6.984876E-15	8.384085E-15	4.717688E-14	99.933021	2.499995
0.71	1.731426E+16	82.833333	1.234286E-06	7.272035E-15	8.503804E-15	4.852463E-14	99.931142	2.499995
0.72	1.731393E+16	84.000000	1.234286E-06	7.566935E-15	8.623521E-15	4.989134E-14	99.929235	2.499994
0.73	1.731359E+16	85.166667	1.234286E-06	7.869680E-15	8.743235E-15	5.127704E-14	99.927298	2.499994
0.74	1.731325E+16	86.333333	1.234286E-06	8.180371E-15	8.862947E-15	5.268170E-14	99.925333	2.499994
0.75	1.731291E+16	87.500000	1.234286E-06	8.499111E-15	8.982657E-15	5.410533E-14	99.923339	2.499994
0.76	1.731256E+16	88.666667	1.234286E-06	8.826003E-15	9.102364E-15	5.554794E-14	99.921316	2.499994
0.77	1.731220E+16	89.833333	1.234286E-06	9.161149E-15	9.222069E-15	5.700952E-14	99.919264	2.499994
0.78	1.731184E+16	91.000000	1.234286E-06	9.504653E-15	9.341771E-15	5.849007E-14	99.917182	2.499993
0.79	1.731148E+16	92.166667	1.234286E-06	9.856616E-15	9.461471E-15	5.998959E-14	99.915071	2.499993
0.80	1.731111E+16	93.333333	1.234286E-06	1.021714E-14	9.581168E-15	6.150808E-14	99.912931	2.499993
0.81	1.731073E+16	94.500000	1.234286E-06	1.058633E-14	9.700863E-15	6.304553E-14	99.910761	2.499993
0.82	1.731035E+16	95.666667	1.234286E-06	1.096429E-14	9.820554E-15	6.460196E-14	99.908561	2.499993
0.83	1.730996E+16	96.833333	1.234286E-06	1.135112E-14	9.940244E-15	6.617736E-14	99.906332	2.499993
0.84	1.730957E+16	98.000000	1.234286E-06	1.174691E-14	1.005993E-14	6.777172E-14	99.904072	2.499992
0.85	1.730917E+16	99.166667	1.234286E-06	1.215179E-14	1.017961E-14	6.938505E-14	99.901783	2.499992
0.86	1.730877E+16	100.333333	1.234286E-06	1.256584E-14	1.029930E-14	7.101735E-14	99.899463	2.499992
0.87	1.730836E+16	101.500000	1.234286E-06	1.298917E-14	1.041897E-14	7.266862E-14	99.897114	2.499992
0.88	1.730795E+16	102.666667	1.234286E-06	1.342189E-14	1.053865E-14	7.433885E-14	99.894733	2.499992
0.89	1.730753E+16	103.833333	1.234286E-06	1.386409E-14	1.065832E-14	7.602805E-14	99.892323	2.499992
0.90	1.730711E+16	105.000000	1.234286E-06	1.431588E-14	1.077799E-14	7.773621E-14	99.889882	2.499991
0.91	1.730668E+16	106.166667	1.234286E-06	1.477736E-14	1.089766E-14	7.946334E-14	99.887410	2.499991
0.92	1.730625E+16	107.333333	1.234286E-06	1.524863E-14	1.101732E-14	8.120943E-14	99.884907	2.499991
0.93	1.730581E+16	108.500000	1.234286E-06	1.572980E-14	1.113698E-14	8.297448E-14	99.882374	2.499991
0.94	1.730537E+16	109.666667	1.234286E-06	1.622096E-14	1.125664E-14	8.475850E-14	99.879809	2.499991
0.95	1.730492E+16	110.833333	1.234286E-06	1.672223E-14	1.137629E-14	8.656148E-14	99.877213	2.499990
0.96	1.730446E+16	112.000000	1.234286E-06	1.723369E-14	1.149595E-14	8.838342E-14	99.874586	2.499990
0.97	1.730400E+16	113.166667	1.234286E-06	1.775547E-14	1.161559E-14	9.022433E-14	99.871928	2.499990
0.98	1.730354E+16	114.333333	1.234286E-06	1.828765E-14	1.173524E-14	9.208420E-14	99.869238	2.499990
0.99	1.730306E+16	115.500000	1.234286E-06	1.883034E-14	1.185488E-14	9.396302E-14	99.866517	2.499990
1.00	1.730259E+16	116.666667	1.234286E-06	1.938365E-14	1.197452E-14	9.586081E-14	99.863764	2.499989



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732616E+16	1.166667	3.509919E-07	1.843223E-19	1.222117E-16	1.936926E-17	99.999848	2.500000
0.02	1.732613E+16	2.333333	4.963766E-07	8.136378E-19	2.444233E-16	5.810773E-17	99.999675	2.500000
0.03	1.732610E+16	3.500000	6.079335E-07	2.076867E-18	3.666346E-16	1.162154E-16	99.999481	2.500000
0.04	1.732606E+16	4.666667	7.019796E-07	4.129816E-18	4.888456E-16	1.936922E-16	99.999265	2.500000
0.05	1.732602E+16	5.833333	7.848352E-07	7.108161E-18	6.110563E-16	2.905381E-16	99.999027	2.500000
0.06	1.732598E+16	7.000000	8.597416E-07	1.113367E-17	7.332667E-16	4.067530E-16	99.998767	2.500000
0.07	1.732593E+16	8.166667	9.286245E-07	1.631777E-17	8.554768E-16	5.423369E-16	99.998486	2.500000
0.08	1.732588E+16	9.333333	9.927383E-07	2.276379E-17	9.776865E-16	6.972898E-16	99.998182	2.500000
0.09	1.732582E+16	10.500000	1.052955E-06	3.056854E-17	1.099896E-15	8.716115E-16	99.997856	2.500000
0.10	1.732576E+16	11.666667	1.109908E-06	3.982335E-17	1.222105E-15	1.065302E-15	99.997508	2.500000
0.11	1.732570E+16	12.833333	1.164077E-06	5.061498E-17	1.344313E-15	1.278361E-15	99.997137	2.500000
0.12	1.732563E+16	14.000000	1.215834E-06	6.302618E-17	1.466521E-15	1.510789E-15	99.996744	2.500000
0.13	1.732556E+16	15.166667	1.234286E-06	7.715301E-17	1.588729E-15	1.762585E-15	99.996329	2.500000
0.14	1.732548E+16	16.333333	1.234286E-06	9.310032E-17	1.710935E-15	2.033750E-15	99.995890	2.500000
0.15	1.732540E+16	17.500000	1.234286E-06	1.109729E-16	1.833142E-15	2.324283E-15	99.995429	2.500000
0.16	1.732532E+16	18.666667	1.234286E-06	1.308756E-16	1.955348E-15	2.634185E-15	99.994945	2.500000
0.17	1.732523E+16	19.833333	1.234286E-06	1.529133E-16	2.077553E-15	2.963455E-15	99.994438	2.500000
0.18	1.732514E+16	21.000000	1.234286E-06	1.771907E-16	2.199757E-15	3.312092E-15	99.993908	2.500000
0.19	1.732504E+16	22.166667	1.234286E-06	2.038126E-16	2.321961E-15	3.680098E-15	99.993354	2.500000
0.20	1.732494E+16	23.333333	1.234286E-06	2.328840E-16	2.444164E-15	4.067472E-15	99.992777	2.500000
0.21	1.732484E+16	24.500000	1.234286E-06	2.645095E-16	2.566367E-15	4.474213E-15	99.992177	2.500000
0.22	1.732473E+16	25.666667	1.234286E-06	2.987941E-16	2.688568E-15	4.900322E-15	99.991553	2.499999
0.23	1.732462E+16	26.833333	1.234286E-06	3.358425E-16	2.810769E-15	5.345798E-15	99.990906	2.499999
0.24	1.732450E+16	28.000000	1.234286E-06	3.757596E-16	2.932969E-15	5.810641E-15	99.990234	2.499999
0.25	1.732438E+16	29.166667	1.234286E-06	4.186502E-16	3.055168E-15	6.294852E-15	99.989539	2.499999
0.26	1.732425E+16	30.333333	1.234286E-06	4.646190E-16	3.177366E-15	6.798430E-15	99.988820	2.499999
0.27	1.732413E+16	31.500000	1.234286E-06	5.137709E-16	3.299564E-15	7.321375E-15	99.988076	2.499999
0.28	1.732399E+16	32.666667	1.234286E-06	5.662106E-16	3.421760E-15	7.863686E-15	99.987308	2.499999
0.29	1.732385E+16	33.833333	1.234286E-06	6.220431E-16	3.543956E-15	8.425364E-15	99.986516	2.499999
0.30	1.732371E+16	35.000000	1.234286E-06	6.813731E-16	3.666150E-15	9.006408E-15	99.985700	2.499999
0.31	1.732357E+16	36.166667	1.234286E-06	7.443054E-16	3.788344E-15	9.606819E-15	99.984858	2.499999
0.32	1.732342E+16	37.333333	1.234286E-06	8.109447E-16	3.910536E-15	1.022660E-14	99.983992	2.499999
0.33	1.732326E+16	38.500000	1.234286E-06	8.813960E-16	4.032727E-15	1.086574E-14	99.983102	2.499999
0.34	1.732310E+16	39.666667	1.234286E-06	9.557640E-16	4.154918E-15	1.152425E-14	99.982186	2.499999
0.35	1.732294E+16	40.833333	1.234286E-06	1.034153E-15	4.277107E-15	1.220212E-14	99.981245	2.499999
0.36	1.732277E+16	42.000000	1.234286E-06	1.116669E-15	4.399295E-15	1.289936E-14	99.980279	2.499999
0.37	1.732260E+16	43.166667	1.234286E-06	1.203416E-15	4.521481E-15	1.361596E-14	99.979288	2.499998
0.38	1.732243E+16	44.333333	1.234286E-06	1.294499E-15	4.643667E-15	1.435193E-14	99.978272	2.499998
0.39	1.732225E+16	45.500000	1.234286E-06	1.390022E-15	4.765851E-15	1.510726E-14	99.977230	2.499998
0.40	1.732206E+16	46.666667	1.234286E-06	1.490091E-15	4.888034E-15	1.588196E-14	99.976162	2.499998
0.41	1.732187E+16	47.833333	1.234286E-06	1.594810E-15	5.010215E-15	1.667602E-14	99.975069	2.499998
0.42	1.732168E+16	49.000000	1.234286E-06	1.704284E-15	5.132395E-15	1.748945E-14	99.973950	2.499998
0.43	1.732148E+16	50.166667	1.234286E-06	1.818618E-15	5.254574E-15	1.832224E-14	99.972805	2.499998
0.44	1.732128E+16	51.333333	1.234286E-06	1.937916E-15	5.376752E-15	1.917439E-14	99.971633	2.499998
0.45	1.732107E+16	52.500000	1.234286E-06	2.062284E-15	5.498927E-15	2.004591E-14	99.970436	2.499998

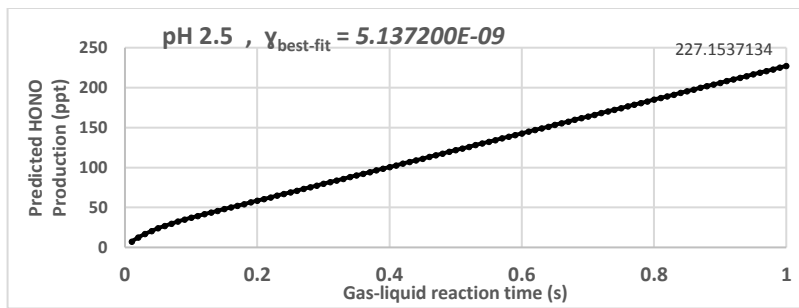
0.46	1.732086E+16	53.666667	1.234286E-06	2.191825E-15	5.621102E-15	2.093679E-14	99.969213	2.499998
0.47	1.732064E+16	54.833333	1.234286E-06	2.326646E-15	5.743275E-15	2.184703E-14	99.967963	2.499998
0.48	1.732042E+16	56.000000	1.234286E-06	2.466850E-15	5.865446E-15	2.277664E-14	99.966686	2.499997
0.49	1.732019E+16	57.166667	1.234286E-06	2.612543E-15	5.987616E-15	2.372561E-14	99.965383	2.499997
0.50	1.731996E+16	58.333333	1.234286E-06	2.763829E-15	6.109784E-15	2.469394E-14	99.964053	2.499997
0.51	1.731973E+16	59.500000	1.234286E-06	2.920813E-15	6.231950E-15	2.568163E-14	99.962697	2.499997
0.52	1.731949E+16	60.666667	1.234286E-06	3.083599E-15	6.354115E-15	2.668868E-14	99.961313	2.499997
0.53	1.731924E+16	61.833333	1.234286E-06	3.252293E-15	6.476278E-15	2.771509E-14	99.959902	2.499997
0.54	1.731899E+16	63.000000	1.234286E-06	3.426999E-15	6.598439E-15	2.876087E-14	99.958465	2.499997
0.55	1.731874E+16	64.166667	1.234286E-06	3.607822E-15	6.720599E-15	2.982600E-14	99.957000	2.499997
0.56	1.731848E+16	65.333333	1.234286E-06	3.794866E-15	6.842756E-15	3.091050E-14	99.955507	2.499997
0.57	1.731822E+16	66.500000	1.234286E-06	3.988237E-15	6.964912E-15	3.201435E-14	99.953987	2.499996
0.58	1.731795E+16	67.666667	1.234286E-06	4.188039E-15	7.087066E-15	3.313757E-14	99.952439	2.499996
0.59	1.731768E+16	68.833333	1.234286E-06	4.394377E-15	7.209218E-15	3.428014E-14	99.950864	2.499996
0.60	1.731740E+16	70.000000	1.234286E-06	4.607356E-15	7.331368E-15	3.544207E-14	99.949261	2.499996
0.61	1.731712E+16	71.166667	1.234286E-06	4.827080E-15	7.453516E-15	3.662337E-14	99.947630	2.499996
0.62	1.731683E+16	72.333333	1.234286E-06	5.053654E-15	7.575662E-15	3.782402E-14	99.945971	2.499996
0.63	1.731654E+16	73.500000	1.234286E-06	5.287182E-15	7.697806E-15	3.904402E-14	99.944283	2.499996
0.64	1.731624E+16	74.666667	1.234286E-06	5.527770E-15	7.819948E-15	4.028339E-14	99.942568	2.499996
0.65	1.731594E+16	75.833333	1.234286E-06	5.775523E-15	7.942088E-15	4.154211E-14	99.940824	2.499995
0.66	1.731563E+16	77.000000	1.234286E-06	6.030544E-15	8.064226E-15	4.282019E-14	99.939051	2.499995
0.67	1.731532E+16	78.166667	1.234286E-06	6.292939E-15	8.186361E-15	4.411763E-14	99.937250	2.499995
0.68	1.731500E+16	79.333333	1.234286E-06	6.562812E-15	8.308494E-15	4.543442E-14	99.935420	2.499995
0.69	1.731468E+16	80.500000	1.234286E-06	6.840268E-15	8.430625E-15	4.677057E-14	99.933561	2.499995
0.70	1.731435E+16	81.666667	1.234286E-06	7.125412E-15	8.552754E-15	4.812607E-14	99.931674	2.499995
0.71	1.731402E+16	82.833333	1.234286E-06	7.418348E-15	8.674880E-15	4.950093E-14	99.929757	2.499994
0.72	1.731368E+16	84.000000	1.234286E-06	7.719181E-15	8.797004E-15	5.089514E-14	99.927811	2.499994
0.73	1.731334E+16	85.166667	1.234286E-06	8.028016E-15	8.919126E-15	5.230871E-14	99.925836	2.499994
0.74	1.731299E+16	86.333333	1.234286E-06	8.344957E-15	9.041245E-15	5.374163E-14	99.923831	2.499994
0.75	1.731264E+16	87.500000	1.234286E-06	8.670110E-15	9.163361E-15	5.519391E-14	99.921797	2.499994
0.76	1.731228E+16	88.666667	1.234286E-06	9.003578E-15	9.285475E-15	5.666553E-14	99.919733	2.499994
0.77	1.731192E+16	89.833333	1.234286E-06	9.345467E-15	9.407587E-15	5.815651E-14	99.917639	2.499994
0.78	1.731155E+16	91.000000	1.234286E-06	9.695880E-15	9.529696E-15	5.966684E-14	99.915516	2.499993
0.79	1.731118E+16	92.166667	1.234286E-06	1.005492E-14	9.651802E-15	6.119653E-14	99.913363	2.499993
0.80	1.731080E+16	93.333333	1.234286E-06	1.042270E-14	9.773906E-15	6.274556E-14	99.911179	2.499993
0.81	1.731042E+16	94.500000	1.234286E-06	1.079932E-14	9.896007E-15	6.431395E-14	99.908966	2.499993
0.82	1.731003E+16	95.666667	1.234286E-06	1.118488E-14	1.001810E-14	6.590168E-14	99.906722	2.499993
0.83	1.730964E+16	96.833333	1.234286E-06	1.157949E-14	1.014020E-14	6.750877E-14	99.904447	2.499992
0.84	1.730924E+16	98.000000	1.234286E-06	1.198325E-14	1.026229E-14	6.913521E-14	99.902142	2.499992
0.85	1.730883E+16	99.166667	1.234286E-06	1.239627E-14	1.038438E-14	7.078099E-14	99.899807	2.499992
0.86	1.730842E+16	100.333333	1.234286E-06	1.281865E-14	1.050647E-14	7.244612E-14	99.897441	2.499992
0.87	1.730801E+16	101.500000	1.234286E-06	1.325050E-14	1.062855E-14	7.413060E-14	99.895044	2.499992
0.88	1.730759E+16	102.666667	1.234286E-06	1.369192E-14	1.075063E-14	7.583443E-14	99.892616	2.499992
0.89	1.730716E+16	103.833333	1.234286E-06	1.414301E-14	1.087271E-14	7.755760E-14	99.890157	2.499991
0.90	1.730673E+16	105.000000	1.234286E-06	1.460389E-14	1.099479E-14	7.930013E-14	99.887666	2.499991
0.91	1.730629E+16	106.166667	1.234286E-06	1.507465E-14	1.111686E-14	8.106199E-14	99.885145	2.499991
0.92	1.730585E+16	107.333333	1.234286E-06	1.555540E-14	1.123893E-14	8.284320E-14	99.882592	2.499991
0.93	1.730540E+16	108.500000	1.234286E-06	1.604625E-14	1.136099E-14	8.464376E-14	99.880007	2.499991
0.94	1.730495E+16	109.666667	1.234286E-06	1.654729E-14	1.148306E-14	8.646366E-14	99.877391	2.499990
0.95	1.730449E+16	110.833333	1.234286E-06	1.705864E-14	1.160512E-14	8.830291E-14	99.874743	2.499990
0.96	1.730402E+16	112.000000	1.234286E-06	1.758040E-14	1.172717E-14	9.016150E-14	99.872063	2.499990
0.97	1.730355E+16	113.166667	1.234286E-06	1.811267E-14	1.184922E-14	9.203943E-14	99.869352	2.499990
0.98	1.730308E+16	114.333333	1.234286E-06	1.865555E-14	1.197127E-14	9.393670E-14	99.866608	2.499990
0.99	1.730260E+16	115.500000	1.234286E-06	1.920916E-14	1.209332E-14	9.585332E-14	99.863832	2.499989
1.00	1.730211E+16	116.666667	1.234286E-06	1.977359E-14	1.221536E-14	9.778927E-14	99.861024	2.499989



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732616E+16	1.166667	3.509918E-07	1.939899E-19	1.286217E-16	2.038517E-17	99.999840	2.500000
0.02	1.732613E+16	2.333333	4.963765E-07	8.563129E-19	2.572432E-16	6.115546E-17	99.999658	2.500000
0.03	1.732610E+16	3.500000	6.079333E-07	2.185798E-18	3.858644E-16	1.223108E-16	99.999453	2.500000
0.04	1.732606E+16	4.666667	7.019793E-07	4.346424E-18	5.144853E-16	2.038512E-16	99.999226	2.500000
0.05	1.732601E+16	5.833333	7.848348E-07	7.480982E-18	6.431059E-16	3.057766E-16	99.998976	2.500000
0.06	1.732597E+16	7.000000	8.597411E-07	1.171763E-17	7.717261E-16	4.280870E-16	99.998703	2.500000
0.07	1.732592E+16	8.166667	9.286238E-07	1.717363E-17	9.003460E-16	5.707822E-16	99.998406	2.500000
0.08	1.732586E+16	9.333333	9.927374E-07	2.395775E-17	1.028965E-15	7.338622E-16	99.998087	2.500000
0.09	1.732580E+16	10.500000	1.052953E-06	3.217185E-17	1.157584E-15	9.173269E-16	99.997744	2.500000
0.10	1.732574E+16	11.666667	1.109906E-06	4.191208E-17	1.286203E-15	1.121176E-15	99.997377	2.500000
0.11	1.732567E+16	12.833333	1.164075E-06	5.326972E-17	1.414821E-15	1.345410E-15	99.996987	2.500000
0.12	1.732560E+16	14.000000	1.215832E-06	6.633188E-17	1.543438E-15	1.590029E-15	99.996573	2.500000
0.13	1.732552E+16	15.166667	1.234286E-06	8.119966E-17	1.672055E-15	1.855031E-15	99.996136	2.500000
0.14	1.732544E+16	16.333333	1.234286E-06	9.798340E-17	1.800672E-15	2.140418E-15	99.995675	2.500000
0.15	1.732536E+16	17.500000	1.234286E-06	1.167934E-16	1.929288E-15	2.446190E-15	99.995189	2.500000
0.16	1.732527E+16	18.666667	1.234286E-06	1.377400E-16	2.057903E-15	2.772345E-15	99.994680	2.500000
0.17	1.732518E+16	19.833333	1.234286E-06	1.609335E-16	2.186517E-15	3.118884E-15	99.994146	2.500000
0.18	1.732508E+16	21.000000	1.234286E-06	1.864842E-16	2.315131E-15	3.485808E-15	99.993588	2.500000
0.19	1.732498E+16	22.166667	1.234286E-06	2.145025E-16	2.443744E-15	3.873114E-15	99.993006	2.500000
0.20	1.732487E+16	23.333333	1.234286E-06	2.450986E-16	2.572356E-15	4.280805E-15	99.992399	2.500000
0.21	1.732476E+16	24.500000	1.234286E-06	2.783829E-16	2.700967E-15	4.708879E-15	99.991767	2.499999
0.22	1.732465E+16	25.666667	1.234286E-06	3.144656E-16	2.829578E-15	5.157336E-15	99.991110	2.499999
0.23	1.732453E+16	26.833333	1.234286E-06	3.534572E-16	2.958187E-15	5.626176E-15	99.990429	2.499999
0.24	1.732441E+16	28.000000	1.234286E-06	3.954679E-16	3.086796E-15	6.115400E-15	99.989722	2.499999
0.25	1.732428E+16	29.166667	1.234286E-06	4.406079E-16	3.215404E-15	6.625006E-15	99.988990	2.499999
0.26	1.732415E+16	30.333333	1.234286E-06	4.889877E-16	3.344010E-15	7.154995E-15	99.988233	2.499999
0.27	1.732402E+16	31.500000	1.234286E-06	5.407175E-16	3.472616E-15	7.705367E-15	99.987451	2.499999
0.28	1.732388E+16	32.666667	1.234286E-06	5.959076E-16	3.601221E-15	8.276120E-15	99.986643	2.499999
0.29	1.732373E+16	33.833333	1.234286E-06	6.546684E-16	3.729825E-15	8.867256E-15	99.985809	2.499999
0.30	1.732358E+16	35.000000	1.234286E-06	7.171101E-16	3.858427E-15	9.478775E-15	99.984950	2.499999
0.31	1.732343E+16	36.166667	1.234286E-06	7.833430E-16	3.987029E-15	1.011067E-14	99.984064	2.499999
0.32	1.732327E+16	37.333333	1.234286E-06	8.534774E-16	4.115629E-15	1.076296E-14	99.983153	2.499999
0.33	1.732311E+16	38.500000	1.234286E-06	9.276236E-16	4.244228E-15	1.143562E-14	99.982215	2.499999
0.34	1.732294E+16	39.666667	1.234286E-06	1.005892E-15	4.372826E-15	1.212866E-14	99.981252	2.499999
0.35	1.732277E+16	40.833333	1.234286E-06	1.088393E-15	4.501423E-15	1.284209E-14	99.980262	2.499999
0.36	1.732260E+16	42.000000	1.234286E-06	1.175236E-15	4.630018E-15	1.357589E-14	99.979245	2.499998
0.37	1.732241E+16	43.166667	1.234286E-06	1.266533E-15	4.758612E-15	1.433008E-14	99.978202	2.499998
0.38	1.732223E+16	44.333333	1.234286E-06	1.362392E-15	4.887204E-15	1.510465E-14	99.977132	2.499998
0.39	1.732204E+16	45.500000	1.234286E-06	1.462925E-15	5.015795E-15	1.589959E-14	99.976036	2.499998
0.40	1.732184E+16	46.666667	1.234286E-06	1.568242E-15	5.144385E-15	1.671492E-14	99.974912	2.499998
0.41	1.732164E+16	47.833333	1.234286E-06	1.678453E-15	5.272973E-15	1.755063E-14	99.973761	2.499998
0.42	1.732144E+16	49.000000	1.234286E-06	1.793669E-15	5.401560E-15	1.840671E-14	99.972583	2.499998
0.43	1.732123E+16	50.166667	1.234286E-06	1.913999E-15	5.530145E-15	1.928318E-14	99.971378	2.499998
0.44	1.732102E+16	51.333333	1.234286E-06	2.039554E-15	5.658729E-15	2.018002E-14	99.970146	2.499998
0.45	1.732080E+16	52.500000	1.234286E-06	2.170444E-15	5.787311E-15	2.109724E-14	99.968886	2.499998

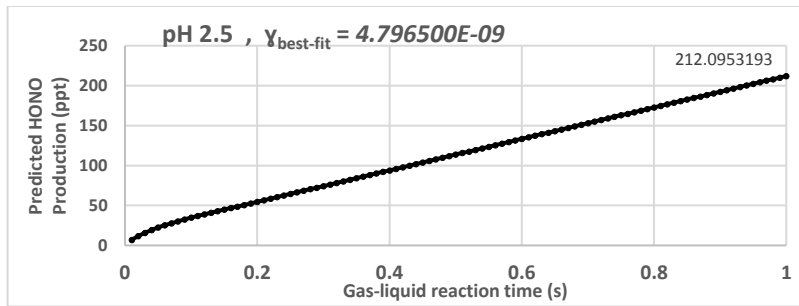


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0.47	1.732035E+16	54.833333	1.234286E-06	2.448671E-15	6.044470E-15	2.299282E-14	99.966282	2.499997
0.48	1.732012E+16	56.000000	1.234286E-06	2.596228E-15	6.173047E-15	2.397118E-14	99.964939	2.499997
0.49	1.731988E+16	57.166667	1.234286E-06	2.749561E-15	6.301622E-15	2.496991E-14	99.963568	2.499997
0.50	1.731964E+16	58.333333	1.234286E-06	2.908781E-15	6.430195E-15	2.598902E-14	99.962168	2.499997
0.51	1.731939E+16	59.500000	1.234286E-06	3.073997E-15	6.558767E-15	2.702851E-14	99.960740	2.499997
0.52	1.731914E+16	60.666667	1.234286E-06	3.245321E-15	6.687336E-15	2.808837E-14	99.959284	2.499997
0.53	1.731888E+16	61.833333	1.234286E-06	3.422861E-15	6.815904E-15	2.916861E-14	99.957800	2.499997
0.54	1.731862E+16	63.000000	1.234286E-06	3.606729E-15	6.944470E-15	3.026923E-14	99.956286	2.499997
0.55	1.731835E+16	64.166667	1.234286E-06	3.797035E-15	7.073034E-15	3.139022E-14	99.954744	2.499997
0.56	1.731808E+16	65.333333	1.234286E-06	3.993888E-15	7.201596E-15	3.253158E-14	99.953174	2.499996
0.57	1.731780E+16	66.500000	1.234286E-06	4.197400E-15	7.330155E-15	3.369333E-14	99.951574	2.499996
0.58	1.731752E+16	67.666667	1.234286E-06	4.407680E-15	7.458713E-15	3.487544E-14	99.949945	2.499996
0.59	1.731723E+16	68.833333	1.234286E-06	4.624839E-15	7.587269E-15	3.607793E-14	99.948287	2.499996
0.60	1.731694E+16	70.000000	1.234286E-06	4.848986E-15	7.715822E-15	3.730080E-14	99.946600	2.499996
0.61	1.731664E+16	71.166667	1.234286E-06	5.080232E-15	7.844373E-15	3.854403E-14	99.944883	2.499996
0.62	1.731634E+16	72.333333	1.234286E-06	5.318688E-15	7.972922E-15	3.980764E-14	99.943137	2.499996
0.63	1.731603E+16	73.500000	1.234286E-06	5.564463E-15	8.101469E-15	4.109163E-14	99.941361	2.499995
0.64	1.731572E+16	74.666667	1.234286E-06	5.817667E-15	8.230013E-15	4.239598E-14	99.939556	2.499995
0.65	1.731540E+16	75.833333	1.234286E-06	6.078411E-15	8.358555E-15	4.372071E-14	99.937720	2.499995
0.66	1.731508E+16	77.000000	1.234286E-06	6.346806E-15	8.487095E-15	4.506581E-14	99.935855	2.499995
0.67	1.731475E+16	78.166667	1.234286E-06	6.622960E-15	8.615632E-15	4.643128E-14	99.933959	2.499995
0.68	1.731442E+16	79.333333	1.234286E-06	6.906985E-15	8.744167E-15	4.781712E-14	99.932033	2.499995
0.69	1.731408E+16	80.500000	1.234286E-06	7.198990E-15	8.872699E-15	4.922333E-14	99.930077	2.499995
0.70	1.731373E+16	81.666667	1.234286E-06	7.499086E-15	9.001229E-15	5.064991E-14	99.928090	2.499994
0.71	1.731338E+16	82.833333	1.234286E-06	7.807383E-15	9.129756E-15	5.209686E-14	99.926073	2.499994
0.72	1.731303E+16	84.000000	1.234286E-06	8.123991E-15	9.258280E-15	5.356417E-14	99.924025	2.499994
0.73	1.731267E+16	85.166667	1.234286E-06	8.449021E-15	9.386802E-15	5.505186E-14	99.921946	2.499994
0.74	1.731230E+16	86.333333	1.234286E-06	8.782581E-15	9.515321E-15	5.655992E-14	99.919836	2.499994
0.75	1.731193E+16	87.500000	1.234286E-06	9.124783E-15	9.643837E-15	5.808834E-14	99.917696	2.499994
0.76	1.731155E+16	88.666667	1.234286E-06	9.475737E-15	9.772351E-15	5.963713E-14	99.915524	2.499993
0.77	1.731117E+16	89.833333	1.234286E-06	9.835553E-15	9.900861E-15	6.120628E-14	99.913320	2.499993
0.78	1.731079E+16	91.000000	1.234286E-06	1.020434E-14	1.002937E-14	6.279581E-14	99.911086	2.499993
0.79	1.731039E+16	92.166667	1.234286E-06	1.058221E-14	1.015787E-14	6.440569E-14	99.908819	2.499993
0.80	1.730999E+16	93.333333	1.234286E-06	1.096927E-14	1.028638E-14	6.603595E-14	99.906521	2.499993
0.81	1.730959E+16	94.500000	1.234286E-06	1.136564E-14	1.041488E-14	6.768656E-14	99.904192	2.499992
0.82	1.730918E+16	95.666667	1.234286E-06	1.177141E-14	1.054337E-14	6.935755E-14	99.901830	2.499992
0.83	1.730877E+16	96.833333	1.234286E-06	1.218671E-14	1.067186E-14	7.104889E-14	99.899437	2.499992
0.84	1.730835E+16	98.000000	1.234286E-06	1.261164E-14	1.080035E-14	7.276060E-14	99.897011	2.499992
0.85	1.730792E+16	99.166667	1.234286E-06	1.304632E-14	1.092884E-14	7.449267E-14	99.894553	2.499992
0.86	1.730749E+16	100.333333	1.234286E-06	1.349085E-14	1.105732E-14	7.624511E-14	99.892063	2.499992
0.87	1.730705E+16	101.500000	1.234286E-06	1.394534E-14	1.118580E-14	7.801790E-14	99.889540	2.499991
0.88	1.730661E+16	102.666667	1.234286E-06	1.440990E-14	1.131428E-14	7.981106E-14	99.886985	2.499991
0.89	1.730616E+16	103.833333	1.234286E-06	1.488465E-14	1.144275E-14	8.162457E-14	99.884397	2.499991
0.90	1.730571E+16	105.000000	1.234286E-06	1.536969E-14	1.157122E-14	8.345845E-14	99.881776	2.499991
0.91	1.730525E+16	106.166667	1.234286E-06	1.586513E-14	1.169969E-14	8.531269E-14	99.879122	2.499991
0.92	1.730478E+16	107.333333	1.234286E-06	1.637109E-14	1.182815E-14	8.718728E-14	99.876435	2.499990
0.93	1.730431E+16	108.500000	1.234286E-06	1.688767E-14	1.195661E-14	8.908223E-14	99.873715	2.499990
0.94	1.730383E+16	109.666667	1.234286E-06	1.741498E-14	1.208507E-14	9.099754E-14	99.870962	2.499990
0.95	1.730335E+16	110.833333	1.234286E-06	1.795314E-14	1.221352E-14	9.293321E-14	99.868175	2.499990
0.96	1.730286E+16	112.000000	1.234286E-06	1.850225E-14	1.234197E-14	9.488923E-14	99.865355	2.499989
0.97	1.730237E+16	113.166667	1.234286E-06	1.906242E-14	1.247042E-14	9.686561E-14	99.862501	2.499989
0.98	1.730187E+16	114.333333	1.234286E-06	1.963377E-14	1.259886E-14	9.886235E-14	99.859613	2.499989
0.99	1.730136E+16	115.500000	1.234286E-06	2.021640E-14	1.272730E-14	1.008794E-13	99.856692	2.499989
1.00	1.730085E+16	116.666667	1.234286E-06	2.081043E-14	1.285573E-14	1.029169E-13	99.853736	2.499989



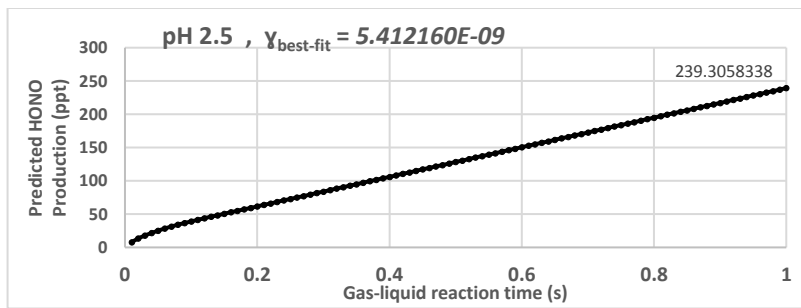
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO2}}$ (mol)	$\Phi_{\text{NO2}}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732616E+16	1.166667	3.509918E-07	1.924203E-19	1.275810E-16	2.022023E-17	99.999842	2.500000
0.02	1.732613E+16	2.333333	4.963765E-07	8.493843E-19	2.551618E-16	6.066064E-17	99.999661	2.500000
0.03	1.732610E+16	3.500000	6.079333E-07	2.168112E-18	3.827423E-16	1.213212E-16	99.999458	2.500000
0.04	1.732606E+16	4.666667	7.019794E-07	4.311256E-18	5.103225E-16	2.022019E-16	99.999232	2.500000
0.05	1.732602E+16	5.833333	7.848349E-07	7.420452E-18	6.379024E-16	3.033026E-16	99.998984	2.500000
0.06	1.732597E+16	7.000000	8.597412E-07	1.162282E-17	7.654820E-16	4.246233E-16	99.998713	2.500000
0.07	1.732592E+16	8.166667	9.286239E-07	1.703467E-17	8.930612E-16	5.661639E-16	99.998419	2.500000
0.08	1.732586E+16	9.333333	9.927375E-07	2.376390E-17	1.020640E-15	7.279244E-16	99.998102	2.500000
0.09	1.732580E+16	10.500000	1.052954E-06	3.191154E-17	1.148218E-15	9.099047E-16	99.997762	2.500000
0.10	1.732574E+16	11.666667	1.109906E-06	4.157296E-17	1.275796E-15	1.112105E-15	99.997398	2.500000
0.11	1.732567E+16	12.833333	1.164075E-06	5.283871E-17	1.403374E-15	1.334524E-15	99.997011	2.500000
0.12	1.732560E+16	14.000000	1.215832E-06	6.579518E-17	1.530950E-15	1.577164E-15	99.996601	2.500000
0.13	1.732553E+16	15.166667	1.234286E-06	8.054267E-17	1.658527E-15	1.840022E-15	99.996167	2.500000
0.14	1.732545E+16	16.333333	1.234286E-06	9.719060E-17	1.786103E-15	2.123100E-15	99.995710	2.500000
0.15	1.732536E+16	17.500000	1.234286E-06	1.158484E-16	1.913678E-15	2.426397E-15	99.995228	2.500000
0.16	1.732528E+16	18.666667	1.234286E-06	1.366255E-16	2.041252E-15	2.749914E-15	99.994723	2.500000
0.17	1.732519E+16	19.833333	1.234286E-06	1.596313E-16	2.168826E-15	3.093649E-15	99.994194	2.500000
0.18	1.732509E+16	21.000000	1.234286E-06	1.849753E-16	2.296399E-15	3.457604E-15	99.993640	2.500000
0.19	1.732499E+16	22.166667	1.234286E-06	2.127669E-16	2.423971E-15	3.841777E-15	99.993062	2.500000
0.20	1.732488E+16	23.333333	1.234286E-06	2.431155E-16	2.551543E-15	4.246169E-15	99.992460	2.500000
0.21	1.732478E+16	24.500000	1.234286E-06	2.761304E-16	2.679114E-15	4.670779E-15	99.991833	2.499999
0.22	1.732466E+16	25.666667	1.234286E-06	3.119213E-16	2.806684E-15	5.115608E-15	99.991182	2.499999
0.23	1.732455E+16	26.833333	1.234286E-06	3.505973E-16	2.934253E-15	5.580655E-15	99.990506	2.499999
0.24	1.732442E+16	28.000000	1.234286E-06	3.922681E-16	3.061821E-15	6.065920E-15	99.989805	2.499999
0.25	1.732430E+16	29.166667	1.234286E-06	4.370429E-16	3.189388E-15	6.571404E-15	99.989079	2.499999
0.26	1.732417E+16	30.333333	1.234286E-06	4.850313E-16	3.316955E-15	7.097105E-15	99.988328	2.499999
0.27	1.732403E+16	31.500000	1.234286E-06	5.363426E-16	3.444520E-15	7.643023E-15	99.987552	2.499999
0.28	1.732390E+16	32.666667	1.234286E-06	5.910862E-16	3.572084E-15	8.209159E-15	99.986751	2.499999
0.29	1.732375E+16	33.833333	1.234286E-06	6.493715E-16	3.699648E-15	8.795512E-15	99.985924	2.499999
0.30	1.732360E+16	35.000000	1.234286E-06	7.113080E-16	3.827210E-15	9.402083E-15	99.985071	2.499999
0.31	1.732345E+16	36.166667	1.234286E-06	7.770050E-16	3.954771E-15	1.002887E-14	99.984193	2.499999
0.32	1.732330E+16	37.333333	1.234286E-06	8.465720E-16	4.082331E-15	1.067587E-14	99.983289	2.499999
0.33	1.732313E+16	38.500000	1.234286E-06	9.201183E-16	4.209890E-15	1.134309E-14	99.982359	2.499999
0.34	1.732297E+16	39.666667	1.234286E-06	9.977534E-16	4.337447E-15	1.203053E-14	99.981403	2.499999
0.35	1.732280E+16	40.833333	1.234286E-06	1.079587E-15	4.465004E-15	1.273819E-14	99.980421	2.499999
0.36	1.732262E+16	42.000000	1.234286E-06	1.165727E-15	4.592559E-15	1.346605E-14	99.979413	2.499999
0.37	1.732244E+16	43.166667	1.234286E-06	1.256285E-15	4.720112E-15	1.421414E-14	99.978378	2.499998
0.38	1.732226E+16	44.333333	1.234286E-06	1.351369E-15	4.847665E-15	1.498244E-14	99.977317	2.499998
0.39	1.732207E+16	45.500000	1.234286E-06	1.451089E-15	4.975216E-15	1.577095E-14	99.976229	2.499998
0.40	1.732188E+16	46.666667	1.234286E-06	1.555554E-15	5.102765E-15	1.657968E-14	99.975115	2.499998
0.41	1.732168E+16	47.833333	1.234286E-06	1.664873E-15	5.230313E-15	1.740863E-14	99.973974	2.499998
0.42	1.732148E+16	49.000000	1.234286E-06	1.779157E-15	5.357860E-15	1.825779E-14	99.972805	2.499998
0.43	1.732127E+16	50.166667	1.234286E-06	1.898513E-15	5.485405E-15	1.912716E-14	99.971610	2.499998
0.44	1.732106E+16	51.333333	1.234286E-06	2.023052E-15	5.612948E-15	2.001675E-14	99.970387	2.499998
0.45	1.732084E+16	52.500000	1.234286E-06	2.152883E-15	5.740490E-15	2.092655E-14	99.969137	2.499998

0.46	1.732062E+16	53.666667	1.234286E-06	2.288116E-15	5.868030E-15	2.185657E-14	99.967860	2.499998
0.47	1.732040E+16	54.833333	1.234286E-06	2.428859E-15	5.995569E-15	2.280680E-14	99.966555	2.499997
0.48	1.732017E+16	56.000000	1.234286E-06	2.575222E-15	6.123106E-15	2.377724E-14	99.965223	2.499997
0.49	1.731993E+16	57.166667	1.234286E-06	2.727315E-15	6.250641E-15	2.476789E-14	99.963862	2.499997
0.50	1.731969E+16	58.333333	1.234286E-06	2.885247E-15	6.378175E-15	2.577876E-14	99.962474	2.499997
0.51	1.731944E+16	59.500000	1.234286E-06	3.049127E-15	6.505706E-15	2.680983E-14	99.961058	2.499997
0.52	1.731919E+16	60.666667	1.234286E-06	3.219064E-15	6.633236E-15	2.786112E-14	99.959614	2.499997
0.53	1.731894E+16	61.833333	1.234286E-06	3.395168E-15	6.760764E-15	2.893262E-14	99.958141	2.499997
0.54	1.731868E+16	63.000000	1.234286E-06	3.577549E-15	6.888290E-15	3.002434E-14	99.956640	2.499997
0.55	1.731841E+16	64.166667	1.234286E-06	3.766315E-15	7.015814E-15	3.113626E-14	99.955111	2.499997
0.56	1.731814E+16	65.333333	1.234286E-06	3.961576E-15	7.143336E-15	3.226839E-14	99.953553	2.499996
0.57	1.731787E+16	66.500000	1.234286E-06	4.163441E-15	7.270856E-15	3.342074E-14	99.951966	2.499996
0.58	1.731759E+16	67.666667	1.234286E-06	4.372020E-15	7.398374E-15	3.459329E-14	99.950350	2.499996
0.59	1.731730E+16	68.833333	1.234286E-06	4.587422E-15	7.525890E-15	3.578605E-14	99.948706	2.499996
0.60	1.731701E+16	70.000000	1.234286E-06	4.809756E-15	7.653404E-15	3.699902E-14	99.947032	2.499996
0.61	1.731672E+16	71.166667	1.234286E-06	5.039131E-15	7.780916E-15	3.823220E-14	99.945329	2.499996
0.62	1.731642E+16	72.333333	1.234286E-06	5.275658E-15	7.908425E-15	3.948559E-14	99.943597	2.499996
0.63	1.731611E+16	73.500000	1.234286E-06	5.519445E-15	8.035932E-15	4.075919E-14	99.941836	2.499995
0.64	1.731580E+16	74.666667	1.234286E-06	5.770601E-15	8.163437E-15	4.205299E-14	99.940045	2.499995
0.65	1.731549E+16	75.833333	1.234286E-06	6.029236E-15	8.290940E-15	4.336700E-14	99.938224	2.499995
0.66	1.731517E+16	77.000000	1.234286E-06	6.295459E-15	8.418440E-15	4.470122E-14	99.936374	2.499995
0.67	1.731484E+16	78.166667	1.234286E-06	6.569379E-15	8.545938E-15	4.605564E-14	99.934493	2.499995
0.68	1.731451E+16	79.333333	1.234286E-06	6.851107E-15	8.673433E-15	4.743027E-14	99.932583	2.499995
0.69	1.731417E+16	80.500000	1.234286E-06	7.140750E-15	8.800926E-15	4.882511E-14	99.930643	2.499995
0.70	1.731383E+16	81.666667	1.234286E-06	7.438418E-15	8.928417E-15	5.024015E-14	99.928672	2.499994
0.71	1.731349E+16	82.833333	1.234286E-06	7.744221E-15	9.055904E-15	5.167539E-14	99.926671	2.499994
0.72	1.731313E+16	84.000000	1.234286E-06	8.058268E-15	9.183390E-15	5.313084E-14	99.924640	2.499994
0.73	1.731278E+16	85.166667	1.234286E-06	8.380668E-15	9.310872E-15	5.460650E-14	99.922578	2.499994
0.74	1.731241E+16	86.333333	1.234286E-06	8.711531E-15	9.438352E-15	5.610235E-14	99.920485	2.499994
0.75	1.731205E+16	87.500000	1.234286E-06	9.050965E-15	9.565830E-15	5.761841E-14	99.918361	2.499994
0.76	1.731167E+16	88.666667	1.234286E-06	9.399080E-15	9.693304E-15	5.915467E-14	99.916207	2.499993
0.77	1.731129E+16	89.833333	1.234286E-06	9.755985E-15	9.820776E-15	6.071114E-14	99.914022	2.499993
0.78	1.731091E+16	91.000000	1.234286E-06	1.012179E-14	9.948245E-15	6.228780E-14	99.911805	2.499993
0.79	1.731052E+16	92.166667	1.234286E-06	1.049660E-14	1.007571E-14	6.388467E-14	99.909557	2.499993
0.80	1.731013E+16	93.333333	1.234286E-06	1.088053E-14	1.020317E-14	6.550174E-14	99.907278	2.499993
0.81	1.730973E+16	94.500000	1.234286E-06	1.127369E-14	1.033063E-14	6.713900E-14	99.904967	2.499993
0.82	1.730932E+16	95.666667	1.234286E-06	1.167619E-14	1.045809E-14	6.879647E-14	99.902624	2.499992
0.83	1.730891E+16	96.833333	1.234286E-06	1.208813E-14	1.058555E-14	7.047414E-14	99.900250	2.499992
0.84	1.730849E+16	98.000000	1.234286E-06	1.250962E-14	1.071300E-14	7.217200E-14	99.897844	2.499992
0.85	1.730807E+16	99.166667	1.234286E-06	1.294078E-14	1.084045E-14	7.389006E-14	99.895406	2.499992
0.86	1.730764E+16	100.333333	1.234286E-06	1.338171E-14	1.096789E-14	7.562832E-14	99.892936	2.499992
0.87	1.730721E+16	101.500000	1.234286E-06	1.383253E-14	1.109533E-14	7.738678E-14	99.890434	2.499991
0.88	1.730677E+16	102.666667	1.234286E-06	1.429333E-14	1.122277E-14	7.916543E-14	99.887899	2.499991
0.89	1.730632E+16	103.833333	1.234286E-06	1.476424E-14	1.135021E-14	8.096428E-14	99.885332	2.499991
0.90	1.730587E+16	105.000000	1.234286E-06	1.524536E-14	1.147764E-14	8.278333E-14	99.882732	2.499991
0.91	1.730542E+16	106.166667	1.234286E-06	1.573679E-14	1.160507E-14	8.462256E-14	99.880100	2.499991
0.92	1.730496E+16	107.333333	1.234286E-06	1.623866E-14	1.173249E-14	8.648200E-14	99.877435	2.499990
0.93	1.730449E+16	108.500000	1.234286E-06	1.675106E-14	1.185991E-14	8.836163E-14	99.874737	2.499990
0.94	1.730401E+16	109.666667	1.234286E-06	1.727411E-14	1.198733E-14	9.026145E-14	99.872006	2.499990
0.95	1.730354E+16	110.833333	1.234286E-06	1.780791E-14	1.211475E-14	9.218146E-14	99.869242	2.499990
0.96	1.730305E+16	112.000000	1.234286E-06	1.835258E-14	1.224216E-14	9.412166E-14	99.866444	2.499990
0.97	1.730256E+16	113.166667	1.234286E-06	1.890822E-14	1.236957E-14	9.608206E-14	99.863613	2.499989
0.98	1.730206E+16	114.333333	1.234286E-06	1.947495E-14	1.249697E-14	9.806264E-14	99.860749	2.499989
0.99	1.730156E+16	115.500000	1.234286E-06	2.005287E-14	1.262437E-14	1.000634E-13	99.857851	2.499989
1.00	1.730105E+16	116.666667	1.234286E-06	2.064209E-14	1.275177E-14	1.020844E-13	99.854919	2.499989



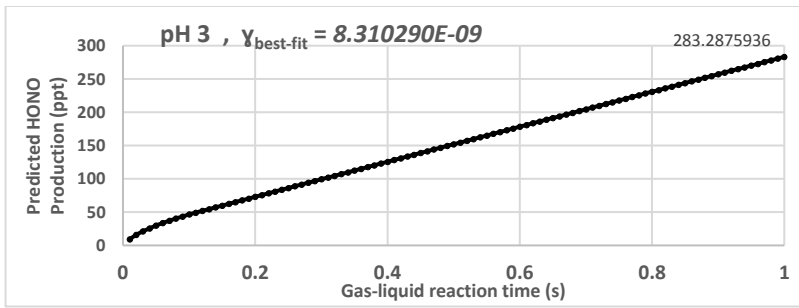
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO2}}$ (mol)	$\Phi_{\text{NO2}}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732617E+16	1.166667	3.509919E-07	1.796590E-19	1.191198E-16	1.887922E-17	99.999852	2.500000
0.02	1.732614E+16	2.333333	4.963766E-07	7.930530E-19	2.382394E-16	5.663762E-17	99.999683	2.500000
0.03	1.732610E+16	3.500000	6.079336E-07	2.024323E-18	3.573588E-16	1.132752E-16	99.999494	2.500000
0.04	1.732607E+16	4.666667	7.019797E-07	4.025333E-18	4.764780E-16	1.887918E-16	99.999283	2.500000
0.05	1.732603E+16	5.833333	7.848354E-07	6.928326E-18	5.955968E-16	2.831876E-16	99.999052	2.500000
0.06	1.732598E+16	7.000000	8.597419E-07	1.085199E-17	7.147154E-16	3.964623E-16	99.998798	2.500000
0.07	1.732594E+16	8.166667	9.286249E-07	1.590493E-17	8.338337E-16	5.286160E-16	99.998524	2.500000
0.08	1.732588E+16	9.333333	9.927388E-07	2.218787E-17	9.529515E-16	6.796486E-16	99.998228	2.500000
0.09	1.732583E+16	10.500000	1.052955E-06	2.979516E-17	1.072069E-15	8.495601E-16	99.997910	2.500000
0.10	1.732577E+16	11.666667	1.109908E-06	3.881583E-17	1.191186E-15	1.038350E-15	99.997571	2.500000
0.11	1.732571E+16	12.833333	1.164078E-06	4.933444E-17	1.310303E-15	1.246019E-15	99.997210	2.500000
0.12	1.732564E+16	14.000000	1.215835E-06	6.143163E-17	1.429419E-15	1.472567E-15	99.996827	2.500000
0.13	1.732557E+16	15.166667	1.234286E-06	7.520106E-17	1.548535E-15	1.717993E-15	99.996421	2.500000
0.14	1.732550E+16	16.333333	1.234286E-06	9.074491E-17	1.667650E-15	1.982298E-15	99.995994	2.500000
0.15	1.732542E+16	17.500000	1.234286E-06	1.081653E-16	1.786765E-15	2.265480E-15	99.995545	2.500000
0.16	1.732534E+16	18.666667	1.234286E-06	1.275645E-16	1.905879E-15	2.567542E-15	99.995073	2.500000
0.17	1.732525E+16	19.833333	1.234286E-06	1.490446E-16	2.024992E-15	2.888481E-15	99.994579	2.500000
0.18	1.732516E+16	21.000000	1.234286E-06	1.727078E-16	2.144105E-15	3.228299E-15	99.994062	2.500000
0.19	1.732507E+16	22.166667	1.234286E-06	1.986562E-16	2.263218E-15	3.586994E-15	99.993522	2.500000
0.20	1.732497E+16	23.333333	1.234286E-06	2.269921E-16	2.382329E-15	3.964568E-15	99.992960	2.500000
0.21	1.732487E+16	24.500000	1.234286E-06	2.578176E-16	2.501440E-15	4.361019E-15	99.992375	2.500000
0.22	1.732476E+16	25.666667	1.234286E-06	2.912348E-16	2.620550E-15	4.776347E-15	99.991767	2.499999
0.23	1.732466E+16	26.833333	1.234286E-06	3.273459E-16	2.739660E-15	5.210554E-15	99.991136	2.499999
0.24	1.732454E+16	28.000000	1.234286E-06	3.662531E-16	2.858769E-15	5.663637E-15	99.990481	2.499999
0.25	1.732442E+16	29.166667	1.234286E-06	4.080586E-16	2.977876E-15	6.135598E-15	99.989804	2.499999
0.26	1.732430E+16	30.333333	1.234286E-06	4.528644E-16	3.096983E-15	6.626436E-15	99.989102	2.499999
0.27	1.732418E+16	31.500000	1.234286E-06	5.007728E-16	3.216090E-15	7.136151E-15	99.988378	2.499999
0.28	1.732405E+16	32.666667	1.234286E-06	5.518859E-16	3.335195E-15	7.664743E-15	99.987629	2.499999
0.29	1.732391E+16	33.833333	1.234286E-06	6.063059E-16	3.454299E-15	8.212211E-15	99.986857	2.499999
0.30	1.732378E+16	35.000000	1.234286E-06	6.641349E-16	3.573403E-15	8.778556E-15	99.986061	2.499999
0.31	1.732363E+16	36.166667	1.234286E-06	7.254751E-16	3.692505E-15	9.363777E-15	99.985241	2.499999
0.32	1.732349E+16	37.333333	1.234286E-06	7.904286E-16	3.811607E-15	9.967875E-15	99.984397	2.499999
0.33	1.732334E+16	38.500000	1.234286E-06	8.590975E-16	3.930707E-15	1.059085E-14	99.983529	2.499999
0.34	1.732318E+16	39.666667	1.234286E-06	9.315841E-16	4.049806E-15	1.123270E-14	99.982637	2.499999
0.35	1.732302E+16	40.833333	1.234286E-06	1.007990E-15	4.168905E-15	1.189342E-14	99.981720	2.499999
0.36	1.732286E+16	42.000000	1.234286E-06	1.088419E-15	4.288002E-15	1.257302E-14	99.980778	2.499999
0.37	1.732269E+16	43.166667	1.234286E-06	1.172971E-15	4.407098E-15	1.327150E-14	99.979812	2.499999
0.38	1.732252E+16	44.333333	1.234286E-06	1.261749E-15	4.526193E-15	1.398885E-14	99.978821	2.499998
0.39	1.732235E+16	45.500000	1.234286E-06	1.354856E-15	4.645286E-15	1.472507E-14	99.977806	2.499998
0.40	1.732217E+16	46.666667	1.234286E-06	1.452394E-15	4.764379E-15	1.548017E-14	99.976765	2.499998
0.41	1.732198E+16	47.833333	1.234286E-06	1.554463E-15	4.883470E-15	1.625415E-14	99.975700	2.499998
0.42	1.732179E+16	49.000000	1.234286E-06	1.661168E-15	5.002560E-15	1.704700E-14	99.974609	2.499998
0.43	1.732160E+16	50.166667	1.234286E-06	1.772609E-15	5.121648E-15	1.785872E-14	99.973493	2.499998
0.44	1.732140E+16	51.333333	1.234286E-06	1.888890E-15	5.240735E-15	1.868932E-14	99.972351	2.499998
0.45	1.732120E+16	52.500000	1.234286E-06	2.010111E-15	5.359821E-15	1.953879E-14	99.971184	2.499998

0.46	1.732099E+16	53.666667	1.234286E-06	2.136376E-15	5.478905E-15	2.040713E-14	99.969991	2.499998
0.47	1.732078E+16	54.833333	1.234286E-06	2.267786E-15	5.597988E-15	2.129435E-14	99.968773	2.499998
0.48	1.732057E+16	56.000000	1.234286E-06	2.404443E-15	5.717070E-15	2.220044E-14	99.967529	2.499998
0.49	1.732035E+16	57.166667	1.234286E-06	2.546451E-15	5.836150E-15	2.312540E-14	99.966259	2.499997
0.50	1.732012E+16	58.333333	1.234286E-06	2.693909E-15	5.955228E-15	2.406923E-14	99.964963	2.499997
0.51	1.731989E+16	59.500000	1.234286E-06	2.846922E-15	6.074305E-15	2.503194E-14	99.963640	2.499997
0.52	1.731966E+16	60.666667	1.234286E-06	3.005590E-15	6.193380E-15	2.601352E-14	99.962292	2.499997
0.53	1.731942E+16	61.833333	1.234286E-06	3.170017E-15	6.312453E-15	2.701397E-14	99.960917	2.499997
0.54	1.731918E+16	63.000000	1.234286E-06	3.340303E-15	6.431525E-15	2.803329E-14	99.959515	2.499997
0.55	1.731893E+16	64.166667	1.234286E-06	3.516552E-15	6.550595E-15	2.907148E-14	99.958087	2.499997
0.56	1.731868E+16	65.333333	1.234286E-06	3.698865E-15	6.669664E-15	3.012854E-14	99.956633	2.499997
0.57	1.731842E+16	66.500000	1.234286E-06	3.887344E-15	6.788731E-15	3.120447E-14	99.955151	2.499997
0.58	1.731816E+16	67.666667	1.234286E-06	4.082092E-15	6.907796E-15	3.229928E-14	99.953643	2.499996
0.59	1.731789E+16	68.833333	1.234286E-06	4.283211E-15	7.026859E-15	3.341295E-14	99.952107	2.499996
0.60	1.731762E+16	70.000000	1.234286E-06	4.490802E-15	7.145920E-15	3.454549E-14	99.950545	2.499996
0.61	1.731735E+16	71.166667	1.234286E-06	4.704968E-15	7.264979E-15	3.569690E-14	99.948955	2.499996
0.62	1.731707E+16	72.333333	1.234286E-06	4.925810E-15	7.384037E-15	3.686718E-14	99.947337	2.499996
0.63	1.731678E+16	73.500000	1.234286E-06	5.153432E-15	7.503092E-15	3.805633E-14	99.945693	2.499996
0.64	1.731649E+16	74.666667	1.234286E-06	5.387934E-15	7.622146E-15	3.926435E-14	99.944021	2.499996
0.65	1.731620E+16	75.833333	1.234286E-06	5.629419E-15	7.741197E-15	4.049123E-14	99.942321	2.499995
0.66	1.731590E+16	77.000000	1.234286E-06	5.877990E-15	7.860246E-15	4.173698E-14	99.940593	2.499995
0.67	1.731559E+16	78.166667	1.234286E-06	6.133747E-15	7.979294E-15	4.300160E-14	99.938837	2.499995
0.68	1.731528E+16	79.333333	1.234286E-06	6.396794E-15	8.098339E-15	4.428509E-14	99.937054	2.499995
0.69	1.731497E+16	80.500000	1.234286E-06	6.667232E-15	8.217382E-15	4.558744E-14	99.935242	2.499995
0.70	1.731465E+16	81.666667	1.234286E-06	6.945163E-15	8.336423E-15	4.690866E-14	99.933402	2.499995
0.71	1.731433E+16	82.833333	1.234286E-06	7.230690E-15	8.455462E-15	4.824874E-14	99.931534	2.499995
0.72	1.731400E+16	84.000000	1.234286E-06	7.523914E-15	8.574498E-15	4.960769E-14	99.929637	2.499994
0.73	1.731367E+16	85.166667	1.234286E-06	7.824937E-15	8.693532E-15	5.098550E-14	99.927712	2.499994
0.74	1.731333E+16	86.333333	1.234286E-06	8.133862E-15	8.812564E-15	5.238218E-14	99.925758	2.499994
0.75	1.731298E+16	87.500000	1.234286E-06	8.450790E-15	8.931593E-15	5.379773E-14	99.923775	2.499994
0.76	1.731264E+16	88.666667	1.234286E-06	8.775824E-15	9.050620E-15	5.523213E-14	99.921763	2.499994
0.77	1.731228E+16	89.833333	1.234286E-06	9.109065E-15	9.169645E-15	5.668540E-14	99.919723	2.499994
0.78	1.731192E+16	91.000000	1.234286E-06	9.450615E-15	9.288667E-15	5.815753E-14	99.917653	2.499994
0.79	1.731156E+16	92.166667	1.234286E-06	9.800578E-15	9.407687E-15	5.964853E-14	99.915554	2.499993
0.80	1.731119E+16	93.333333	1.234286E-06	1.015905E-14	9.526704E-15	6.115839E-14	99.913426	2.499993
0.81	1.731082E+16	94.500000	1.234286E-06	1.052614E-14	9.645718E-15	6.268711E-14	99.911268	2.499993
0.82	1.731044E+16	95.666667	1.234286E-06	1.090195E-14	9.764730E-15	6.423469E-14	99.909081	2.499993
0.83	1.731005E+16	96.833333	1.234286E-06	1.128658E-14	9.883740E-15	6.580113E-14	99.906864	2.499993
0.84	1.730967E+16	98.000000	1.234286E-06	1.168013E-14	1.000275E-14	6.738643E-14	99.904618	2.499993
0.85	1.730927E+16	99.166667	1.234286E-06	1.208270E-14	1.012175E-14	6.899059E-14	99.902341	2.499992
0.86	1.730887E+16	100.333333	1.234286E-06	1.249440E-14	1.024075E-14	7.061361E-14	99.900035	2.499992
0.87	1.730847E+16	101.500000	1.234286E-06	1.291533E-14	1.035975E-14	7.225549E-14	99.897699	2.499992
0.88	1.730806E+16	102.666667	1.234286E-06	1.334559E-14	1.047875E-14	7.391623E-14	99.895332	2.499992
0.89	1.730764E+16	103.833333	1.234286E-06	1.378527E-14	1.059774E-14	7.559582E-14	99.892935	2.499992
0.90	1.730722E+16	105.000000	1.234286E-06	1.423449E-14	1.071673E-14	7.729427E-14	99.890508	2.499991
0.91	1.730679E+16	106.166667	1.234286E-06	1.469335E-14	1.083572E-14	7.901158E-14	99.888050	2.499991
0.92	1.730636E+16	107.333333	1.234286E-06	1.516194E-14	1.095470E-14	8.074775E-14	99.885561	2.499991
0.93	1.730593E+16	108.500000	1.234286E-06	1.564037E-14	1.107368E-14	8.250277E-14	99.883042	2.499991
0.94	1.730549E+16	109.666667	1.234286E-06	1.612875E-14	1.119266E-14	8.427665E-14	99.880492	2.499991
0.95	1.730504E+16	110.833333	1.234286E-06	1.662716E-14	1.131163E-14	8.606939E-14	99.877911	2.499990
0.96	1.730459E+16	112.000000	1.234286E-06	1.713572E-14	1.143060E-14	8.788097E-14	99.875299	2.499990
0.97	1.730413E+16	113.166667	1.234286E-06	1.765453E-14	1.154957E-14	8.971142E-14	99.872656	2.499990
0.98	1.730366E+16	114.333333	1.234286E-06	1.818369E-14	1.166854E-14	9.156071E-14	99.869982	2.499990
0.99	1.730320E+16	115.500000	1.234286E-06	1.872329E-14	1.178750E-14	9.342886E-14	99.867276	2.499990
1.00	1.730272E+16	116.666667	1.234286E-06	1.927345E-14	1.190646E-14	9.531586E-14	99.864539	2.499989



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732616E+16	1.166667	3.509918E-07	2.027193E-19	1.344095E-16	2.130248E-17	99.999833	2.500000
0.02	1.732613E+16	2.333333	4.963764E-07	8.948462E-19	2.688188E-16	6.390739E-17	99.999643	2.500000
0.03	1.732609E+16	3.500000	6.079332E-07	2.284157E-18	4.032278E-16	1.278147E-16	99.999429	2.500000
0.04	1.732605E+16	4.666667	7.019791E-07	4.542009E-18	5.376365E-16	2.130243E-16	99.999191	2.500000
0.05	1.732601E+16	5.833333	7.848344E-07	7.817619E-18	6.720449E-16	3.195363E-16	99.998930	2.500000
0.06	1.732596E+16	7.000000	8.597406E-07	1.224491E-17	8.064528E-16	4.473504E-16	99.998644	2.500000
0.07	1.732590E+16	8.166667	9.286231E-07	1.794643E-17	9.408604E-16	5.964667E-16	99.998334	2.500000
0.08	1.732584E+16	9.333333	9.927365E-07	2.503582E-17	1.075267E-15	7.668850E-16	99.998000	2.500000
0.09	1.732578E+16	10.500000	1.052952E-06	3.361955E-17	1.209674E-15	9.586054E-16	99.997642	2.500000
0.10	1.732572E+16	11.666667	1.109905E-06	4.379808E-17	1.344080E-15	1.171628E-15	99.997259	2.500000
0.11	1.732565E+16	12.833333	1.164073E-06	5.566681E-17	1.478486E-15	1.405952E-15	99.996852	2.500000
0.12	1.732557E+16	14.000000	1.215830E-06	6.931675E-17	1.612891E-15	1.661578E-15	99.996419	2.500000
0.13	1.732549E+16	15.166667	1.234286E-06	8.485357E-17	1.747295E-15	1.938505E-15	99.995962	2.500000
0.14	1.732541E+16	16.333333	1.234286E-06	1.023926E-16	1.881699E-15	2.236734E-15	99.995480	2.500000
0.15	1.732532E+16	17.500000	1.234286E-06	1.220490E-16	2.016102E-15	2.556264E-15	99.994973	2.500000
0.16	1.732523E+16	18.666667	1.234286E-06	1.439381E-16	2.150504E-15	2.897096E-15	99.994441	2.500000
0.17	1.732513E+16	19.833333	1.234286E-06	1.681753E-16	2.284906E-15	3.259229E-15	99.993883	2.500000
0.18	1.732503E+16	21.000000	1.234286E-06	1.948758E-16	2.419306E-15	3.642663E-15	99.993300	2.500000
0.19	1.732492E+16	22.166667	1.234286E-06	2.241548E-16	2.553706E-15	4.047398E-15	99.992691	2.500000
0.20	1.732481E+16	23.333333	1.234286E-06	2.561277E-16	2.688106E-15	4.473433E-15	99.992057	2.500000
0.21	1.732470E+16	24.500000	1.234286E-06	2.909097E-16	2.822504E-15	4.920769E-15	99.991396	2.499999
0.22	1.732458E+16	25.666667	1.234286E-06	3.286162E-16	2.956901E-15	5.389406E-15	99.990710	2.499999
0.23	1.732446E+16	26.833333	1.234286E-06	3.693623E-16	3.091297E-15	5.879343E-15	99.989998	2.499999
0.24	1.732433E+16	28.000000	1.234286E-06	4.132633E-16	3.225693E-15	6.390580E-15	99.989260	2.499999
0.25	1.732420E+16	29.166667	1.234286E-06	4.604346E-16	3.360087E-15	6.923117E-15	99.988495	2.499999
0.26	1.732406E+16	30.333333	1.234286E-06	5.109913E-16	3.494480E-15	7.476953E-15	99.987704	2.499999
0.27	1.732392E+16	31.500000	1.234286E-06	5.650489E-16	3.628873E-15	8.052090E-15	99.986886	2.499999
0.28	1.732377E+16	32.666667	1.234286E-06	6.227224E-16	3.763264E-15	8.648526E-15	99.986042	2.499999
0.29	1.732362E+16	33.833333	1.234286E-06	6.841272E-16	3.897654E-15	9.266261E-15	99.985170	2.499999
0.30	1.732347E+16	35.000000	1.234286E-06	7.493786E-16	4.032042E-15	9.905295E-15	99.984272	2.499999
0.31	1.732331E+16	36.166667	1.234286E-06	8.185918E-16	4.166430E-15	1.056563E-14	99.983347	2.499999
0.32	1.732314E+16	37.333333	1.234286E-06	8.918820E-16	4.300816E-15	1.124726E-14	99.982395	2.499999
0.33	1.732297E+16	38.500000	1.234286E-06	9.693646E-16	4.435201E-15	1.195019E-14	99.981415	2.499999
0.34	1.732280E+16	39.666667	1.234286E-06	1.051155E-15	4.569584E-15	1.267442E-14	99.980408	2.499999
0.35	1.732262E+16	40.833333	1.234286E-06	1.137368E-15	4.703966E-15	1.341994E-14	99.979374	2.499999
0.36	1.732243E+16	42.000000	1.234286E-06	1.228119E-15	4.838347E-15	1.418677E-14	99.978311	2.499998
0.37	1.732224E+16	43.166667	1.234286E-06	1.323523E-15	4.972726E-15	1.497489E-14	99.977221	2.499998
0.38	1.732205E+16	44.333333	1.234286E-06	1.423696E-15	5.107104E-15	1.578431E-14	99.976103	2.499998
0.39	1.732185E+16	45.500000	1.234286E-06	1.528753E-15	5.241480E-15	1.661502E-14	99.974957	2.499998
0.40	1.732165E+16	46.666667	1.234286E-06	1.638808E-15	5.375855E-15	1.746703E-14	99.973783	2.499998
0.41	1.732144E+16	47.833333	1.234286E-06	1.753979E-15	5.510228E-15	1.834034E-14	99.972581	2.499998
0.42	1.732123E+16	49.000000	1.234286E-06	1.874378E-15	5.644599E-15	1.923494E-14	99.971350	2.499998
0.43	1.732101E+16	50.166667	1.234286E-06	2.000122E-15	5.778969E-15	2.015084E-14	99.970090	2.499998
0.44	1.732079E+16	51.333333	1.234286E-06	2.131327E-15	5.913337E-15	2.108804E-14	99.968802	2.499998
0.45	1.732056E+16	52.500000	1.234286E-06	2.268106E-15	6.047703E-15	2.204653E-14	99.967486	2.499998

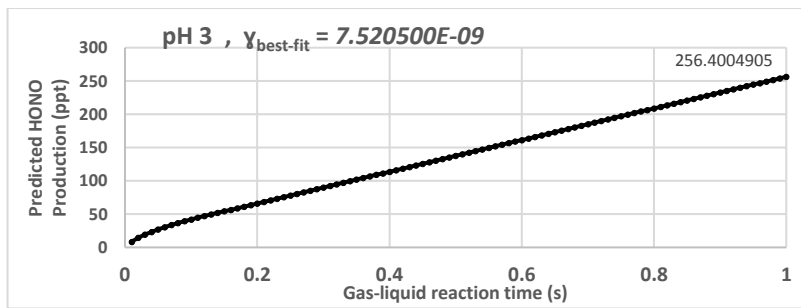
0.46	1.732032E+16	53.666667	1.234286E-06	2.410576E-15	6.182067E-15	2.302632E-14	99.966140	2.499997
0.47	1.732009E+16	54.833333	1.234286E-06	2.558851E-15	6.316430E-15	2.402740E-14	99.964765	2.499997
0.48	1.731984E+16	56.000000	1.234286E-06	2.713048E-15	6.450790E-15	2.504977E-14	99.963361	2.499997
0.49	1.731959E+16	57.166667	1.234286E-06	2.873280E-15	6.585149E-15	2.609344E-14	99.961928	2.499997
0.50	1.731934E+16	58.333333	1.234286E-06	3.039664E-15	6.719506E-15	2.715840E-14	99.960466	2.499997
0.51	1.731908E+16	59.500000	1.234286E-06	3.212314E-15	6.853861E-15	2.824466E-14	99.958974	2.499997
0.52	1.731882E+16	60.666667	1.234286E-06	3.391346E-15	6.988213E-15	2.935221E-14	99.957452	2.499997
0.53	1.731855E+16	61.833333	1.234286E-06	3.576874E-15	7.122564E-15	3.048105E-14	99.955901	2.499997
0.54	1.731828E+16	63.000000	1.234286E-06	3.769015E-15	7.256913E-15	3.163118E-14	99.954319	2.499996
0.55	1.731800E+16	64.166667	1.234286E-06	3.967883E-15	7.391259E-15	3.280261E-14	99.952708	2.499996
0.56	1.731771E+16	65.333333	1.234286E-06	4.173593E-15	7.525603E-15	3.399533E-14	99.951067	2.499996
0.57	1.731742E+16	66.500000	1.234286E-06	4.386261E-15	7.659945E-15	3.520933E-14	99.949395	2.499996
0.58	1.731713E+16	67.666667	1.234286E-06	4.606002E-15	7.794285E-15	3.644463E-14	99.947693	2.499996
0.59	1.731683E+16	68.833333	1.234286E-06	4.832931E-15	7.928622E-15	3.770122E-14	99.945961	2.499996
0.60	1.731652E+16	70.000000	1.234286E-06	5.067163E-15	8.062957E-15	3.897910E-14	99.944197	2.499996
0.61	1.731621E+16	71.166667	1.234286E-06	5.308813E-15	8.197289E-15	4.027827E-14	99.942404	2.499996
0.62	1.731590E+16	72.333333	1.234286E-06	5.557997E-15	8.331620E-15	4.159873E-14	99.940579	2.499995
0.63	1.731557E+16	73.500000	1.234286E-06	5.814829E-15	8.465947E-15	4.294048E-14	99.938723	2.499995
0.64	1.731525E+16	74.666667	1.234286E-06	6.079426E-15	8.600272E-15	4.430352E-14	99.936836	2.499995
0.65	1.731491E+16	75.833333	1.234286E-06	6.351901E-15	8.734595E-15	4.568784E-14	99.934918	2.499995
0.66	1.731458E+16	77.000000	1.234286E-06	6.632370E-15	8.868915E-15	4.709345E-14	99.932969	2.499995
0.67	1.731423E+16	78.166667	1.234286E-06	6.920948E-15	9.003232E-15	4.852035E-14	99.930988	2.499995
0.68	1.731389E+16	79.333333	1.234286E-06	7.217751E-15	9.137546E-15	4.996853E-14	99.928975	2.499994
0.69	1.731353E+16	80.500000	1.234286E-06	7.522893E-15	9.271858E-15	5.143800E-14	99.926931	2.499994
0.70	1.731317E+16	81.666667	1.234286E-06	7.836490E-15	9.406167E-15	5.292876E-14	99.924855	2.499994
0.71	1.731281E+16	82.833333	1.234286E-06	8.158657E-15	9.540473E-15	5.444080E-14	99.922747	2.499994
0.72	1.731244E+16	84.000000	1.234286E-06	8.489509E-15	9.674777E-15	5.597413E-14	99.920607	2.499994
0.73	1.731206E+16	85.166667	1.234286E-06	8.829160E-15	9.809077E-15	5.752874E-14	99.918435	2.499994
0.74	1.731168E+16	86.333333	1.234286E-06	9.177727E-15	9.943375E-15	5.910464E-14	99.916230	2.499993
0.75	1.731129E+16	87.500000	1.234286E-06	9.535323E-15	1.007767E-14	6.070181E-14	99.913993	2.499993
0.76	1.731090E+16	88.666667	1.234286E-06	9.902065E-15	1.021196E-14	6.232028E-14	99.911723	2.499993
0.77	1.731050E+16	89.833333	1.234286E-06	1.027807E-14	1.034625E-14	6.396002E-14	99.909421	2.499993
0.78	1.731009E+16	91.000000	1.234286E-06	1.066345E-14	1.048053E-14	6.562104E-14	99.907085	2.499993
0.79	1.730968E+16	92.166667	1.234286E-06	1.105831E-14	1.061482E-14	6.730335E-14	99.904717	2.499993
0.80	1.730927E+16	93.333333	1.234286E-06	1.146279E-14	1.074909E-14	6.900694E-14	99.902316	2.499992
0.81	1.730884E+16	94.500000	1.234286E-06	1.187698E-14	1.088337E-14	7.073180E-14	99.899881	2.499992
0.82	1.730842E+16	95.666667	1.234286E-06	1.230101E-14	1.101764E-14	7.247795E-14	99.897414	2.499992
0.83	1.730798E+16	96.833333	1.234286E-06	1.273499E-14	1.115191E-14	7.424537E-14	99.894912	2.499992
0.84	1.730754E+16	98.000000	1.234286E-06	1.317904E-14	1.128618E-14	7.603408E-14	99.892378	2.499992
0.85	1.730710E+16	99.166667	1.234286E-06	1.363327E-14	1.142044E-14	7.784406E-14	99.889809	2.499991
0.86	1.730665E+16	100.333333	1.234286E-06	1.409779E-14	1.155470E-14	7.967532E-14	99.887207	2.499991
0.87	1.730619E+16	101.500000	1.234286E-06	1.457273E-14	1.168895E-14	8.152785E-14	99.884571	2.499991
0.88	1.730573E+16	102.666667	1.234286E-06	1.505819E-14	1.182320E-14	8.340166E-14	99.881900	2.499991
0.89	1.730526E+16	103.833333	1.234286E-06	1.555429E-14	1.195745E-14	8.529675E-14	99.879196	2.499991
0.90	1.730479E+16	105.000000	1.234286E-06	1.606115E-14	1.209170E-14	8.721311E-14	99.876457	2.499990
0.91	1.730431E+16	106.166667	1.234286E-06	1.657888E-14	1.222594E-14	8.915075E-14	99.873684	2.499990
0.92	1.730382E+16	107.333333	1.234286E-06	1.710759E-14	1.236017E-14	9.110966E-14	99.870876	2.499990
0.93	1.730333E+16	108.500000	1.234286E-06	1.764741E-14	1.249441E-14	9.308984E-14	99.868034	2.499990
0.94	1.730283E+16	109.666667	1.234286E-06	1.819844E-14	1.262863E-14	9.509130E-14	99.865157	2.499989
0.95	1.730232E+16	110.833333	1.234286E-06	1.876080E-14	1.276286E-14	9.711402E-14	99.862245	2.499989
0.96	1.730181E+16	112.000000	1.234286E-06	1.933461E-14	1.289708E-14	9.915802E-14	99.859298	2.499989
0.97	1.730130E+16	113.166667	1.234286E-06	1.991998E-14	1.303130E-14	1.012233E-13	99.856316	2.499989
0.98	1.730077E+16	114.333333	1.234286E-06	2.051703E-14	1.316551E-14	1.033098E-13	99.853298	2.499989
0.99	1.730024E+16	115.500000	1.234286E-06	2.112586E-14	1.329972E-14	1.054176E-13	99.850245	2.499988
1.00	1.729971E+16	116.666667	1.234286E-06	2.174660E-14	1.343393E-14	1.075467E-13	99.847157	2.499988



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732615E+16	1.166667	3.509915E-07	2.402137E-19	1.592695E-16	7.982380E-17	99.999744	3.000000
0.02	1.732609E+16	2.333333	4.963752E-07	1.060355E-18	3.185384E-16	2.394711E-16	99.999401	3.000000
0.03	1.732601E+16	3.500000	6.079304E-07	2.706629E-18	4.778066E-16	4.789415E-16	99.998973	3.000000
0.04	1.732592E+16	4.666667	7.019739E-07	5.382088E-18	6.370741E-16	7.982345E-16	99.998457	3.000000
0.05	1.732582E+16	5.833333	7.848260E-07	9.263547E-18	7.963406E-16	1.197350E-15	99.997855	2.999999
0.06	1.732570E+16	7.000000	8.597279E-07	1.450970E-17	9.556060E-16	1.676286E-15	99.997166	2.999999
0.07	1.732557E+16	8.166667	9.286050E-07	2.126576E-17	1.114870E-15	2.235044E-15	99.996390	2.999999
0.08	1.732542E+16	9.333333	9.927120E-07	2.966639E-17	1.274133E-15	2.873621E-15	99.995526	2.999999
0.09	1.732525E+16	10.500000	1.052920E-06	3.983775E-17	1.433395E-15	3.592018E-15	99.994576	2.999999
0.10	1.732507E+16	11.666667	1.109864E-06	5.189888E-17	1.592654E-15	4.390233E-15	99.993537	2.999998
0.11	1.732488E+16	12.833333	1.164022E-06	6.596282E-17	1.751912E-15	5.268265E-15	99.992412	2.999998
0.12	1.732467E+16	14.000000	1.215766E-06	8.213743E-17	1.911168E-15	6.226113E-15	99.991198	2.999998
0.13	1.732444E+16	15.166667	1.234286E-06	1.005479E-16	2.070422E-15	7.263776E-15	99.989897	2.999997
0.14	1.732420E+16	16.333333	1.234286E-06	1.213307E-16	2.229674E-15	8.381253E-15	99.988507	2.999997
0.15	1.732394E+16	17.500000	1.234286E-06	1.446225E-16	2.388924E-15	9.578542E-15	99.987029	2.999997
0.16	1.732367E+16	18.666667	1.234286E-06	1.705599E-16	2.548171E-15	1.085564E-14	99.985464	2.999996
0.17	1.732339E+16	19.833333	1.234286E-06	1.992795E-16	2.707416E-15	1.221255E-14	99.983809	2.999996
0.18	1.732308E+16	21.000000	1.234286E-06	2.309178E-16	2.866658E-15	1.364927E-14	99.982066	2.999995
0.19	1.732277E+16	22.166667	1.234286E-06	2.656115E-16	3.025897E-15	1.516579E-14	99.980235	2.999995
0.20	1.732243E+16	23.333333	1.234286E-06	3.034970E-16	3.185133E-15	1.676211E-14	99.978314	2.999994
0.21	1.732209E+16	24.500000	1.234286E-06	3.447109E-16	3.344366E-15	1.843824E-14	99.976304	2.999994
0.22	1.732172E+16	25.666667	1.234286E-06	3.893898E-16	3.503595E-15	2.019417E-14	99.974206	2.999993
0.23	1.732134E+16	26.833333	1.234286E-06	4.376703E-16	3.662821E-15	2.202990E-14	99.972018	2.999992
0.24	1.732095E+16	28.000000	1.234286E-06	4.896889E-16	3.822044E-15	2.394542E-14	99.969740	2.999992
0.25	1.732054E+16	29.166667	1.234286E-06	5.455821E-16	3.981263E-15	2.594074E-14	99.967373	2.999991
0.26	1.732011E+16	30.333333	1.234286E-06	6.054864E-16	4.140478E-15	2.801584E-14	99.964916	2.999990
0.27	1.731967E+16	31.500000	1.234286E-06	6.695385E-16	4.299690E-15	3.017074E-14	99.962369	2.999989
0.28	1.731921E+16	32.666667	1.234286E-06	7.378747E-16	4.458897E-15	3.240543E-14	99.959733	2.999989
0.29	1.731874E+16	33.833333	1.234286E-06	8.106317E-16	4.618100E-15	3.471989E-14	99.957006	2.999988
0.30	1.731825E+16	35.000000	1.234286E-06	8.879459E-16	4.777298E-15	3.711414E-14	99.954189	2.999987
0.31	1.731775E+16	36.166667	1.234286E-06	9.699537E-16	4.936492E-15	3.958817E-14	99.951281	2.999986
0.32	1.731723E+16	37.333333	1.234286E-06	1.056792E-15	5.095681E-15	4.214197E-14	99.948283	2.999985
0.33	1.731670E+16	38.500000	1.234286E-06	1.148597E-15	5.254866E-15	4.477555E-14	99.945194	2.999984
0.34	1.731614E+16	39.666667	1.234286E-06	1.245505E-15	5.414045E-15	4.748889E-14	99.942014	2.999983
0.35	1.731558E+16	40.833333	1.234286E-06	1.347652E-15	5.573220E-15	5.028201E-14	99.938743	2.999982
0.36	1.731500E+16	42.000000	1.234286E-06	1.455176E-15	5.732389E-15	5.315488E-14	99.935381	2.999981
0.37	1.731440E+16	43.166667	1.234286E-06	1.568212E-15	5.891553E-15	5.610752E-14	99.931927	2.999980
0.38	1.731378E+16	44.333333	1.234286E-06	1.686897E-15	6.050711E-15	5.913991E-14	99.928382	2.999979
0.39	1.731315E+16	45.500000	1.234286E-06	1.811368E-15	6.209864E-15	6.225206E-14	99.924746	2.999978
0.40	1.731251E+16	46.666667	1.234286E-06	1.941760E-15	6.369011E-15	6.544396E-14	99.921018	2.999977
0.41	1.731184E+16	47.833333	1.234286E-06	2.078211E-15	6.528152E-15	6.871560E-14	99.917198	2.999976
0.42	1.731117E+16	49.000000	1.234286E-06	2.220856E-15	6.687286E-15	7.206699E-14	99.913286	2.999975
0.43	1.731047E+16	50.166667	1.234286E-06	2.369832E-15	6.846415E-15	7.549812E-14	99.909281	2.999973
0.44	1.730976E+16	51.333333	1.234286E-06	2.525276E-15	7.005537E-15	7.900898E-14	99.905185	2.999972
0.45	1.730904E+16	52.500000	1.234286E-06	2.687323E-15	7.164653E-15	8.259957E-14	99.900996	2.999971

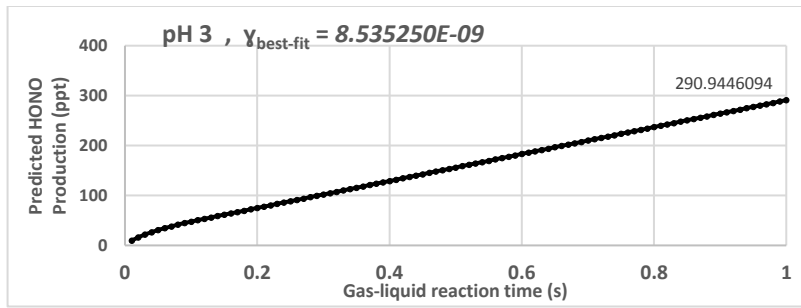


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0.47	1.730754E+16	54.833333	1.234286E-06	3.031775E-15	7.482864E-15	9.001993E-14	99.892340	2.999968
0.48	1.730676E+16	56.000000	1.234286E-06	3.214451E-15	7.641960E-15	9.384969E-14	99.887873	2.999967
0.49	1.730597E+16	57.166667	1.234286E-06	3.404277E-15	7.801048E-15	9.775917E-14	99.883312	2.999966
0.50	1.730517E+16	58.333333	1.234286E-06	3.601388E-15	7.960129E-15	1.017484E-13	99.878659	2.999964
0.51	1.730434E+16	59.500000	1.234286E-06	3.805921E-15	8.119202E-15	1.058172E-13	99.873912	2.999963
0.52	1.730351E+16	60.666667	1.234286E-06	4.018012E-15	8.278268E-15	1.099658E-13	99.869072	2.999961
0.53	1.730265E+16	61.833333	1.234286E-06	4.237797E-15	8.437327E-15	1.141941E-13	99.864139	2.999960
0.54	1.730178E+16	63.000000	1.234286E-06	4.465413E-15	8.596377E-15	1.185021E-13	99.859111	2.999958
0.55	1.730089E+16	64.166667	1.234286E-06	4.700996E-15	8.755420E-15	1.228898E-13	99.853990	2.999957
0.56	1.729999E+16	65.333333	1.234286E-06	4.944681E-15	8.914454E-15	1.273571E-13	99.848775	2.999955
0.57	1.729907E+16	66.500000	1.234286E-06	5.196606E-15	9.073481E-15	1.319042E-13	99.843465	2.999954
0.58	1.729813E+16	67.666667	1.234286E-06	5.456906E-15	9.232498E-15	1.365309E-13	99.838062	2.999952
0.59	1.729718E+16	68.833333	1.234286E-06	5.725717E-15	9.391508E-15	1.412372E-13	99.832564	2.999950
0.60	1.729621E+16	70.000000	1.234286E-06	6.003177E-15	9.550508E-15	1.460232E-13	99.826971	2.999949
0.61	1.729523E+16	71.166667	1.234286E-06	6.289420E-15	9.709500E-15	1.508889E-13	99.821284	2.999947
0.62	1.729422E+16	72.333333	1.234286E-06	6.584583E-15	9.868483E-15	1.558343E-13	99.815501	2.999945
0.63	1.729321E+16	73.500000	1.234286E-06	6.888803E-15	1.002746E-14	1.608592E-13	99.809624	2.999943
0.64	1.729217E+16	74.666667	1.234286E-06	7.202215E-15	1.018642E-14	1.659639E-13	99.803652	2.999942
0.65	1.729112E+16	75.833333	1.234286E-06	7.524955E-15	1.034538E-14	1.711481E-13	99.797585	2.999940
0.66	1.729005E+16	77.000000	1.234286E-06	7.857159E-15	1.050432E-14	1.764120E-13	99.791422	2.999938
0.67	1.728897E+16	78.166667	1.234286E-06	8.198964E-15	1.066326E-14	1.817555E-13	99.785163	2.999936
0.68	1.728787E+16	79.333333	1.234286E-06	8.550506E-15	1.082218E-14	1.871786E-13	99.778809	2.999934
0.69	1.728675E+16	80.500000	1.234286E-06	8.911921E-15	1.098110E-14	1.926813E-13	99.772359	2.999932
0.70	1.728562E+16	81.666667	1.234286E-06	9.283343E-15	1.114000E-14	1.982637E-13	99.765813	2.999930
0.71	1.728446E+16	82.833333	1.234286E-06	9.664911E-15	1.129890E-14	2.039256E-13	99.759171	2.999928
0.72	1.728330E+16	84.000000	1.234286E-06	1.005676E-14	1.145778E-14	2.096671E-13	99.752433	2.999926
0.73	1.728211E+16	85.166667	1.234286E-06	1.045902E-14	1.161666E-14	2.154882E-13	99.745598	2.999924
0.74	1.728091E+16	86.333333	1.234286E-06	1.087184E-14	1.177552E-14	2.213889E-13	99.738667	2.999922
0.75	1.727969E+16	87.500000	1.234286E-06	1.129535E-14	1.193437E-14	2.273691E-13	99.731639	2.999920
0.76	1.727846E+16	88.666667	1.234286E-06	1.172968E-14	1.209321E-14	2.334290E-13	99.724515	2.999918
0.77	1.727721E+16	89.833333	1.234286E-06	1.217497E-14	1.225204E-14	2.395683E-13	99.717294	2.999916
0.78	1.727594E+16	91.000000	1.234286E-06	1.263135E-14	1.241086E-14	2.457873E-13	99.709975	2.999914
0.79	1.727466E+16	92.166667	1.234286E-06	1.309897E-14	1.256967E-14	2.520857E-13	99.702559	2.999911
0.80	1.727335E+16	93.333333	1.234286E-06	1.357795E-14	1.272846E-14	2.584637E-13	99.695046	2.999909
0.81	1.727204E+16	94.500000	1.234286E-06	1.406844E-14	1.288725E-14	2.649213E-13	99.687436	2.999907
0.82	1.727070E+16	95.666667	1.234286E-06	1.457057E-14	1.304602E-14	2.714583E-13	99.679728	2.999904
0.83	1.726935E+16	96.833333	1.234286E-06	1.508447E-14	1.320478E-14	2.780749E-13	99.671922	2.999902
0.84	1.726798E+16	98.000000	1.234286E-06	1.561029E-14	1.336352E-14	2.847710E-13	99.664018	2.999900
0.85	1.726659E+16	99.166667	1.234286E-06	1.614815E-14	1.352226E-14	2.915466E-13	99.656016	2.999897
0.86	1.726519E+16	100.333333	1.234286E-06	1.669819E-14	1.368098E-14	2.984017E-13	99.647916	2.999895
0.87	1.726377E+16	101.500000	1.234286E-06	1.726055E-14	1.383969E-14	3.053362E-13	99.639718	2.999893
0.88	1.726233E+16	102.666667	1.234286E-06	1.783536E-14	1.399839E-14	3.123503E-13	99.631421	2.999890
0.89	1.726088E+16	103.833333	1.234286E-06	1.842277E-14	1.415707E-14	3.194438E-13	99.623026	2.999888
0.90	1.725940E+16	105.000000	1.234286E-06	1.902290E-14	1.431574E-14	3.266167E-13	99.614532	2.999885
0.91	1.725792E+16	106.166667	1.234286E-06	1.963588E-14	1.447440E-14	3.338691E-13	99.605939	2.999883
0.92	1.725641E+16	107.333333	1.234286E-06	2.026187E-14	1.463304E-14	3.412010E-13	99.597248	2.999880
0.93	1.725489E+16	108.500000	1.234286E-06	2.090098E-14	1.479167E-14	3.486123E-13	99.588457	2.999877
0.94	1.725335E+16	109.666667	1.234286E-06	2.155336E-14	1.495028E-14	3.561030E-13	99.579567	2.999875
0.95	1.725179E+16	110.833333	1.234286E-06	2.221915E-14	1.510888E-14	3.636732E-13	99.570577	2.999872
0.96	1.725021E+16	112.000000	1.234286E-06	2.289847E-14	1.526747E-14	3.713228E-13	99.561488	2.999869
0.97	1.724862E+16	113.166667	1.234286E-06	2.359147E-14	1.542605E-14	3.790517E-13	99.552299	2.999867
0.98	1.724701E+16	114.333333	1.234286E-06	2.429827E-14	1.558460E-14	3.868601E-13	99.543011	2.999864
0.99	1.724539E+16	115.500000	1.234286E-06	2.501902E-14	1.574315E-14	3.947478E-13	99.533622	2.999861
1.00	1.724374E+16	116.666667	1.234286E-06	2.575385E-14	1.590168E-14	4.027149E-13	99.524134	2.999858



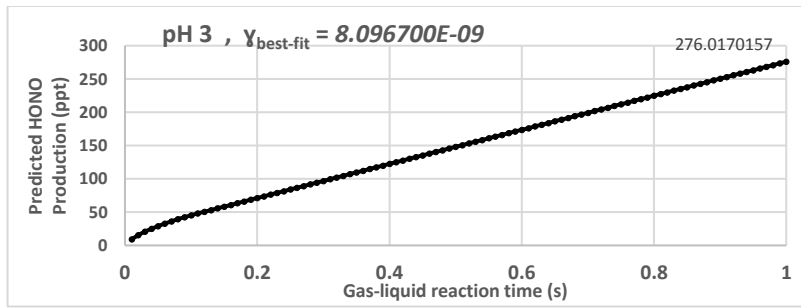
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732615E+16	1.166667	3.509916E-07	2.173844E-19	1.441329E-16	7.223756E-17	99.999768	3.000000
0.02	1.732610E+16	2.333333	4.963755E-07	9.595811E-19	2.882654E-16	2.167124E-16	99.999458	3.000000
0.03	1.732603E+16	3.500000	6.079310E-07	2.449397E-18	4.323973E-16	4.334243E-16	99.999070	3.000000
0.04	1.732595E+16	4.666667	7.019750E-07	4.870587E-18	5.765286E-16	7.223727E-16	99.998604	3.000000
0.05	1.732585E+16	5.833333	7.848276E-07	8.383162E-18	7.206590E-16	1.083557E-15	99.998059	2.999999
0.06	1.732575E+16	7.000000	8.597302E-07	1.313073E-17	8.647887E-16	1.516978E-15	99.997435	2.999999
0.07	1.732563E+16	8.166667	9.286082E-07	1.924471E-17	1.008917E-15	2.022633E-15	99.996733	2.999999
0.08	1.732549E+16	9.333333	9.927162E-07	2.684697E-17	1.153045E-15	2.600523E-15	99.995952	2.999999
0.09	1.732534E+16	10.500000	1.052925E-06	3.605166E-17	1.297171E-15	3.250646E-15	99.995091	2.999999
0.10	1.732518E+16	11.666667	1.109870E-06	4.696653E-17	1.441296E-15	3.973003E-15	99.994152	2.999998
0.11	1.732500E+16	12.833333	1.164030E-06	5.969387E-17	1.585420E-15	4.767592E-15	99.993133	2.999998
0.12	1.732481E+16	14.000000	1.215776E-06	7.433129E-17	1.729542E-15	5.634412E-15	99.992035	2.999998
0.13	1.732461E+16	15.166667	1.234286E-06	9.099204E-17	1.873662E-15	6.573462E-15	99.990857	2.999998
0.14	1.732439E+16	16.333333	1.234286E-06	1.097997E-16	2.017780E-15	7.584742E-15	99.989599	2.999997
0.15	1.732416E+16	17.500000	1.234286E-06	1.308780E-16	2.161897E-15	8.668249E-15	99.988262	2.999997
0.16	1.732391E+16	18.666667	1.234286E-06	1.543504E-16	2.306012E-15	9.823984E-15	99.986845	2.999997
0.17	1.732365E+16	19.833333	1.234286E-06	1.803406E-16	2.450124E-15	1.105194E-14	99.985348	2.999996
0.18	1.732338E+16	21.000000	1.234286E-06	2.089722E-16	2.594235E-15	1.235213E-14	99.983771	2.999996
0.19	1.732309E+16	22.166667	1.234286E-06	2.403687E-16	2.738343E-15	1.372454E-14	99.982113	2.999995
0.20	1.732279E+16	23.333333	1.234286E-06	2.746538E-16	2.882448E-15	1.516916E-14	99.980375	2.999995
0.21	1.732248E+16	24.500000	1.234286E-06	3.119511E-16	3.026551E-15	1.668601E-14	99.978556	2.999994
0.22	1.732215E+16	25.666667	1.234286E-06	3.523841E-16	3.170651E-15	1.827508E-14	99.976657	2.999994
0.23	1.732180E+16	26.833333	1.234286E-06	3.960763E-16	3.314749E-15	1.993636E-14	99.974677	2.999993
0.24	1.732145E+16	28.000000	1.234286E-06	4.431515E-16	3.458843E-15	2.166986E-14	99.972616	2.999992
0.25	1.732108E+16	29.166667	1.234286E-06	4.937331E-16	3.602935E-15	2.347557E-14	99.970474	2.999992
0.26	1.732069E+16	30.333333	1.234286E-06	5.479448E-16	3.747023E-15	2.535349E-14	99.968250	2.999991
0.27	1.732029E+16	31.500000	1.234286E-06	6.059100E-16	3.891109E-15	2.730362E-14	99.965945	2.999990
0.28	1.731988E+16	32.666667	1.234286E-06	6.677523E-16	4.035191E-15	2.932596E-14	99.963559	2.999990
0.29	1.731945E+16	33.833333	1.234286E-06	7.335953E-16	4.179269E-15	3.142050E-14	99.961091	2.999989
0.30	1.731901E+16	35.000000	1.234286E-06	8.035625E-16	4.323344E-15	3.358725E-14	99.958542	2.999988
0.31	1.731855E+16	36.166667	1.234286E-06	8.777775E-16	4.467415E-15	3.582619E-14	99.955911	2.999987
0.32	1.731808E+16	37.333333	1.234286E-06	9.563638E-16	4.611482E-15	3.813734E-14	99.953197	2.999987
0.33	1.731760E+16	38.500000	1.234286E-06	1.039445E-15	4.755545E-15	4.052068E-14	99.950402	2.999986
0.34	1.731710E+16	39.666667	1.234286E-06	1.127144E-15	4.899605E-15	4.297621E-14	99.947524	2.999985
0.35	1.731659E+16	40.833333	1.234286E-06	1.219585E-15	5.043660E-15	4.550394E-14	99.944564	2.999984
0.36	1.731606E+16	42.000000	1.234286E-06	1.316892E-15	5.187710E-15	4.810385E-14	99.941521	2.999983
0.37	1.731552E+16	43.166667	1.234286E-06	1.419187E-15	5.331757E-15	5.077595E-14	99.938396	2.999982
0.38	1.731496E+16	44.333333	1.234286E-06	1.526595E-15	5.475799E-15	5.352023E-14	99.935188	2.999981
0.39	1.731439E+16	45.500000	1.234286E-06	1.639238E-15	5.619836E-15	5.633669E-14	99.931897	2.999980
0.40	1.731381E+16	46.666667	1.234286E-06	1.757241E-15	5.763869E-15	5.922533E-14	99.928523	2.999979
0.41	1.731321E+16	47.833333	1.234286E-06	1.880727E-15	5.907896E-15	6.218614E-14	99.925066	2.999978
0.42	1.731259E+16	49.000000	1.234286E-06	2.009818E-15	6.051919E-15	6.521913E-14	99.921525	2.999977
0.43	1.731197E+16	50.166667	1.234286E-06	2.144640E-15	6.195936E-15	6.832428E-14	99.917901	2.999976
0.44	1.731132E+16	51.333333	1.234286E-06	2.285314E-15	6.339949E-15	7.150160E-14	99.914194	2.999975
0.45	1.731067E+16	52.500000	1.234286E-06	2.431965E-15	6.483956E-15	7.475108E-14	99.910403	2.999974

0.46	1.731000E+16	53.666667	1.234286E-06	2.584715E-15	6.627957E-15	7.807271E-14	99.906528	2.999973
0.47	1.730931E+16	54.833333	1.234286E-06	2.743689E-15	6.771953E-15	8.146651E-14	99.902569	2.999971
0.48	1.730861E+16	56.000000	1.234286E-06	2.909010E-15	6.915944E-15	8.493245E-14	99.898526	2.999970
0.49	1.730789E+16	57.166667	1.234286E-06	3.080801E-15	7.059928E-15	8.847054E-14	99.894399	2.999969
0.50	1.730716E+16	58.333333	1.234286E-06	3.259185E-15	7.203907E-15	9.208078E-14	99.890188	2.999968
0.51	1.730642E+16	59.500000	1.234286E-06	3.444286E-15	7.347879E-15	9.576316E-14	99.885892	2.999966
0.52	1.730566E+16	60.666667	1.234286E-06	3.636228E-15	7.491845E-15	9.951767E-14	99.881512	2.999965
0.53	1.730489E+16	61.833333	1.234286E-06	3.835133E-15	7.635805E-15	1.033443E-13	99.877047	2.999964
0.54	1.730410E+16	63.000000	1.234286E-06	4.041125E-15	7.779759E-15	1.072431E-13	99.872497	2.999962
0.55	1.730330E+16	64.166667	1.234286E-06	4.254327E-15	7.923706E-15	1.112140E-13	99.867862	2.999961
0.56	1.730248E+16	65.333333	1.234286E-06	4.474862E-15	8.067647E-15	1.152570E-13	99.863142	2.999959
0.57	1.730165E+16	66.500000	1.234286E-06	4.702855E-15	8.211580E-15	1.193722E-13	99.858337	2.999958
0.58	1.730080E+16	67.666667	1.234286E-06	4.938427E-15	8.355507E-15	1.235594E-13	99.853447	2.999957
0.59	1.729994E+16	68.833333	1.234286E-06	5.181703E-15	8.499427E-15	1.278188E-13	99.848471	2.999955
0.60	1.729906E+16	70.000000	1.234286E-06	5.432806E-15	8.643340E-15	1.321502E-13	99.843410	2.999954
0.61	1.729817E+16	71.166667	1.234286E-06	5.691859E-15	8.787245E-15	1.365538E-13	99.838262	2.999952
0.62	1.729726E+16	72.333333	1.234286E-06	5.958985E-15	8.931143E-15	1.410295E-13	99.833029	2.999950
0.63	1.729634E+16	73.500000	1.234286E-06	6.234307E-15	9.075034E-15	1.455772E-13	99.827710	2.999949
0.64	1.729540E+16	74.666667	1.234286E-06	6.517949E-15	9.218917E-15	1.501971E-13	99.822305	2.999947
0.65	1.729445E+16	75.833333	1.234286E-06	6.810033E-15	9.362792E-15	1.548890E-13	99.816814	2.999946
0.66	1.729349E+16	77.000000	1.234286E-06	7.110684E-15	9.506659E-15	1.596530E-13	99.811236	2.999944
0.67	1.729250E+16	78.166667	1.234286E-06	7.420024E-15	9.650519E-15	1.644891E-13	99.805572	2.999942
0.68	1.729151E+16	79.333333	1.234286E-06	7.738177E-15	9.794370E-15	1.693972E-13	99.799821	2.999940
0.69	1.729050E+16	80.500000	1.234286E-06	8.065264E-15	9.938213E-15	1.743774E-13	99.793984	2.999939
0.70	1.728947E+16	81.666667	1.234286E-06	8.401411E-15	1.008205E-14	1.794297E-13	99.788059	2.999937
0.71	1.728843E+16	82.833333	1.234286E-06	8.746739E-15	1.022587E-14	1.845540E-13	99.782048	2.999935
0.72	1.728737E+16	84.000000	1.234286E-06	9.101372E-15	1.036969E-14	1.897503E-13	99.775950	2.999933
0.73	1.728630E+16	85.166667	1.234286E-06	9.465434E-15	1.051350E-14	1.950187E-13	99.769764	2.999931
0.74	1.728521E+16	86.333333	1.234286E-06	9.839046E-15	1.065730E-14	2.003592E-13	99.763491	2.999930
0.75	1.728411E+16	87.500000	1.234286E-06	1.022233E-14	1.080109E-14	2.057716E-13	99.757130	2.999928
0.76	1.728299E+16	88.666667	1.234286E-06	1.061542E-14	1.094487E-14	2.112561E-13	99.750682	2.999926
0.77	1.728186E+16	89.833333	1.234286E-06	1.101842E-14	1.108865E-14	2.168126E-13	99.744146	2.999924
0.78	1.728071E+16	91.000000	1.234286E-06	1.143147E-14	1.123241E-14	2.224412E-13	99.737523	2.999922
0.79	1.727955E+16	92.166667	1.234286E-06	1.185468E-14	1.137616E-14	2.281417E-13	99.730811	2.999920
0.80	1.727837E+16	93.333333	1.234286E-06	1.228818E-14	1.151991E-14	2.339142E-13	99.724011	2.999918
0.81	1.727718E+16	94.500000	1.234286E-06	1.273210E-14	1.166364E-14	2.397588E-13	99.717123	2.999916
0.82	1.727597E+16	95.666667	1.234286E-06	1.318655E-14	1.180737E-14	2.456753E-13	99.710147	2.999914
0.83	1.727475E+16	96.833333	1.234286E-06	1.365165E-14	1.195108E-14	2.516638E-13	99.703082	2.999911
0.84	1.727351E+16	98.000000	1.234286E-06	1.412754E-14	1.209479E-14	2.577243E-13	99.695928	2.999909
0.85	1.727225E+16	99.166667	1.234286E-06	1.461433E-14	1.223848E-14	2.638568E-13	99.688686	2.999907
0.86	1.727098E+16	100.333333	1.234286E-06	1.511215E-14	1.238217E-14	2.700612E-13	99.681355	2.999905
0.87	1.726970E+16	101.500000	1.234286E-06	1.562112E-14	1.252584E-14	2.763376E-13	99.673935	2.999903
0.88	1.726840E+16	102.666667	1.234286E-06	1.614136E-14	1.266951E-14	2.826859E-13	99.666425	2.999901
0.89	1.726708E+16	103.833333	1.234286E-06	1.667300E-14	1.281316E-14	2.891062E-13	99.658827	2.999898
0.90	1.726575E+16	105.000000	1.234286E-06	1.721615E-14	1.295680E-14	2.955984E-13	99.651139	2.999896
0.91	1.726440E+16	106.166667	1.234286E-06	1.777095E-14	1.310043E-14	3.021626E-13	99.643362	2.999894
0.92	1.726304E+16	107.333333	1.234286E-06	1.833751E-14	1.324405E-14	3.087987E-13	99.635495	2.999891
0.93	1.726166E+16	108.500000	1.234286E-06	1.891595E-14	1.338766E-14	3.155067E-13	99.627538	2.999889
0.94	1.726026E+16	109.666667	1.234286E-06	1.950640E-14	1.353126E-14	3.222866E-13	99.619491	2.999887
0.95	1.725885E+16	110.833333	1.234286E-06	2.010899E-14	1.367484E-14	3.291384E-13	99.611355	2.999884
0.96	1.725743E+16	112.000000	1.234286E-06	2.072383E-14	1.381842E-14	3.360622E-13	99.603128	2.999882
0.97	1.725599E+16	113.166667	1.234286E-06	2.135105E-14	1.396198E-14	3.430578E-13	99.594811	2.999879
0.98	1.725453E+16	114.333333	1.234286E-06	2.199076E-14	1.410553E-14	3.501253E-13	99.586404	2.999877
0.99	1.725306E+16	115.500000	1.234286E-06	2.264310E-14	1.424907E-14	3.572647E-13	99.577907	2.999874
1.00	1.725157E+16	116.666667	1.234286E-06	2.330819E-14	1.439260E-14	3.644759E-13	99.569318	2.999872



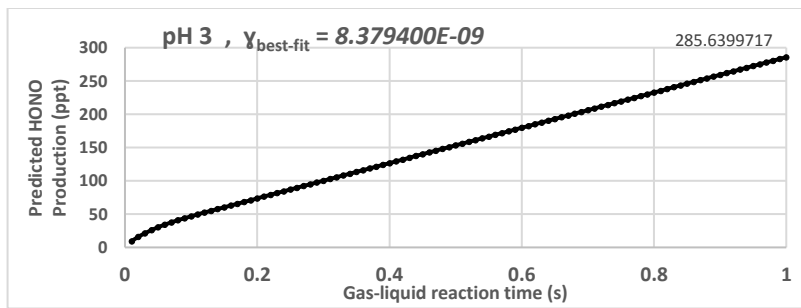
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732615E+16	1.166667	3.509915E-07	2.467163E-19	1.635809E-16	8.198463E-17	99.999737	3.000000
0.02	1.732608E+16	2.333333	4.963751E-07	1.089059E-18	3.271612E-16	2.459536E-16	99.999385	3.000000
0.03	1.732601E+16	3.500000	6.079302E-07	2.779897E-18	4.907408E-16	4.919064E-16	99.998945	3.000000
0.04	1.732592E+16	4.666667	7.019736E-07	5.527782E-18	6.543196E-16	8.198426E-16	99.998415	2.999999
0.05	1.732581E+16	5.833333	7.848255E-07	9.514312E-18	8.178973E-16	1.229762E-15	99.997797	2.999999
0.06	1.732569E+16	7.000000	8.597272E-07	1.490248E-17	9.814740E-16	1.721663E-15	99.997089	2.999999
0.07	1.732555E+16	8.166667	9.286041E-07	2.184142E-17	1.145049E-15	2.295546E-15	99.996292	2.999999
0.08	1.732540E+16	9.333333	9.927108E-07	3.046946E-17	1.308623E-15	2.951409E-15	99.995405	2.999999
0.09	1.732523E+16	10.500000	1.052918E-06	4.091616E-17	1.472196E-15	3.689252E-15	99.994429	2.999998
0.10	1.732504E+16	11.666667	1.109862E-06	5.330379E-17	1.635766E-15	4.509074E-15	99.993363	2.999998
0.11	1.732484E+16	12.833333	1.164019E-06	6.774844E-17	1.799335E-15	5.410873E-15	99.992206	2.999998
0.12	1.732462E+16	14.000000	1.215763E-06	8.436090E-17	1.962902E-15	6.394650E-15	99.990960	2.999998
0.13	1.732439E+16	15.166667	1.234286E-06	1.032697E-16	2.126467E-15	7.460401E-15	99.989623	2.999997
0.14	1.732415E+16	16.333333	1.234286E-06	1.246151E-16	2.290029E-15	8.608126E-15	99.988196	2.999997
0.15	1.732388E+16	17.500000	1.234286E-06	1.485375E-16	2.453589E-15	9.837824E-15	99.986678	2.999997
0.16	1.732360E+16	18.666667	1.234286E-06	1.751770E-16	2.617146E-15	1.114949E-14	99.985070	2.999996
0.17	1.732331E+16	19.833333	1.234286E-06	2.046740E-16	2.780701E-15	1.254313E-14	99.983371	2.999996
0.18	1.732300E+16	21.000000	1.234286E-06	2.371687E-16	2.944253E-15	1.401874E-14	99.981581	2.999995
0.19	1.732267E+16	22.166667	1.234286E-06	2.728015E-16	3.107801E-15	1.557631E-14	99.979699	2.999995
0.20	1.732233E+16	23.333333	1.234286E-06	3.117125E-16	3.271347E-15	1.721584E-14	99.977727	2.999994
0.21	1.732197E+16	24.500000	1.234286E-06	3.540420E-16	3.434889E-15	1.893734E-14	99.975663	2.999993
0.22	1.732160E+16	25.666667	1.234286E-06	3.999304E-16	3.598428E-15	2.074079E-14	99.973507	2.999993
0.23	1.732121E+16	26.833333	1.234286E-06	4.495177E-16	3.761964E-15	2.262621E-14	99.971260	2.999992
0.24	1.732081E+16	28.000000	1.234286E-06	5.029443E-16	3.925495E-15	2.459358E-14	99.968921	2.999991
0.25	1.732039E+16	29.166667	1.234286E-06	5.603504E-16	4.089023E-15	2.664290E-14	99.966490	2.999991
0.26	1.731995E+16	30.333333	1.234286E-06	6.218762E-16	4.252546E-15	2.877417E-14	99.963967	2.999990
0.27	1.731949E+16	31.500000	1.234286E-06	6.876620E-16	4.416066E-15	3.098739E-14	99.961351	2.999989
0.28	1.731903E+16	32.666667	1.234286E-06	7.578479E-16	4.579581E-15	3.328255E-14	99.958643	2.999988
0.29	1.731854E+16	33.833333	1.234286E-06	8.325742E-16	4.743092E-15	3.565966E-14	99.955842	2.999987
0.30	1.731804E+16	35.000000	1.234286E-06	9.119810E-16	4.906598E-15	3.811871E-14	99.952949	2.999987
0.31	1.731752E+16	36.166667	1.234286E-06	9.962086E-16	5.070099E-15	4.065970E-14	99.949962	2.999986
0.32	1.731699E+16	37.333333	1.234286E-06	1.085397E-15	5.233595E-15	4.328262E-14	99.946883	2.999985
0.33	1.731644E+16	38.500000	1.234286E-06	1.179687E-15	5.397086E-15	4.598747E-14	99.943710	2.999984
0.34	1.731587E+16	39.666667	1.234286E-06	1.279217E-15	5.560572E-15	4.877424E-14	99.940444	2.999983
0.35	1.731529E+16	40.833333	1.234286E-06	1.384130E-15	5.724053E-15	5.164295E-14	99.937085	2.999982
0.36	1.731469E+16	42.000000	1.234286E-06	1.494563E-15	5.887528E-15	5.459357E-14	99.933632	2.999981
0.37	1.731408E+16	43.166667	1.234286E-06	1.610659E-15	6.050998E-15	5.762611E-14	99.930085	2.999980
0.38	1.731345E+16	44.333333	1.234286E-06	1.732556E-15	6.214461E-15	6.074057E-14	99.926444	2.999979
0.39	1.731280E+16	45.500000	1.234286E-06	1.860396E-15	6.377919E-15	6.393693E-14	99.922709	2.999978
0.40	1.731214E+16	46.666667	1.234286E-06	1.994317E-15	6.541371E-15	6.721520E-14	99.918880	2.999976
0.41	1.731146E+16	47.833333	1.234286E-06	2.134460E-15	6.704816E-15	7.057538E-14	99.914957	2.999975
0.42	1.731076E+16	49.000000	1.234286E-06	2.280966E-15	6.868255E-15	7.401746E-14	99.910939	2.999974
0.43	1.731005E+16	50.166667	1.234286E-06	2.433974E-15	7.031687E-15	7.754143E-14	99.906826	2.999973
0.44	1.730932E+16	51.333333	1.234286E-06	2.593624E-15	7.195113E-15	8.114729E-14	99.902619	2.999971
0.45	1.730857E+16	52.500000	1.234286E-06	2.760057E-15	7.358531E-15	8.483504E-14	99.898316	2.999970

0.46	1.730781E+16	53.666667	1.234286E-06	2.933412E-15	7.521943E-15	8.860467E-14	99.893919	2.999969
0.47	1.730703E+16	54.833333	1.234286E-06	3.113830E-15	7.685348E-15	9.245618E-14	99.889426	2.999967
0.48	1.730624E+16	56.000000	1.234286E-06	3.301450E-15	7.848745E-15	9.638956E-14	99.884838	2.999966
0.49	1.730543E+16	57.166667	1.234286E-06	3.496412E-15	8.012134E-15	1.004048E-13	99.880155	2.999965
0.50	1.730460E+16	58.333333	1.234286E-06	3.698857E-15	8.175516E-15	1.045019E-13	99.875375	2.999963
0.51	1.730375E+16	59.500000	1.234286E-06	3.908925E-15	8.338891E-15	1.086809E-13	99.870500	2.999962
0.52	1.730289E+16	60.666667	1.234286E-06	4.126755E-15	8.502257E-15	1.129417E-13	99.865529	2.999960
0.53	1.730201E+16	61.833333	1.234286E-06	4.352487E-15	8.665615E-15	1.172844E-13	99.860462	2.999959
0.54	1.730112E+16	63.000000	1.234286E-06	4.586262E-15	8.828965E-15	1.217090E-13	99.855299	2.999957
0.55	1.730021E+16	64.166667	1.234286E-06	4.828219E-15	8.992307E-15	1.262153E-13	99.850039	2.999956
0.56	1.729928E+16	65.333333	1.234286E-06	5.078498E-15	9.155640E-15	1.308035E-13	99.844683	2.999954
0.57	1.729834E+16	66.500000	1.234286E-06	5.337239E-15	9.318964E-15	1.354736E-13	99.839230	2.999952
0.58	1.729737E+16	67.666667	1.234286E-06	5.604581E-15	9.482279E-15	1.402254E-13	99.833680	2.999951
0.59	1.729640E+16	68.833333	1.234286E-06	5.880666E-15	9.645586E-15	1.450591E-13	99.828033	2.999949
0.60	1.729540E+16	70.000000	1.234286E-06	6.165632E-15	9.808883E-15	1.499746E-13	99.822289	2.999947
0.61	1.729439E+16	71.166667	1.234286E-06	6.459620E-15	9.972171E-15	1.549719E-13	99.816448	2.999945
0.62	1.729336E+16	72.333333	1.234286E-06	6.762769E-15	1.013545E-14	1.600510E-13	99.810509	2.999944
0.63	1.729231E+16	73.500000	1.234286E-06	7.075219E-15	1.029872E-14	1.652119E-13	99.804473	2.999942
0.64	1.729125E+16	74.666667	1.234286E-06	7.397109E-15	1.046198E-14	1.704546E-13	99.798339	2.999940
0.65	1.729017E+16	75.833333	1.234286E-06	7.728580E-15	1.062523E-14	1.757790E-13	99.792108	2.999938
0.66	1.728907E+16	77.000000	1.234286E-06	8.069772E-15	1.078846E-14	1.811853E-13	99.785778	2.999936
0.67	1.728796E+16	78.166667	1.234286E-06	8.420824E-15	1.095169E-14	1.866733E-13	99.779350	2.999934
0.68	1.728683E+16	79.333333	1.234286E-06	8.781875E-15	1.111491E-14	1.922431E-13	99.772824	2.999932
0.69	1.728568E+16	80.500000	1.234286E-06	9.153066E-15	1.127812E-14	1.978946E-13	99.766200	2.999930
0.70	1.728452E+16	81.666667	1.234286E-06	9.534536E-15	1.144132E-14	2.036279E-13	99.759477	2.999928
0.71	1.728334E+16	82.833333	1.234286E-06	9.926425E-15	1.160450E-14	2.094430E-13	99.752655	2.999926
0.72	1.728214E+16	84.000000	1.234286E-06	1.032887E-14	1.176768E-14	2.153397E-13	99.745735	2.999924
0.73	1.728092E+16	85.166667	1.234286E-06	1.074202E-14	1.193084E-14	2.213183E-13	99.738716	2.999922
0.74	1.727969E+16	86.333333	1.234286E-06	1.116600E-14	1.209399E-14	2.273785E-13	99.731597	2.999920
0.75	1.727844E+16	87.500000	1.234286E-06	1.160096E-14	1.225713E-14	2.335204E-13	99.724379	2.999918
0.76	1.727717E+16	88.666667	1.234286E-06	1.204704E-14	1.242026E-14	2.397441E-13	99.717062	2.999916
0.77	1.727588E+16	89.833333	1.234286E-06	1.250437E-14	1.258338E-14	2.460495E-13	99.709645	2.999913
0.78	1.727458E+16	91.000000	1.234286E-06	1.297310E-14	1.274648E-14	2.524366E-13	99.702129	2.999911
0.79	1.727326E+16	92.166667	1.234286E-06	1.345336E-14	1.290958E-14	2.589053E-13	99.694513	2.999909
0.80	1.727192E+16	93.333333	1.234286E-06	1.394530E-14	1.307266E-14	2.654558E-13	99.686797	2.999907
0.81	1.727057E+16	94.500000	1.234286E-06	1.444906E-14	1.323573E-14	2.720879E-13	99.678980	2.999904
0.82	1.726920E+16	95.666667	1.234286E-06	1.496476E-14	1.339878E-14	2.788017E-13	99.671064	2.999902
0.83	1.726781E+16	96.833333	1.234286E-06	1.549256E-14	1.356182E-14	2.855971E-13	99.663047	2.999900
0.84	1.726640E+16	98.000000	1.234286E-06	1.603260E-14	1.372485E-14	2.924742E-13	99.654930	2.999897
0.85	1.726498E+16	99.166667	1.234286E-06	1.658500E-14	1.388787E-14	2.994329E-13	99.646712	2.999895
0.86	1.726354E+16	100.333333	1.234286E-06	1.714992E-14	1.405087E-14	3.064733E-13	99.638393	2.999892
0.87	1.726208E+16	101.500000	1.234286E-06	1.772748E-14	1.421386E-14	3.135953E-13	99.629973	2.999890
0.88	1.726060E+16	102.666667	1.234286E-06	1.831784E-14	1.437684E-14	3.207989E-13	99.621452	2.999887
0.89	1.725911E+16	103.833333	1.234286E-06	1.892112E-14	1.453980E-14	3.280841E-13	99.612830	2.999885
0.90	1.725760E+16	105.000000	1.234286E-06	1.953748E-14	1.470275E-14	3.354510E-13	99.604106	2.999882
0.91	1.725607E+16	106.166667	1.234286E-06	2.016704E-14	1.486569E-14	3.428994E-13	99.595281	2.999879
0.92	1.725452E+16	107.333333	1.234286E-06	2.080994E-14	1.502861E-14	3.504294E-13	99.586355	2.999877
0.93	1.725296E+16	108.500000	1.234286E-06	2.146634E-14	1.519151E-14	3.580410E-13	99.577326	2.999874
0.94	1.725138E+16	109.666667	1.234286E-06	2.213636E-14	1.535440E-14	3.657341E-13	99.568196	2.999871
0.95	1.724978E+16	110.833333	1.234286E-06	2.282014E-14	1.551728E-14	3.735088E-13	99.558963	2.999869
0.96	1.724816E+16	112.000000	1.234286E-06	2.351782E-14	1.568014E-14	3.813651E-13	99.549629	2.999866
0.97	1.724652E+16	113.166667	1.234286E-06	2.422955E-14	1.584299E-14	3.893029E-13	99.540192	2.999863
0.98	1.724487E+16	114.333333	1.234286E-06	2.495546E-14	1.600582E-14	3.973222E-13	99.530652	2.999860
0.99	1.724320E+16	115.500000	1.234286E-06	2.569569E-14	1.616863E-14	4.054231E-13	99.521010	2.999857
1.00	1.724151E+16	116.666667	1.234286E-06	2.645038E-14	1.633143E-14	4.136054E-13	99.511265	2.999854



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO2}}$ (mol)	$\Phi_{\text{NO2}}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732615E+16	1.166667	3.509915E-07	2.340398E-19	1.551759E-16	7.777218E-17	99.999750	3.000000
0.02	1.732609E+16	2.333333	4.963753E-07	1.033102E-18	3.103514E-16	2.333163E-16	99.999417	3.000000
0.03	1.732602E+16	3.500000	6.079306E-07	2.637063E-18	4.655262E-16	4.666319E-16	99.998999	3.000000
0.04	1.732593E+16	4.666667	7.019742E-07	5.243758E-18	6.207002E-16	7.777185E-16	99.998497	3.000000
0.05	1.732583E+16	5.833333	7.848264E-07	9.025456E-18	7.758734E-16	1.166576E-15	99.997910	2.999999
0.06	1.732571E+16	7.000000	8.597285E-07	1.413677E-17	9.310455E-16	1.633203E-15	99.997239	2.999999
0.07	1.732558E+16	8.166667	9.286059E-07	2.071919E-17	1.086216E-15	2.177600E-15	99.996483	2.999999
0.08	1.732544E+16	9.333333	9.927131E-07	2.890391E-17	1.241386E-15	2.799765E-15	99.995641	2.999999
0.09	1.732528E+16	10.500000	1.052922E-06	3.881384E-17	1.396554E-15	3.499698E-15	99.994715	2.999999
0.10	1.732510E+16	11.666667	1.109865E-06	5.056498E-17	1.551721E-15	4.277398E-15	99.993704	2.999998
0.11	1.732491E+16	12.833333	1.164024E-06	6.426745E-17	1.706886E-15	5.132863E-15	99.992607	2.999998
0.12	1.732471E+16	14.000000	1.215769E-06	8.002635E-17	1.862050E-15	6.066094E-15	99.991424	2.999998
0.13	1.732449E+16	15.166667	1.234286E-06	9.796359E-17	2.017211E-15	7.077089E-15	99.990156	2.999998
0.14	1.732425E+16	16.333333	1.234286E-06	1.182123E-16	2.172370E-15	8.165846E-15	99.988802	2.999997
0.15	1.732400E+16	17.500000	1.234286E-06	1.409055E-16	2.327527E-15	9.332364E-15	99.987363	2.999997
0.16	1.732374E+16	18.666667	1.234286E-06	1.661763E-16	2.482682E-15	1.057664E-14	99.985837	2.999996
0.17	1.732346E+16	19.833333	1.234286E-06	1.941577E-16	2.637834E-15	1.189868E-14	99.984225	2.999996
0.18	1.732316E+16	21.000000	1.234286E-06	2.249829E-16	2.792984E-15	1.329847E-14	99.982527	2.999995
0.19	1.732285E+16	22.166667	1.234286E-06	2.587849E-16	2.948131E-15	1.477602E-14	99.980742	2.999995
0.20	1.732253E+16	23.333333	1.234286E-06	2.956967E-16	3.103275E-15	1.633132E-14	99.978871	2.999994
0.21	1.732219E+16	24.500000	1.234286E-06	3.358514E-16	3.258417E-15	1.796437E-14	99.976913	2.999994
0.22	1.732184E+16	25.666667	1.234286E-06	3.793821E-16	3.413555E-15	1.967518E-14	99.974869	2.999993
0.23	1.732147E+16	26.833333	1.234286E-06	4.264217E-16	3.568690E-15	2.146373E-14	99.972737	2.999992
0.24	1.732108E+16	28.000000	1.234286E-06	4.771034E-16	3.723821E-15	2.333002E-14	99.970518	2.999992
0.25	1.732068E+16	29.166667	1.234286E-06	5.315601E-16	3.878949E-15	2.527406E-14	99.968211	2.999991
0.26	1.732027E+16	30.333333	1.234286E-06	5.899250E-16	4.034074E-15	2.729584E-14	99.965818	2.999990
0.27	1.731984E+16	31.500000	1.234286E-06	6.523309E-16	4.189194E-15	2.939537E-14	99.963337	2.999990
0.28	1.731939E+16	32.666667	1.234286E-06	7.189110E-16	4.344311E-15	3.157262E-14	99.960768	2.999989
0.29	1.731893E+16	33.833333	1.234286E-06	7.897981E-16	4.499424E-15	3.382762E-14	99.958111	2.999988
0.30	1.731846E+16	35.000000	1.234286E-06	8.651254E-16	4.654532E-15	3.616034E-14	99.955366	2.999987
0.31	1.731797E+16	36.166667	1.234286E-06	9.450258E-16	4.809637E-15	3.857079E-14	99.952533	2.999986
0.32	1.731746E+16	37.333333	1.234286E-06	1.029632E-15	4.964737E-15	4.105897E-14	99.949612	2.999986
0.33	1.731694E+16	38.500000	1.234286E-06	1.119078E-15	5.119832E-15	4.362488E-14	99.946602	2.999985
0.34	1.731640E+16	39.666667	1.234286E-06	1.213496E-15	5.274922E-15	4.626850E-14	99.943504	2.999984
0.35	1.731585E+16	40.833333	1.234286E-06	1.313018E-15	5.430008E-15	4.898984E-14	99.940317	2.999983
0.36	1.731528E+16	42.000000	1.234286E-06	1.417779E-15	5.585089E-15	5.178890E-14	99.937041	2.999982
0.37	1.731470E+16	43.166667	1.234286E-06	1.527910E-15	5.740165E-15	5.466567E-14	99.933677	2.999981
0.38	1.731410E+16	44.333333	1.234286E-06	1.643546E-15	5.895235E-15	5.762015E-14	99.930223	2.999980
0.39	1.731349E+16	45.500000	1.234286E-06	1.764818E-15	6.050300E-15	6.065233E-14	99.926680	2.999979
0.40	1.731286E+16	46.666667	1.234286E-06	1.891859E-15	6.205360E-15	6.376222E-14	99.923047	2.999978
0.41	1.731221E+16	47.833333	1.234286E-06	2.024804E-15	6.360414E-15	6.694981E-14	99.919325	2.999976
0.42	1.731155E+16	49.000000	1.234286E-06	2.163784E-15	6.515462E-15	7.021509E-14	99.915514	2.999975
0.43	1.731088E+16	50.166667	1.234286E-06	2.308932E-15	6.670504E-15	7.355806E-14	99.911613	2.999974
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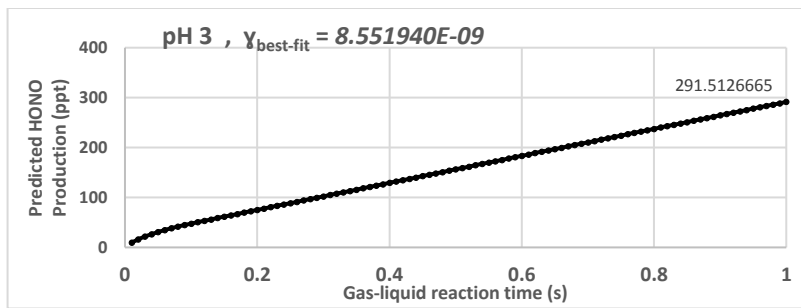
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0.48	1.730726E+16	56.000000	1.234286E-06	3.131849E-15	7.445622E-15	9.143816E-14	99.890754	2.999968
0.49	1.730649E+16	57.166667	1.234286E-06	3.316798E-15	7.600626E-15	9.524721E-14	99.886311	2.999966
0.50	1.730571E+16	58.333333	1.234286E-06	3.508845E-15	7.755623E-15	9.913391E-14	99.881777	2.999965
0.51	1.730491E+16	59.500000	1.234286E-06	3.708123E-15	7.910613E-15	1.030983E-13	99.877152	2.999964
0.52	1.730409E+16	60.666667	1.234286E-06	3.914764E-15	8.065596E-15	1.071403E-13	99.872436	2.999962
0.53	1.730326E+16	61.833333	1.234286E-06	4.128903E-15	8.220571E-15	1.112600E-13	99.867630	2.999961
0.54	1.730241E+16	63.000000	1.234286E-06	4.350671E-15	8.375539E-15	1.154573E-13	99.862731	2.999959
0.55	1.730154E+16	64.166667	1.234286E-06	4.580201E-15	8.530500E-15	1.197323E-13	99.857742	2.999958
0.56	1.730066E+16	65.333333	1.234286E-06	4.817626E-15	8.685453E-15	1.240849E-13	99.852660	2.999956
0.57	1.729977E+16	66.500000	1.234286E-06	5.063079E-15	8.840398E-15	1.285151E-13	99.847487	2.999955
0.58	1.729885E+16	67.666667	1.234286E-06	5.316692E-15	8.995335E-15	1.330230E-13	99.842222	2.999953
0.59	1.729793E+16	68.833333	1.234286E-06	5.578598E-15	9.150264E-15	1.376084E-13	99.836866	2.999952
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0.61	1.729602E+16	71.166667	1.234286E-06	6.127820E-15	9.460097E-15	1.470123E-13	99.825875	2.999948
0.62	1.729505E+16	72.333333	1.234286E-06	6.415401E-15	9.615001E-15	1.518306E-13	99.820242	2.999947
0.63	1.729405E+16	73.500000	1.234286E-06	6.711806E-15	9.769896E-15	1.567265E-13	99.814515	2.999945
0.64	1.729305E+16	74.666667	1.234286E-06	7.017167E-15	9.924782E-15	1.617000E-13	99.808696	2.999943
0.65	1.729202E+16	75.833333	1.234286E-06	7.331617E-15	1.007966E-14	1.667511E-13	99.802785	2.999941
0.66	1.729098E+16	77.000000	1.234286E-06	7.655289E-15	1.023453E-14	1.718798E-13	99.796780	2.999940
0.67	1.728992E+16	78.166667	1.234286E-06	7.988314E-15	1.038939E-14	1.770861E-13	99.790682	2.999938
0.68	1.728885E+16	79.333333	1.234286E-06	8.330827E-15	1.054424E-14	1.823700E-13	99.784491	2.999936
0.69	1.728776E+16	80.500000	1.234286E-06	8.682958E-15	1.069908E-14	1.877314E-13	99.778207	2.999934
0.70	1.728666E+16	81.666667	1.234286E-06	9.044841E-15	1.085391E-14	1.931704E-13	99.771829	2.999932
0.71	1.728554E+16	82.833333	1.234286E-06	9.416609E-15	1.100873E-14	1.986869E-13	99.765358	2.999930
0.72	1.728440E+16	84.000000	1.234286E-06	9.798393E-15	1.116354E-14	2.042810E-13	99.758793	2.999928
0.73	1.728325E+16	85.166667	1.234286E-06	1.019033E-14	1.131834E-14	2.099527E-13	99.752133	2.999926
0.74	1.728208E+16	86.333333	1.234286E-06	1.059254E-14	1.147313E-14	2.157019E-13	99.745380	2.999924
0.75	1.728089E+16	87.500000	1.234286E-06	1.100517E-14	1.162791E-14	2.215286E-13	99.738533	2.999922
0.76	1.727969E+16	88.666667	1.234286E-06	1.142835E-14	1.178268E-14	2.274328E-13	99.731591	2.999920
0.77	1.727847E+16	89.833333	1.234286E-06	1.186220E-14	1.193744E-14	2.334146E-13	99.724555	2.999918
0.78	1.727723E+16	91.000000	1.234286E-06	1.230687E-14	1.209218E-14	2.394738E-13	99.717425	2.999916
0.79	1.727598E+16	92.166667	1.234286E-06	1.276248E-14	1.224692E-14	2.456106E-13	99.710199	2.999914
0.80	1.727471E+16	93.333333	1.234286E-06	1.322916E-14	1.240165E-14	2.518249E-13	99.702879	2.999911
0.81	1.727343E+16	94.500000	1.234286E-06	1.370706E-14	1.255636E-14	2.581167E-13	99.695464	2.999909
0.82	1.727213E+16	95.666667	1.234286E-06	1.419629E-14	1.271106E-14	2.644859E-13	99.687954	2.999907
0.83	1.727081E+16	96.833333	1.234286E-06	1.469700E-14	1.286576E-14	2.709327E-13	99.680348	2.999905
0.84	1.726947E+16	98.000000	1.234286E-06	1.520931E-14	1.302044E-14	2.774569E-13	99.672647	2.999902
0.85	1.726812E+16	99.166667	1.234286E-06	1.573336E-14	1.317510E-14	2.840586E-13	99.664851	2.999900
0.86	1.726676E+16	100.333333	1.234286E-06	1.626928E-14	1.332976E-14	2.907377E-13	99.656959	2.999898
0.87	1.726537E+16	101.500000	1.234286E-06	1.681721E-14	1.348440E-14	2.974943E-13	99.648971	2.999895
0.88	1.726397E+16	102.666667	1.234286E-06	1.737726E-14	1.363904E-14	3.043283E-13	99.640887	2.999893
0.89	1.726255E+16	103.833333	1.234286E-06	1.794958E-14	1.379366E-14	3.112398E-13	99.632707	2.999891
0.90	1.726112E+16	105.000000	1.234286E-06	1.853431E-14	1.394826E-14	3.182286E-13	99.624432	2.999888
0.91	1.725967E+16	106.166667	1.234286E-06	1.913156E-14	1.410286E-14	3.252949E-13	99.616059	2.999886
0.92	1.725820E+16	107.333333	1.234286E-06	1.974147E-14	1.425744E-14	3.324387E-13	99.607590	2.999883
0.93	1.725672E+16	108.500000	1.234286E-06	2.036418E-14	1.441201E-14	3.396598E-13	99.599025	2.999881
0.94	1.725522E+16	109.666667	1.234286E-06	2.099982E-14	1.456656E-14	3.469583E-13	99.590363	2.999878
0.95	1.725370E+16	110.833333	1.234286E-06	2.164851E-14	1.472110E-14	3.543342E-13	99.581604	2.999875
0.96	1.725216E+16	112.000000	1.234286E-06	2.231040E-14	1.487563E-14	3.617875E-13	99.572748	2.999873
0.97	1.725061E+16	113.166667	1.234286E-06	2.298560E-14	1.503015E-14	3.693182E-13	99.563796	2.999870
0.98	1.724905E+16	114.333333	1.234286E-06	2.367427E-14	1.518465E-14	3.769262E-13	99.554745	2.999867
0.99	1.724746E+16	115.500000	1.234286E-06	2.437652E-14	1.533913E-14	3.846116E-13	99.545598	2.999865
1.00	1.724586E+16	116.666667	1.234286E-06	2.509248E-14	1.549361E-14	3.923743E-13	99.536353	2.999862



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732615E+16	1.166667	3.509915E-07	2.422114E-19	1.605940E-16	8.048763E-17	99.999742	3.000000
0.02	1.732609E+16	2.333333	4.963752E-07	1.069173E-18	3.211874E-16	2.414626E-16	99.999396	3.000000
0.03	1.732601E+16	3.500000	6.079303E-07	2.729137E-18	4.817801E-16	4.829244E-16	99.998964	3.000000
0.04	1.732592E+16	4.666667	7.019738E-07	5.426847E-18	6.423721E-16	8.048727E-16	99.998444	3.000000
0.05	1.732582E+16	5.833333	7.848259E-07	9.340584E-18	8.029631E-16	1.207307E-15	99.997837	2.999999
0.06	1.732570E+16	7.000000	8.597277E-07	1.463036E-17	9.635529E-16	1.690226E-15	99.997142	2.999999
0.07	1.732556E+16	8.166667	9.286048E-07	2.144261E-17	1.124142E-15	2.253630E-15	99.996360	2.999999
0.08	1.732541E+16	9.333333	9.927116E-07	2.991310E-17	1.284729E-15	2.897518E-15	99.995489	2.999999
0.09	1.732524E+16	10.500000	1.052920E-06	4.016905E-17	1.445315E-15	3.621889E-15	99.994531	2.999999
0.10	1.732506E+16	11.666667	1.109863E-06	5.233048E-17	1.605899E-15	4.426742E-15	99.993484	2.999998
0.11	1.732487E+16	12.833333	1.164021E-06	6.651138E-17	1.766481E-15	5.312076E-15	99.992349	2.999998
0.12	1.732465E+16	14.000000	1.215765E-06	8.282051E-17	1.927061E-15	6.277889E-15	99.991125	2.999998
0.13	1.732443E+16	15.166667	1.234286E-06	1.013840E-16	2.087640E-15	7.324181E-15	99.989813	2.999997
0.14	1.732418E+16	16.333333	1.234286E-06	1.223397E-16	2.248216E-15	8.450951E-15	99.988411	2.999997
0.15	1.732393E+16	17.500000	1.234286E-06	1.458252E-16	2.408790E-15	9.658196E-15	99.986922	2.999997
0.16	1.732365E+16	18.666667	1.234286E-06	1.719783E-16	2.569361E-15	1.094592E-14	99.985343	2.999996
0.17	1.732336E+16	19.833333	1.234286E-06	2.009368E-16	2.729930E-15	1.231411E-14	99.983675	2.999996
0.18	1.732306E+16	21.000000	1.234286E-06	2.328382E-16	2.890496E-15	1.376277E-14	99.981917	2.999995
0.19	1.732274E+16	22.166667	1.234286E-06	2.678203E-16	3.051059E-15	1.529190E-14	99.980070	2.999995
0.20	1.732240E+16	23.333333	1.234286E-06	3.060209E-16	3.211619E-15	1.690150E-14	99.978134	2.999994
0.21	1.732205E+16	24.500000	1.234286E-06	3.475775E-16	3.372175E-15	1.859157E-14	99.976107	2.999993
0.22	1.732168E+16	25.666667	1.234286E-06	3.926280E-16	3.532729E-15	2.036210E-14	99.973991	2.999993
0.23	1.732130E+16	26.833333	1.234286E-06	4.413100E-16	3.693279E-15	2.221309E-14	99.971785	2.999992
0.24	1.732090E+16	28.000000	1.234286E-06	4.937611E-16	3.853825E-15	2.414454E-14	99.969488	2.999992
0.25	1.732049E+16	29.166667	1.234286E-06	5.501191E-16	4.014368E-15	2.615645E-14	99.967102	2.999991
0.26	1.732006E+16	30.333333	1.234286E-06	6.105216E-16	4.174907E-15	2.824881E-14	99.964624	2.999990
0.27	1.731962E+16	31.500000	1.234286E-06	6.751062E-16	4.335442E-15	3.042162E-14	99.962057	2.999989
0.28	1.731916E+16	32.666667	1.234286E-06	7.440107E-16	4.495972E-15	3.267489E-14	99.959398	2.999989
0.29	1.731868E+16	33.833333	1.234286E-06	8.173726E-16	4.656498E-15	3.500860E-14	99.956648	2.999988
0.30	1.731819E+16	35.000000	1.234286E-06	8.953297E-16	4.817020E-15	3.742276E-14	99.953808	2.999987
0.31	1.731768E+16	36.166667	1.234286E-06	9.780195E-16	4.977537E-15	3.991735E-14	99.950876	2.999986
0.32	1.731716E+16	37.333333	1.234286E-06	1.065580E-15	5.138050E-15	4.249239E-14	99.947853	2.999985
0.33	1.731662E+16	38.500000	1.234286E-06	1.158148E-15	5.298558E-15	4.514786E-14	99.944738	2.999984
0.34	1.731606E+16	39.666667	1.234286E-06	1.255862E-15	5.459060E-15	4.788377E-14	99.941532	2.999983
0.35	1.731549E+16	40.833333	1.234286E-06	1.358858E-15	5.619557E-15	5.070010E-14	99.938233	2.999982
0.36	1.731490E+16	42.000000	1.234286E-06	1.467276E-15	5.780050E-15	5.359686E-14	99.934843	2.999981
0.37	1.731430E+16	43.166667	1.234286E-06	1.581252E-15	5.940536E-15	5.657405E-14	99.931361	2.999980
0.38	1.731368E+16	44.333333	1.234286E-06	1.700924E-15	6.101017E-15	5.963165E-14	99.927787	2.999979
0.39	1.731304E+16	45.500000	1.234286E-06	1.826430E-15	6.261492E-15	6.276967E-14	99.924120	2.999978
0.40	1.731239E+16	46.666667	1.234286E-06	1.957906E-15	6.421962E-15	6.598811E-14	99.920361	2.999977
0.41	1.731173E+16	47.833333	1.234286E-06	2.095491E-15	6.582425E-15	6.928695E-14	99.916509	2.999976
0.42	1.731104E+16	49.000000	1.234286E-06	2.239322E-15	6.742882E-15	7.266620E-14	99.912565	2.999974
0.43	1.731034E+16	50.166667	1.234286E-06	2.389537E-15	6.903333E-15	7.612584E-14	99.908527	2.999973
0.44	1.730963E+16	51.333333	1.234286E-06	2.546273E-15	7.063777E-15	7.966589E-14	99.904396	2.999972
0.45	1.730889E+16	52.500000	1.234286E-06	2.709668E-15	7.224215E-15	8.328633E-14	99.900173	2.999971

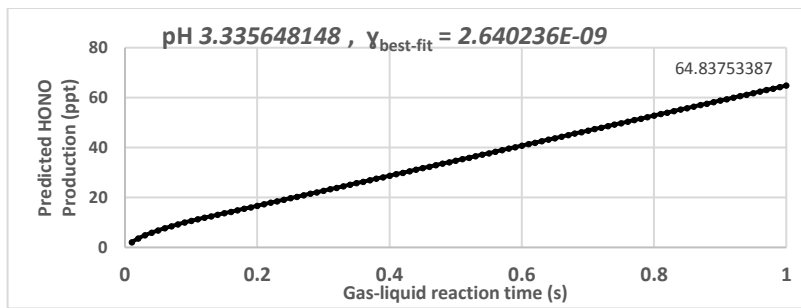


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0.47	1.730738E+16	54.833333	1.234286E-06	3.056983E-15	7.545070E-15	9.076837E-14	99.891445	2.999968
0.48	1.730660E+16	56.000000	1.234286E-06	3.241178E-15	7.705487E-15	9.462997E-14	99.886940	2.999967
0.49	1.730581E+16	57.166667	1.234286E-06	3.432582E-15	7.865896E-15	9.857194E-14	99.882342	2.999965
0.50	1.730499E+16	58.333333	1.234286E-06	3.631332E-15	8.026299E-15	1.025943E-13	99.877650	2.999964
0.51	1.730416E+16	59.500000	1.234286E-06	3.837565E-15	8.186693E-15	1.066970E-13	99.872864	2.999962
0.52	1.730332E+16	60.666667	1.234286E-06	4.051419E-15	8.347081E-15	1.108801E-13	99.867984	2.999961
0.53	1.730246E+16	61.833333	1.234286E-06	4.273031E-15	8.507460E-15	1.151435E-13	99.863009	2.999959
0.54	1.730158E+16	63.000000	1.234286E-06	4.502539E-15	8.667831E-15	1.194873E-13	99.857940	2.999958
0.55	1.730068E+16	64.166667	1.234286E-06	4.740080E-15	8.828195E-15	1.239114E-13	99.852776	2.999956
0.56	1.729977E+16	65.333333	1.234286E-06	4.985791E-15	8.988550E-15	1.284159E-13	99.847518	2.999955
0.57	1.729884E+16	66.500000	1.234286E-06	5.239810E-15	9.148896E-15	1.330007E-13	99.842164	2.999953
0.58	1.729790E+16	67.666667	1.234286E-06	5.502273E-15	9.309235E-15	1.376659E-13	99.836716	2.999952
0.59	1.729694E+16	68.833333	1.234286E-06	5.773319E-15	9.469564E-15	1.424113E-13	99.831172	2.999950
0.60	1.729596E+16	70.000000	1.234286E-06	6.053085E-15	9.629884E-15	1.472371E-13	99.825533	2.999948
0.61	1.729497E+16	71.166667	1.234286E-06	6.341707E-15	9.790196E-15	1.521433E-13	99.819798	2.999946
0.62	1.729396E+16	72.333333	1.234286E-06	6.639324E-15	9.950498E-15	1.571297E-13	99.813968	2.999945
0.63	1.729293E+16	73.500000	1.234286E-06	6.946072E-15	1.011079E-14	1.621964E-13	99.808042	2.999943
0.64	1.729189E+16	74.666667	1.234286E-06	7.262089E-15	1.027108E-14	1.673435E-13	99.802020	2.999941
0.65	1.729083E+16	75.833333	1.234286E-06	7.587511E-15	1.043135E-14	1.725708E-13	99.795902	2.999939
0.66	1.728975E+16	77.000000	1.234286E-06	7.922477E-15	1.059161E-14	1.778784E-13	99.789688	2.999937
0.67	1.728866E+16	78.166667	1.234286E-06	8.267122E-15	1.075187E-14	1.832663E-13	99.783377	2.999936
0.68	1.728755E+16	79.333333	1.234286E-06	8.621586E-15	1.091211E-14	1.887345E-13	99.776970	2.999934
0.69	1.728642E+16	80.500000	1.234286E-06	8.986003E-15	1.107235E-14	1.942829E-13	99.770467	2.999932
0.70	1.728528E+16	81.666667	1.234286E-06	9.360513E-15	1.123257E-14	1.999116E-13	99.763867	2.999930
0.71	1.728412E+16	82.833333	1.234286E-06	9.745251E-15	1.139278E-14	2.056206E-13	99.757169	2.999928
0.72	1.728294E+16	84.000000	1.234286E-06	1.014036E-14	1.155299E-14	2.114098E-13	99.750375	2.999926
0.73	1.728175E+16	85.166667	1.234286E-06	1.054596E-14	1.171318E-14	2.172793E-13	99.743484	2.999924
0.74	1.728054E+16	86.333333	1.234286E-06	1.096221E-14	1.187336E-14	2.232290E-13	99.736495	2.999921
0.75	1.727931E+16	87.500000	1.234286E-06	1.138923E-14	1.203353E-14	2.292589E-13	99.729409	2.999919
0.76	1.727806E+16	88.666667	1.234286E-06	1.182717E-14	1.219369E-14	2.353691E-13	99.722225	2.999917
0.77	1.727680E+16	89.833333	1.234286E-06	1.227616E-14	1.235383E-14	2.415594E-13	99.714944	2.999915
0.78	1.727552E+16	91.000000	1.234286E-06	1.273634E-14	1.251397E-14	2.478300E-13	99.707565	2.999913
0.79	1.727423E+16	92.166667	1.234286E-06	1.320784E-14	1.267409E-14	2.541808E-13	99.700087	2.999911
0.80	1.727292E+16	93.333333	1.234286E-06	1.369081E-14	1.283421E-14	2.606118E-13	99.692512	2.999908
0.81	1.727159E+16	94.500000	1.234286E-06	1.418537E-14	1.299431E-14	2.671230E-13	99.684838	2.999906
0.82	1.727024E+16	95.666667	1.234286E-06	1.469167E-14	1.315439E-14	2.737143E-13	99.677066	2.999904
0.83	1.726888E+16	96.833333	1.234286E-06	1.520984E-14	1.331447E-14	2.803858E-13	99.669195	2.999901
0.84	1.726749E+16	98.000000	1.234286E-06	1.574003E-14	1.347453E-14	2.871375E-13	99.661226	2.999899
0.85	1.726610E+16	99.166667	1.234286E-06	1.628235E-14	1.363458E-14	2.939694E-13	99.653158	2.999897
0.86	1.726468E+16	100.333333	1.234286E-06	1.683697E-14	1.379462E-14	3.008814E-13	99.644990	2.999894
0.87	1.726325E+16	101.500000	1.234286E-06	1.740400E-14	1.395464E-14	3.078735E-13	99.636724	2.999892
0.88	1.726180E+16	102.666667	1.234286E-06	1.798359E-14	1.411465E-14	3.149458E-13	99.628359	2.999889
0.89	1.726033E+16	103.833333	1.234286E-06	1.857587E-14	1.427465E-14	3.220982E-13	99.619894	2.999887
0.90	1.725885E+16	105.000000	1.234286E-06	1.918098E-14	1.443464E-14	3.293307E-13	99.611329	2.999884
0.91	1.725735E+16	106.166667	1.234286E-06	1.979906E-14	1.459461E-14	3.366434E-13	99.602665	2.999882
0.92	1.725583E+16	107.333333	1.234286E-06	2.043024E-14	1.475456E-14	3.440361E-13	99.593901	2.999879
0.93	1.725429E+16	108.500000	1.234286E-06	2.107467E-14	1.491451E-14	3.515089E-13	99.585037	2.999876
0.94	1.725274E+16	109.666667	1.234286E-06	2.173247E-14	1.507444E-14	3.590619E-13	99.576073	2.999874
0.95	1.725117E+16	110.833333	1.234286E-06	2.240378E-14	1.523435E-14	3.666949E-13	99.567009	2.999871
0.96	1.724958E+16	112.000000	1.234286E-06	2.308874E-14	1.539425E-14	3.744079E-13	99.557845	2.999868
0.97	1.724798E+16	113.166667	1.234286E-06	2.378750E-14	1.555414E-14	3.822010E-13	99.548580	2.999866
0.98	1.724635E+16	114.333333	1.234286E-06	2.450017E-14	1.571401E-14	3.900742E-13	99.539214	2.999863
0.99	1.724471E+16	115.500000	1.234286E-06	2.522690E-14	1.587387E-14	3.980274E-13	99.529748	2.999860
1.00	1.724306E+16	116.666667	1.234286E-06	2.596783E-14	1.603371E-14	4.060607E-13	99.520181	2.999857



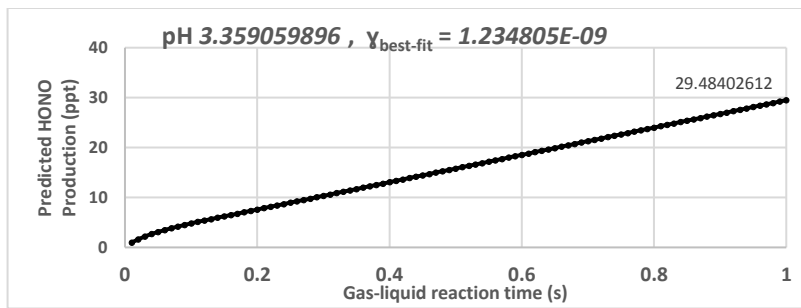
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732615E+16	1.166667	3.509915E-07	2.471988E-19	1.639007E-16	8.214494E-17	99.999736	3.000000
0.02	1.732608E+16	2.333333	4.963751E-07	1.091188E-18	3.278009E-16	2.464345E-16	99.999384	3.000000
0.03	1.732601E+16	3.500000	6.079302E-07	2.785333E-18	4.917004E-16	4.928683E-16	99.998943	3.000000
0.04	1.732592E+16	4.666667	7.019736E-07	5.538591E-18	6.555990E-16	8.214457E-16	99.998412	2.999999
0.05	1.732581E+16	5.833333	7.848255E-07	9.532916E-18	8.194967E-16	1.232166E-15	99.997793	2.999999
0.06	1.732569E+16	7.000000	8.597272E-07	1.493162E-17	9.833932E-16	1.725029E-15	99.997084	2.999999
0.07	1.732555E+16	8.166667	9.286041E-07	2.188413E-17	1.147288E-15	2.300034E-15	99.996285	2.999999
0.08	1.732539E+16	9.333333	9.927107E-07	3.052904E-17	1.311182E-15	2.957180E-15	99.995396	2.999999
0.09	1.732522E+16	10.500000	1.052918E-06	4.099617E-17	1.475074E-15	3.696466E-15	99.994418	2.999998
0.10	1.732504E+16	11.666667	1.109862E-06	5.340802E-17	1.638965E-15	4.517891E-15	99.993350	2.999998
0.11	1.732484E+16	12.833333	1.164019E-06	6.788092E-17	1.802853E-15	5.421454E-15	99.992191	2.999998
0.12	1.732462E+16	14.000000	1.215763E-06	8.452586E-17	1.966740E-15	6.407154E-15	99.990942	2.999998
0.13	1.732439E+16	15.166667	1.234286E-06	1.034716E-16	2.130625E-15	7.474989E-15	99.989603	2.999997
0.14	1.732414E+16	16.333333	1.234286E-06	1.248588E-16	2.294507E-15	8.624958E-15	99.988173	2.999997
0.15	1.732388E+16	17.500000	1.234286E-06	1.488279E-16	2.458386E-15	9.857060E-15	99.986652	2.999997
0.16	1.732360E+16	18.666667	1.234286E-06	1.755195E-16	2.622264E-15	1.117129E-14	99.985041	2.999996
0.17	1.732330E+16	19.833333	1.234286E-06	2.050742E-16	2.786138E-15	1.256766E-14	99.983338	2.999996
0.18	1.732299E+16	21.000000	1.234286E-06	2.376325E-16	2.950009E-15	1.404615E-14	99.981545	2.999995
0.19	1.732267E+16	22.166667	1.234286E-06	2.733349E-16	3.113878E-15	1.560676E-14	99.979660	2.999995
0.20	1.732232E+16	23.333333	1.234286E-06	3.123220E-16	3.277743E-15	1.724950E-14	99.977683	2.999994
0.21	1.732197E+16	24.500000	1.234286E-06	3.547343E-16	3.441605E-15	1.897436E-14	99.975615	2.999993
0.22	1.732159E+16	25.666667	1.234286E-06	4.007124E-16	3.605464E-15	2.078135E-14	99.973456	2.999993
0.23	1.732120E+16	26.833333	1.234286E-06	4.503967E-16	3.769319E-15	2.267045E-14	99.971204	2.999992
0.24	1.732080E+16	28.000000	1.234286E-06	5.039277E-16	3.933170E-15	2.464166E-14	99.968860	2.999991
0.25	1.732037E+16	29.166667	1.234286E-06	5.614461E-16	4.097017E-15	2.669499E-14	99.966424	2.999991
0.26	1.731994E+16	30.333333	1.234286E-06	6.230922E-16	4.260861E-15	2.883043E-14	99.963896	2.999990
0.27	1.731948E+16	31.500000	1.234286E-06	6.890066E-16	4.424700E-15	3.104798E-14	99.961275	2.999989
0.28	1.731901E+16	32.666667	1.234286E-06	7.593297E-16	4.588535E-15	3.334763E-14	99.958562	2.999988
0.29	1.731853E+16	33.833333	1.234286E-06	8.342021E-16	4.752365E-15	3.572939E-14	99.955756	2.999987
0.30	1.731802E+16	35.000000	1.234286E-06	9.137642E-16	4.916190E-15	3.819324E-14	99.952857	2.999987
0.31	1.731750E+16	36.166667	1.234286E-06	9.981564E-16	5.080011E-15	4.073919E-14	99.949864	2.999986
0.32	1.731697E+16	37.333333	1.234286E-06	1.087519E-15	5.243827E-15	4.336724E-14	99.946779	2.999985
0.33	1.731642E+16	38.500000	1.234286E-06	1.181993E-15	5.407638E-15	4.607738E-14	99.943600	2.999984
0.34	1.731585E+16	39.666667	1.234286E-06	1.281719E-15	5.571443E-15	4.886960E-14	99.940328	2.999983
0.35	1.731527E+16	40.833333	1.234286E-06	1.386836E-15	5.735243E-15	5.174391E-14	99.936962	2.999982
0.36	1.731467E+16	42.000000	1.234286E-06	1.497486E-15	5.899038E-15	5.470031E-14	99.933502	2.999981
0.37	1.731405E+16	43.166667	1.234286E-06	1.613808E-15	6.062827E-15	5.773878E-14	99.929948	2.999980
0.38	1.731342E+16	44.333333	1.234286E-06	1.735944E-15	6.226610E-15	6.085932E-14	99.926300	2.999979
0.39	1.731277E+16	45.500000	1.234286E-06	1.864033E-15	6.390387E-15	6.406193E-14	99.922558	2.999977
0.40	1.731211E+16	46.666667	1.234286E-06	1.998216E-15	6.554158E-15	6.734661E-14	99.918722	2.999976
0.41	1.731143E+16	47.833333	1.234286E-06	2.138633E-15	6.717923E-15	7.071336E-14	99.914790	2.999975
0.42	1.731073E+16	49.000000	1.234286E-06	2.285426E-15	6.881681E-15	7.416216E-14	99.910765	2.999974
0.43	1.731002E+16	50.166667	1.234286E-06	2.438733E-15	7.045432E-15	7.769302E-14	99.906644	2.999973
0.44	1.730929E+16	51.333333	1.234286E-06	2.598695E-15	7.209177E-15	8.130593E-14	99.902428	2.999971
0.45	1.730854E+16	52.500000	1.234286E-06	2.765453E-15	7.372915E-15	8.500089E-14	99.898118	2.999970

0.46	1.730778E+16	53.666667	1.234286E-06	2.939147E-15	7.536646E-15	8.877789E-14	99.893712	2.999969
0.47	1.730700E+16	54.833333	1.234286E-06	3.119917E-15	7.700370E-15	9.263692E-14	99.889210	2.999967
0.48	1.730620E+16	56.000000	1.234286E-06	3.307904E-15	7.864086E-15	9.657799E-14	99.884613	2.999966
0.49	1.730539E+16	57.166667	1.234286E-06	3.503248E-15	8.027795E-15	1.006011E-13	99.879920	2.999965
0.50	1.730456E+16	58.333333	1.234286E-06	3.706089E-15	8.191496E-15	1.047062E-13	99.875132	2.999963
0.51	1.730371E+16	59.500000	1.234286E-06	3.916567E-15	8.355189E-15	1.088934E-13	99.870247	2.999962
0.52	1.730285E+16	60.666667	1.234286E-06	4.134823E-15	8.518875E-15	1.131625E-13	99.865266	2.999960
0.53	1.730197E+16	61.833333	1.234286E-06	4.360996E-15	8.682552E-15	1.175137E-13	99.860189	2.999959
0.54	1.730107E+16	63.000000	1.234286E-06	4.595228E-15	8.846221E-15	1.219469E-13	99.855016	2.999957
0.55	1.730016E+16	64.166667	1.234286E-06	4.837657E-15	9.009881E-15	1.264620E-13	99.849746	2.999956
0.56	1.729923E+16	65.333333	1.234286E-06	5.088425E-15	9.173533E-15	1.310592E-13	99.844379	2.999954
0.57	1.729828E+16	66.500000	1.234286E-06	5.347672E-15	9.337176E-15	1.357384E-13	99.838915	2.999952
0.58	1.729732E+16	67.666667	1.234286E-06	5.615537E-15	9.500811E-15	1.404995E-13	99.833355	2.999951
0.59	1.729634E+16	68.833333	1.234286E-06	5.892162E-15	9.664436E-15	1.453426E-13	99.827697	2.999949
0.60	1.729534E+16	70.000000	1.234286E-06	6.177685E-15	9.828052E-15	1.502677E-13	99.821942	2.999947
0.61	1.729433E+16	71.166667	1.234286E-06	6.472247E-15	9.991658E-15	1.552748E-13	99.816089	2.999945
0.62	1.729330E+16	72.333333	1.234286E-06	6.775988E-15	1.015526E-14	1.603638E-13	99.810139	2.999944
0.63	1.729225E+16	73.500000	1.234286E-06	7.089049E-15	1.031884E-14	1.655348E-13	99.804091	2.999942
0.64	1.729118E+16	74.666667	1.234286E-06	7.411569E-15	1.048242E-14	1.707877E-13	99.797945	2.999940
0.65	1.729010E+16	75.833333	1.234286E-06	7.743688E-15	1.064599E-14	1.761226E-13	99.791701	2.999938
0.66	1.728900E+16	77.000000	1.234286E-06	8.085546E-15	1.080955E-14	1.815394E-13	99.785359	2.999936
0.67	1.728789E+16	78.166667	1.234286E-06	8.437284E-15	1.097309E-14	1.870381E-13	99.778919	2.999934
0.68	1.728675E+16	79.333333	1.234286E-06	8.799040E-15	1.113663E-14	1.926188E-13	99.772380	2.999932
0.69	1.728560E+16	80.500000	1.234286E-06	9.170957E-15	1.130016E-14	1.982814E-13	99.765743	2.999930
0.70	1.728444E+16	81.666667	1.234286E-06	9.553172E-15	1.146367E-14	2.040259E-13	99.759007	2.999928
0.71	1.728325E+16	82.833333	1.234286E-06	9.945826E-15	1.162717E-14	2.098523E-13	99.752172	2.999926
0.72	1.728205E+16	84.000000	1.234286E-06	1.034906E-14	1.179067E-14	2.157606E-13	99.745238	2.999924
0.73	1.728083E+16	85.166667	1.234286E-06	1.076301E-14	1.195415E-14	2.217508E-13	99.738205	2.999922
0.74	1.727960E+16	86.333333	1.234286E-06	1.118782E-14	1.211762E-14	2.278229E-13	99.731073	2.999920
0.75	1.727834E+16	87.500000	1.234286E-06	1.162363E-14	1.228108E-14	2.339768E-13	99.723841	2.999918
0.76	1.727707E+16	88.666667	1.234286E-06	1.207058E-14	1.244453E-14	2.402126E-13	99.716509	2.999915
0.77	1.727579E+16	89.833333	1.234286E-06	1.252881E-14	1.260796E-14	2.465303E-13	99.709078	2.999913
0.78	1.727448E+16	91.000000	1.234286E-06	1.299845E-14	1.277138E-14	2.529299E-13	99.701547	2.999911
0.79	1.727316E+16	92.166667	1.234286E-06	1.347966E-14	1.293480E-14	2.594113E-13	99.693916	2.999909
0.80	1.727182E+16	93.333333	1.234286E-06	1.397256E-14	1.309819E-14	2.659745E-13	99.686185	2.999906
0.81	1.727046E+16	94.500000	1.234286E-06	1.447729E-14	1.326158E-14	2.726196E-13	99.678353	2.999904
0.82	1.726909E+16	95.666667	1.234286E-06	1.499401E-14	1.342495E-14	2.793465E-13	99.670421	2.999902
0.83	1.726770E+16	96.833333	1.234286E-06	1.552284E-14	1.358831E-14	2.861552E-13	99.662389	2.999899
0.84	1.726629E+16	98.000000	1.234286E-06	1.606393E-14	1.375166E-14	2.930457E-13	99.654255	2.999897
0.85	1.726486E+16	99.166667	1.234286E-06	1.661741E-14	1.391500E-14	3.000180E-13	99.646021	2.999894
0.86	1.726342E+16	100.333333	1.234286E-06	1.718343E-14	1.407832E-14	3.070721E-13	99.637686	2.999892
0.87	1.726195E+16	101.500000	1.234286E-06	1.776212E-14	1.424162E-14	3.142080E-13	99.629250	2.999889
0.88	1.726048E+16	102.666667	1.234286E-06	1.835363E-14	1.440492E-14	3.214257E-13	99.620712	2.999887
0.89	1.725898E+16	103.833333	1.234286E-06	1.895809E-14	1.456820E-14	3.287252E-13	99.612073	2.999884
0.90	1.725746E+16	105.000000	1.234286E-06	1.957565E-14	1.473146E-14	3.361064E-13	99.603333	2.999882
0.91	1.725593E+16	106.166667	1.234286E-06	2.020644E-14	1.489471E-14	3.435693E-13	99.594491	2.999879
0.92	1.725438E+16	107.333333	1.234286E-06	2.085060E-14	1.505795E-14	3.511140E-13	99.585546	2.999876
0.93	1.725281E+16	108.500000	1.234286E-06	2.150828E-14	1.522118E-14	3.587405E-13	99.576500	2.999874
0.94	1.725123E+16	109.666667	1.234286E-06	2.217961E-14	1.538438E-14	3.664486E-13	99.567352	2.999871
0.95	1.724963E+16	110.833333	1.234286E-06	2.286472E-14	1.554758E-14	3.742385E-13	99.558102	2.999868
0.96	1.724801E+16	112.000000	1.234286E-06	2.356377E-14	1.571076E-14	3.821101E-13	99.548749	2.999866
0.97	1.724637E+16	113.166667	1.234286E-06	2.427689E-14	1.587392E-14	3.900634E-13	99.539294	2.999863
0.98	1.724471E+16	114.333333	1.234286E-06	2.500422E-14	1.603707E-14	3.980984E-13	99.529735	2.999860
0.99	1.724304E+16	115.500000	1.234286E-06	2.574589E-14	1.620020E-14	4.062151E-13	99.520075	2.999857
1.00	1.724135E+16	116.666667	1.234286E-06	2.650206E-14	1.636332E-14	4.144134E-13	99.510311	2.999854



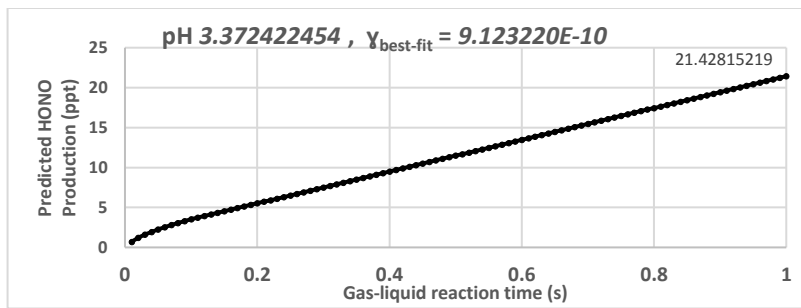
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732618E+16	1.166667	3.509921E-07	5.493379E-20	3.642294E-17	3.953876E-17	99.999919	3.335648
0.02	1.732616E+16	2.333333	4.963772E-07	2.424895E-19	7.284584E-17	1.186162E-16	99.999795	3.335648
0.03	1.732613E+16	3.500000	6.079344E-07	6.189712E-19	1.092687E-16	2.372323E-16	99.999628	3.335648
0.04	1.732609E+16	4.666667	7.019807E-07	1.230814E-18	1.456915E-16	3.953868E-16	99.999419	3.335648
0.05	1.732605E+16	5.833333	7.848363E-07	2.118454E-18	1.821142E-16	5.930798E-16	99.999168	3.335647
0.06	1.732600E+16	7.000000	8.597426E-07	3.318182E-18	2.185367E-16	8.303109E-16	99.998873	3.335647
0.07	1.732594E+16	8.166667	9.286250E-07	4.863206E-18	2.549592E-16	1.107080E-15	99.998536	3.335647
0.08	1.732587E+16	9.333333	9.927381E-07	6.784323E-18	2.913816E-16	1.423387E-15	99.998156	3.335647
0.09	1.732580E+16	10.500000	1.052953E-06	9.110382E-18	3.278038E-16	1.779232E-15	99.997734	3.335647
0.10	1.732572E+16	11.666667	1.109905E-06	1.186861E-17	3.642258E-16	2.174614E-15	99.997269	3.335646
0.11	1.732563E+16	12.833333	1.164072E-06	1.508485E-17	4.006477E-16	2.609533E-15	99.996760	3.335646
0.12	1.732553E+16	14.000000	1.215827E-06	1.878378E-17	4.370694E-16	3.083990E-15	99.996209	3.335646
0.13	1.732543E+16	15.166667	1.234286E-06	2.299402E-17	4.734909E-16	3.597982E-15	99.995615	3.335645
0.14	1.732532E+16	16.333333	1.234286E-06	2.774682E-17	5.099122E-16	4.151511E-15	99.994978	3.335645
0.15	1.732520E+16	17.500000	1.234286E-06	3.307341E-17	5.463332E-16	4.744576E-15	99.994299	3.335645
0.16	1.732508E+16	18.666667	1.234286E-06	3.900503E-17	5.827540E-16	5.377176E-15	99.993576	3.335644
0.17	1.732495E+16	19.833333	1.234286E-06	4.557293E-17	6.191746E-16	6.049312E-15	99.992810	3.335644
0.18	1.732481E+16	21.000000	1.234286E-06	5.280835E-17	6.555948E-16	6.760981E-15	99.992001	3.335643
0.19	1.732466E+16	22.166667	1.234286E-06	6.074251E-17	6.920148E-16	7.512185E-15	99.991149	3.335642
0.20	1.732450E+16	23.333333	1.234286E-06	6.940666E-17	7.284345E-16	8.302923E-15	99.990254	3.335642
0.21	1.732434E+16	24.500000	1.234286E-06	7.883204E-17	7.648539E-16	9.133193E-15	99.989316	3.335641
0.22	1.732417E+16	25.666667	1.234286E-06	8.904988E-17	8.012730E-16	1.000300E-14	99.988335	3.335641
0.23	1.732399E+16	26.833333	1.234286E-06	1.000914E-16	8.376917E-16	1.091233E-14	99.987310	3.335640
0.24	1.732381E+16	28.000000	1.234286E-06	1.119879E-16	8.741100E-16	1.186120E-14	99.986242	3.335639
0.25	1.732361E+16	29.166667	1.234286E-06	1.247705E-16	9.105280E-16	1.284960E-14	99.985131	3.335638
0.26	1.732341E+16	30.333333	1.234286E-06	1.384706E-16	9.469456E-16	1.387752E-14	99.983977	3.335638
0.27	1.732321E+16	31.500000	1.234286E-06	1.531193E-16	9.833628E-16	1.494498E-14	99.982779	3.335637
0.28	1.732299E+16	32.666667	1.234286E-06	1.687478E-16	1.019780E-15	1.605197E-14	99.981538	3.335636
0.29	1.732277E+16	33.833333	1.234286E-06	1.853875E-16	1.056196E-15	1.719848E-14	99.980253	3.335635
0.30	1.732254E+16	35.000000	1.234286E-06	2.030695E-16	1.092612E-15	1.838452E-14	99.978925	3.335634
0.31	1.732230E+16	36.166667	1.234286E-06	2.218250E-16	1.129027E-15	1.961009E-14	99.977553	3.335633
0.32	1.732206E+16	37.333333	1.234286E-06	2.416854E-16	1.165442E-15	2.087519E-14	99.976138	3.335632
0.33	1.732180E+16	38.500000	1.234286E-06	2.626817E-16	1.201857E-15	2.217981E-14	99.974680	3.335631
0.34	1.732154E+16	39.666667	1.234286E-06	2.848454E-16	1.238271E-15	2.352395E-14	99.973178	3.335630
0.35	1.732128E+16	40.833333	1.234286E-06	3.082075E-16	1.274684E-15	2.490762E-14	99.971632	3.335629
0.36	1.732100E+16	42.000000	1.234286E-06	3.327993E-16	1.311097E-15	2.633081E-14	99.970043	3.335628
0.37	1.732072E+16	43.166667	1.234286E-06	3.586520E-16	1.347509E-15	2.779352E-14	99.968409	3.335627
0.38	1.732043E+16	44.333333	1.234286E-06	3.857969E-16	1.383921E-15	2.929575E-14	99.966733	3.335626
0.39	1.732013E+16	45.500000	1.234286E-06	4.142652E-16	1.420332E-15	3.083751E-14	99.965012	3.335625
0.40	1.731982E+16	46.666667	1.234286E-06	4.440881E-16	1.456743E-15	3.241878E-14	99.963248	3.335623
0.41	1.731951E+16	47.833333	1.234286E-06	4.752968E-16	1.493153E-15	3.403957E-14	99.961440	3.335622
0.42	1.731919E+16	49.000000	1.234286E-06	5.079225E-16	1.529563E-15	3.569987E-14	99.959588	3.335621
0.43	1.731886E+16	50.166667	1.234286E-06	5.419966E-16	1.565971E-15	3.739969E-14	99.957692	3.335620
0.44	1.731852E+16	51.333333	1.234286E-06	5.775501E-16	1.602380E-15	3.913903E-14	99.955752	3.335618
0.45	1.731818E+16	52.500000	1.234286E-06	6.146143E-16	1.638787E-15	4.091788E-14	99.953769	3.335617





$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732618E+16	1.166667	3.509923E-07	2.497191E-20	1.655722E-17	1.896912E-17	99.999962	3.359060
0.02	1.732617E+16	2.333333	4.963777E-07	1.102313E-19	3.311443E-17	5.690735E-17	99.999903	3.359060
0.03	1.732616E+16	3.500000	6.079356E-07	2.813731E-19	4.967163E-17	1.138147E-16	99.999825	3.359060
0.04	1.732614E+16	4.666667	7.019828E-07	5.595060E-19	6.622881E-17	1.896910E-16	99.999725	3.359060
0.05	1.732612E+16	5.833333	7.848397E-07	9.630110E-19	8.278598E-17	2.845364E-16	99.999606	3.359060
0.06	1.732610E+16	7.000000	8.597476E-07	1.508385E-18	9.934312E-17	3.983509E-16	99.999465	3.359059
0.07	1.732607E+16	8.166667	9.286321E-07	2.210725E-18	1.159002E-16	5.311342E-16	99.999305	3.359059
0.08	1.732604E+16	9.333333	9.927477E-07	3.084030E-18	1.324573E-16	6.828865E-16	99.999124	3.359059
0.09	1.732600E+16	10.500000	1.052966E-06	4.141415E-18	1.490144E-16	8.536076E-16	99.998922	3.359059
0.10	1.732597E+16	11.666667	1.109921E-06	5.395254E-18	1.655714E-16	1.043298E-15	99.998700	3.359059
0.11	1.732592E+16	12.833333	1.164092E-06	6.857300E-18	1.821284E-16	1.251956E-15	99.998457	3.359059
0.12	1.732588E+16	14.000000	1.215851E-06	8.538765E-18	1.986854E-16	1.479584E-15	99.998194	3.359059
0.13	1.732583E+16	15.166667	1.234286E-06	1.045267E-17	2.152423E-16	1.726180E-15	99.997910	3.359059
0.14	1.732578E+16	16.333333	1.234286E-06	1.261320E-17	2.317991E-16	1.991744E-15	99.997605	3.359058
0.15	1.732572E+16	17.500000	1.234286E-06	1.503458E-17	2.483559E-16	2.276277E-15	99.997280	3.359058
0.16	1.732566E+16	18.666667	1.234286E-06	1.773101E-17	2.649127E-16	2.579779E-15	99.996935	3.359058
0.17	1.732560E+16	19.833333	1.234286E-06	2.071667E-17	2.814694E-16	2.902248E-15	99.996568	3.359058
0.18	1.732553E+16	21.000000	1.234286E-06	2.400578E-17	2.980260E-16	3.243686E-15	99.996182	3.359057
0.19	1.732546E+16	22.166667	1.234286E-06	2.761254E-17	3.145826E-16	3.604092E-15	99.995774	3.359057
0.20	1.732538E+16	23.333333	1.234286E-06	3.155114E-17	3.311391E-16	3.983465E-15	99.995346	3.359057
0.21	1.732531E+16	24.500000	1.234286E-06	3.583579E-17	3.476956E-16	4.381807E-15	99.994897	3.359056
0.22	1.732523E+16	25.666667	1.234286E-06	4.048070E-17	3.642520E-16	4.799116E-15	99.994427	3.359056
0.23	1.732514E+16	26.833333	1.234286E-06	4.550005E-17	3.808083E-16	5.235393E-15	99.993937	3.359056
0.24	1.732505E+16	28.000000	1.234286E-06	5.090806E-17	3.973645E-16	5.690637E-15	99.993426	3.359055
0.25	1.732496E+16	29.166667	1.234286E-06	5.671892E-17	4.139207E-16	6.164848E-15	99.992894	3.359055
0.26	1.732486E+16	30.333333	1.234286E-06	6.294683E-17	4.304767E-16	6.658027E-15	99.992342	3.359055
0.27	1.732476E+16	31.500000	1.234286E-06	6.960600E-17	4.470327E-16	7.170173E-15	99.991768	3.359054
0.28	1.732466E+16	32.666667	1.234286E-06	7.671062E-17	4.635886E-16	7.701285E-15	99.991174	3.359054
0.29	1.732456E+16	33.833333	1.234286E-06	8.427489E-17	4.801444E-16	8.251364E-15	99.990559	3.359053
0.30	1.732445E+16	35.000000	1.234286E-06	9.231302E-17	4.967001E-16	8.820410E-15	99.989924	3.359053
0.31	1.732433E+16	36.166667	1.234286E-06	1.008392E-16	5.132557E-16	9.408421E-15	99.989267	3.359052
0.32	1.732421E+16	37.333333	1.234286E-06	1.098676E-16	5.298112E-16	1.001540E-14	99.988590	3.359052
0.33	1.732409E+16	38.500000	1.234286E-06	1.194125E-16	5.463666E-16	1.064134E-14	99.987891	3.359051
0.34	1.732397E+16	39.666667	1.234286E-06	1.294881E-16	5.629219E-16	1.128625E-14	99.987172	3.359051
0.35	1.732384E+16	40.833333	1.234286E-06	1.401085E-16	5.794770E-16	1.195013E-14	99.986432	3.359050
0.36	1.732371E+16	42.000000	1.234286E-06	1.512879E-16	5.960321E-16	1.263297E-14	99.985671	3.359050
0.37	1.732357E+16	43.166667	1.234286E-06	1.630406E-16	6.125870E-16	1.333477E-14	99.984889	3.359049
0.38	1.732343E+16	44.333333	1.234286E-06	1.753808E-16	6.291418E-16	1.405555E-14	99.984087	3.359049
0.39	1.732329E+16	45.500000	1.234286E-06	1.883226E-16	6.456965E-16	1.479528E-14	99.983263	3.359048
0.40	1.732314E+16	46.666667	1.234286E-06	2.018802E-16	6.622511E-16	1.555398E-14	99.982418	3.359047
0.41	1.732299E+16	47.833333	1.234286E-06	2.160679E-16	6.788055E-16	1.633165E-14	99.981553	3.359047
0.42	1.732284E+16	49.000000	1.234286E-06	2.308998E-16	6.953599E-16	1.712827E-14	99.980666	3.359046
0.43	1.732268E+16	50.166667	1.234286E-06	2.463901E-16	7.119140E-16	1.794387E-14	99.979758	3.359045
0.44	1.732252E+16	51.333333	1.234286E-06	2.625531E-16	7.284680E-16	1.877842E-14	99.978829	3.359045
0.45	1.732236E+16	52.500000	1.234286E-06	2.794030E-16	7.450219E-16	1.963194E-14	99.977880	3.359044

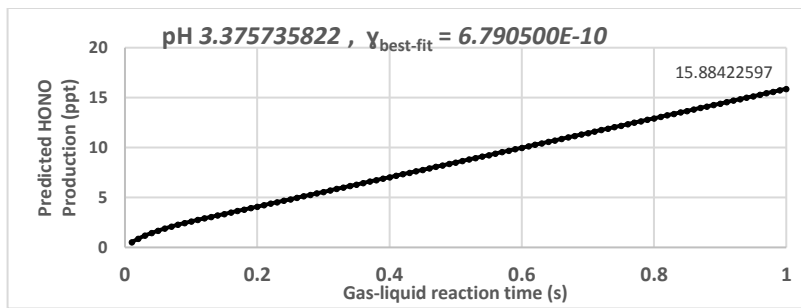




$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO2}}$ (mol)	$\Phi_{\text{NO2}}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732619E+16	1.166667	3.509923E-07	1.814745E-20	1.203237E-17	1.421588E-17	99.999972	3.372422
0.02	1.732618E+16	2.333333	4.963778E-07	8.010671E-20	2.406474E-17	4.264762E-17	99.999928	3.372422
0.03	1.732617E+16	3.500000	6.079359E-07	2.044779E-19	3.609710E-17	8.529521E-17	99.999870	3.372422
0.04	1.732616E+16	4.666667	7.019833E-07	4.066011E-19	4.812945E-17	1.421587E-16	99.999796	3.372422
0.05	1.732614E+16	5.833333	7.848405E-07	6.998339E-19	6.016179E-17	2.132379E-16	99.999706	3.372422
0.06	1.732612E+16	7.000000	8.597488E-07	1.096165E-18	7.219412E-17	2.985330E-16	99.999602	3.372422
0.07	1.732610E+16	8.166667	9.286337E-07	1.606566E-18	8.422644E-17	3.980438E-16	99.999482	3.372422
0.08	1.732608E+16	9.333333	9.927499E-07	2.241209E-18	9.625874E-17	5.117704E-16	99.999346	3.372422
0.09	1.732605E+16	10.500000	1.052969E-06	3.009625E-18	1.082910E-16	6.397128E-16	99.999196	3.372422
0.10	1.732602E+16	11.666667	1.109925E-06	3.920809E-18	1.203233E-16	7.818708E-16	99.999030	3.372422
0.11	1.732599E+16	12.833333	1.164097E-06	4.983298E-18	1.323555E-16	9.382445E-16	99.998848	3.372422
0.12	1.732596E+16	14.000000	1.215857E-06	6.205243E-18	1.443878E-16	1.108834E-15	99.998651	3.372422
0.13	1.732592E+16	15.166667	1.234286E-06	7.596102E-18	1.564200E-16	1.293639E-15	99.998439	3.372421
0.14	1.732588E+16	16.333333	1.234286E-06	9.166198E-18	1.684521E-16	1.492659E-15	99.998211	3.372421
0.15	1.732584E+16	17.500000	1.234286E-06	1.092585E-17	1.804843E-16	1.705895E-15	99.997968	3.372421
0.16	1.732579E+16	18.666667	1.234286E-06	1.288538E-17	1.925164E-16	1.933347E-15	99.997710	3.372421
0.17	1.732575E+16	19.833333	1.234286E-06	1.505511E-17	2.045485E-16	2.175013E-15	99.997436	3.372421
0.18	1.732570E+16	21.000000	1.234286E-06	1.744536E-17	2.165806E-16	2.430896E-15	99.997146	3.372420
0.19	1.732564E+16	22.166667	1.234286E-06	2.006644E-17	2.286126E-16	2.700993E-15	99.996841	3.372420
0.20	1.732559E+16	23.333333	1.234286E-06	2.292869E-17	2.406446E-16	2.985306E-15	99.996521	3.372420
0.21	1.732553E+16	24.500000	1.234286E-06	2.604241E-17	2.526765E-16	3.283833E-15	99.996185	3.372420
0.22	1.732547E+16	25.666667	1.234286E-06	2.941794E-17	2.647085E-16	3.596576E-15	99.995834	3.372419
0.23	1.732541E+16	26.833333	1.234286E-06	3.306559E-17	2.767403E-16	3.923534E-15	99.995467	3.372419
0.24	1.732534E+16	28.000000	1.234286E-06	3.699568E-17	2.887722E-16	4.264706E-15	99.995084	3.372419
0.25	1.732527E+16	29.166667	1.234286E-06	4.121853E-17	3.008040E-16	4.620094E-15	99.994686	3.372419
0.26	1.732520E+16	30.333333	1.234286E-06	4.574447E-17	3.128357E-16	4.989696E-15	99.994273	3.372418
0.27	1.732512E+16	31.500000	1.234286E-06	5.058380E-17	3.248674E-16	5.373513E-15	99.993844	3.372418
0.28	1.732505E+16	32.666667	1.234286E-06	5.574686E-17	3.368991E-16	5.771545E-15	99.993399	3.372418
0.29	1.732497E+16	33.833333	1.234286E-06	6.124396E-17	3.489307E-16	6.183791E-15	99.992939	3.372417
0.30	1.732489E+16	35.000000	1.234286E-06	6.708542E-17	3.609622E-16	6.610251E-15	99.992463	3.372417
0.31	1.732480E+16	36.166667	1.234286E-06	7.328157E-17	3.729937E-16	7.050926E-15	99.991971	3.372417
0.32	1.732471E+16	37.333333	1.234286E-06	7.984271E-17	3.850251E-16	7.505815E-15	99.991464	3.372416
0.33	1.732462E+16	38.500000	1.234286E-06	8.677917E-17	3.970565E-16	7.974918E-15	99.990942	3.372416
0.34	1.732453E+16	39.666667	1.234286E-06	9.410128E-17	4.090878E-16	8.458234E-15	99.990403	3.372415
0.35	1.732443E+16	40.833333	1.234286E-06	1.018193E-16	4.211191E-16	8.955765E-15	99.989849	3.372415
0.36	1.732433E+16	42.000000	1.234286E-06	1.099437E-16	4.331503E-16	9.467510E-15	99.989280	3.372415
0.37	1.732423E+16	43.166667	1.234286E-06	1.184846E-16	4.451814E-16	9.993468E-15	99.988695	3.372414
0.38	1.732413E+16	44.333333	1.234286E-06	1.274525E-16	4.572125E-16	1.053364E-14	99.988094	3.372414
0.39	1.732402E+16	45.500000	1.234286E-06	1.368576E-16	4.692435E-16	1.108802E-14	99.987477	3.372413
0.40	1.732391E+16	46.666667	1.234286E-06	1.467102E-16	4.812745E-16	1.165662E-14	99.986845	3.372413
0.41	1.732380E+16	47.833333	1.234286E-06	1.570207E-16	4.933053E-16	1.223943E-14	99.986197	3.372412
0.42	1.732368E+16	49.000000	1.234286E-06	1.677994E-16	5.053361E-16	1.283646E-14	99.985533	3.372412
0.43	1.732357E+16	50.166667	1.234286E-06	1.790567E-16	5.173668E-16	1.344770E-14	99.984853	3.372411
0.44	1.732345E+16	51.333333	1.234286E-06	1.908027E-16	5.293975E-16	1.407315E-14	99.984158	3.372411
0.45	1.732332E+16	52.500000	1.234286E-06	2.030479E-16	5.414280E-16	1.471281E-14	99.983447	3.372410

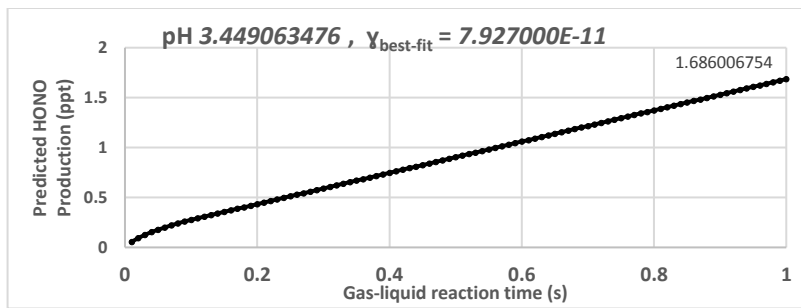


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0.47	1.732307E+16	54.833333	1.234286E-06	2.290770E-16	5.654889E-16	1.603477E-14	99.981978	3.372409
0.48	1.732294E+16	56.000000	1.234286E-06	2.428815E-16	5.775192E-16	1.671707E-14	99.981220	3.372409
0.49	1.732280E+16	57.166667	1.234286E-06	2.572265E-16	5.895495E-16	1.741358E-14	99.980445	3.372408
0.50	1.732267E+16	58.333333	1.234286E-06	2.721222E-16	6.015796E-16	1.812431E-14	99.979655	3.372407
0.51	1.732253E+16	59.500000	1.234286E-06	2.875789E-16	6.136097E-16	1.884924E-14	99.978850	3.372407
0.52	1.732238E+16	60.666667	1.234286E-06	3.036070E-16	6.256397E-16	1.958839E-14	99.978028	3.372406
0.53	1.732224E+16	61.833333	1.234286E-06	3.202168E-16	6.376696E-16	2.034174E-14	99.977191	3.372406
0.54	1.732209E+16	63.000000	1.234286E-06	3.374187E-16	6.496993E-16	2.110931E-14	99.976337	3.372405
0.55	1.732194E+16	64.166667	1.234286E-06	3.552228E-16	6.617290E-16	2.189109E-14	99.975468	3.372404
0.56	1.732179E+16	65.333333	1.234286E-06	3.736395E-16	6.737586E-16	2.268708E-14	99.974583	3.372404
0.57	1.732163E+16	66.500000	1.234286E-06	3.926793E-16	6.857881E-16	2.349729E-14	99.973682	3.372403
0.58	1.732147E+16	67.666667	1.234286E-06	4.123522E-16	6.978175E-16	2.432170E-14	99.972766	3.372402
0.59	1.732131E+16	68.833333	1.234286E-06	4.326688E-16	7.098468E-16	2.516032E-14	99.971833	3.372402
0.60	1.732115E+16	70.000000	1.234286E-06	4.536393E-16	7.218760E-16	2.601315E-14	99.970884	3.372401
0.61	1.732098E+16	71.166667	1.234286E-06	4.752740E-16	7.339051E-16	2.688019E-14	99.969920	3.372400
0.62	1.732081E+16	72.333333	1.234286E-06	4.975832E-16	7.459341E-16	2.776144E-14	99.968939	3.372399
0.63	1.732064E+16	73.500000	1.234286E-06	5.205772E-16	7.579630E-16	2.865691E-14	99.967943	3.372399
0.64	1.732046E+16	74.666667	1.234286E-06	5.442665E-16	7.699917E-16	2.956658E-14	99.966930	3.372398
0.65	1.732028E+16	75.833333	1.234286E-06	5.686612E-16	7.820204E-16	3.049046E-14	99.965902	3.372397
0.66	1.732010E+16	77.000000	1.234286E-06	5.937717E-16	7.940489E-16	3.142854E-14	99.964858	3.372396
0.67	1.731992E+16	78.166667	1.234286E-06	6.196083E-16	8.060773E-16	3.238084E-14	99.963797	3.372396
0.68	1.731973E+16	79.333333	1.234286E-06	6.461813E-16	8.181056E-16	3.334735E-14	99.962721	3.372395
0.69	1.731954E+16	80.500000	1.234286E-06	6.735010E-16	8.301338E-16	3.432806E-14	99.961629	3.372394
0.70	1.731935E+16	81.666667	1.234286E-06	7.015778E-16	8.421619E-16	3.532298E-14	99.960520	3.372393
0.71	1.731916E+16	82.833333	1.234286E-06	7.304220E-16	8.541898E-16	3.633211E-14	99.959396	3.372392
0.72	1.731896E+16	84.000000	1.234286E-06	7.600439E-16	8.662176E-16	3.735545E-14	99.958255	3.372391
0.73	1.731876E+16	85.166667	1.234286E-06	7.904537E-16	8.782453E-16	3.839299E-14	99.957099	3.372391
0.74	1.731855E+16	86.333333	1.234286E-06	8.216618E-16	8.902729E-16	3.944474E-14	99.955926	3.372390
0.75	1.731835E+16	87.500000	1.234286E-06	8.536786E-16	9.023003E-16	4.051070E-14	99.954738	3.372389
0.76	1.731814E+16	88.666667	1.234286E-06	8.865143E-16	9.143276E-16	4.159086E-14	99.953533	3.372388
0.77	1.731793E+16	89.833333	1.234286E-06	9.201792E-16	9.263548E-16	4.268523E-14	99.952312	3.372387
0.78	1.731771E+16	91.000000	1.234286E-06	9.546837E-16	9.383818E-16	4.379381E-14	99.951075	3.372386
0.79	1.731750E+16	92.166667	1.234286E-06	9.900380E-16	9.504087E-16	4.491659E-14	99.949822	3.372385
0.80	1.731728E+16	93.333333	1.234286E-06	1.026253E-15	9.624355E-16	4.605358E-14	99.948553	3.372384
0.81	1.731705E+16	94.500000	1.234286E-06	1.063338E-15	9.744621E-16	4.720477E-14	99.947267	3.372383
0.82	1.731683E+16	95.666667	1.234286E-06	1.101303E-15	9.864885E-16	4.837017E-14	99.945966	3.372382
0.83	1.731660E+16	96.833333	1.234286E-06	1.140160E-15	9.985149E-16	4.954977E-14	99.944648	3.372381
0.84	1.731637E+16	98.000000	1.234286E-06	1.179919E-15	1.010541E-15	5.074358E-14	99.943314	3.372380
0.85	1.731614E+16	99.166667	1.234286E-06	1.220589E-15	1.022567E-15	5.195159E-14	99.941964	3.372379
0.86	1.731590E+16	100.333333	1.234286E-06	1.262181E-15	1.034593E-15	5.317381E-14	99.940598	3.372378
0.87	1.731566E+16	101.500000	1.234286E-06	1.304705E-15	1.046619E-15	5.441023E-14	99.939215	3.372377
0.88	1.731542E+16	102.666667	1.234286E-06	1.348172E-15	1.058644E-15	5.566085E-14	99.937817	3.372376
0.89	1.731517E+16	103.833333	1.234286E-06	1.392592E-15	1.070670E-15	5.692568E-14	99.936402	3.372375
0.90	1.731492E+16	105.000000	1.234286E-06	1.437976E-15	1.082695E-15	5.820471E-14	99.934971	3.372374
0.91	1.731467E+16	106.166667	1.234286E-06	1.484333E-15	1.094720E-15	5.949794E-14	99.933523	3.372373
0.92	1.731442E+16	107.333333	1.234286E-06	1.531673E-15	1.106745E-15	6.080537E-14	99.932060	3.372372
0.93	1.731416E+16	108.500000	1.234286E-06	1.580009E-15	1.118770E-15	6.212701E-14	99.930580	3.372371
0.94	1.731390E+16	109.666667	1.234286E-06	1.629348E-15	1.130794E-15	6.346284E-14	99.929083	3.372370
0.95	1.731364E+16	110.833333	1.234286E-06	1.679702E-15	1.142819E-15	6.481288E-14	99.927571	3.372369
0.96	1.731338E+16	112.000000	1.234286E-06	1.731082E-15	1.154843E-15	6.617712E-14	99.926042	3.372368
0.97	1.731311E+16	113.166667	1.234286E-06	1.783497E-15	1.166867E-15	6.755556E-14	99.924497	3.372366
0.98	1.731284E+16	114.333333	1.234286E-06	1.836958E-15	1.178891E-15	6.894820E-14	99.922935	3.372365
0.99	1.731257E+16	115.500000	1.234286E-06	1.891474E-15	1.190915E-15	7.035504E-14	99.921358	3.372364
1.00	1.731229E+16	116.666667	1.234286E-06	1.947057E-15	1.202939E-15	7.177608E-14	99.919763	3.372363



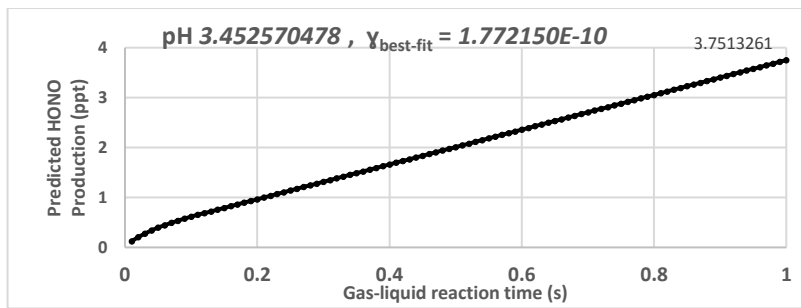
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732619E+16	1.166667	3.509923E-07	1.345152E-20	8.918816E-18	1.061801E-17	99.999979	3.375736
0.02	1.732618E+16	2.333333	4.963779E-07	5.937790E-20	1.783763E-17	3.185401E-17	99.999947	3.375736
0.03	1.732617E+16	3.500000	6.079361E-07	1.515662E-19	2.675644E-17	6.370802E-17	99.999903	3.375736
0.04	1.732616E+16	4.666667	7.019837E-07	3.013870E-19	3.567524E-17	1.061800E-16	99.999848	3.375736
0.05	1.732615E+16	5.833333	7.848411E-07	5.187415E-19	4.459404E-17	1.592700E-16	99.999781	3.375736
0.06	1.732614E+16	7.000000	8.597497E-07	8.125162E-19	5.351284E-17	2.229779E-16	99.999703	3.375736
0.07	1.732612E+16	8.166667	9.286350E-07	1.190843E-18	6.243162E-17	2.973038E-16	99.999613	3.375735
0.08	1.732611E+16	9.333333	9.927515E-07	1.661263E-18	7.135040E-17	3.822476E-16	99.999512	3.375735
0.09	1.732609E+16	10.500000	1.052971E-06	2.230840E-18	8.026917E-17	4.778094E-16	99.999400	3.375735
0.10	1.732607E+16	11.666667	1.109927E-06	2.906241E-18	8.918793E-17	5.839891E-16	99.999276	3.375735
0.11	1.732604E+16	12.833333	1.164100E-06	3.693795E-18	9.810668E-17	7.007866E-16	99.999141	3.375735
0.12	1.732602E+16	14.000000	1.215861E-06	4.599543E-18	1.070254E-16	8.282020E-16	99.998994	3.375735
0.13	1.732599E+16	15.166667	1.234286E-06	5.630497E-18	1.159441E-16	9.662353E-16	99.998835	3.375735
0.14	1.732596E+16	16.333333	1.234286E-06	6.794308E-18	1.248628E-16	1.114886E-15	99.998665	3.375735
0.15	1.732593E+16	17.500000	1.234286E-06	8.098624E-18	1.337815E-16	1.274155E-15	99.998484	3.375735
0.16	1.732589E+16	18.666667	1.234286E-06	9.551098E-18	1.427002E-16	1.444042E-15	99.998291	3.375735
0.17	1.732586E+16	19.833333	1.234286E-06	1.115938E-17	1.516189E-16	1.624546E-15	99.998086	3.375734
0.18	1.732582E+16	21.000000	1.234286E-06	1.293111E-17	1.605375E-16	1.815668E-15	99.997870	3.375734
0.19	1.732578E+16	22.166667	1.234286E-06	1.487396E-17	1.694561E-16	2.017408E-15	99.997642	3.375734
0.20	1.732574E+16	23.333333	1.234286E-06	1.699556E-17	1.783748E-16	2.229766E-15	99.997403	3.375734
0.21	1.732570E+16	24.500000	1.234286E-06	1.930357E-17	1.872933E-16	2.452740E-15	99.997152	3.375734
0.22	1.732565E+16	25.666667	1.234286E-06	2.180563E-17	1.962119E-16	2.686333E-15	99.996890	3.375734
0.23	1.732560E+16	26.833333	1.234286E-06	2.450940E-17	2.051304E-16	2.930543E-15	99.996616	3.375733
0.24	1.732556E+16	28.000000	1.234286E-06	2.742253E-17	2.140490E-16	3.185371E-15	99.996330	3.375733
0.25	1.732550E+16	29.166667	1.234286E-06	3.055267E-17	2.229675E-16	3.450815E-15	99.996033	3.375733
0.26	1.732545E+16	30.333333	1.234286E-06	3.390746E-17	2.318859E-16	3.726878E-15	99.995724	3.375733
0.27	1.732539E+16	31.500000	1.234286E-06	3.749456E-17	2.408044E-16	4.013557E-15	99.995404	3.375732
0.28	1.732534E+16	32.666667	1.234286E-06	4.132161E-17	2.497228E-16	4.310854E-15	99.995072	3.375732
0.29	1.732528E+16	33.833333	1.234286E-06	4.539627E-17	2.586412E-16	4.618768E-15	99.994728	3.375732
0.30	1.732522E+16	35.000000	1.234286E-06	4.972619E-17	2.675595E-16	4.937300E-15	99.994373	3.375732
0.31	1.732515E+16	36.166667	1.234286E-06	5.431901E-17	2.764779E-16	5.266448E-15	99.994006	3.375731
0.32	1.732509E+16	37.333333	1.234286E-06	5.918239E-17	2.853962E-16	5.606214E-15	99.993627	3.375731
0.33	1.732502E+16	38.500000	1.234286E-06	6.432397E-17	2.943144E-16	5.956596E-15	99.993237	3.375731
0.34	1.732495E+16	39.666667	1.234286E-06	6.975140E-17	3.032327E-16	6.317596E-15	99.992835	3.375731
0.35	1.732488E+16	40.833333	1.234286E-06	7.547234E-17	3.121509E-16	6.689212E-15	99.992422	3.375730
0.36	1.732480E+16	42.000000	1.234286E-06	8.149442E-17	3.210691E-16	7.071445E-15	99.991996	3.375730
0.37	1.732473E+16	43.166667	1.234286E-06	8.782531E-17	3.299872E-16	7.464295E-15	99.991559	3.375730
0.38	1.732465E+16	44.333333	1.234286E-06	9.447266E-17	3.389053E-16	7.867762E-15	99.991111	3.375729
0.39	1.732457E+16	45.500000	1.234286E-06	1.014441E-16	3.478233E-16	8.281845E-15	99.990650	3.375729
0.40	1.732449E+16	46.666667	1.234286E-06	1.087473E-16	3.567414E-16	8.706545E-15	99.990178	3.375729
0.41	1.732441E+16	47.833333	1.234286E-06	1.163899E-16	3.656594E-16	9.141861E-15	99.989694	3.375728
0.42	1.732432E+16	49.000000	1.234286E-06	1.243795E-16	3.745773E-16	9.587794E-15	99.989198	3.375728
0.43	1.732423E+16	50.166667	1.234286E-06	1.327238E-16	3.834952E-16	1.004434E-14	99.988691	3.375727
0.44	1.732414E+16	51.333333	1.234286E-06	1.414305E-16	3.924131E-16	1.051151E-14	99.988172	3.375727
0.45	1.732405E+16	52.500000	1.234286E-06	1.505072E-16	4.013309E-16	1.098929E-14	99.987641	3.375727

0.46	1.732396E+16	53.666667	1.234286E-06	1.599615E-16	4.102487E-16	1.147769E-14	99.987098	3.375726
0.47	1.732386E+16	54.833333	1.234286E-06	1.698011E-16	4.191664E-16	1.197670E-14	99.986544	3.375726
0.48	1.732376E+16	56.000000	1.234286E-06	1.800336E-16	4.280841E-16	1.248633E-14	99.985977	3.375725
0.49	1.732366E+16	57.166667	1.234286E-06	1.906668E-16	4.370017E-16	1.300657E-14	99.985399	3.375725
0.50	1.732356E+16	58.333333	1.234286E-06	2.017081E-16	4.459193E-16	1.353744E-14	99.984810	3.375725
0.51	1.732345E+16	59.500000	1.234286E-06	2.131654E-16	4.548368E-16	1.407891E-14	99.984208	3.375724
0.52	1.732335E+16	60.666667	1.234286E-06	2.250462E-16	4.637543E-16	1.463100E-14	99.983594	3.375724
0.53	1.732324E+16	61.833333	1.234286E-06	2.373581E-16	4.726718E-16	1.519371E-14	99.982969	3.375723
0.54	1.732313E+16	63.000000	1.234286E-06	2.501089E-16	4.815891E-16	1.576703E-14	99.982332	3.375723
0.55	1.732302E+16	64.166667	1.234286E-06	2.633062E-16	4.905065E-16	1.635097E-14	99.981683	3.375722
0.56	1.732290E+16	65.333333	1.234286E-06	2.769576E-16	4.994238E-16	1.694553E-14	99.981022	3.375722
0.57	1.732279E+16	66.500000	1.234286E-06	2.910707E-16	5.083410E-16	1.755069E-14	99.980349	3.375721
0.58	1.732267E+16	67.666667	1.234286E-06	3.056533E-16	5.172582E-16	1.816648E-14	99.979665	3.375721
0.59	1.732255E+16	68.833333	1.234286E-06	3.207130E-16	5.261753E-16	1.879288E-14	99.978968	3.375720
0.60	1.732242E+16	70.000000	1.234286E-06	3.362573E-16	5.350923E-16	1.942989E-14	99.978260	3.375720
0.61	1.732230E+16	71.166667	1.234286E-06	3.522941E-16	5.440093E-16	2.007752E-14	99.977540	3.375719
0.62	1.732217E+16	72.333333	1.234286E-06	3.688308E-16	5.529263E-16	2.073576E-14	99.976807	3.375718
0.63	1.732204E+16	73.500000	1.234286E-06	3.858752E-16	5.618432E-16	2.140462E-14	99.976063	3.375718
0.64	1.732191E+16	74.666667	1.234286E-06	4.034349E-16	5.707600E-16	2.208409E-14	99.975307	3.375717
0.65	1.732178E+16	75.833333	1.234286E-06	4.215175E-16	5.796767E-16	2.277417E-14	99.974540	3.375717
0.66	1.732164E+16	77.000000	1.234286E-06	4.401308E-16	5.885934E-16	2.347487E-14	99.973760	3.375716
0.67	1.732151E+16	78.166667	1.234286E-06	4.592823E-16	5.975101E-16	2.418618E-14	99.972968	3.375716
0.68	1.732137E+16	79.333333	1.234286E-06	4.789796E-16	6.064266E-16	2.490811E-14	99.972164	3.375715
0.69	1.732123E+16	80.500000	1.234286E-06	4.992306E-16	6.153431E-16	2.564065E-14	99.971348	3.375714
0.70	1.732108E+16	81.666667	1.234286E-06	5.200427E-16	6.242596E-16	2.638381E-14	99.970521	3.375714
0.71	1.732094E+16	82.833333	1.234286E-06	5.414236E-16	6.331759E-16	2.713757E-14	99.969681	3.375713
0.72	1.732079E+16	84.000000	1.234286E-06	5.633810E-16	6.420922E-16	2.790196E-14	99.968830	3.375713
0.73	1.732064E+16	85.166667	1.234286E-06	5.859225E-16	6.510085E-16	2.867695E-14	99.967966	3.375712
0.74	1.732049E+16	86.333333	1.234286E-06	6.090558E-16	6.599246E-16	2.946256E-14	99.967090	3.375711
0.75	1.732034E+16	87.500000	1.234286E-06	6.327885E-16	6.688407E-16	3.025878E-14	99.966203	3.375711
0.76	1.732018E+16	88.666667	1.234286E-06	6.571283E-16	6.777567E-16	3.106561E-14	99.965303	3.375710
0.77	1.732002E+16	89.833333	1.234286E-06	6.820828E-16	6.866727E-16	3.188306E-14	99.964391	3.375709
0.78	1.731986E+16	91.000000	1.234286E-06	7.076596E-16	6.955885E-16	3.271111E-14	99.963468	3.375708
0.79	1.731970E+16	92.166667	1.234286E-06	7.338664E-16	7.045043E-16	3.354978E-14	99.962532	3.375708
0.80	1.731954E+16	93.333333	1.234286E-06	7.607109E-16	7.134200E-16	3.439907E-14	99.961584	3.375707
0.81	1.731937E+16	94.500000	1.234286E-06	7.882006E-16	7.223357E-16	3.525896E-14	99.960624	3.375706
0.82	1.731920E+16	95.666667	1.234286E-06	8.163433E-16	7.312512E-16	3.612947E-14	99.959653	3.375706
0.83	1.731903E+16	96.833333	1.234286E-06	8.451465E-16	7.401667E-16	3.701059E-14	99.958669	3.375705
0.84	1.731886E+16	98.000000	1.234286E-06	8.746180E-16	7.490821E-16	3.790232E-14	99.957673	3.375704
0.85	1.731868E+16	99.166667	1.234286E-06	9.047654E-16	7.579974E-16	3.880466E-14	99.956664	3.375703
0.86	1.731851E+16	100.333333	1.234286E-06	9.355962E-16	7.669126E-16	3.971761E-14	99.955644	3.375703
0.87	1.731833E+16	101.500000	1.234286E-06	9.671182E-16	7.758278E-16	4.064118E-14	99.954612	3.375702
0.88	1.731815E+16	102.666667	1.234286E-06	9.993390E-16	7.847428E-16	4.157535E-14	99.953567	3.375701
0.89	1.731796E+16	103.833333	1.234286E-06	1.032266E-15	7.936578E-16	4.252014E-14	99.952511	3.375700
0.90	1.731778E+16	105.000000	1.234286E-06	1.065908E-15	8.025727E-16	4.347554E-14	99.951442	3.375699
0.91	1.731759E+16	106.166667	1.234286E-06	1.100271E-15	8.114875E-16	4.444154E-14	99.950361	3.375699
0.92	1.731740E+16	107.333333	1.234286E-06	1.135363E-15	8.204022E-16	4.541816E-14	99.949268	3.375698
0.93	1.731721E+16	108.500000	1.234286E-06	1.171192E-15	8.293169E-16	4.640539E-14	99.948163	3.375697
0.94	1.731702E+16	109.666667	1.234286E-06	1.207767E-15	8.382314E-16	4.740323E-14	99.947046	3.375696
0.95	1.731682E+16	110.833333	1.234286E-06	1.245093E-15	8.471458E-16	4.841168E-14	99.945917	3.375695
0.96	1.731662E+16	112.000000	1.234286E-06	1.283179E-15	8.560602E-16	4.943073E-14	99.944775	3.375695
0.97	1.731642E+16	113.166667	1.234286E-06	1.322033E-15	8.649745E-16	5.046040E-14	99.943621	3.375694
0.98	1.731622E+16	114.333333	1.234286E-06	1.361662E-15	8.738886E-16	5.150068E-14	99.942455	3.375693
0.99	1.731602E+16	115.500000	1.234286E-06	1.402074E-15	8.828027E-16	5.255156E-14	99.941277	3.375692
1.00	1.731581E+16	116.666667	1.234286E-06	1.443277E-15	8.917167E-16	5.361306E-14	99.940087	3.375691



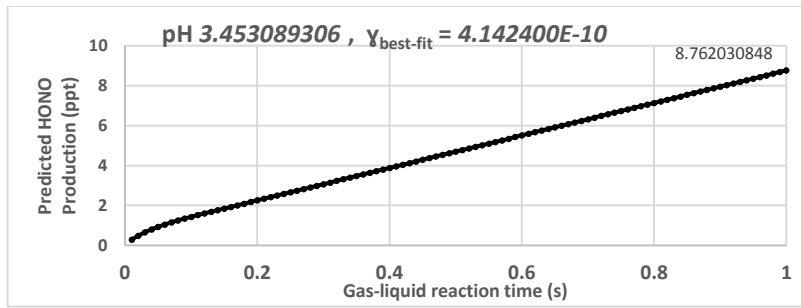
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO2}}$ (mol)	$\Phi_{\text{NO2}}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732619E+16	1.166667	3.509924E-07	1.427576E-21	9.465316E-19	1.334131E-18	99.999998	3.449063
0.02	1.732619E+16	2.333333	4.963782E-07	6.301627E-21	1.893063E-18	4.002394E-18	99.999994	3.449063
0.03	1.732619E+16	3.500000	6.079366E-07	1.608534E-20	2.839595E-18	8.004788E-18	99.999988	3.449063
0.04	1.732619E+16	4.666667	7.019846E-07	3.198544E-20	3.786126E-18	1.334131E-17	99.999982	3.449063
0.05	1.732619E+16	5.833333	7.848426E-07	5.505272E-20	4.732658E-18	2.001197E-17	99.999973	3.449063
0.06	1.732618E+16	7.000000	8.597519E-07	8.623029E-20	5.679189E-18	2.801675E-17	99.999964	3.449063
0.07	1.732618E+16	8.166667	9.286381E-07	1.263811E-19	6.625720E-18	3.735567E-17	99.999953	3.449063
0.08	1.732618E+16	9.333333	9.927558E-07	1.763056E-19	7.572251E-18	4.802872E-17	99.999940	3.449063
0.09	1.732618E+16	10.500000	1.052976E-06	2.367534E-19	8.518782E-18	6.003590E-17	99.999926	3.449063
0.10	1.732618E+16	11.666667	1.109934E-06	3.084320E-19	9.465313E-18	7.337720E-17	99.999911	3.449063
0.11	1.732617E+16	12.833333	1.164109E-06	3.920131E-19	1.041184E-17	8.805264E-17	99.999894	3.449063
0.12	1.732617E+16	14.000000	1.215872E-06	4.881379E-19	1.135837E-17	1.040622E-16	99.999876	3.449063
0.13	1.732617E+16	15.166667	1.234286E-06	5.975504E-19	1.230490E-17	1.214059E-16	99.999856	3.449063
0.14	1.732616E+16	16.333333	1.234286E-06	7.210628E-19	1.325143E-17	1.400837E-16	99.999835	3.449063
0.15	1.732616E+16	17.500000	1.234286E-06	8.594868E-19	1.419796E-17	1.600957E-16	99.999812	3.449063
0.16	1.732615E+16	18.666667	1.234286E-06	1.013634E-18	1.514449E-17	1.814417E-16	99.999788	3.449063
0.17	1.732615E+16	19.833333	1.234286E-06	1.184317E-18	1.609102E-17	2.041220E-16	99.999763	3.449063
0.18	1.732615E+16	21.000000	1.234286E-06	1.372348E-18	1.703755E-17	2.281363E-16	99.999736	3.449063
0.19	1.732614E+16	22.166667	1.234286E-06	1.578538E-18	1.798408E-17	2.534847E-16	99.999708	3.449063
0.20	1.732614E+16	23.333333	1.234286E-06	1.803699E-18	1.893061E-17	2.801673E-16	99.999678	3.449063
0.21	1.732613E+16	24.500000	1.234286E-06	2.048643E-18	1.987714E-17	3.081840E-16	99.999646	3.449063
0.22	1.732612E+16	25.666667	1.234286E-06	2.314182E-18	2.082367E-17	3.375349E-16	99.999614	3.449063
0.23	1.732612E+16	26.833333	1.234286E-06	2.601129E-18	2.177020E-17	3.682198E-16	99.999580	3.449063
0.24	1.732611E+16	28.000000	1.234286E-06	2.910294E-18	2.271672E-17	4.002389E-16	99.999544	3.449063
0.25	1.732611E+16	29.166667	1.234286E-06	3.242490E-18	2.366325E-17	4.335921E-16	99.999507	3.449063
0.26	1.732610E+16	30.333333	1.234286E-06	3.598528E-18	2.460978E-17	4.682794E-16	99.999468	3.449063
0.27	1.732609E+16	31.500000	1.234286E-06	3.979222E-18	2.555631E-17	5.043008E-16	99.999428	3.449063
0.28	1.732608E+16	32.666667	1.234286E-06	4.385381E-18	2.650283E-17	5.416564E-16	99.999387	3.449063
0.29	1.732608E+16	33.833333	1.234286E-06	4.817819E-18	2.744936E-17	5.803461E-16	99.999344	3.449063
0.30	1.732607E+16	35.000000	1.234286E-06	5.277348E-18	2.839588E-17	6.203699E-16	99.999300	3.449063
0.31	1.732606E+16	36.166667	1.234286E-06	5.764779E-18	2.934241E-17	6.617278E-16	99.999254	3.449063
0.32	1.732605E+16	37.333333	1.234286E-06	6.280924E-18	3.028893E-17	7.044198E-16	99.999206	3.449063
0.33	1.732605E+16	38.500000	1.234286E-06	6.826595E-18	3.123546E-17	7.484460E-16	99.999158	3.449063
0.34	1.732604E+16	39.666667	1.234286E-06	7.402603E-18	3.218198E-17	7.938062E-16	99.999108	3.449063
0.35	1.732603E+16	40.833333	1.234286E-06	8.009762E-18	3.312851E-17	8.405006E-16	99.999056	3.449063
0.36	1.732602E+16	42.000000	1.234286E-06	8.648883E-18	3.407503E-17	8.885291E-16	99.999003	3.449063
0.37	1.732601E+16	43.166667	1.234286E-06	9.320777E-18	3.502155E-17	9.378917E-16	99.998948	3.449063
0.38	1.732600E+16	44.333333	1.234286E-06	1.002626E-17	3.596808E-17	9.885884E-16	99.998892	3.449062
0.39	1.732599E+16	45.500000	1.234286E-06	1.076613E-17	3.691460E-17	1.040619E-15	99.998835	3.449062
0.40	1.732598E+16	46.666667	1.234286E-06	1.154122E-17	3.786112E-17	1.093984E-15	99.998776	3.449062
0.41	1.732597E+16	47.833333	1.234286E-06	1.235233E-17	3.880764E-17	1.148683E-15	99.998715	3.449062
0.42	1.732596E+16	49.000000	1.234286E-06	1.320027E-17	3.975416E-17	1.204716E-15	99.998653	3.449062
0.43	1.732595E+16	50.166667	1.234286E-06	1.408586E-17	4.070068E-17	1.262083E-15	99.998590	3.449062
0.44	1.732594E+16	51.333333	1.234286E-06	1.500990E-17	4.164720E-17	1.320785E-15	99.998525	3.449062
0.45	1.732592E+16	52.500000	1.234286E-06	1.597321E-17	4.259372E-17	1.380820E-15	99.998459	3.449062

0.46	1.732591E+16	53.666667	1.234286E-06	1.697660E-17	4.354024E-17	1.442190E-15	99.998391	3.449062
0.47	1.732590E+16	54.833333	1.234286E-06	1.802089E-17	4.448675E-17	1.504893E-15	99.998322	3.449062
0.48	1.732589E+16	56.000000	1.234286E-06	1.910688E-17	4.543327E-17	1.568931E-15	99.998251	3.449062
0.49	1.732588E+16	57.166667	1.234286E-06	2.023538E-17	4.637979E-17	1.634303E-15	99.998179	3.449062
0.50	1.732586E+16	58.333333	1.234286E-06	2.140722E-17	4.732630E-17	1.701009E-15	99.998105	3.449062
0.51	1.732585E+16	59.500000	1.234286E-06	2.262319E-17	4.827282E-17	1.769049E-15	99.998030	3.449062
0.52	1.732584E+16	60.666667	1.234286E-06	2.388412E-17	4.921933E-17	1.838423E-15	99.997953	3.449062
0.53	1.732582E+16	61.833333	1.234286E-06	2.519081E-17	5.016585E-17	1.909131E-15	99.997875	3.449062
0.54	1.732581E+16	63.000000	1.234286E-06	2.654408E-17	5.111236E-17	1.981173E-15	99.997795	3.449062
0.55	1.732580E+16	64.166667	1.234286E-06	2.794473E-17	5.205887E-17	2.054550E-15	99.997714	3.449061
0.56	1.732578E+16	65.333333	1.234286E-06	2.939359E-17	5.300538E-17	2.129260E-15	99.997632	3.449061
0.57	1.732577E+16	66.500000	1.234286E-06	3.089145E-17	5.395190E-17	2.205305E-15	99.997548	3.449061
0.58	1.732575E+16	67.666667	1.234286E-06	3.243914E-17	5.489841E-17	2.282683E-15	99.997462	3.449061
0.59	1.732574E+16	68.833333	1.234286E-06	3.403746E-17	5.584492E-17	2.361396E-15	99.997375	3.449061
0.60	1.732572E+16	70.000000	1.234286E-06	3.568723E-17	5.679143E-17	2.441443E-15	99.997286	3.449061
0.61	1.732571E+16	71.166667	1.234286E-06	3.738927E-17	5.773793E-17	2.522824E-15	99.997196	3.449061
0.62	1.732569E+16	72.333333	1.234286E-06	3.914437E-17	5.868444E-17	2.605539E-15	99.997105	3.449061
0.63	1.732567E+16	73.500000	1.234286E-06	4.095335E-17	5.963095E-17	2.689588E-15	99.997012	3.449061
0.64	1.732566E+16	74.666667	1.234286E-06	4.281703E-17	6.057745E-17	2.774971E-15	99.996918	3.449061
0.65	1.732564E+16	75.833333	1.234286E-06	4.473621E-17	6.152396E-17	2.861688E-15	99.996822	3.449061
0.66	1.732562E+16	77.000000	1.234286E-06	4.671172E-17	6.247046E-17	2.949739E-15	99.996724	3.449061
0.67	1.732561E+16	78.166667	1.234286E-06	4.874435E-17	6.341697E-17	3.039124E-15	99.996625	3.449060
0.68	1.732559E+16	79.333333	1.234286E-06	5.083493E-17	6.436347E-17	3.129844E-15	99.996525	3.449060
0.69	1.732557E+16	80.500000	1.234286E-06	5.298426E-17	6.530997E-17	3.221897E-15	99.996423	3.449060
0.70	1.732555E+16	81.666667	1.234286E-06	5.519315E-17	6.625647E-17	3.315285E-15	99.996320	3.449060
0.71	1.732554E+16	82.833333	1.234286E-06	5.746243E-17	6.720297E-17	3.410006E-15	99.996215	3.449060
0.72	1.732552E+16	84.000000	1.234286E-06	5.979289E-17	6.814947E-17	3.506062E-15	99.996108	3.449060
0.73	1.732550E+16	85.166667	1.234286E-06	6.218535E-17	6.909597E-17	3.603451E-15	99.996001	3.449060
0.74	1.732548E+16	86.333333	1.234286E-06	6.464063E-17	7.004247E-17	3.702175E-15	99.995891	3.449060
0.75	1.732546E+16	87.500000	1.234286E-06	6.715954E-17	7.098896E-17	3.802233E-15	99.995780	3.449060
0.76	1.732544E+16	88.666667	1.234286E-06	6.974288E-17	7.193546E-17	3.903624E-15	99.995668	3.449060
0.77	1.732542E+16	89.833333	1.234286E-06	7.239146E-17	7.288195E-17	4.006350E-15	99.995554	3.449060
0.78	1.732540E+16	91.000000	1.234286E-06	7.510611E-17	7.382845E-17	4.110410E-15	99.995439	3.449059
0.79	1.732538E+16	92.166667	1.234286E-06	7.788764E-17	7.477494E-17	4.215804E-15	99.995322	3.449059
0.80	1.732536E+16	93.333333	1.234286E-06	8.073684E-17	7.572143E-17	4.322532E-15	99.995204	3.449059
0.81	1.732534E+16	94.500000	1.234286E-06	8.365455E-17	7.666792E-17	4.430594E-15	99.995084	3.449059
0.82	1.732532E+16	95.666667	1.234286E-06	8.664156E-17	7.761441E-17	4.539990E-15	99.994962	3.449059
0.83	1.732530E+16	96.833333	1.234286E-06	8.969869E-17	7.856090E-17	4.650720E-15	99.994839	3.449059
0.84	1.732528E+16	98.000000	1.234286E-06	9.282675E-17	7.950739E-17	4.762784E-15	99.994715	3.449059
0.85	1.732525E+16	99.166667	1.234286E-06	9.602656E-17	8.045387E-17	4.876182E-15	99.994589	3.449059
0.86	1.732523E+16	100.333333	1.234286E-06	9.929892E-17	8.140036E-17	4.990914E-15	99.994462	3.449059
0.87	1.732521E+16	101.500000	1.234286E-06	1.026446E-16	8.234684E-17	5.106980E-15	99.994333	3.449058
0.88	1.732519E+16	102.666667	1.234286E-06	1.060646E-16	8.329333E-17	5.224380E-15	99.994203	3.449058
0.89	1.732516E+16	103.833333	1.234286E-06	1.095595E-16	8.423981E-17	5.343114E-15	99.994071	3.449058
0.90	1.732514E+16	105.000000	1.234286E-06	1.131302E-16	8.518629E-17	5.463182E-15	99.993937	3.449058
0.91	1.732512E+16	106.166667	1.234286E-06	1.167775E-16	8.613277E-17	5.584584E-15	99.993802	3.449058
0.92	1.732509E+16	107.333333	1.234286E-06	1.205022E-16	8.707925E-17	5.707321E-15	99.993666	3.449058
0.93	1.732507E+16	108.500000	1.234286E-06	1.243052E-16	8.802573E-17	5.831391E-15	99.993528	3.449058
0.94	1.732505E+16	109.666667	1.234286E-06	1.281872E-16	8.897220E-17	5.956795E-15	99.993388	3.449058
0.95	1.732502E+16	110.833333	1.234286E-06	1.321491E-16	8.991868E-17	6.083533E-15	99.993247	3.449057
0.96	1.732500E+16	112.000000	1.234286E-06	1.361917E-16	9.086515E-17	6.211605E-15	99.993105	3.449057
0.97	1.732497E+16	113.166667	1.234286E-06	1.403157E-16	9.181163E-17	6.341011E-15	99.992961	3.449057
0.98	1.732495E+16	114.333333	1.234286E-06	1.445221E-16	9.275810E-17	6.471751E-15	99.992815	3.449057
0.99	1.732492E+16	115.500000	1.234286E-06	1.488116E-16	9.370457E-17	6.603826E-15	99.992668	3.449057
1.00	1.732490E+16	116.666667	1.234286E-06	1.531849E-16	9.465104E-17	6.737234E-15	99.992520	3.449057



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732619E+16	1.166667	3.509924E-07	3.176406E-21	2.106065E-18	2.992556E-18	99.999995	3.452570
0.02	1.732619E+16	2.333333	4.963781E-07	1.402133E-20	4.212130E-18	8.977667E-18	99.999986	3.452570
0.03	1.732619E+16	3.500000	6.079365E-07	3.579042E-20	6.318195E-18	1.795533E-17	99.999974	3.452570
0.04	1.732618E+16	4.666667	7.019845E-07	7.116869E-20	8.424259E-18	2.992555E-17	99.999959	3.452570
0.05	1.732618E+16	5.833333	7.848424E-07	1.224942E-19	1.053032E-17	4.488833E-17	99.999941	3.452570
0.06	1.732618E+16	7.000000	8.597515E-07	1.918653E-19	1.263639E-17	6.284365E-17	99.999919	3.452570
0.07	1.732617E+16	8.166667	9.286376E-07	2.812024E-19	1.474245E-17	8.379153E-17	99.999894	3.452570
0.08	1.732617E+16	9.333333	9.927551E-07	3.922860E-19	1.684851E-17	1.077320E-16	99.999866	3.452570
0.09	1.732616E+16	10.500000	1.052975E-06	5.267844E-19	1.895457E-17	1.346649E-16	99.999835	3.452570
0.10	1.732616E+16	11.666667	1.109933E-06	6.862717E-19	2.106064E-17	1.645905E-16	99.999800	3.452570
0.11	1.732615E+16	12.833333	1.164107E-06	8.722426E-19	2.316670E-17	1.975085E-16	99.999763	3.452570
0.12	1.732614E+16	14.000000	1.215870E-06	1.086123E-18	2.527276E-17	2.334191E-16	99.999722	3.452570
0.13	1.732614E+16	15.166667	1.234286E-06	1.329570E-18	2.737882E-17	2.723223E-16	99.999678	3.452570
0.14	1.732613E+16	16.333333	1.234286E-06	1.604389E-18	2.948487E-17	3.142180E-16	99.999630	3.452570
0.15	1.732612E+16	17.500000	1.234286E-06	1.912387E-18	3.159093E-17	3.591062E-16	99.999580	3.452570
0.16	1.732611E+16	18.666667	1.234286E-06	2.255371E-18	3.369699E-17	4.069870E-16	99.999526	3.452570
0.17	1.732610E+16	19.833333	1.234286E-06	2.635147E-18	3.580304E-17	4.578603E-16	99.999469	3.452570
0.18	1.732609E+16	21.000000	1.234286E-06	3.053521E-18	3.790910E-17	5.117262E-16	99.999408	3.452570
0.19	1.732608E+16	22.166667	1.234286E-06	3.512300E-18	4.001515E-17	5.685845E-16	99.999345	3.452570
0.20	1.732607E+16	23.333333	1.234286E-06	4.013290E-18	4.212120E-17	6.284354E-16	99.999278	3.452570
0.21	1.732605E+16	24.500000	1.234286E-06	4.558299E-18	4.422725E-17	6.912788E-16	99.999207	3.452570
0.22	1.732604E+16	25.666667	1.234286E-06	5.149133E-18	4.633330E-17	7.571148E-16	99.999134	3.452570
0.23	1.732603E+16	26.833333	1.234286E-06	5.787597E-18	4.843935E-17	8.259432E-16	99.999057	3.452570
0.24	1.732601E+16	28.000000	1.234286E-06	6.475499E-18	5.054539E-17	8.977641E-16	99.998978	3.452570
0.25	1.732600E+16	29.166667	1.234286E-06	7.214646E-18	5.265144E-17	9.725776E-16	99.998894	3.452570
0.26	1.732598E+16	30.333333	1.234286E-06	8.006843E-18	5.475748E-17	1.050384E-15	99.998808	3.452569
0.27	1.732597E+16	31.500000	1.234286E-06	8.853897E-18	5.686352E-17	1.131182E-15	99.998718	3.452569
0.28	1.732595E+16	32.666667	1.234286E-06	9.757615E-18	5.896956E-17	1.214973E-15	99.998625	3.452569
0.29	1.732594E+16	33.833333	1.234286E-06	1.071980E-17	6.107560E-17	1.301756E-15	99.998529	3.452569
0.30	1.732592E+16	35.000000	1.234286E-06	1.174227E-17	6.318164E-17	1.391532E-15	99.998430	3.452569
0.31	1.732590E+16	36.166667	1.234286E-06	1.282681E-17	6.528767E-17	1.484301E-15	99.998327	3.452569
0.32	1.732588E+16	37.333333	1.234286E-06	1.397525E-17	6.739370E-17	1.580062E-15	99.998221	3.452569
0.33	1.732586E+16	38.500000	1.234286E-06	1.518939E-17	6.949973E-17	1.678815E-15	99.998112	3.452569
0.34	1.732584E+16	39.666667	1.234286E-06	1.647102E-17	7.160576E-17	1.780561E-15	99.997999	3.452569
0.35	1.732582E+16	40.833333	1.234286E-06	1.782197E-17	7.371179E-17	1.885299E-15	99.997883	3.452569
0.36	1.732580E+16	42.000000	1.234286E-06	1.924403E-17	7.581781E-17	1.993030E-15	99.997764	3.452568
0.37	1.732578E+16	43.166667	1.234286E-06	2.073901E-17	7.792383E-17	2.103753E-15	99.997641	3.452568
0.38	1.732576E+16	44.333333	1.234286E-06	2.230872E-17	8.002985E-17	2.217469E-15	99.997516	3.452568
0.39	1.732574E+16	45.500000	1.234286E-06	2.395497E-17	8.213587E-17	2.334177E-15	99.997387	3.452568
0.40	1.732572E+16	46.666667	1.234286E-06	2.567955E-17	8.424188E-17	2.453878E-15	99.997254	3.452568
0.41	1.732569E+16	47.833333	1.234286E-06	2.748429E-17	8.634789E-17	2.576570E-15	99.997119	3.452568
0.42	1.732567E+16	49.000000	1.234286E-06	2.937098E-17	8.845390E-17	2.702256E-15	99.996980	3.452568
0.43	1.732564E+16	50.166667	1.234286E-06	3.134143E-17	9.055991E-17	2.830934E-15	99.996838	3.452568
0.44	1.732562E+16	51.333333	1.234286E-06	3.339745E-17	9.266591E-17	2.962604E-15	99.996692	3.452568
0.45	1.732559E+16	52.500000	1.234286E-06	3.554084E-17	9.477192E-17	3.097267E-15	99.996544	3.452567

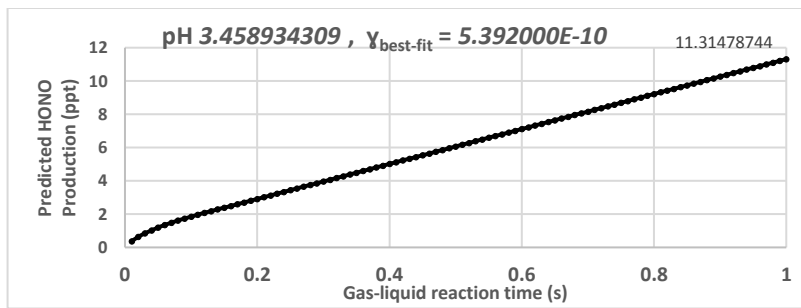
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0.47	1.732554E+16	54.833333	1.234286E-06	4.009697E-17	9.898391E-17	3.375569E-15	99.996236	3.452567
0.48	1.732551E+16	56.000000	1.234286E-06	4.251332E-17	1.010899E-16	3.519209E-15	99.996078	3.452567
0.49	1.732548E+16	57.166667	1.234286E-06	4.502427E-17	1.031959E-16	3.665841E-15	99.995916	3.452567
0.50	1.732545E+16	58.333333	1.234286E-06	4.763162E-17	1.053019E-16	3.815465E-15	99.995750	3.452567
0.51	1.732543E+16	59.500000	1.234286E-06	5.033719E-17	1.074079E-16	3.968082E-15	99.995582	3.452567
0.52	1.732540E+16	60.666667	1.234286E-06	5.314278E-17	1.095138E-16	4.123692E-15	99.995410	3.452566
0.53	1.732537E+16	61.833333	1.234286E-06	5.605019E-17	1.116198E-16	4.282293E-15	99.995235	3.452566
0.54	1.732533E+16	63.000000	1.234286E-06	5.906123E-17	1.137258E-16	4.443887E-15	99.995056	3.452566
0.55	1.732530E+16	64.166667	1.234286E-06	6.217771E-17	1.158318E-16	4.608473E-15	99.994874	3.452566
0.56	1.732527E+16	65.333333	1.234286E-06	6.540144E-17	1.179377E-16	4.776052E-15	99.994689	3.452566
0.57	1.732524E+16	66.500000	1.234286E-06	6.873421E-17	1.200437E-16	4.946623E-15	99.994501	3.452566
0.58	1.732521E+16	67.666667	1.234286E-06	7.217784E-17	1.221497E-16	5.120186E-15	99.994309	3.452565
0.59	1.732517E+16	68.833333	1.234286E-06	7.573414E-17	1.242556E-16	5.296741E-15	99.994114	3.452565
0.60	1.732514E+16	70.000000	1.234286E-06	7.940490E-17	1.263616E-16	5.476289E-15	99.993915	3.452565
0.61	1.732510E+16	71.166667	1.234286E-06	8.319194E-17	1.284675E-16	5.658829E-15	99.993713	3.452565
0.62	1.732507E+16	72.333333	1.234286E-06	8.709707E-17	1.305735E-16	5.844361E-15	99.993508	3.452565
0.63	1.732503E+16	73.500000	1.234286E-06	9.112208E-17	1.326794E-16	6.032886E-15	99.993300	3.452564
0.64	1.732499E+16	74.666667	1.234286E-06	9.526878E-17	1.347853E-16	6.224403E-15	99.993088	3.452564
0.65	1.732496E+16	75.833333	1.234286E-06	9.953899E-17	1.368913E-16	6.418912E-15	99.992873	3.452564
0.66	1.732492E+16	77.000000	1.234286E-06	1.039345E-16	1.389972E-16	6.616413E-15	99.992654	3.452564
0.67	1.732488E+16	78.166667	1.234286E-06	1.084571E-16	1.411031E-16	6.816907E-15	99.992433	3.452564
0.68	1.732484E+16	79.333333	1.234286E-06	1.131087E-16	1.432090E-16	7.020392E-15	99.992208	3.452563
0.69	1.732480E+16	80.500000	1.234286E-06	1.178910E-16	1.453150E-16	7.226870E-15	99.991979	3.452563
0.70	1.732476E+16	81.666667	1.234286E-06	1.228058E-16	1.474209E-16	7.436340E-15	99.991747	3.452563
0.71	1.732472E+16	82.833333	1.234286E-06	1.278549E-16	1.495268E-16	7.648803E-15	99.991512	3.452563
0.72	1.732468E+16	84.000000	1.234286E-06	1.330402E-16	1.516327E-16	7.864257E-15	99.991273	3.452563
0.73	1.732464E+16	85.166667	1.234286E-06	1.383634E-16	1.537386E-16	8.082704E-15	99.991032	3.452562
0.74	1.732459E+16	86.333333	1.234286E-06	1.438264E-16	1.558445E-16	8.304142E-15	99.990786	3.452562
0.75	1.732455E+16	87.500000	1.234286E-06	1.494310E-16	1.579504E-16	8.528573E-15	99.990538	3.452562
0.76	1.732451E+16	88.666667	1.234286E-06	1.551789E-16	1.600563E-16	8.755996E-15	99.990286	3.452562
0.77	1.732446E+16	89.833333	1.234286E-06	1.610721E-16	1.621621E-16	8.986411E-15	99.990031	3.452562
0.78	1.732442E+16	91.000000	1.234286E-06	1.671122E-16	1.642680E-16	9.219819E-15	99.989772	3.452561
0.79	1.732437E+16	92.166667	1.234286E-06	1.733010E-16	1.663739E-16	9.456218E-15	99.989510	3.452561
0.80	1.732433E+16	93.333333	1.234286E-06	1.796405E-16	1.684797E-16	9.695609E-15	99.989244	3.452561
0.81	1.732428E+16	94.500000	1.234286E-06	1.861324E-16	1.705856E-16	9.937993E-15	99.988976	3.452561
0.82	1.732423E+16	95.666667	1.234286E-06	1.927785E-16	1.726915E-16	1.018337E-14	99.988703	3.452560
0.83	1.732419E+16	96.833333	1.234286E-06	1.995806E-16	1.747973E-16	1.043174E-14	99.988428	3.452560
0.84	1.732414E+16	98.000000	1.234286E-06	2.065405E-16	1.769032E-16	1.068310E-14	99.988149	3.452560
0.85	1.732409E+16	99.166667	1.234286E-06	2.136601E-16	1.790090E-16	1.093745E-14	99.987867	3.452560
0.86	1.732404E+16	100.333333	1.234286E-06	2.209410E-16	1.811148E-16	1.119479E-14	99.987581	3.452559
0.87	1.732399E+16	101.500000	1.234286E-06	2.283853E-16	1.832207E-16	1.145513E-14	99.987292	3.452559
0.88	1.732394E+16	102.666667	1.234286E-06	2.359945E-16	1.853265E-16	1.171845E-14	99.987000	3.452559
0.89	1.732389E+16	103.833333	1.234286E-06	2.437706E-16	1.874323E-16	1.198477E-14	99.986704	3.452559
0.90	1.732384E+16	105.000000	1.234286E-06	2.517154E-16	1.895381E-16	1.225408E-14	99.986405	3.452558
0.91	1.732378E+16	106.166667	1.234286E-06	2.598306E-16	1.916439E-16	1.252639E-14	99.986102	3.452558
0.92	1.732373E+16	107.333333	1.234286E-06	2.681181E-16	1.937497E-16	1.280168E-14	99.985796	3.452558
0.93	1.732368E+16	108.500000	1.234286E-06	2.765797E-16	1.958555E-16	1.307997E-14	99.985487	3.452557
0.94	1.732362E+16	109.666667	1.234286E-06	2.852172E-16	1.979613E-16	1.336125E-14	99.985174	3.452557
0.95	1.732357E+16	110.833333	1.234286E-06	2.940323E-16	2.000671E-16	1.364552E-14	99.984858	3.452557
0.96	1.732351E+16	112.000000	1.234286E-06	3.030270E-16	2.021729E-16	1.393278E-14	99.984539	3.452557
0.97	1.732346E+16	113.166667	1.234286E-06	3.122029E-16	2.042787E-16	1.422304E-14	99.984216	3.452556
0.98	1.732340E+16	114.333333	1.234286E-06	3.215619E-16	2.063844E-16	1.451628E-14	99.983889	3.452556
0.99	1.732334E+16	115.500000	1.234286E-06	3.311059E-16	2.084902E-16	1.481252E-14	99.983560	3.452556
1.00	1.732328E+16	116.666667	1.234286E-06	3.408366E-16	2.105959E-16	1.511175E-14	99.983227	3.452555



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO2}}$ (mol)	$\Phi_{\text{NO2}}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732619E+16	1.166667	3.509923E-07	7.419643E-21	4.919475E-18	6.998549E-18	99.999987	3.453089
0.02	1.732619E+16	2.333333	4.963780E-07	3.275189E-20	9.838948E-18	2.099564E-17	99.999967	3.453089
0.03	1.732618E+16	3.500000	6.079363E-07	8.360145E-20	1.475842E-17	4.199128E-17	99.999939	3.453089
0.04	1.732617E+16	4.666667	7.019841E-07	1.662402E-19	1.967789E-17	6.998546E-17	99.999904	3.453089
0.05	1.732617E+16	5.833333	7.848417E-07	2.861294E-19	2.459736E-17	1.049782E-16	99.999861	3.453089
0.06	1.732616E+16	7.000000	8.597506E-07	4.481708E-19	2.951683E-17	1.469694E-16	99.999811	3.453089
0.07	1.732615E+16	8.166667	9.286363E-07	6.568496E-19	3.443629E-17	1.959592E-16	99.999753	3.453089
0.08	1.732614E+16	9.333333	9.927533E-07	9.163256E-19	3.935575E-17	2.519475E-16	99.999687	3.453089
0.09	1.732612E+16	10.500000	1.052973E-06	1.230495E-18	4.427521E-17	3.149343E-16	99.999614	3.453089
0.10	1.732611E+16	11.666667	1.109930E-06	1.603035E-18	4.919467E-17	3.849196E-16	99.999533	3.453089
0.11	1.732610E+16	12.833333	1.164104E-06	2.037438E-18	5.411412E-17	4.619034E-16	99.999445	3.453089
0.12	1.732608E+16	14.000000	1.215865E-06	2.537034E-18	5.903357E-17	5.458857E-16	99.999349	3.453089
0.13	1.732606E+16	15.166667	1.234286E-06	3.105691E-18	6.395301E-17	6.368665E-16	99.999246	3.453089
0.14	1.732604E+16	16.333333	1.234286E-06	3.747630E-18	6.887244E-17	7.348457E-16	99.999135	3.453089
0.15	1.732602E+16	17.500000	1.234286E-06	4.467071E-18	7.379188E-17	8.398234E-16	99.999017	3.453088
0.16	1.732600E+16	18.666667	1.234286E-06	5.268232E-18	7.871130E-17	9.517996E-16	99.998891	3.453088
0.17	1.732598E+16	19.833333	1.234286E-06	6.155334E-18	8.363072E-17	1.070774E-15	99.998757	3.453088
0.18	1.732595E+16	21.000000	1.234286E-06	7.132596E-18	8.855014E-17	1.196747E-15	99.998616	3.453088
0.19	1.732593E+16	22.166667	1.234286E-06	8.204239E-18	9.346955E-17	1.329718E-15	99.998467	3.453088
0.20	1.732590E+16	23.333333	1.234286E-06	9.374482E-18	9.838895E-17	1.469688E-15	99.998311	3.453088
0.21	1.732587E+16	24.500000	1.234286E-06	1.064754E-17	1.033083E-16	1.616656E-15	99.998147	3.453088
0.22	1.732584E+16	25.666667	1.234286E-06	1.202765E-17	1.082277E-16	1.770623E-15	99.997975	3.453088
0.23	1.732581E+16	26.833333	1.234286E-06	1.351901E-17	1.131471E-16	1.931588E-15	99.997796	3.453087
0.24	1.732578E+16	28.000000	1.234286E-06	1.512585E-17	1.180665E-16	2.099551E-15	99.997609	3.453087
0.25	1.732574E+16	29.166667	1.234286E-06	1.685238E-17	1.229858E-16	2.274512E-15	99.997415	3.453087
0.26	1.732571E+16	30.333333	1.234286E-06	1.870284E-17	1.279052E-16	2.456472E-15	99.997212	3.453087
0.27	1.732567E+16	31.500000	1.234286E-06	2.068143E-17	1.328245E-16	2.645429E-15	99.997003	3.453087
0.28	1.732563E+16	32.666667	1.234286E-06	2.279238E-17	1.377439E-16	2.841386E-15	99.996785	3.453086
0.29	1.732560E+16	33.833333	1.234286E-06	2.503991E-17	1.426632E-16	3.044340E-15	99.996560	3.453086
0.30	1.732555E+16	35.000000	1.234286E-06	2.742823E-17	1.475825E-16	3.254292E-15	99.996328	3.453086
0.31	1.732551E+16	36.166667	1.234286E-06	2.996157E-17	1.525018E-16	3.471243E-15	99.996087	3.453086
0.32	1.732547E+16	37.333333	1.234286E-06	3.264415E-17	1.574211E-16	3.695192E-15	99.995839	3.453086
0.33	1.732543E+16	38.500000	1.234286E-06	3.548018E-17	1.623404E-16	3.926139E-15	99.995584	3.453085
0.34	1.732538E+16	39.666667	1.234286E-06	3.847388E-17	1.672597E-16	4.164083E-15	99.995320	3.453085
0.35	1.732533E+16	40.833333	1.234286E-06	4.162948E-17	1.721789E-16	4.409026E-15	99.995050	3.453085
0.36	1.732529E+16	42.000000	1.234286E-06	4.495119E-17	1.770982E-16	4.660967E-15	99.994771	3.453085
0.37	1.732524E+16	43.166667	1.234286E-06	4.844323E-17	1.820174E-16	4.919906E-15	99.994485	3.453084
0.38	1.732518E+16	44.333333	1.234286E-06	5.210983E-17	1.869366E-16	5.185843E-15	99.994191	3.453084
0.39	1.732513E+16	45.500000	1.234286E-06	5.595520E-17	1.918559E-16	5.458778E-15	99.993889	3.453084
0.40	1.732508E+16	46.666667	1.234286E-06	5.998356E-17	1.967751E-16	5.738711E-15	99.993580	3.453084
0.41	1.732502E+16	47.833333	1.234286E-06	6.419913E-17	2.016942E-16	6.025641E-15	99.993263	3.453083
0.42	1.732497E+16	49.000000	1.234286E-06	6.860613E-17	2.066134E-16	6.319570E-15	99.992938	3.453083
0.43	1.732491E+16	50.166667	1.234286E-06	7.320877E-17	2.115326E-16	6.620496E-15	99.992605	3.453083
0.44	1.732485E+16	51.333333	1.234286E-06	7.801129E-17	2.164517E-16	6.928420E-15	99.992265	3.453082
0.45	1.732479E+16	52.500000	1.234286E-06	8.301789E-17	2.213708E-16	7.243341E-15	99.991917	3.453082

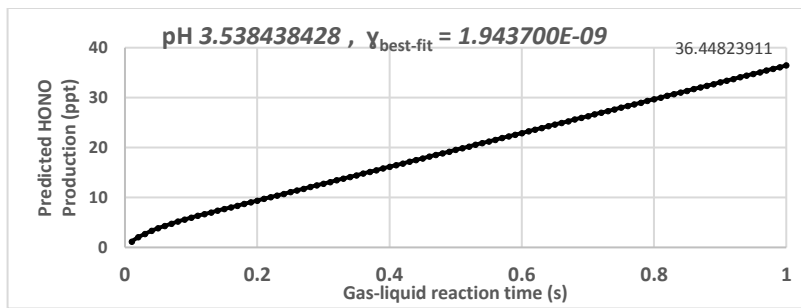


0.46	1.732473E+16	53.666667	1.234286E-06	8.823281E-17	2.262899E-16	7.565260E-15	99.991562	3.453082
0.47	1.732467E+16	54.833333	1.234286E-06	9.366024E-17	2.312090E-16	7.894177E-15	99.991198	3.453081
0.48	1.732460E+16	56.000000	1.234286E-06	9.930442E-17	2.361281E-16	8.230092E-15	99.990827	3.453081
0.49	1.732454E+16	57.166667	1.234286E-06	1.051696E-16	2.410472E-16	8.573004E-15	99.990449	3.453081
0.50	1.732447E+16	58.333333	1.234286E-06	1.112599E-16	2.459662E-16	8.922914E-15	99.990062	3.453080
0.51	1.732440E+16	59.500000	1.234286E-06	1.175796E-16	2.508852E-16	9.279821E-15	99.989668	3.453080
0.52	1.732433E+16	60.666667	1.234286E-06	1.241330E-16	2.558043E-16	9.643725E-15	99.989266	3.453080
0.53	1.732426E+16	61.833333	1.234286E-06	1.309242E-16	2.607233E-16	1.001463E-14	99.988856	3.453079
0.54	1.732419E+16	63.000000	1.234286E-06	1.379574E-16	2.656422E-16	1.039253E-14	99.988439	3.453079
0.55	1.732411E+16	64.166667	1.234286E-06	1.452370E-16	2.705612E-16	1.077742E-14	99.988013	3.453079
0.56	1.732404E+16	65.333333	1.234286E-06	1.527670E-16	2.754801E-16	1.116932E-14	99.987580	3.453078
0.57	1.732396E+16	66.500000	1.234286E-06	1.605517E-16	2.803990E-16	1.156821E-14	99.987140	3.453078
0.58	1.732389E+16	67.666667	1.234286E-06	1.685954E-16	2.853179E-16	1.197410E-14	99.986691	3.453077
0.59	1.732381E+16	68.833333	1.234286E-06	1.769023E-16	2.902368E-16	1.238698E-14	99.986235	3.453077
0.60	1.732373E+16	70.000000	1.234286E-06	1.854765E-16	2.951557E-16	1.280686E-14	99.985771	3.453077
0.61	1.732364E+16	71.166667	1.234286E-06	1.943223E-16	3.000745E-16	1.323374E-14	99.985299	3.453076
0.62	1.732356E+16	72.333333	1.234286E-06	2.034439E-16	3.049933E-16	1.366762E-14	99.984819	3.453076
0.63	1.732348E+16	73.500000	1.234286E-06	2.128455E-16	3.099121E-16	1.410849E-14	99.984332	3.453075
0.64	1.732339E+16	74.666667	1.234286E-06	2.225314E-16	3.148309E-16	1.455636E-14	99.983836	3.453075
0.65	1.732330E+16	75.833333	1.234286E-06	2.325058E-16	3.197497E-16	1.501123E-14	99.983333	3.453074
0.66	1.732321E+16	77.000000	1.234286E-06	2.427728E-16	3.246684E-16	1.547309E-14	99.982823	3.453074
0.67	1.732313E+16	78.166667	1.234286E-06	2.533367E-16	3.295871E-16	1.594195E-14	99.982304	3.453073
0.68	1.732303E+16	79.333333	1.234286E-06	2.642018E-16	3.345058E-16	1.641781E-14	99.981777	3.453073
0.69	1.732294E+16	80.500000	1.234286E-06	2.753722E-16	3.394245E-16	1.690067E-14	99.981243	3.453072
0.70	1.732285E+16	81.666667	1.234286E-06	2.868522E-16	3.443431E-16	1.739052E-14	99.980701	3.453072
0.71	1.732275E+16	82.833333	1.234286E-06	2.986459E-16	3.492617E-16	1.788736E-14	99.980151	3.453071
0.72	1.732266E+16	84.000000	1.234286E-06	3.107576E-16	3.541803E-16	1.839121E-14	99.979593	3.453071
0.73	1.732256E+16	85.166667	1.234286E-06	3.231916E-16	3.590989E-16	1.890204E-14	99.979028	3.453070
0.74	1.732246E+16	86.333333	1.234286E-06	3.359520E-16	3.640174E-16	1.941988E-14	99.978454	3.453070
0.75	1.732236E+16	87.500000	1.234286E-06	3.490430E-16	3.689359E-16	1.994471E-14	99.977873	3.453069
0.76	1.732226E+16	88.666667	1.234286E-06	3.624689E-16	3.738544E-16	2.047654E-14	99.977284	3.453069
0.77	1.732215E+16	89.833333	1.234286E-06	3.762339E-16	3.787729E-16	2.101537E-14	99.976687	3.453068
0.78	1.732205E+16	91.000000	1.234286E-06	3.903422E-16	3.836914E-16	2.156119E-14	99.976082	3.453068
0.79	1.732194E+16	92.166667	1.234286E-06	4.047980E-16	3.886098E-16	2.211400E-14	99.975469	3.453067
0.80	1.732183E+16	93.333333	1.234286E-06	4.196056E-16	3.935282E-16	2.267381E-14	99.974848	3.453067
0.81	1.732172E+16	94.500000	1.234286E-06	4.347691E-16	3.984465E-16	2.324062E-14	99.974220	3.453066
0.82	1.732161E+16	95.666667	1.234286E-06	4.502928E-16	4.033648E-16	2.381443E-14	99.973584	3.453066
0.83	1.732150E+16	96.833333	1.234286E-06	4.661809E-16	4.082832E-16	2.439523E-14	99.972939	3.453065
0.84	1.732139E+16	98.000000	1.234286E-06	4.824376E-16	4.132014E-16	2.498302E-14	99.972287	3.453064
0.85	1.732128E+16	99.166667	1.234286E-06	4.990671E-16	4.181197E-16	2.557781E-14	99.971627	3.453064
0.86	1.732116E+16	100.333333	1.234286E-06	5.160737E-16	4.230379E-16	2.617960E-14	99.970959	3.453063
0.87	1.732104E+16	101.500000	1.234286E-06	5.334615E-16	4.279561E-16	2.678838E-14	99.970283	3.453063
0.88	1.732092E+16	102.666667	1.234286E-06	5.512349E-16	4.328743E-16	2.740416E-14	99.969600	3.453062
0.89	1.732080E+16	103.833333	1.234286E-06	5.693979E-16	4.377924E-16	2.802693E-14	99.968908	3.453061
0.90	1.732068E+16	105.000000	1.234286E-06	5.879548E-16	4.427105E-16	2.865670E-14	99.968208	3.453061
0.91	1.732056E+16	106.166667	1.234286E-06	6.069099E-16	4.476286E-16	2.929346E-14	99.967501	3.453060
0.92	1.732044E+16	107.333333	1.234286E-06	6.262673E-16	4.525466E-16	2.993722E-14	99.966786	3.453059
0.93	1.732031E+16	108.500000	1.234286E-06	6.460314E-16	4.574646E-16	3.058797E-14	99.966062	3.453059
0.94	1.732018E+16	109.666667	1.234286E-06	6.662061E-16	4.623826E-16	3.124572E-14	99.965331	3.453058
0.95	1.732006E+16	110.833333	1.234286E-06	6.867959E-16	4.673005E-16	3.191046E-14	99.964592	3.453057
0.96	1.731993E+16	112.000000	1.234286E-06	7.078050E-16	4.722184E-16	3.258220E-14	99.963845	3.453057
0.97	1.731980E+16	113.166667	1.234286E-06	7.292374E-16	4.771363E-16	3.326093E-14	99.963090	3.453056
0.98	1.731966E+16	114.333333	1.234286E-06	7.510975E-16	4.820542E-16	3.394666E-14	99.962327	3.453055
0.99	1.731953E+16	115.500000	1.234286E-06	7.733895E-16	4.869720E-16	3.463938E-14	99.961556	3.453055
1.00	1.731940E+16	116.666667	1.234286E-06	7.961176E-16	4.918898E-16	3.533910E-14	99.960777	3.453054



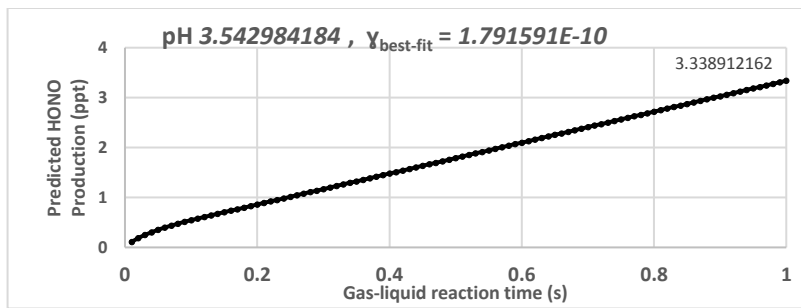
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732619E+16	1.166667	3.509923E-07	9.581621E-21	6.352939E-18	9.160285E-18	99.999983	3.458934
0.02	1.732618E+16	2.333333	4.963780E-07	4.229532E-20	1.270588E-17	2.748085E-17	99.999957	3.458934
0.03	1.732618E+16	3.500000	6.079362E-07	1.079617E-19	1.905881E-17	5.496169E-17	99.999921	3.458934
0.04	1.732617E+16	4.666667	7.019839E-07	2.146802E-19	2.541175E-17	9.160281E-17	99.999874	3.458934
0.05	1.732616E+16	5.833333	7.848414E-07	3.695034E-19	3.176468E-17	1.374042E-16	99.999818	3.458934
0.06	1.732615E+16	7.000000	8.597501E-07	5.787614E-19	3.811760E-17	1.923658E-16	99.999753	3.458934
0.07	1.732614E+16	8.166667	9.286356E-07	8.482463E-19	4.447053E-17	2.564877E-16	99.999677	3.458934
0.08	1.732612E+16	9.333333	9.927523E-07	1.183330E-18	5.082344E-17	3.297698E-16	99.999591	3.458934
0.09	1.732610E+16	10.500000	1.052972E-06	1.589044E-18	5.717636E-17	4.122121E-16	99.999496	3.458934
0.10	1.732609E+16	11.666667	1.109929E-06	2.070137E-18	6.352926E-17	5.038147E-16	99.999390	3.458934
0.11	1.732607E+16	12.833333	1.164102E-06	2.631118E-18	6.988216E-17	6.045774E-16	99.999275	3.458934
0.12	1.732604E+16	14.000000	1.215863E-06	3.276289E-18	7.623505E-17	7.145004E-16	99.999150	3.458934
0.13	1.732602E+16	15.166667	1.234286E-06	4.010646E-18	8.258794E-17	8.335835E-16	99.999015	3.458933
0.14	1.732600E+16	16.333333	1.234286E-06	4.839636E-18	8.894082E-17	9.618267E-16	99.998870	3.458933
0.15	1.732597E+16	17.500000	1.234286E-06	5.768711E-18	9.529368E-17	1.099230E-15	99.998715	3.458933
0.16	1.732594E+16	18.666667	1.234286E-06	6.803319E-18	1.016465E-16	1.245793E-15	99.998550	3.458933
0.17	1.732591E+16	19.833333	1.234286E-06	7.948910E-18	1.079994E-16	1.401517E-15	99.998375	3.458933
0.18	1.732588E+16	21.000000	1.234286E-06	9.210932E-18	1.143522E-16	1.566401E-15	99.998190	3.458933
0.19	1.732584E+16	22.166667	1.234286E-06	1.059484E-17	1.207051E-16	1.740444E-15	99.997996	3.458933
0.20	1.732581E+16	23.333333	1.234286E-06	1.210607E-17	1.270579E-16	1.923648E-15	99.997791	3.458932
0.21	1.732577E+16	24.500000	1.234286E-06	1.375008E-17	1.334107E-16	2.116011E-15	99.997576	3.458932
0.22	1.732573E+16	25.666667	1.234286E-06	1.553232E-17	1.397635E-16	2.317535E-15	99.997352	3.458932
0.23	1.732569E+16	26.833333	1.234286E-06	1.745824E-17	1.461162E-16	2.528218E-15	99.997117	3.458932
0.24	1.732565E+16	28.000000	1.234286E-06	1.953329E-17	1.524690E-16	2.748061E-15	99.996873	3.458932
0.25	1.732561E+16	29.166667	1.234286E-06	2.176291E-17	1.588218E-16	2.977064E-15	99.996619	3.458931
0.26	1.732556E+16	30.333333	1.234286E-06	2.415256E-17	1.651745E-16	3.215227E-15	99.996354	3.458931
0.27	1.732551E+16	31.500000	1.234286E-06	2.670768E-17	1.715272E-16	3.462550E-15	99.996080	3.458931
0.28	1.732546E+16	32.666667	1.234286E-06	2.943373E-17	1.778799E-16	3.719032E-15	99.995795	3.458931
0.29	1.732541E+16	33.833333	1.234286E-06	3.233614E-17	1.842326E-16	3.984674E-15	99.995501	3.458930
0.30	1.732536E+16	35.000000	1.234286E-06	3.542038E-17	1.905853E-16	4.259476E-15	99.995197	3.458930
0.31	1.732530E+16	36.166667	1.234286E-06	3.869189E-17	1.969379E-16	4.543437E-15	99.994882	3.458930
0.32	1.732525E+16	37.333333	1.234286E-06	4.215612E-17	2.032906E-16	4.836558E-15	99.994558	3.458929
0.33	1.732519E+16	38.500000	1.234286E-06	4.581852E-17	2.096432E-16	5.138838E-15	99.994223	3.458929
0.34	1.732513E+16	39.666667	1.234286E-06	4.968453E-17	2.159958E-16	5.450278E-15	99.993879	3.458929
0.35	1.732507E+16	40.833333	1.234286E-06	5.375961E-17	2.223484E-16	5.770877E-15	99.993524	3.458928
0.36	1.732501E+16	42.000000	1.234286E-06	5.804920E-17	2.287009E-16	6.100636E-15	99.993160	3.458928
0.37	1.732494E+16	43.166667	1.234286E-06	6.255876E-17	2.350535E-16	6.439554E-15	99.992785	3.458928
0.38	1.732487E+16	44.333333	1.234286E-06	6.729373E-17	2.414060E-16	6.787631E-15	99.992401	3.458927
0.39	1.732481E+16	45.500000	1.234286E-06	7.225956E-17	2.477585E-16	7.144867E-15	99.992006	3.458927
0.40	1.732474E+16	46.666667	1.234286E-06	7.746170E-17	2.541110E-16	7.511263E-15	99.991601	3.458927
0.41	1.732466E+16	47.833333	1.234286E-06	8.290560E-17	2.604634E-16	7.886817E-15	99.991186	3.458926
0.42	1.732459E+16	49.000000	1.234286E-06	8.859671E-17	2.668158E-16	8.271531E-15	99.990762	3.458926
0.43	1.732452E+16	50.166667	1.234286E-06	9.454047E-17	2.731682E-16	8.665403E-15	99.990327	3.458926
0.44	1.732444E+16	51.333333	1.234286E-06	1.007423E-16	2.795206E-16	9.068435E-15	99.989882	3.458925
0.45	1.732436E+16	52.500000	1.234286E-06	1.072077E-16	2.858730E-16	9.480625E-15	99.989426	3.458925

0.46	1.732428E+16	53.666667	1.234286E-06	1.139422E-16	2.922253E-16	9.901974E-15	99.988961	3.458924
0.47	1.732420E+16	54.833333	1.234286E-06	1.209510E-16	2.985776E-16	1.033248E-14	99.988486	3.458924
0.48	1.732411E+16	56.000000	1.234286E-06	1.282398E-16	3.049299E-16	1.077215E-14	99.988000	3.458923
0.49	1.732403E+16	57.166667	1.234286E-06	1.358139E-16	3.112821E-16	1.122097E-14	99.987505	3.458923
0.50	1.732394E+16	58.333333	1.234286E-06	1.436788E-16	3.176343E-16	1.167896E-14	99.986999	3.458922
0.51	1.732385E+16	59.500000	1.234286E-06	1.518399E-16	3.239865E-16	1.214610E-14	99.986483	3.458922
0.52	1.732376E+16	60.666667	1.234286E-06	1.603028E-16	3.303387E-16	1.262240E-14	99.985958	3.458922
0.53	1.732367E+16	61.833333	1.234286E-06	1.690728E-16	3.366908E-16	1.310786E-14	99.985421	3.458921
0.54	1.732357E+16	63.000000	1.234286E-06	1.781553E-16	3.430429E-16	1.360248E-14	99.984875	3.458921
0.55	1.732347E+16	64.166667	1.234286E-06	1.875559E-16	3.493950E-16	1.410625E-14	99.984319	3.458920
0.56	1.732338E+16	65.333333	1.234286E-06	1.972800E-16	3.557470E-16	1.461918E-14	99.983752	3.458920
0.57	1.732328E+16	66.500000	1.234286E-06	2.073330E-16	3.620990E-16	1.514127E-14	99.983176	3.458919
0.58	1.732317E+16	67.666667	1.234286E-06	2.177204E-16	3.684510E-16	1.567252E-14	99.982589	3.458918
0.59	1.732307E+16	68.833333	1.234286E-06	2.284476E-16	3.748029E-16	1.621293E-14	99.981992	3.458918
0.60	1.732297E+16	70.000000	1.234286E-06	2.395201E-16	3.811548E-16	1.676250E-14	99.981385	3.458917
0.61	1.732286E+16	71.166667	1.234286E-06	2.509433E-16	3.875067E-16	1.732122E-14	99.980767	3.458917
0.62	1.732275E+16	72.333333	1.234286E-06	2.627226E-16	3.938585E-16	1.788910E-14	99.980140	3.458916
0.63	1.732264E+16	73.500000	1.234286E-06	2.748636E-16	4.002103E-16	1.846613E-14	99.979502	3.458916
0.64	1.732253E+16	74.666667	1.234286E-06	2.873717E-16	4.065621E-16	1.905233E-14	99.978854	3.458915
0.65	1.732241E+16	75.833333	1.234286E-06	3.002522E-16	4.129138E-16	1.964768E-14	99.978196	3.458914
0.66	1.732230E+16	77.000000	1.234286E-06	3.135108E-16	4.192655E-16	2.025219E-14	99.977528	3.458914
0.67	1.732218E+16	78.166667	1.234286E-06	3.271527E-16	4.256171E-16	2.086586E-14	99.976849	3.458913
0.68	1.732206E+16	79.333333	1.234286E-06	3.411835E-16	4.319688E-16	2.148868E-14	99.976160	3.458913
0.69	1.732194E+16	80.500000	1.234286E-06	3.556086E-16	4.383203E-16	2.212066E-14	99.975461	3.458912
0.70	1.732182E+16	81.666667	1.234286E-06	3.704334E-16	4.446719E-16	2.276180E-14	99.974752	3.458911
0.71	1.732169E+16	82.833333	1.234286E-06	3.856634E-16	4.510234E-16	2.341209E-14	99.974033	3.458911
0.72	1.732157E+16	84.000000	1.234286E-06	4.013041E-16	4.573748E-16	2.407154E-14	99.973303	3.458910
0.73	1.732144E+16	85.166667	1.234286E-06	4.173608E-16	4.637262E-16	2.474015E-14	99.972563	3.458909
0.74	1.732131E+16	86.333333	1.234286E-06	4.338391E-16	4.700776E-16	2.541791E-14	99.971813	3.458909
0.75	1.732118E+16	87.500000	1.234286E-06	4.507444E-16	4.764289E-16	2.610483E-14	99.971052	3.458908
0.76	1.732104E+16	88.666667	1.234286E-06	4.680820E-16	4.827802E-16	2.680091E-14	99.970281	3.458907
0.77	1.732091E+16	89.833333	1.234286E-06	4.858576E-16	4.891315E-16	2.750614E-14	99.969500	3.458906
0.78	1.732077E+16	91.000000	1.234286E-06	5.040765E-16	4.954827E-16	2.822053E-14	99.968709	3.458906
0.79	1.732063E+16	92.166667	1.234286E-06	5.227442E-16	5.018338E-16	2.894407E-14	99.967907	3.458905
0.80	1.732049E+16	93.333333	1.234286E-06	5.418660E-16	5.081849E-16	2.967677E-14	99.967095	3.458904
0.81	1.732035E+16	94.500000	1.234286E-06	5.614475E-16	5.145360E-16	3.041863E-14	99.966273	3.458904
0.82	1.732020E+16	95.666667	1.234286E-06	5.814942E-16	5.208870E-16	3.116964E-14	99.965441	3.458903
0.83	1.732006E+16	96.833333	1.234286E-06	6.020114E-16	5.272380E-16	3.192980E-14	99.964598	3.458902
0.84	1.731991E+16	98.000000	1.234286E-06	6.230046E-16	5.335889E-16	3.269913E-14	99.963745	3.458901
0.85	1.731976E+16	99.166667	1.234286E-06	6.444792E-16	5.399398E-16	3.347760E-14	99.962881	3.458900
0.86	1.731961E+16	100.333333	1.234286E-06	6.664407E-16	5.462906E-16	3.426524E-14	99.962007	3.458900
0.87	1.731946E+16	101.500000	1.234286E-06	6.888946E-16	5.526414E-16	3.506202E-14	99.961123	3.458899
0.88	1.731930E+16	102.666667	1.234286E-06	7.118462E-16	5.589921E-16	3.586796E-14	99.960229	3.458898
0.89	1.731914E+16	103.833333	1.234286E-06	7.353011E-16	5.653428E-16	3.668306E-14	99.959324	3.458897
0.90	1.731899E+16	105.000000	1.234286E-06	7.592646E-16	5.716934E-16	3.750731E-14	99.958409	3.458896
0.91	1.731882E+16	106.166667	1.234286E-06	7.837423E-16	5.780440E-16	3.834072E-14	99.957484	3.458895
0.92	1.731866E+16	107.333333	1.234286E-06	8.087395E-16	5.843945E-16	3.918328E-14	99.956548	3.458895
0.93	1.731850E+16	108.500000	1.234286E-06	8.342617E-16	5.907450E-16	4.003499E-14	99.955601	3.458894
0.94	1.731833E+16	109.666667	1.234286E-06	8.603144E-16	5.970954E-16	4.089586E-14	99.954645	3.458893
0.95	1.731817E+16	110.833333	1.234286E-06	8.869030E-16	6.034457E-16	4.176588E-14	99.953678	3.458892
0.96	1.731800E+16	112.000000	1.234286E-06	9.140329E-16	6.097960E-16	4.264506E-14	99.952701	3.458891
0.97	1.731782E+16	113.166667	1.234286E-06	9.417096E-16	6.161463E-16	4.353339E-14	99.951713	3.458890
0.98	1.731765E+16	114.333333	1.234286E-06	9.699386E-16	6.224965E-16	4.443087E-14	99.950715	3.458889
0.99	1.731748E+16	115.500000	1.234286E-06	9.987252E-16	6.288466E-16	4.533751E-14	99.949706	3.458888
1.00	1.731730E+16	116.666667	1.234286E-06	1.028075E-15	6.351967E-16	4.625330E-14	99.948687	3.458887



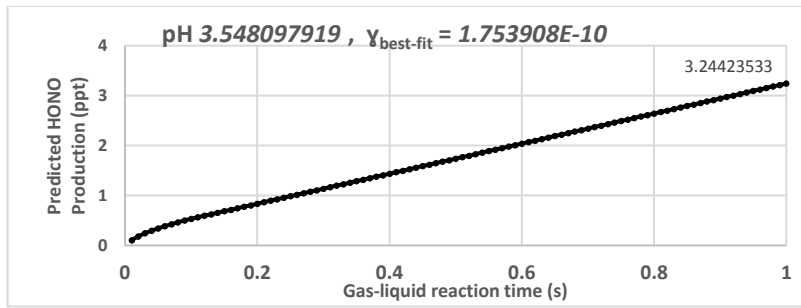
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732618E+16	1.166667	3.509922E-07	3.087696E-20	2.047246E-17	3.544935E-17	99.999940	3.538438
0.02	1.732616E+16	2.333333	4.963774E-07	1.362975E-19	4.094490E-17	1.063480E-16	99.999842	3.538438
0.03	1.732614E+16	3.500000	6.079349E-07	3.479088E-19	6.141733E-17	2.126959E-16	99.999706	3.538438
0.04	1.732611E+16	4.666667	7.019815E-07	6.918111E-19	8.188972E-17	3.544929E-16	99.999532	3.538438
0.05	1.732607E+16	5.833333	7.848375E-07	1.190732E-18	1.023621E-16	5.317389E-16	99.999320	3.538437
0.06	1.732603E+16	7.000000	8.597442E-07	1.865070E-18	1.228344E-16	7.444338E-16	99.999069	3.538437
0.07	1.732598E+16	8.166667	9.286272E-07	2.733491E-18	1.433067E-16	9.925775E-16	99.998781	3.538437
0.08	1.732592E+16	9.333333	9.927410E-07	3.813305E-18	1.637789E-16	1.276170E-15	99.998454	3.538436
0.09	1.732586E+16	10.500000	1.052957E-06	5.120728E-18	1.842510E-16	1.595210E-15	99.998089	3.538436
0.10	1.732579E+16	11.666667	1.109910E-06	6.671061E-18	2.047231E-16	1.949699E-15	99.997686	3.538436
0.11	1.732571E+16	12.833333	1.164078E-06	8.478835E-18	2.251951E-16	2.339636E-15	99.997244	3.538435
0.12	1.732563E+16	14.000000	1.215834E-06	1.055791E-17	2.456670E-16	2.765021E-15	99.996765	3.538435
0.13	1.732554E+16	15.166667	1.234286E-06	1.292439E-17	2.661388E-16	3.225853E-15	99.996247	3.538435
0.14	1.732544E+16	16.333333	1.234286E-06	1.559583E-17	2.866105E-16	3.722132E-15	99.995690	3.538434
0.15	1.732534E+16	17.500000	1.234286E-06	1.858978E-17	3.070821E-16	4.253858E-15	99.995096	3.538433
0.16	1.732523E+16	18.666667	1.234286E-06	2.192381E-17	3.275536E-16	4.821030E-15	99.994463	3.538433
0.17	1.732512E+16	19.833333	1.234286E-06	2.561548E-17	3.480250E-16	5.423649E-15	99.993792	3.538432
0.18	1.732499E+16	21.000000	1.234286E-06	2.968234E-17	3.684963E-16	6.061712E-15	99.993082	3.538431
0.19	1.732486E+16	22.166667	1.234286E-06	3.414196E-17	3.889675E-16	6.735222E-15	99.992334	3.538430
0.20	1.732473E+16	23.333333	1.234286E-06	3.901189E-17	4.094385E-16	7.444176E-15	99.991548	3.538429
0.21	1.732458E+16	24.500000	1.234286E-06	4.430970E-17	4.299093E-16	8.188574E-15	99.990723	3.538428
0.22	1.732443E+16	25.666667	1.234286E-06	5.005293E-17	4.503800E-16	8.968416E-15	99.989860	3.538428
0.23	1.732428E+16	26.833333	1.234286E-06	5.625915E-17	4.708506E-16	9.783701E-15	99.988958	3.538427
0.24	1.732412E+16	28.000000	1.234286E-06	6.294591E-17	4.913210E-16	1.063443E-14	99.988018	3.538426
0.25	1.732395E+16	29.166667	1.234286E-06	7.013078E-17	5.117912E-16	1.152060E-14	99.987040	3.538424
0.26	1.732377E+16	30.333333	1.234286E-06	7.783131E-17	5.322613E-16	1.244221E-14	99.986023	3.538423
0.27	1.732359E+16	31.500000	1.234286E-06	8.606505E-17	5.527312E-16	1.339927E-14	99.984967	3.538422
0.28	1.732340E+16	32.666667	1.234286E-06	9.484956E-17	5.732009E-16	1.439176E-14	99.983873	3.538421
0.29	1.732320E+16	33.833333	1.234286E-06	1.042024E-16	5.936704E-16	1.541969E-14	99.982740	3.538420
0.30	1.732300E+16	35.000000	1.234286E-06	1.141411E-16	6.141396E-16	1.648307E-14	99.981569	3.538418
0.31	1.732279E+16	36.166667	1.234286E-06	1.246833E-16	6.346087E-16	1.758188E-14	99.980359	3.538417
0.32	1.732257E+16	37.333333	1.234286E-06	1.358465E-16	6.550776E-16	1.871613E-14	99.979110	3.538416
0.33	1.732235E+16	38.500000	1.234286E-06	1.476482E-16	6.755463E-16	1.988581E-14	99.977823	3.538414
0.34	1.732212E+16	39.666667	1.234286E-06	1.601060E-16	6.960147E-16	2.109093E-14	99.976497	3.538413
0.35	1.732188E+16	40.833333	1.234286E-06	1.732375E-16	7.164829E-16	2.233149E-14	99.975133	3.538411
0.36	1.732164E+16	42.000000	1.234286E-06	1.870601E-16	7.369508E-16	2.360749E-14	99.973730	3.538410
0.37	1.732139E+16	43.166667	1.234286E-06	2.015916E-16	7.574185E-16	2.491891E-14	99.972288	3.538408
0.38	1.732113E+16	44.333333	1.234286E-06	2.168494E-16	7.778860E-16	2.626577E-14	99.970807	3.538406
0.39	1.732087E+16	45.500000	1.234286E-06	2.328510E-16	7.983531E-16	2.764806E-14	99.969288	3.538405
0.40	1.732060E+16	46.666667	1.234286E-06	2.496140E-16	8.188201E-16	2.906579E-14	99.967730	3.538403
0.41	1.732032E+16	47.833333	1.234286E-06	2.671561E-16	8.392867E-16	3.051894E-14	99.966133	3.538401
0.42	1.732004E+16	49.000000	1.234286E-06	2.854946E-16	8.597531E-16	3.200753E-14	99.964497	3.538400
0.43	1.731975E+16	50.166667	1.234286E-06	3.046472E-16	8.802191E-16	3.353154E-14	99.962823	3.538398
0.44	1.731945E+16	51.333333	1.234286E-06	3.246315E-16	9.006849E-16	3.509098E-14	99.961110	3.538396
0.45	1.731915E+16	52.500000	1.234286E-06	3.454649E-16	9.211504E-16	3.668584E-14	99.959358	3.538394

0.46	1.731884E+16	53.666667	1.234286E-06	3.671650E-16	9.416156E-16	3.831614E-14	99.957567	3.538392
0.47	1.731852E+16	54.833333	1.234286E-06	3.897494E-16	9.620804E-16	3.998185E-14	99.955737	3.538390
0.48	1.731820E+16	56.000000	1.234286E-06	4.132357E-16	9.825450E-16	4.168299E-14	99.953868	3.538388
0.49	1.731787E+16	57.166667	1.234286E-06	4.376413E-16	1.003009E-15	4.341956E-14	99.951960	3.538386
0.50	1.731753E+16	58.333333	1.234286E-06	4.629838E-16	1.023473E-15	4.519154E-14	99.950014	3.538383
0.51	1.731719E+16	59.500000	1.234286E-06	4.892807E-16	1.043937E-15	4.699895E-14	99.948028	3.538381
0.52	1.731684E+16	60.666667	1.234286E-06	5.165497E-16	1.064400E-15	4.884177E-14	99.946003	3.538379
0.53	1.731648E+16	61.833333	1.234286E-06	5.448082E-16	1.084863E-15	5.072001E-14	99.943940	3.538377
0.54	1.731611E+16	63.000000	1.234286E-06	5.740738E-16	1.105325E-15	5.263367E-14	99.941837	3.538374
0.55	1.731574E+16	64.166667	1.234286E-06	6.043640E-16	1.125787E-15	5.458274E-14	99.939696	3.538372
0.56	1.731536E+16	65.333333	1.234286E-06	6.356964E-16	1.146249E-15	5.656723E-14	99.937515	3.538370
0.57	1.731498E+16	66.500000	1.234286E-06	6.680886E-16	1.166710E-15	5.858713E-14	99.935296	3.538367
0.58	1.731459E+16	67.666667	1.234286E-06	7.015580E-16	1.187171E-15	6.064245E-14	99.933037	3.538365
0.59	1.731419E+16	68.833333	1.234286E-06	7.361222E-16	1.207632E-15	6.273317E-14	99.930739	3.538362
0.60	1.731379E+16	70.000000	1.234286E-06	7.717987E-16	1.228092E-15	6.485931E-14	99.928402	3.538360
0.61	1.731337E+16	71.166667	1.234286E-06	8.086051E-16	1.248552E-15	6.702085E-14	99.926026	3.538357
0.62	1.731296E+16	72.333333	1.234286E-06	8.465590E-16	1.269011E-15	6.921779E-14	99.923611	3.538354
0.63	1.731253E+16	73.500000	1.234286E-06	8.856778E-16	1.289470E-15	7.145015E-14	99.921156	3.538352
0.64	1.731210E+16	74.666667	1.234286E-06	9.259791E-16	1.309928E-15	7.371790E-14	99.918663	3.538349
0.65	1.731166E+16	75.833333	1.234286E-06	9.674805E-16	1.330386E-15	7.602106E-14	99.916130	3.538346
0.66	1.731121E+16	77.000000	1.234286E-06	1.010199E-15	1.350844E-15	7.835962E-14	99.913558	3.538343
0.67	1.731076E+16	78.166667	1.234286E-06	1.054153E-15	1.371301E-15	8.073358E-14	99.910947	3.538340
0.68	1.731030E+16	79.333333	1.234286E-06	1.099360E-15	1.391758E-15	8.314294E-14	99.908296	3.538337
0.69	1.730984E+16	80.500000	1.234286E-06	1.145837E-15	1.412214E-15	8.558769E-14	99.905607	3.538334
0.70	1.730936E+16	81.666667	1.234286E-06	1.193601E-15	1.432670E-15	8.806784E-14	99.902878	3.538331
0.71	1.730888E+16	82.833333	1.234286E-06	1.242671E-15	1.453125E-15	9.058338E-14	99.900109	3.538328
0.72	1.730840E+16	84.000000	1.234286E-06	1.293064E-15	1.473580E-15	9.313431E-14	99.897302	3.538325
0.73	1.730790E+16	85.166667	1.234286E-06	1.344797E-15	1.494034E-15	9.572063E-14	99.894455	3.538322
0.74	1.730740E+16	86.333333	1.234286E-06	1.397887E-15	1.514488E-15	9.834234E-14	99.891569	3.538319
0.75	1.730690E+16	87.500000	1.234286E-06	1.452353E-15	1.534942E-15	1.009994E-13	99.888643	3.538316
0.76	1.730638E+16	88.666667	1.234286E-06	1.508212E-15	1.555394E-15	1.036919E-13	99.885678	3.538312
0.77	1.730586E+16	89.833333	1.234286E-06	1.565482E-15	1.575847E-15	1.064198E-13	99.882674	3.538309
0.78	1.730534E+16	91.000000	1.234286E-06	1.624179E-15	1.596299E-15	1.091830E-13	99.879630	3.538306
0.79	1.730480E+16	92.166667	1.234286E-06	1.684322E-15	1.616750E-15	1.119817E-13	99.876546	3.538302
0.80	1.730426E+16	93.333333	1.234286E-06	1.745927E-15	1.637201E-15	1.148157E-13	99.873424	3.538299
0.81	1.730371E+16	94.500000	1.234286E-06	1.809014E-15	1.657651E-15	1.176851E-13	99.870261	3.538295
0.82	1.730316E+16	95.666667	1.234286E-06	1.873598E-15	1.678100E-15	1.205898E-13	99.867060	3.538292
0.83	1.730260E+16	96.833333	1.234286E-06	1.939698E-15	1.698549E-15	1.235299E-13	99.863819	3.538288
0.84	1.730203E+16	98.000000	1.234286E-06	2.007331E-15	1.718998E-15	1.265054E-13	99.860538	3.538285
0.85	1.730145E+16	99.166667	1.234286E-06	2.076514E-15	1.739446E-15	1.295163E-13	99.857218	3.538281
0.86	1.730087E+16	100.333333	1.234286E-06	2.147266E-15	1.759893E-15	1.325625E-13	99.853858	3.538277
0.87	1.730028E+16	101.500000	1.234286E-06	2.219603E-15	1.780340E-15	1.356441E-13	99.850458	3.538274
0.88	1.729969E+16	102.666667	1.234286E-06	2.293544E-15	1.800786E-15	1.387611E-13	99.847019	3.538270
0.89	1.729908E+16	103.833333	1.234286E-06	2.369105E-15	1.821232E-15	1.419134E-13	99.843541	3.538266
0.90	1.729847E+16	105.000000	1.234286E-06	2.446304E-15	1.841677E-15	1.451011E-13	99.840023	3.538262
0.91	1.729786E+16	106.166667	1.234286E-06	2.525159E-15	1.862121E-15	1.483242E-13	99.836465	3.538258
0.92	1.729723E+16	107.333333	1.234286E-06	2.605687E-15	1.882565E-15	1.515826E-13	99.832867	3.538254
0.93	1.729660E+16	108.500000	1.234286E-06	2.687906E-15	1.903008E-15	1.548763E-13	99.829230	3.538250
0.94	1.729597E+16	109.666667	1.234286E-06	2.771833E-15	1.923450E-15	1.582054E-13	99.825553	3.538246
0.95	1.729532E+16	110.833333	1.234286E-06	2.857486E-15	1.943892E-15	1.615699E-13	99.821837	3.538242
0.96	1.729467E+16	112.000000	1.234286E-06	2.944882E-15	1.964333E-15	1.649697E-13	99.818081	3.538238
0.97	1.729401E+16	113.166667	1.234286E-06	3.034039E-15	1.984774E-15	1.684048E-13	99.814285	3.538234
0.98	1.729335E+16	114.333333	1.234286E-06	3.124974E-15	2.005214E-15	1.718753E-13	99.810449	3.538230
0.99	1.729268E+16	115.500000	1.234286E-06	3.217705E-15	2.025653E-15	1.753811E-13	99.806573	3.538225
1.00	1.729200E+16	116.666667	1.234286E-06	3.312249E-15	2.046092E-15	1.789223E-13	99.802658	3.538221



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732619E+16	1.166667	3.509924E-07	2.827203E-21	1.874531E-18	3.280023E-18	99.999994	3.542984
0.02	1.732619E+16	2.333333	4.963781E-07	1.247988E-20	3.749062E-18	9.840068E-18	99.999985	3.542984
0.03	1.732619E+16	3.500000	6.079365E-07	3.185575E-20	5.623593E-18	1.968013E-17	99.999973	3.542984
0.04	1.732618E+16	4.666667	7.019845E-07	6.334464E-20	7.498124E-18	3.280022E-17	99.999957	3.542984
0.05	1.732618E+16	5.833333	7.848423E-07	1.090276E-19	9.372655E-18	4.920033E-17	99.999937	3.542984
0.06	1.732618E+16	7.000000	8.597515E-07	1.707723E-19	1.124718E-17	6.888046E-17	99.999914	3.542984
0.07	1.732617E+16	8.166667	9.286375E-07	2.502879E-19	1.312171E-17	9.184060E-17	99.999887	3.542984
0.08	1.732617E+16	9.333333	9.927550E-07	3.491594E-19	1.499624E-17	1.180808E-16	99.999857	3.542984
0.09	1.732616E+16	10.500000	1.052975E-06	4.688715E-19	1.687077E-17	1.476009E-16	99.999823	3.542984
0.10	1.732615E+16	11.666667	1.109933E-06	6.108253E-19	1.874530E-17	1.804011E-16	99.999786	3.542984
0.11	1.732615E+16	12.833333	1.164107E-06	7.763512E-19	2.061983E-17	2.164813E-16	99.999745	3.542984
0.12	1.732614E+16	14.000000	1.215870E-06	9.667187E-19	2.249435E-17	2.558415E-16	99.999701	3.542984
0.13	1.732613E+16	15.166667	1.234286E-06	1.183402E-18	2.436888E-17	2.984817E-16	99.999653	3.542984
0.14	1.732612E+16	16.333333	1.234286E-06	1.428008E-18	2.624341E-17	3.444020E-16	99.999602	3.542984
0.15	1.732611E+16	17.500000	1.234286E-06	1.702146E-18	2.811793E-17	3.936022E-16	99.999547	3.542984
0.16	1.732610E+16	18.666667	1.234286E-06	2.007423E-18	2.999245E-17	4.460824E-16	99.999488	3.542984
0.17	1.732609E+16	19.833333	1.234286E-06	2.345447E-18	3.186697E-17	5.018426E-16	99.999426	3.542984
0.18	1.732608E+16	21.000000	1.234286E-06	2.717827E-18	3.374150E-17	5.608828E-16	99.999360	3.542983
0.19	1.732607E+16	22.166667	1.234286E-06	3.126169E-18	3.561602E-17	6.232030E-16	99.999291	3.542983
0.20	1.732606E+16	23.333333	1.234286E-06	3.572083E-18	3.749054E-17	6.888032E-16	99.999218	3.542983
0.21	1.732604E+16	24.500000	1.234286E-06	4.057175E-18	3.936505E-17	7.576833E-16	99.999142	3.542983
0.22	1.732603E+16	25.666667	1.234286E-06	4.583054E-18	4.123957E-17	8.298435E-16	99.999062	3.542983
0.23	1.732601E+16	26.833333	1.234286E-06	5.151328E-18	4.311408E-17	9.052836E-16	99.998979	3.542983
0.24	1.732600E+16	28.000000	1.234286E-06	5.763605E-18	4.498860E-17	9.840036E-16	99.998892	3.542983
0.25	1.732598E+16	29.166667	1.234286E-06	6.421492E-18	4.686311E-17	1.066004E-15	99.998801	3.542983
0.26	1.732597E+16	30.333333	1.234286E-06	7.126597E-18	4.873762E-17	1.151284E-15	99.998707	3.542983
0.27	1.732595E+16	31.500000	1.234286E-06	7.880529E-18	5.061213E-17	1.239844E-15	99.998610	3.542983
0.28	1.732593E+16	32.666667	1.234286E-06	8.684895E-18	5.248664E-17	1.331683E-15	99.998508	3.542983
0.29	1.732591E+16	33.833333	1.234286E-06	9.541303E-18	5.436115E-17	1.426803E-15	99.998404	3.542982
0.30	1.732590E+16	35.000000	1.234286E-06	1.045136E-17	5.623565E-17	1.525203E-15	99.998295	3.542982
0.31	1.732588E+16	36.166667	1.234286E-06	1.141668E-17	5.811015E-17	1.626883E-15	99.998183	3.542982
0.32	1.732586E+16	37.333333	1.234286E-06	1.243886E-17	5.998465E-17	1.731842E-15	99.998068	3.542982
0.33	1.732584E+16	38.500000	1.234286E-06	1.351951E-17	6.185915E-17	1.840082E-15	99.997949	3.542982
0.34	1.732581E+16	39.666667	1.234286E-06	1.466025E-17	6.373365E-17	1.951601E-15	99.997826	3.542982
0.35	1.732579E+16	40.833333	1.234286E-06	1.586268E-17	6.560815E-17	2.066401E-15	99.997700	3.542982
0.36	1.732577E+16	42.000000	1.234286E-06	1.712840E-17	6.748264E-17	2.184480E-15	99.997570	3.542982
0.37	1.732575E+16	43.166667	1.234286E-06	1.845903E-17	6.935713E-17	2.305839E-15	99.997437	3.542981
0.38	1.732572E+16	44.333333	1.234286E-06	1.985617E-17	7.123162E-17	2.430478E-15	99.997300	3.542981
0.39	1.732570E+16	45.500000	1.234286E-06	2.132144E-17	7.310611E-17	2.558397E-15	99.997159	3.542981
0.40	1.732567E+16	46.666667	1.234286E-06	2.285643E-17	7.498059E-17	2.689596E-15	99.997015	3.542981
0.41	1.732565E+16	47.833333	1.234286E-06	2.446276E-17	7.685507E-17	2.824074E-15	99.996867	3.542981
0.42	1.732562E+16	49.000000	1.234286E-06	2.614203E-17	7.872955E-17	2.961833E-15	99.996716	3.542981
0.43	1.732560E+16	50.166667	1.234286E-06	2.789585E-17	8.060403E-17	3.102871E-15	99.996561	3.542980
0.44	1.732557E+16	51.333333	1.234286E-06	2.972584E-17	8.247850E-17	3.247189E-15	99.996403	3.542980
0.45	1.732554E+16	52.500000	1.234286E-06	3.163359E-17	8.435298E-17	3.394787E-15	99.996240	3.542980

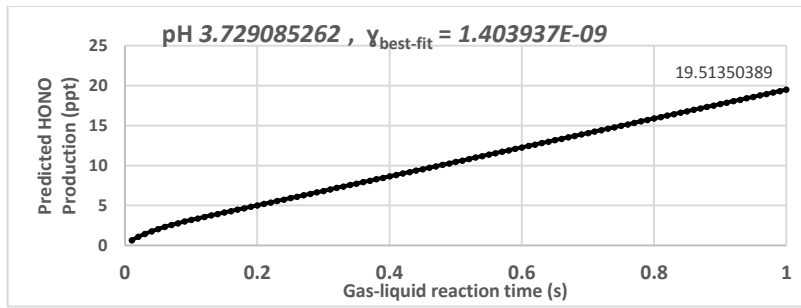
0.46	1.732551E+16	53.666667	1.234286E-06	3.362072E-17	8.622745E-17	3.545665E-15	99.996075	3.542980
0.47	1.732548E+16	54.833333	1.234286E-06	3.568884E-17	8.810191E-17	3.699823E-15	99.995905	3.542980
0.48	1.732545E+16	56.000000	1.234286E-06	3.783954E-17	8.997638E-17	3.857260E-15	99.995732	3.542979
0.49	1.732542E+16	57.166667	1.234286E-06	4.007444E-17	9.185084E-17	4.017977E-15	99.995556	3.542979
0.50	1.732539E+16	58.333333	1.234286E-06	4.239515E-17	9.372530E-17	4.181974E-15	99.995376	3.542979
0.51	1.732536E+16	59.500000	1.234286E-06	4.480328E-17	9.559975E-17	4.349251E-15	99.995192	3.542979
0.52	1.732533E+16	60.666667	1.234286E-06	4.730043E-17	9.747421E-17	4.519808E-15	99.995005	3.542979
0.53	1.732529E+16	61.833333	1.234286E-06	4.988821E-17	9.934866E-17	4.693644E-15	99.994814	3.542978
0.54	1.732526E+16	63.000000	1.234286E-06	5.256822E-17	1.012231E-16	4.870760E-15	99.994619	3.542978
0.55	1.732522E+16	64.166667	1.234286E-06	5.534209E-17	1.030975E-16	5.051156E-15	99.994421	3.542978
0.56	1.732519E+16	65.333333	1.234286E-06	5.821141E-17	1.049720E-16	5.234831E-15	99.994219	3.542978
0.57	1.732515E+16	66.500000	1.234286E-06	6.117779E-17	1.068464E-16	5.421786E-15	99.994014	3.542978
0.58	1.732512E+16	67.666667	1.234286E-06	6.424283E-17	1.087209E-16	5.612021E-15	99.993805	3.542977
0.59	1.732508E+16	68.833333	1.234286E-06	6.740816E-17	1.105953E-16	5.805536E-15	99.993592	3.542977
0.60	1.732504E+16	70.000000	1.234286E-06	7.067537E-17	1.124697E-16	6.002330E-15	99.993376	3.542977
0.61	1.732501E+16	71.166667	1.234286E-06	7.404607E-17	1.143441E-16	6.202404E-15	99.993156	3.542977
0.62	1.732497E+16	72.333333	1.234286E-06	7.752188E-17	1.162186E-16	6.405758E-15	99.992933	3.542976
0.63	1.732493E+16	73.500000	1.234286E-06	8.110439E-17	1.180930E-16	6.612391E-15	99.992706	3.542976
0.64	1.732489E+16	74.666667	1.234286E-06	8.479522E-17	1.199674E-16	6.822304E-15	99.992475	3.542976
0.65	1.732485E+16	75.833333	1.234286E-06	8.859597E-17	1.218418E-16	7.035496E-15	99.992240	3.542976
0.66	1.732481E+16	77.000000	1.234286E-06	9.250826E-17	1.237162E-16	7.251968E-15	99.992002	3.542975
0.67	1.732476E+16	78.166667	1.234286E-06	9.653368E-17	1.255906E-16	7.471720E-15	99.991761	3.542975
0.68	1.732472E+16	79.333333	1.234286E-06	1.006738E-16	1.274650E-16	7.694751E-15	99.991516	3.542975
0.69	1.732468E+16	80.500000	1.234286E-06	1.049304E-16	1.293394E-16	7.921062E-15	99.991267	3.542974
0.70	1.732463E+16	81.666667	1.234286E-06	1.093049E-16	1.312138E-16	8.150652E-15	99.991014	3.542974
0.71	1.732459E+16	82.833333	1.234286E-06	1.137989E-16	1.330882E-16	8.383522E-15	99.990758	3.542974
0.72	1.732454E+16	84.000000	1.234286E-06	1.184142E-16	1.349626E-16	8.619672E-15	99.990498	3.542974
0.73	1.732450E+16	85.166667	1.234286E-06	1.231522E-16	1.368369E-16	8.859101E-15	99.990235	3.542973
0.74	1.732445E+16	86.333333	1.234286E-06	1.280146E-16	1.387113E-16	9.101809E-15	99.989967	3.542973
0.75	1.732441E+16	87.500000	1.234286E-06	1.330030E-16	1.405857E-16	9.347797E-15	99.989697	3.542973
0.76	1.732436E+16	88.666667	1.234286E-06	1.381190E-16	1.424600E-16	9.597064E-15	99.989422	3.542972
0.77	1.732431E+16	89.833333	1.234286E-06	1.433643E-16	1.443344E-16	9.849611E-15	99.989144	3.542972
0.78	1.732426E+16	91.000000	1.234286E-06	1.487403E-16	1.462088E-16	1.010544E-14	99.988862	3.542972
0.79	1.732421E+16	92.166667	1.234286E-06	1.542488E-16	1.480831E-16	1.036454E-14	99.988577	3.542971
0.80	1.732416E+16	93.333333	1.234286E-06	1.598913E-16	1.499575E-16	1.062693E-14	99.988288	3.542971
0.81	1.732411E+16	94.500000	1.234286E-06	1.656695E-16	1.518318E-16	1.089259E-14	99.987995	3.542971
0.82	1.732406E+16	95.666667	1.234286E-06	1.715850E-16	1.537061E-16	1.116154E-14	99.987699	3.542970
0.83	1.732401E+16	96.833333	1.234286E-06	1.776392E-16	1.555805E-16	1.143376E-14	99.987399	3.542970
0.84	1.732396E+16	98.000000	1.234286E-06	1.838340E-16	1.574548E-16	1.170926E-14	99.987095	3.542970
0.85	1.732390E+16	99.166667	1.234286E-06	1.901709E-16	1.593291E-16	1.198804E-14	99.986788	3.542969
0.86	1.732385E+16	100.333333	1.234286E-06	1.966514E-16	1.612035E-16	1.227011E-14	99.986477	3.542969
0.87	1.732379E+16	101.500000	1.234286E-06	2.032772E-16	1.630778E-16	1.255545E-14	99.986162	3.542969
0.88	1.732374E+16	102.666667	1.234286E-06	2.100499E-16	1.649521E-16	1.284407E-14	99.985844	3.542968
0.89	1.732368E+16	103.833333	1.234286E-06	2.169711E-16	1.668264E-16	1.313597E-14	99.985522	3.542968
0.90	1.732363E+16	105.000000	1.234286E-06	2.240425E-16	1.687007E-16	1.343114E-14	99.985196	3.542968
0.91	1.732357E+16	106.166667	1.234286E-06	2.312655E-16	1.705750E-16	1.372960E-14	99.984867	3.542967
0.92	1.732351E+16	107.333333	1.234286E-06	2.386419E-16	1.724493E-16	1.403134E-14	99.984534	3.542967
0.93	1.732345E+16	108.500000	1.234286E-06	2.461733E-16	1.743235E-16	1.433635E-14	99.984197	3.542967
0.94	1.732339E+16	109.666667	1.234286E-06	2.538611E-16	1.761978E-16	1.464465E-14	99.983857	3.542966
0.95	1.732333E+16	110.833333	1.234286E-06	2.617072E-16	1.780721E-16	1.495622E-14	99.983513	3.542966
0.96	1.732327E+16	112.000000	1.234286E-06	2.697129E-16	1.799464E-16	1.527108E-14	99.983165	3.542965
0.97	1.732321E+16	113.166667	1.234286E-06	2.778801E-16	1.818206E-16	1.558921E-14	99.982814	3.542965
0.98	1.732315E+16	114.333333	1.234286E-06	2.862102E-16	1.836949E-16	1.591062E-14	99.982458	3.542965
0.99	1.732309E+16	115.500000	1.234286E-06	2.947049E-16	1.855691E-16	1.623531E-14	99.982100	3.542964
1.00	1.732303E+16	116.666667	1.234286E-06	3.033658E-16	1.874434E-16	1.656328E-14	99.981737	3.542964



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732619E+16	1.166667	3.509924E-07	2.747033E-21	1.821376E-18	3.224761E-18	99.999995	3.548098
0.02	1.732619E+16	2.333333	4.963781E-07	1.212599E-20	3.642752E-18	9.674282E-18	99.999986	3.548098
0.03	1.732619E+16	3.500000	6.079365E-07	3.095243E-20	5.464128E-18	1.934856E-17	99.999973	3.548098
0.04	1.732618E+16	4.666667	7.019845E-07	6.154841E-20	7.285503E-18	3.224760E-17	99.999958	3.548098
0.05	1.732618E+16	5.833333	7.848423E-07	1.059359E-19	9.106879E-18	4.837140E-17	99.999938	3.548098
0.06	1.732618E+16	7.000000	8.597515E-07	1.659298E-19	1.092825E-17	6.771996E-17	99.999916	3.548098
0.07	1.732617E+16	8.166667	9.286375E-07	2.431906E-19	1.274963E-17	9.029327E-17	99.999889	3.548098
0.08	1.732617E+16	9.333333	9.927550E-07	3.392585E-19	1.457100E-17	1.160913E-16	99.999860	3.548098
0.09	1.732616E+16	10.500000	1.052975E-06	4.555759E-19	1.639238E-17	1.451142E-16	99.999827	3.548098
0.10	1.732615E+16	11.666667	1.109933E-06	5.935044E-19	1.821375E-17	1.773617E-16	99.999790	3.548098
0.11	1.732615E+16	12.833333	1.164107E-06	7.543366E-19	2.003512E-17	2.128340E-16	99.999750	3.548098
0.12	1.732614E+16	14.000000	1.215870E-06	9.393059E-19	2.185649E-17	2.515311E-16	99.999706	3.548098
0.13	1.732613E+16	15.166667	1.234286E-06	1.149845E-18	2.367786E-17	2.934529E-16	99.999659	3.548098
0.14	1.732612E+16	16.333333	1.234286E-06	1.387515E-18	2.549923E-17	3.385995E-16	99.999609	3.548097
0.15	1.732611E+16	17.500000	1.234286E-06	1.653879E-18	2.732060E-17	3.869708E-16	99.999555	3.548097
0.16	1.732610E+16	18.666667	1.234286E-06	1.950499E-18	2.914197E-17	4.385668E-16	99.999497	3.548097
0.17	1.732609E+16	19.833333	1.234286E-06	2.278939E-18	3.096334E-17	4.933876E-16	99.999436	3.548097
0.18	1.732608E+16	21.000000	1.234286E-06	2.640759E-18	3.278471E-17	5.514331E-16	99.999372	3.548097
0.19	1.732607E+16	22.166667	1.234286E-06	3.037522E-18	3.460607E-17	6.127033E-16	99.999304	3.548097
0.20	1.732606E+16	23.333333	1.234286E-06	3.470791E-18	3.642744E-17	6.771982E-16	99.999232	3.548097
0.21	1.732605E+16	24.500000	1.234286E-06	3.942128E-18	3.824880E-17	7.449179E-16	99.999157	3.548097
0.22	1.732603E+16	25.666667	1.234286E-06	4.453095E-18	4.007016E-17	8.158623E-16	99.999079	3.548097
0.23	1.732602E+16	26.833333	1.234286E-06	5.005254E-18	4.189152E-17	8.900314E-16	99.998997	3.548097
0.24	1.732600E+16	28.000000	1.234286E-06	5.600169E-18	4.371288E-17	9.674252E-16	99.998911	3.548097
0.25	1.732599E+16	29.166667	1.234286E-06	6.239401E-18	4.553424E-17	1.048044E-15	99.998822	3.548097
0.26	1.732597E+16	30.333333	1.234286E-06	6.924512E-18	4.735560E-17	1.131887E-15	99.998730	3.548097
0.27	1.732595E+16	31.500000	1.234286E-06	7.657065E-18	4.917695E-17	1.218955E-15	99.998634	3.548096
0.28	1.732594E+16	32.666667	1.234286E-06	8.438622E-18	5.099830E-17	1.309247E-15	99.998534	3.548096
0.29	1.732592E+16	33.833333	1.234286E-06	9.270745E-18	5.281966E-17	1.402765E-15	99.998431	3.548096
0.30	1.732590E+16	35.000000	1.234286E-06	1.015500E-17	5.464101E-17	1.499506E-15	99.998325	3.548096
0.31	1.732588E+16	36.166667	1.234286E-06	1.109294E-17	5.646236E-17	1.599473E-15	99.998215	3.548096
0.32	1.732586E+16	37.333333	1.234286E-06	1.208614E-17	5.828370E-17	1.702664E-15	99.998101	3.548096
0.33	1.732584E+16	38.500000	1.234286E-06	1.313615E-17	6.010505E-17	1.809080E-15	99.997984	3.548096
0.34	1.732582E+16	39.666667	1.234286E-06	1.424454E-17	6.192639E-17	1.918721E-15	99.997864	3.548096
0.35	1.732580E+16	40.833333	1.234286E-06	1.541287E-17	6.374773E-17	2.031586E-15	99.997740	3.548095
0.36	1.732578E+16	42.000000	1.234286E-06	1.664270E-17	6.556907E-17	2.147676E-15	99.997612	3.548095
0.37	1.732575E+16	43.166667	1.234286E-06	1.793560E-17	6.739041E-17	2.266990E-15	99.997481	3.548095
0.38	1.732573E+16	44.333333	1.234286E-06	1.929312E-17	6.921175E-17	2.389530E-15	99.997346	3.548095
0.39	1.732571E+16	45.500000	1.234286E-06	2.071684E-17	7.103308E-17	2.515293E-15	99.997208	3.548095
0.40	1.732568E+16	46.666667	1.234286E-06	2.220830E-17	7.285441E-17	2.644282E-15	99.997066	3.548095
0.41	1.732566E+16	47.833333	1.234286E-06	2.376908E-17	7.467574E-17	2.776495E-15	99.996921	3.548094
0.42	1.732563E+16	49.000000	1.234286E-06	2.540073E-17	7.649707E-17	2.911932E-15	99.996773	3.548094
0.43	1.732561E+16	50.166667	1.234286E-06	2.710483E-17	7.831839E-17	3.050594E-15	99.996620	3.548094
0.44	1.732558E+16	51.333333	1.234286E-06	2.888292E-17	8.013972E-17	3.192481E-15	99.996464	3.548094
0.45	1.732555E+16	52.500000	1.234286E-06	3.073658E-17	8.196104E-17	3.337592E-15	99.996305	3.548094

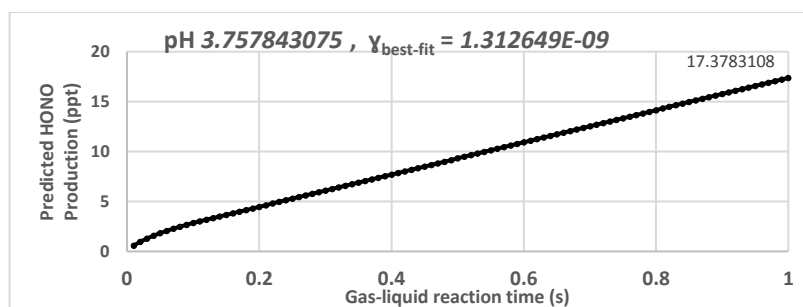


0.46	1.732552E+16	53.666667	1.234286E-06	3.266736E-17	8.378235E-17	3.485928E-15	99.996142	3.548094
0.47	1.732549E+16	54.833333	1.234286E-06	3.467683E-17	8.560367E-17	3.637489E-15	99.995976	3.548093
0.48	1.732546E+16	56.000000	1.234286E-06	3.676655E-17	8.742498E-17	3.792274E-15	99.995806	3.548093
0.49	1.732543E+16	57.166667	1.234286E-06	3.893808E-17	8.924629E-17	3.950283E-15	99.995632	3.548093
0.50	1.732540E+16	58.333333	1.234286E-06	4.119298E-17	9.106760E-17	4.111517E-15	99.995455	3.548093
0.51	1.732537E+16	59.500000	1.234286E-06	4.353282E-17	9.288890E-17	4.275976E-15	99.995275	3.548093
0.52	1.732534E+16	60.666667	1.234286E-06	4.595916E-17	9.471020E-17	4.443659E-15	99.995091	3.548092
0.53	1.732531E+16	61.833333	1.234286E-06	4.847356E-17	9.653150E-17	4.614566E-15	99.994903	3.548092
0.54	1.732527E+16	63.000000	1.234286E-06	5.107758E-17	9.835280E-17	4.788698E-15	99.994712	3.548092
0.55	1.732524E+16	64.166667	1.234286E-06	5.377279E-17	1.001741E-16	4.966055E-15	99.994517	3.548092
0.56	1.732521E+16	65.333333	1.234286E-06	5.656074E-17	1.019954E-16	5.146636E-15	99.994319	3.548092
0.57	1.732517E+16	66.500000	1.234286E-06	5.944301E-17	1.038167E-16	5.330441E-15	99.994117	3.548091
0.58	1.732514E+16	67.666667	1.234286E-06	6.242114E-17	1.056380E-16	5.517471E-15	99.993911	3.548091
0.59	1.732510E+16	68.833333	1.234286E-06	6.549671E-17	1.074592E-16	5.707725E-15	99.993703	3.548091
0.60	1.732506E+16	70.000000	1.234286E-06	6.867128E-17	1.092805E-16	5.901204E-15	99.993490	3.548091
0.61	1.732503E+16	71.166667	1.234286E-06	7.194640E-17	1.111018E-16	6.097907E-15	99.993274	3.548090
0.62	1.732499E+16	72.333333	1.234286E-06	7.532364E-17	1.129231E-16	6.297835E-15	99.993054	3.548090
0.63	1.732495E+16	73.500000	1.234286E-06	7.880457E-17	1.147443E-16	6.500987E-15	99.992831	3.548090
0.64	1.732491E+16	74.666667	1.234286E-06	8.239074E-17	1.165656E-16	6.707363E-15	99.992604	3.548090
0.65	1.732487E+16	75.833333	1.234286E-06	8.608372E-17	1.183868E-16	6.916964E-15	99.992374	3.548089
0.66	1.732483E+16	77.000000	1.234286E-06	8.988506E-17	1.202081E-16	7.129789E-15	99.992140	3.548089
0.67	1.732479E+16	78.166667	1.234286E-06	9.379634E-17	1.220294E-16	7.345838E-15	99.991902	3.548089
0.68	1.732475E+16	79.333333	1.234286E-06	9.781911E-17	1.238506E-16	7.565112E-15	99.991661	3.548089
0.69	1.732470E+16	80.500000	1.234286E-06	1.019549E-16	1.256718E-16	7.787610E-15	99.991417	3.548088
0.70	1.732466E+16	81.666667	1.234286E-06	1.062054E-16	1.274931E-16	8.013333E-15	99.991168	3.548088
0.71	1.732462E+16	82.833333	1.234286E-06	1.105720E-16	1.293143E-16	8.242279E-15	99.990917	3.548088
0.72	1.732457E+16	84.000000	1.234286E-06	1.150564E-16	1.311356E-16	8.474450E-15	99.990661	3.548087
0.73	1.732453E+16	85.166667	1.234286E-06	1.196600E-16	1.329568E-16	8.709845E-15	99.990402	3.548087
0.74	1.732448E+16	86.333333	1.234286E-06	1.243846E-16	1.347780E-16	8.948465E-15	99.990140	3.548087
0.75	1.732444E+16	87.500000	1.234286E-06	1.292315E-16	1.365992E-16	9.190309E-15	99.989874	3.548086
0.76	1.732439E+16	88.666667	1.234286E-06	1.342025E-16	1.384205E-16	9.435377E-15	99.989604	3.548086
0.77	1.732434E+16	89.833333	1.234286E-06	1.392990E-16	1.402417E-16	9.683669E-15	99.989331	3.548086
0.78	1.732429E+16	91.000000	1.234286E-06	1.445226E-16	1.420629E-16	9.935185E-15	99.989054	3.548086
0.79	1.732425E+16	92.166667	1.234286E-06	1.498749E-16	1.438841E-16	1.018993E-14	99.988773	3.548085
0.80	1.732420E+16	93.333333	1.234286E-06	1.553574E-16	1.457053E-16	1.044789E-14	99.988489	3.548085
0.81	1.732415E+16	94.500000	1.234286E-06	1.609718E-16	1.475265E-16	1.070908E-14	99.988202	3.548085
0.82	1.732410E+16	95.666667	1.234286E-06	1.667195E-16	1.493477E-16	1.097349E-14	99.987910	3.548084
0.83	1.732405E+16	96.833333	1.234286E-06	1.726021E-16	1.511689E-16	1.124113E-14	99.987615	3.548084
0.84	1.732399E+16	98.000000	1.234286E-06	1.786212E-16	1.529901E-16	1.151199E-14	99.987317	3.548084
0.85	1.732394E+16	99.166667	1.234286E-06	1.847783E-16	1.548112E-16	1.178608E-14	99.987015	3.548083
0.86	1.732389E+16	100.333333	1.234286E-06	1.910751E-16	1.566324E-16	1.206339E-14	99.986709	3.548083
0.87	1.732383E+16	101.500000	1.234286E-06	1.975130E-16	1.584536E-16	1.234392E-14	99.986400	3.548083
0.88	1.732378E+16	102.666667	1.234286E-06	2.040937E-16	1.602747E-16	1.262768E-14	99.986087	3.548082
0.89	1.732373E+16	103.833333	1.234286E-06	2.108187E-16	1.620959E-16	1.291466E-14	99.985771	3.548082
0.90	1.732367E+16	105.000000	1.234286E-06	2.176895E-16	1.639171E-16	1.320486E-14	99.985451	3.548082
0.91	1.732361E+16	106.166667	1.234286E-06	2.247078E-16	1.657382E-16	1.349829E-14	99.985127	3.548081
0.92	1.732356E+16	107.333333	1.234286E-06	2.318750E-16	1.675594E-16	1.379495E-14	99.984800	3.548081
0.93	1.732350E+16	108.500000	1.234286E-06	2.391928E-16	1.693805E-16	1.409482E-14	99.984469	3.548080
0.94	1.732344E+16	109.666667	1.234286E-06	2.466626E-16	1.712016E-16	1.439792E-14	99.984134	3.548080
0.95	1.732338E+16	110.833333	1.234286E-06	2.542862E-16	1.730228E-16	1.470425E-14	99.983796	3.548080
0.96	1.732332E+16	112.000000	1.234286E-06	2.620649E-16	1.748439E-16	1.501380E-14	99.983454	3.548079
0.97	1.732326E+16	113.166667	1.234286E-06	2.700005E-16	1.766650E-16	1.532657E-14	99.983109	3.548079
0.98	1.732320E+16	114.333333	1.234286E-06	2.780944E-16	1.784861E-16	1.564257E-14	99.982760	3.548078
0.99	1.732314E+16	115.500000	1.234286E-06	2.863483E-16	1.803072E-16	1.596179E-14	99.982407	3.548078
1.00	1.732308E+16	116.666667	1.234286E-06	2.947636E-16	1.821283E-16	1.628423E-14	99.982051	3.548078



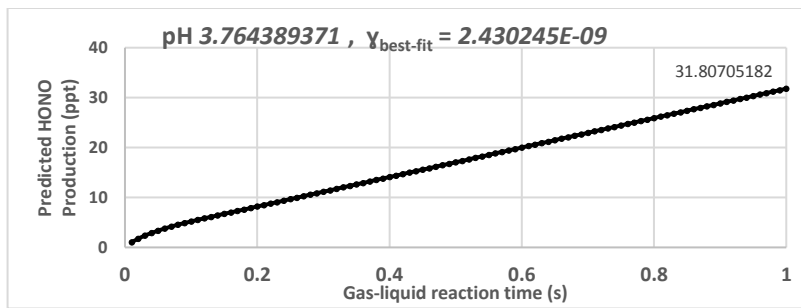
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732618E+16	1.166667	3.509922E-07	1.652814E-20	1.095871E-17	2.943369E-17	99.999957	3.729085
0.02	1.732617E+16	2.333333	4.963776E-07	7.295875E-20	2.191742E-17	8.830102E-17	99.999882	3.729085
0.03	1.732615E+16	3.500000	6.079353E-07	1.862323E-19	3.287613E-17	1.766019E-16	99.999775	3.729085
0.04	1.732613E+16	4.666667	7.019822E-07	3.703200E-19	4.383482E-17	2.943364E-16	99.999637	3.729084
0.05	1.732610E+16	5.833333	7.848387E-07	6.373877E-19	5.479350E-17	4.415043E-16	99.999468	3.729084
0.06	1.732606E+16	7.000000	8.597459E-07	9.983546E-19	6.575217E-17	6.181055E-16	99.999267	3.729084
0.07	1.732602E+16	8.166667	9.286296E-07	1.463212E-18	7.671082E-17	8.241399E-16	99.999034	3.729083
0.08	1.732598E+16	9.333333	9.927442E-07	2.041227E-18	8.766944E-17	1.059607E-15	99.998769	3.729083
0.09	1.732593E+16	10.500000	1.052961E-06	2.741078E-18	9.862805E-17	1.324508E-15	99.998473	3.729082
0.10	1.732587E+16	11.666667	1.109915E-06	3.570957E-18	1.095866E-16	1.618841E-15	99.998145	3.729082
0.11	1.732581E+16	12.833333	1.164084E-06	4.538642E-18	1.205452E-16	1.942607E-15	99.997786	3.729081
0.12	1.732574E+16	14.000000	1.215842E-06	5.651554E-18	1.315037E-16	2.295806E-15	99.997395	3.729081
0.13	1.732567E+16	15.166667	1.234286E-06	6.918308E-18	1.424622E-16	2.678436E-15	99.996972	3.729080
0.14	1.732559E+16	16.333333	1.234286E-06	8.348305E-18	1.534206E-16	3.090499E-15	99.996517	3.729079
0.15	1.732550E+16	17.500000	1.234286E-06	9.950943E-18	1.643790E-16	3.531993E-15	99.996031	3.729079
0.16	1.732541E+16	18.666667	1.234286E-06	1.173562E-17	1.753374E-16	4.002918E-15	99.995513	3.729078
0.17	1.732532E+16	19.833333	1.234286E-06	1.371174E-17	1.862957E-16	4.503275E-15	99.994963	3.729077
0.18	1.732522E+16	21.000000	1.234286E-06	1.588871E-17	1.972540E-16	5.033062E-15	99.994382	3.729076
0.19	1.732511E+16	22.166667	1.234286E-06	1.827591E-17	2.082122E-16	5.592280E-15	99.993769	3.729075
0.20	1.732500E+16	23.333333	1.234286E-06	2.088275E-17	2.191704E-16	6.180927E-15	99.993124	3.729074
0.21	1.732488E+16	24.500000	1.234286E-06	2.371863E-17	2.301285E-16	6.799005E-15	99.992447	3.729072
0.22	1.732476E+16	25.666667	1.234286E-06	2.679295E-17	2.410866E-16	7.446511E-15	99.991739	3.729071
0.23	1.732463E+16	26.833333	1.234286E-06	3.011510E-17	2.520446E-16	8.123447E-15	99.990999	3.729070
0.24	1.732450E+16	28.000000	1.234286E-06	3.369449E-17	2.630025E-16	8.829811E-15	99.990227	3.729069
0.25	1.732436E+16	29.166667	1.234286E-06	3.754051E-17	2.739604E-16	9.565603E-15	99.989423	3.729067
0.26	1.732421E+16	30.333333	1.234286E-06	4.166257E-17	2.849182E-16	1.033082E-14	99.988587	3.729066
0.27	1.732406E+16	31.500000	1.234286E-06	4.607006E-17	2.958760E-16	1.112547E-14	99.987720	3.729064
0.28	1.732391E+16	32.666667	1.234286E-06	5.077238E-17	3.068337E-16	1.194954E-14	99.986821	3.729063
0.29	1.732375E+16	33.833333	1.234286E-06	5.577893E-17	3.177913E-16	1.280304E-14	99.985889	3.729061
0.30	1.732358E+16	35.000000	1.234286E-06	6.109910E-17	3.287488E-16	1.368597E-14	99.984927	3.729059
0.31	1.732341E+16	36.166667	1.234286E-06	6.674230E-17	3.397063E-16	1.459832E-14	99.983932	3.729058
0.32	1.732323E+16	37.333333	1.234286E-06	7.271793E-17	3.506637E-16	1.554009E-14	99.982905	3.729056
0.33	1.732305E+16	38.500000	1.234286E-06	7.903537E-17	3.616210E-16	1.651129E-14	99.981847	3.729054
0.34	1.732286E+16	39.666667	1.234286E-06	8.570404E-17	3.725782E-16	1.751191E-14	99.980756	3.729052
0.35	1.732266E+16	40.833333	1.234286E-06	9.273332E-17	3.835353E-16	1.854195E-14	99.979634	3.729050
0.36	1.732246E+16	42.000000	1.234286E-06	1.001326E-16	3.944923E-16	1.960142E-14	99.978480	3.729048
0.37	1.732226E+16	43.166667	1.234286E-06	1.079113E-16	4.054493E-16	2.069030E-14	99.977293	3.729046
0.38	1.732205E+16	44.333333	1.234286E-06	1.160788E-16	4.164061E-16	2.180861E-14	99.976075	3.729044
0.39	1.732183E+16	45.500000	1.234286E-06	1.246445E-16	4.273629E-16	2.295634E-14	99.974825	3.729042
0.40	1.732161E+16	46.666667	1.234286E-06	1.336179E-16	4.383195E-16	2.413349E-14	99.973544	3.729040
0.41	1.732138E+16	47.833333	1.234286E-06	1.430082E-16	4.492761E-16	2.534005E-14	99.972230	3.729037
0.42	1.732115E+16	49.000000	1.234286E-06	1.528249E-16	4.602325E-16	2.657603E-14	99.970884	3.729035
0.43	1.732091E+16	50.166667	1.234286E-06	1.630774E-16	4.711889E-16	2.784143E-14	99.969506	3.729033
0.44	1.732066E+16	51.333333	1.234286E-06	1.737751E-16	4.821451E-16	2.913625E-14	99.968096	3.729030
0.45	1.732041E+16	52.500000	1.234286E-06	1.849274E-16	4.931012E-16	3.046048E-14	99.966654	3.729028

0.46	1.732016E+16	53.666667	1.234286E-06	1.965436E-16	5.040572E-16	3.181413E-14	99.965181	3.729025
0.47	1.731990E+16	54.833333	1.234286E-06	2.086333E-16	5.150131E-16	3.319719E-14	99.963675	3.729023
0.48	1.731963E+16	56.000000	1.234286E-06	2.212056E-16	5.259689E-16	3.460966E-14	99.962137	3.729020
0.49	1.731936E+16	57.166667	1.234286E-06	2.342702E-16	5.369245E-16	3.605154E-14	99.960567	3.729017
0.50	1.731908E+16	58.333333	1.234286E-06	2.478363E-16	5.478800E-16	3.752284E-14	99.958966	3.729015
0.51	1.731880E+16	59.500000	1.234286E-06	2.619134E-16	5.588354E-16	3.902355E-14	99.957332	3.729012
0.52	1.731851E+16	60.666667	1.234286E-06	2.765108E-16	5.697907E-16	4.055366E-14	99.955666	3.729009
0.53	1.731822E+16	61.833333	1.234286E-06	2.916380E-16	5.807458E-16	4.211319E-14	99.953968	3.729006
0.54	1.731792E+16	63.000000	1.234286E-06	3.073043E-16	5.917008E-16	4.370212E-14	99.952238	3.729003
0.55	1.731761E+16	64.166667	1.234286E-06	3.235191E-16	6.026557E-16	4.532045E-14	99.950476	3.729000
0.56	1.731730E+16	65.333333	1.234286E-06	3.402919E-16	6.136104E-16	4.696820E-14	99.948681	3.728997
0.57	1.731698E+16	66.500000	1.234286E-06	3.576320E-16	6.245650E-16	4.864534E-14	99.946855	3.728994
0.58	1.731666E+16	67.666667	1.234286E-06	3.755488E-16	6.355194E-16	5.035189E-14	99.944997	3.728990
0.59	1.731633E+16	68.833333	1.234286E-06	3.940516E-16	6.464737E-16	5.208785E-14	99.943106	3.728987
0.60	1.731600E+16	70.000000	1.234286E-06	4.131500E-16	6.574278E-16	5.385320E-14	99.941183	3.728984
0.61	1.731566E+16	71.166667	1.234286E-06	4.328533E-16	6.683818E-16	5.564796E-14	99.939229	3.728980
0.62	1.731532E+16	72.333333	1.234286E-06	4.531709E-16	6.793356E-16	5.747211E-14	99.937242	3.728977
0.63	1.731497E+16	73.500000	1.234286E-06	4.741121E-16	6.902893E-16	5.932566E-14	99.935223	3.728973
0.64	1.731461E+16	74.666667	1.234286E-06	4.956864E-16	7.012428E-16	6.120861E-14	99.933171	3.728970
0.65	1.731425E+16	75.833333	1.234286E-06	5.179031E-16	7.121962E-16	6.312095E-14	99.931088	3.728966
0.66	1.731388E+16	77.000000	1.234286E-06	5.407717E-16	7.231494E-16	6.506269E-14	99.928972	3.728963
0.67	1.731351E+16	78.166667	1.234286E-06	5.643015E-16	7.341024E-16	6.703382E-14	99.926825	3.728959
0.68	1.731313E+16	79.333333	1.234286E-06	5.885020E-16	7.450552E-16	6.903434E-14	99.924645	3.728955
0.69	1.731275E+16	80.500000	1.234286E-06	6.133824E-16	7.560079E-16	7.106426E-14	99.922432	3.728951
0.70	1.731236E+16	81.666667	1.234286E-06	6.389523E-16	7.669604E-16	7.312356E-14	99.920188	3.728947
0.71	1.731197E+16	82.833333	1.234286E-06	6.652210E-16	7.779127E-16	7.521225E-14	99.917912	3.728943
0.72	1.731157E+16	84.000000	1.234286E-06	6.921978E-16	7.888649E-16	7.733033E-14	99.915603	3.728939
0.73	1.731116E+16	85.166667	1.234286E-06	7.198923E-16	7.998168E-16	7.947779E-14	99.913262	3.728935
0.74	1.731075E+16	86.333333	1.234286E-06	7.483136E-16	8.107686E-16	8.165464E-14	99.910888	3.728931
0.75	1.731033E+16	87.500000	1.234286E-06	7.774714E-16	8.217202E-16	8.386088E-14	99.908483	3.728927
0.76	1.730991E+16	88.666667	1.234286E-06	8.073748E-16	8.326716E-16	8.609649E-14	99.906045	3.728923
0.77	1.730948E+16	89.833333	1.234286E-06	8.380334E-16	8.436228E-16	8.836148E-14	99.903575	3.728919
0.78	1.730905E+16	91.000000	1.234286E-06	8.694566E-16	8.545738E-16	9.065586E-14	99.901073	3.728914
0.79	1.730861E+16	92.166667	1.234286E-06	9.016536E-16	8.655247E-16	9.297961E-14	99.898538	3.728910
0.80	1.730817E+16	93.333333	1.234286E-06	9.346339E-16	8.764753E-16	9.533273E-14	99.895971	3.728906
0.81	1.730772E+16	94.500000	1.234286E-06	9.684068E-16	8.874257E-16	9.771523E-14	99.893372	3.728901
0.82	1.730726E+16	95.666667	1.234286E-06	1.002982E-15	8.983759E-16	1.001271E-13	99.890740	3.728897
0.83	1.730680E+16	96.833333	1.234286E-06	1.038368E-15	9.093259E-16	1.025684E-13	99.888076	3.728892
0.84	1.730633E+16	98.000000	1.234286E-06	1.074576E-15	9.202757E-16	1.050390E-13	99.885380	3.728887
0.85	1.730586E+16	99.166667	1.234286E-06	1.111613E-15	9.312253E-16	1.075390E-13	99.882651	3.728883
0.86	1.730538E+16	100.333333	1.234286E-06	1.149490E-15	9.421746E-16	1.100683E-13	99.879890	3.728878
0.87	1.730490E+16	101.500000	1.234286E-06	1.188216E-15	9.531238E-16	1.126270E-13	99.877097	3.728873
0.88	1.730441E+16	102.666667	1.234286E-06	1.227801E-15	9.640727E-16	1.152151E-13	99.874272	3.728868
0.89	1.730391E+16	103.833333	1.234286E-06	1.268253E-15	9.750214E-16	1.178325E-13	99.871414	3.728863
0.90	1.730341E+16	105.000000	1.234286E-06	1.309582E-15	9.859699E-16	1.204793E-13	99.868523	3.728858
0.91	1.730290E+16	106.166667	1.234286E-06	1.351798E-15	9.969181E-16	1.231555E-13	99.865600	3.728853
0.92	1.730239E+16	107.333333	1.234286E-06	1.394910E-15	1.007866E-15	1.258610E-13	99.862645	3.728848
0.93	1.730188E+16	108.500000	1.234286E-06	1.438927E-15	1.018814E-15	1.285959E-13	99.859658	3.728843
0.94	1.730135E+16	109.666667	1.234286E-06	1.483859E-15	1.029762E-15	1.313601E-13	99.856638	3.728838
0.95	1.730082E+16	110.833333	1.234286E-06	1.529714E-15	1.040709E-15	1.341537E-13	99.853558	3.728832
0.96	1.730029E+16	112.000000	1.234286E-06	1.576504E-15	1.051656E-15	1.369767E-13	99.850500	3.728827
0.97	1.729975E+16	113.166667	1.234286E-06	1.624236E-15	1.062603E-15	1.398289E-13	99.847383	3.728822
0.98	1.729920E+16	114.333333	1.234286E-06	1.672920E-15	1.073549E-15	1.427106E-13	99.844233	3.728816
0.99	1.729865E+16	115.500000	1.234286E-06	1.722565E-15	1.084496E-15	1.456215E-13	99.841051	3.728811
1.00	1.729809E+16	116.666667	1.234286E-06	1.773182E-15	1.095442E-15	1.485619E-13	99.837837	3.728805



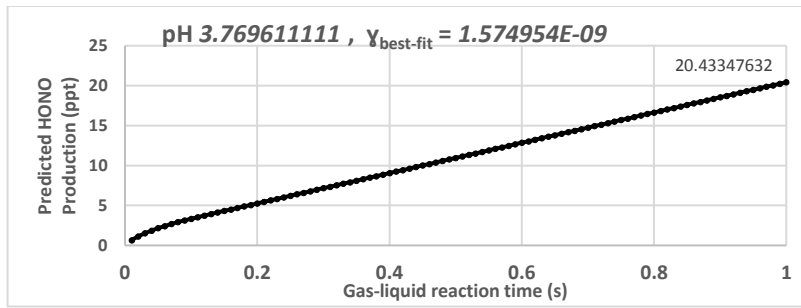
$t_{reac}$ (s)	$Z_{collisions}$ (/mol)	$t_{diffusion}$ (s)	$V_{film,diff}$ (L)	$\Phi_{HONO}$ (mol)	$\Phi_{HNO2}$ (mol)	$\Phi_{NO2}$ (mol)	% $NO_2$ left	film pH
0.01	1.732618E+16	1.166667	3.509922E-07	1.471916E-20	9.759300E-18	2.800667E-17	99.999960	3.757843
0.02	1.732617E+16	2.333333	4.963776E-07	6.497353E-20	1.951860E-17	8.401998E-17	99.999889	3.757843
0.03	1.732615E+16	3.500000	6.079354E-07	1.658494E-19	2.927789E-17	1.680399E-16	99.999789	3.757842
0.04	1.732613E+16	4.666667	7.019824E-07	3.297890E-19	3.903717E-17	2.800663E-16	99.999658	3.757842
0.05	1.732610E+16	5.833333	7.848389E-07	5.676266E-19	4.879645E-17	4.200991E-16	99.999497	3.757842
0.06	1.732607E+16	7.000000	8.597463E-07	8.890862E-19	5.855571E-17	5.881383E-16	99.999307	3.757841
0.07	1.732603E+16	8.166667	9.286301E-07	1.303066E-18	6.831495E-17	7.841838E-16	99.999086	3.757841
0.08	1.732599E+16	9.333333	9.927448E-07	1.817818E-18	7.807418E-17	1.008235E-15	99.998835	3.757841
0.09	1.732594E+16	10.500000	1.052962E-06	2.441071E-18	8.783339E-17	1.260293E-15	99.998554	3.757840
0.10	1.732589E+16	11.666667	1.109916E-06	3.180121E-18	9.759258E-17	1.540356E-15	99.998243	3.757840
0.11	1.732583E+16	12.833333	1.164086E-06	4.041894E-18	1.073517E-16	1.848426E-15	99.997901	3.757839
0.12	1.732576E+16	14.000000	1.215843E-06	5.033000E-18	1.171109E-16	2.184500E-15	99.997530	3.757839
0.13	1.732569E+16	15.166667	1.234286E-06	6.161110E-18	1.268700E-16	2.548580E-15	99.997128	3.757838
0.14	1.732562E+16	16.333333	1.234286E-06	7.434596E-18	1.366291E-16	2.940665E-15	99.996697	3.757837
0.15	1.732554E+16	17.500000	1.234286E-06	8.861829E-18	1.463881E-16	3.360755E-15	99.996235	3.757836
0.16	1.732545E+16	18.666667	1.234286E-06	1.045118E-17	1.561471E-16	3.808849E-15	99.995743	3.757835
0.17	1.732536E+16	19.833333	1.234286E-06	1.221102E-17	1.659061E-16	4.284948E-15	99.995221	3.757834
0.18	1.732527E+16	21.000000	1.234286E-06	1.414972E-17	1.756650E-16	4.789050E-15	99.994668	3.757833
0.19	1.732517E+16	22.166667	1.234286E-06	1.627564E-17	1.854239E-16	5.321156E-15	99.994086	3.757832
0.20	1.732506E+16	23.333333	1.234286E-06	1.859717E-17	1.951828E-16	5.881265E-15	99.993473	3.757831
0.21	1.732495E+16	24.500000	1.234286E-06	2.112267E-17	2.049416E-16	6.469377E-15	99.992830	3.757830
0.22	1.732483E+16	25.666667	1.234286E-06	2.386051E-17	2.147004E-16	7.085492E-15	99.992157	3.757829
0.23	1.732471E+16	26.833333	1.234286E-06	2.681906E-17	2.244591E-16	7.729609E-15	99.991453	3.757828
0.24	1.732458E+16	28.000000	1.234286E-06	3.000670E-17	2.342178E-16	8.401728E-15	99.990720	3.757826
0.25	1.732445E+16	29.166667	1.234286E-06	3.343179E-17	2.439764E-16	9.101848E-15	99.989956	3.757825
0.26	1.732431E+16	30.333333	1.234286E-06	3.710270E-17	2.537350E-16	9.829969E-15	99.989162	3.757823
0.27	1.732417E+16	31.500000	1.234286E-06	4.102780E-17	2.634935E-16	1.058609E-14	99.988337	3.757822
0.28	1.732402E+16	32.666667	1.234286E-06	4.521547E-17	2.732520E-16	1.137021E-14	99.987483	3.757820
0.29	1.732387E+16	33.833333	1.234286E-06	4.967407E-17	2.830104E-16	1.218233E-14	99.986598	3.757819
0.30	1.732371E+16	35.000000	1.234286E-06	5.441197E-17	2.927687E-16	1.302245E-14	99.985683	3.757817
0.31	1.732355E+16	36.166667	1.234286E-06	5.943754E-17	3.025270E-16	1.389057E-14	99.984737	3.757815
0.32	1.732338E+16	37.333333	1.234286E-06	6.475916E-17	3.122852E-16	1.478669E-14	99.983762	3.757813
0.33	1.732320E+16	38.500000	1.234286E-06	7.038519E-17	3.220433E-16	1.571080E-14	99.982755	3.757811
0.34	1.732302E+16	39.666667	1.234286E-06	7.632399E-17	3.318014E-16	1.666292E-14	99.981719	3.757810
0.35	1.732284E+16	40.833333	1.234286E-06	8.258395E-17	3.415594E-16	1.764302E-14	99.980652	3.757808
0.36	1.732265E+16	42.000000	1.234286E-06	8.917343E-17	3.513174E-16	1.865113E-14	99.979555	3.757805
0.37	1.732245E+16	43.166667	1.234286E-06	9.610079E-17	3.610752E-16	1.968723E-14	99.978428	3.757803
0.38	1.732225E+16	44.333333	1.234286E-06	1.033744E-16	3.708330E-16	2.075132E-14	99.977270	3.757801
0.39	1.732205E+16	45.500000	1.234286E-06	1.110027E-16	3.805907E-16	2.184341E-14	99.976082	3.757799
0.40	1.732184E+16	46.666667	1.234286E-06	1.189939E-16	3.903483E-16	2.296349E-14	99.974863	3.757797
0.41	1.732162E+16	47.833333	1.234286E-06	1.273565E-16	4.001058E-16	2.411156E-14	99.973615	3.757794
0.42	1.732140E+16	49.000000	1.234286E-06	1.360988E-16	4.098633E-16	2.528762E-14	99.972335	3.757792
0.43	1.732117E+16	50.166667	1.234286E-06	1.452293E-16	4.196207E-16	2.649168E-14	99.971026	3.757790
0.44	1.732094E+16	51.333333	1.234286E-06	1.547562E-16	4.293779E-16	2.772372E-14	99.969686	3.757787
0.45	1.732070E+16	52.500000	1.234286E-06	1.646879E-16	4.391351E-16	2.898376E-14	99.968315	3.757785

0.46	1.732046E+16	53.666667	1.234286E-06	1.750328E-16	4.488922E-16	3.027178E-14	99.966915	3.757782
0.47	1.732021E+16	54.833333	1.234286E-06	1.857993E-16	4.586492E-16	3.158780E-14	99.965483	3.757779
0.48	1.731996E+16	56.000000	1.234286E-06	1.969958E-16	4.684061E-16	3.293180E-14	99.964022	3.757777
0.49	1.731970E+16	57.166667	1.234286E-06	2.086305E-16	4.781629E-16	3.430378E-14	99.962529	3.757774
0.50	1.731944E+16	58.333333	1.234286E-06	2.207119E-16	4.879196E-16	3.570376E-14	99.961007	3.757771
0.51	1.731917E+16	59.500000	1.234286E-06	2.332484E-16	4.976762E-16	3.713171E-14	99.959454	3.757768
0.52	1.731889E+16	60.666667	1.234286E-06	2.462483E-16	5.074326E-16	3.858765E-14	99.957870	3.757765
0.53	1.731861E+16	61.833333	1.234286E-06	2.597199E-16	5.171890E-16	4.007158E-14	99.956256	3.757762
0.54	1.731833E+16	63.000000	1.234286E-06	2.736717E-16	5.269453E-16	4.158348E-14	99.954612	3.757759
0.55	1.731804E+16	64.166667	1.234286E-06	2.881119E-16	5.367014E-16	4.312337E-14	99.952937	3.757756
0.56	1.731774E+16	65.333333	1.234286E-06	3.030491E-16	5.464575E-16	4.469124E-14	99.951231	3.757753
0.57	1.731744E+16	66.500000	1.234286E-06	3.184915E-16	5.562134E-16	4.628709E-14	99.949496	3.757750
0.58	1.731713E+16	67.666667	1.234286E-06	3.344474E-16	5.659692E-16	4.791091E-14	99.947729	3.757747
0.59	1.731682E+16	68.833333	1.234286E-06	3.509254E-16	5.757249E-16	4.956271E-14	99.945932	3.757743
0.60	1.731651E+16	70.000000	1.234286E-06	3.679337E-16	5.854805E-16	5.124249E-14	99.944105	3.757740
0.61	1.731618E+16	71.166667	1.234286E-06	3.854806E-16	5.952359E-16	5.295025E-14	99.942247	3.757736
0.62	1.731586E+16	72.333333	1.234286E-06	4.035747E-16	6.049912E-16	5.468598E-14	99.940358	3.757733
0.63	1.731552E+16	73.500000	1.234286E-06	4.222241E-16	6.147464E-16	5.644968E-14	99.938439	3.757729
0.64	1.731519E+16	74.666667	1.234286E-06	4.414374E-16	6.245015E-16	5.824136E-14	99.936489	3.757726
0.65	1.731484E+16	75.833333	1.234286E-06	4.612228E-16	6.342564E-16	6.006100E-14	99.934509	3.757722
0.66	1.731450E+16	77.000000	1.234286E-06	4.815887E-16	6.440112E-16	6.190862E-14	99.932498	3.757718
0.67	1.731414E+16	78.166667	1.234286E-06	5.025435E-16	6.537658E-16	6.378420E-14	99.930457	3.757715
0.68	1.731378E+16	79.333333	1.234286E-06	5.240955E-16	6.635203E-16	6.568776E-14	99.928385	3.757711
0.69	1.731342E+16	80.500000	1.234286E-06	5.462532E-16	6.732747E-16	6.761928E-14	99.926282	3.757707
0.70	1.731305E+16	81.666667	1.234286E-06	5.690248E-16	6.830290E-16	6.957876E-14	99.924149	3.757703
0.71	1.731267E+16	82.833333	1.234286E-06	5.924188E-16	6.927830E-16	7.156621E-14	99.921985	3.757699
0.72	1.731229E+16	84.000000	1.234286E-06	6.164434E-16	7.025370E-16	7.358162E-14	99.919791	3.757695
0.73	1.731191E+16	85.166667	1.234286E-06	6.411071E-16	7.122908E-16	7.562500E-14	99.917566	3.757691
0.74	1.731152E+16	86.333333	1.234286E-06	6.664183E-16	7.220444E-16	7.769633E-14	99.915310	3.757687
0.75	1.731112E+16	87.500000	1.234286E-06	6.923852E-16	7.317979E-16	7.979563E-14	99.913024	3.757682
0.76	1.731072E+16	88.666667	1.234286E-06	7.190162E-16	7.415512E-16	8.192288E-14	99.910707	3.757678
0.77	1.731031E+16	89.833333	1.234286E-06	7.463198E-16	7.513044E-16	8.407809E-14	99.908359	3.757674
0.78	1.730990E+16	91.000000	1.234286E-06	7.743042E-16	7.610574E-16	8.626126E-14	99.905981	3.757669
0.79	1.730948E+16	92.166667	1.234286E-06	8.029778E-16	7.708103E-16	8.847238E-14	99.903572	3.757665
0.80	1.730906E+16	93.333333	1.234286E-06	8.323490E-16	7.805630E-16	9.071145E-14	99.901132	3.757660
0.81	1.730863E+16	94.500000	1.234286E-06	8.624262E-16	7.903155E-16	9.297848E-14	99.898662	3.757656
0.82	1.730820E+16	95.666667	1.234286E-06	8.932177E-16	8.000679E-16	9.527345E-14	99.896161	3.757651
0.83	1.730776E+16	96.833333	1.234286E-06	9.247318E-16	8.098201E-16	9.759638E-14	99.893629	3.757646
0.84	1.730732E+16	98.000000	1.234286E-06	9.569770E-16	8.195721E-16	9.994725E-14	99.891066	3.757642
0.85	1.730687E+16	99.166667	1.234286E-06	9.899615E-16	8.293239E-16	1.023261E-13	99.888473	3.757637
0.86	1.730641E+16	100.333333	1.234286E-06	1.023694E-15	8.390756E-16	1.047328E-13	99.885849	3.757632
0.87	1.730595E+16	101.500000	1.234286E-06	1.058182E-15	8.488271E-16	1.071675E-13	99.883195	3.757627
0.88	1.730549E+16	102.666667	1.234286E-06	1.093435E-15	8.585784E-16	1.096302E-13	99.880509	3.757622
0.89	1.730502E+16	103.833333	1.234286E-06	1.129461E-15	8.683295E-16	1.121208E-13	99.877793	3.757617
0.90	1.730454E+16	105.000000	1.234286E-06	1.166267E-15	8.780805E-16	1.146393E-13	99.875046	3.757612
0.91	1.730406E+16	106.166667	1.234286E-06	1.203864E-15	8.878313E-16	1.171858E-13	99.872269	3.757607
0.92	1.730357E+16	107.333333	1.234286E-06	1.242258E-15	8.975818E-16	1.197602E-13	99.869460	3.757602
0.93	1.730308E+16	108.500000	1.234286E-06	1.281458E-15	9.073322E-16	1.223625E-13	99.866621	3.757597
0.94	1.730258E+16	109.666667	1.234286E-06	1.321474E-15	9.170824E-16	1.249928E-13	99.863751	3.757591
0.95	1.730208E+16	110.833333	1.234286E-06	1.362312E-15	9.268324E-16	1.276510E-13	99.860850	3.757586
0.96	1.730157E+16	112.000000	1.234286E-06	1.403981E-15	9.365822E-16	1.303371E-13	99.857919	3.757581
0.97	1.730106E+16	113.166667	1.234286E-06	1.446490E-15	9.463318E-16	1.330511E-13	99.854956	3.757575
0.98	1.730054E+16	114.333333	1.234286E-06	1.489847E-15	9.560812E-16	1.357931E-13	99.851963	3.757570
0.99	1.730002E+16	115.500000	1.234286E-06	1.534060E-15	9.658304E-16	1.385630E-13	99.848939	3.757564
1.00	1.729949E+16	116.666667	1.234286E-06	1.579138E-15	9.755794E-16	1.413609E-13	99.845884	3.757558



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732618E+16	1.166667	3.509921E-07	2.694763E-20	1.786718E-17	5.205291E-17	99.999925	3.764389
0.02	1.732616E+16	2.333333	4.963772E-07	1.189526E-19	3.573435E-17	1.561586E-16	99.999794	3.764389
0.03	1.732612E+16	3.500000	6.079343E-07	3.036348E-19	5.360150E-17	3.123169E-16	99.999608	3.764388
0.04	1.732608E+16	4.666667	7.019803E-07	6.037732E-19	7.146863E-17	5.205275E-16	99.999365	3.764387
0.05	1.732603E+16	5.833333	7.848355E-07	1.039203E-18	8.933572E-17	7.807903E-16	99.999067	3.764387
0.06	1.732597E+16	7.000000	8.597412E-07	1.627727E-18	1.072028E-16	1.093105E-15	99.998713	3.764386
0.07	1.732590E+16	8.166667	9.286228E-07	2.385636E-18	1.250698E-16	1.457471E-15	99.998303	3.764385
0.08	1.732582E+16	9.333333	9.927349E-07	3.328037E-18	1.429367E-16	1.873888E-15	99.997837	3.764385
0.09	1.732573E+16	10.500000	1.052949E-06	4.469082E-18	1.608036E-16	2.342355E-15	99.997315	3.764384
0.10	1.732563E+16	11.666667	1.109899E-06	5.822127E-18	1.786704E-16	2.862873E-15	99.996737	3.764383
0.11	1.732552E+16	12.833333	1.164065E-06	7.399852E-18	1.965371E-16	3.435440E-15	99.996103	3.764382
0.12	1.732540E+16	14.000000	1.215818E-06	9.214358E-18	2.144037E-16	4.060056E-15	99.995413	3.764381
0.13	1.732527E+16	15.166667	1.234286E-06	1.127969E-17	2.322702E-16	4.736721E-15	99.994667	3.764380
0.14	1.732513E+16	16.333333	1.234286E-06	1.361117E-17	2.501367E-16	5.465432E-15	99.993865	3.764378
0.15	1.732498E+16	17.500000	1.234286E-06	1.622412E-17	2.680030E-16	6.246190E-15	99.993007	3.764377
0.16	1.732482E+16	18.666667	1.234286E-06	1.913388E-17	2.858692E-16	7.078993E-15	99.992093	3.764375
0.17	1.732465E+16	19.833333	1.234286E-06	2.235576E-17	3.037353E-16	7.963840E-15	99.991123	3.764373
0.18	1.732448E+16	21.000000	1.234286E-06	2.590508E-17	3.216013E-16	8.900731E-15	99.990096	3.764371
0.19	1.732429E+16	22.166667	1.234286E-06	2.979718E-17	3.394671E-16	9.889664E-15	99.989014	3.764369
0.20	1.732409E+16	23.333333	1.234286E-06	3.404737E-17	3.573328E-16	1.093064E-14	99.987876	3.764367
0.21	1.732388E+16	24.500000	1.234286E-06	3.867099E-17	3.751984E-16	1.202365E-14	99.986681	3.764365
0.22	1.732367E+16	25.666667	1.234286E-06	4.368334E-17	3.930638E-16	1.316870E-14	99.985430	3.764362
0.23	1.732344E+16	26.833333	1.234286E-06	4.909977E-17	4.109290E-16	1.436579E-14	99.984123	3.764360
0.24	1.732320E+16	28.000000	1.234286E-06	5.493558E-17	4.287941E-16	1.561492E-14	99.982760	3.764357
0.25	1.732296E+16	29.166667	1.234286E-06	6.120610E-17	4.466590E-16	1.691608E-14	99.981341	3.764355
0.26	1.732270E+16	30.333333	1.234286E-06	6.792665E-17	4.645237E-16	1.826927E-14	99.979866	3.764352
0.27	1.732244E+16	31.500000	1.234286E-06	7.511256E-17	4.823883E-16	1.967450E-14	99.978334	3.764349
0.28	1.732216E+16	32.666667	1.234286E-06	8.277914E-17	5.002526E-16	2.113175E-14	99.976746	3.764346
0.29	1.732188E+16	33.833333	1.234286E-06	9.094173E-17	5.181168E-16	2.264104E-14	99.975102	3.764343
0.30	1.732158E+16	35.000000	1.234286E-06	9.961563E-17	5.359807E-16	2.420235E-14	99.973402	3.764340
0.31	1.732128E+16	36.166667	1.234286E-06	1.088162E-16	5.538445E-16	2.581568E-14	99.971645	3.764337
0.32	1.732096E+16	37.333333	1.234286E-06	1.185587E-16	5.717080E-16	2.748104E-14	99.969832	3.764333
0.33	1.732064E+16	38.500000	1.234286E-06	1.288584E-16	5.895713E-16	2.919842E-14	99.967963	3.764330
0.34	1.732031E+16	39.666667	1.234286E-06	1.397308E-16	6.074343E-16	3.096781E-14	99.966037	3.764326
0.35	1.731996E+16	40.833333	1.234286E-06	1.511911E-16	6.252971E-16	3.278923E-14	99.964055	3.764322
0.36	1.731961E+16	42.000000	1.234286E-06	1.632546E-16	6.431597E-16	3.466266E-14	99.962017	3.764318
0.37	1.731925E+16	43.166667	1.234286E-06	1.759367E-16	6.610220E-16	3.658810E-14	99.959922	3.764315
0.38	1.731887E+16	44.333333	1.234286E-06	1.892527E-16	6.788841E-16	3.856555E-14	99.957771	3.764311
0.39	1.731849E+16	45.500000	1.234286E-06	2.032178E-16	6.967458E-16	4.059501E-14	99.955564	3.764306
0.40	1.731810E+16	46.666667	1.234286E-06	2.178475E-16	7.146074E-16	4.267648E-14	99.953300	3.764302
0.41	1.731770E+16	47.833333	1.234286E-06	2.331570E-16	7.324686E-16	4.480995E-14	99.950980	3.764298
0.42	1.731729E+16	49.000000	1.234286E-06	2.491616E-16	7.503295E-16	4.699542E-14	99.948603	3.764293
0.43	1.731686E+16	50.166667	1.234286E-06	2.658766E-16	7.681902E-16	4.923290E-14	99.946170	3.764289
0.44	1.731643E+16	51.333333	1.234286E-06	2.833175E-16	7.860505E-16	5.152236E-14	99.943681	3.764284
0.45	1.731599E+16	52.500000	1.234286E-06	3.014994E-16	8.039106E-16	5.386382E-14	99.941135	3.764279

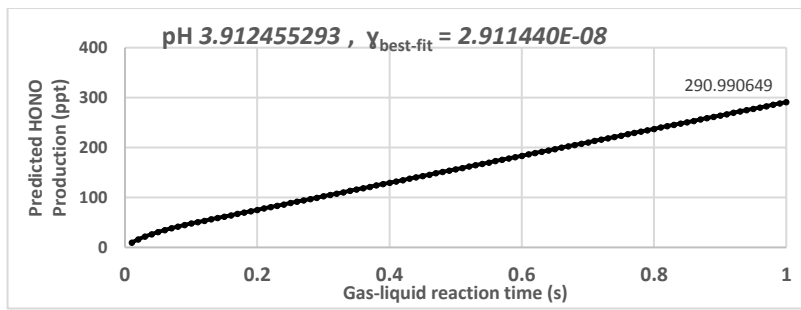
0.46	1.731554E+16	53.666667	1.234286E-06	3.204377E-16	8.217703E-16	5.625728E-14	99.938532	3.764274
0.47	1.731508E+16	54.833333	1.234286E-06	3.401477E-16	8.396297E-16	5.870272E-14	99.935873	3.764269
0.48	1.731461E+16	56.000000	1.234286E-06	3.606448E-16	8.574888E-16	6.120014E-14	99.933158	3.764264
0.49	1.731413E+16	57.166667	1.234286E-06	3.819441E-16	8.753475E-16	6.374955E-14	99.930386	3.764259
0.50	1.731364E+16	58.333333	1.234286E-06	4.040612E-16	8.932059E-16	6.635094E-14	99.927557	3.764254
0.51	1.731314E+16	59.500000	1.234286E-06	4.270111E-16	9.110639E-16	6.900431E-14	99.924672	3.764248
0.52	1.731263E+16	60.666667	1.234286E-06	4.508094E-16	9.289216E-16	7.170965E-14	99.921730	3.764243
0.53	1.731211E+16	61.833333	1.234286E-06	4.754712E-16	9.467789E-16	7.446696E-14	99.918732	3.764237
0.54	1.731158E+16	63.000000	1.234286E-06	5.010119E-16	9.646359E-16	7.727623E-14	99.915677	3.764231
0.55	1.731104E+16	64.166667	1.234286E-06	5.274468E-16	9.824925E-16	8.013748E-14	99.912566	3.764225
0.56	1.731049E+16	65.333333	1.234286E-06	5.547912E-16	1.000349E-15	8.305068E-14	99.909398	3.764220
0.57	1.730993E+16	66.500000	1.234286E-06	5.830604E-16	1.018204E-15	8.601584E-14	99.906173	3.764213
0.58	1.730937E+16	67.666667	1.234286E-06	6.122698E-16	1.036060E-15	8.903296E-14	99.902892	3.764207
0.59	1.730879E+16	68.833333	1.234286E-06	6.424345E-16	1.053915E-15	9.210203E-14	99.899553	3.764201
0.60	1.730820E+16	70.000000	1.234286E-06	6.735700E-16	1.071769E-15	9.522305E-14	99.896159	3.764195
0.61	1.730760E+16	71.166667	1.234286E-06	7.056915E-16	1.089624E-15	9.839601E-14	99.892707	3.764188
0.62	1.730699E+16	72.333333	1.234286E-06	7.388143E-16	1.107477E-15	1.016209E-13	99.889199	3.764182
0.63	1.730638E+16	73.500000	1.234286E-06	7.729538E-16	1.125331E-15	1.048977E-13	99.885635	3.764175
0.64	1.730575E+16	74.666667	1.234286E-06	8.081252E-16	1.143184E-15	1.082265E-13	99.882013	3.764168
0.65	1.730511E+16	75.833333	1.234286E-06	8.443439E-16	1.161036E-15	1.116072E-13	99.878335	3.764161
0.66	1.730446E+16	77.000000	1.234286E-06	8.816251E-16	1.178888E-15	1.150398E-13	99.874600	3.764154
0.67	1.730381E+16	78.166667	1.234286E-06	9.199841E-16	1.196739E-15	1.185244E-13	99.870808	3.764147
0.68	1.730314E+16	79.333333	1.234286E-06	9.594363E-16	1.214590E-15	1.220609E-13	99.866960	3.764140
0.69	1.730246E+16	80.500000	1.234286E-06	9.999969E-16	1.232441E-15	1.256492E-13	99.863054	3.764132
0.70	1.730178E+16	81.666667	1.234286E-06	1.041681E-15	1.250291E-15	1.292895E-13	99.859092	3.764125
0.71	1.730108E+16	82.833333	1.234286E-06	1.084505E-15	1.268141E-15	1.329817E-13	99.855074	3.764117
0.72	1.730037E+16	84.000000	1.234286E-06	1.128482E-15	1.285990E-15	1.367258E-13	99.850998	3.764110
0.73	1.729966E+16	85.166667	1.234286E-06	1.173630E-15	1.303838E-15	1.405218E-13	99.846865	3.764102
0.74	1.729893E+16	86.333333	1.234286E-06	1.219962E-15	1.321687E-15	1.443697E-13	99.842676	3.764094
0.75	1.729820E+16	87.500000	1.234286E-06	1.267495E-15	1.339534E-15	1.482695E-13	99.838430	3.764086
0.76	1.729745E+16	88.666667	1.234286E-06	1.316242E-15	1.357381E-15	1.522212E-13	99.834127	3.764078
0.77	1.729670E+16	89.833333	1.234286E-06	1.366221E-15	1.375228E-15	1.562247E-13	99.829767	3.764070
0.78	1.729593E+16	91.000000	1.234286E-06	1.417446E-15	1.393074E-15	1.602801E-13	99.825350	3.764062
0.79	1.729516E+16	92.166667	1.234286E-06	1.469932E-15	1.410919E-15	1.643874E-13	99.820876	3.764053
0.80	1.729437E+16	93.333333	1.234286E-06	1.523695E-15	1.428764E-15	1.685466E-13	99.816346	3.764045
0.81	1.729358E+16	94.500000	1.234286E-06	1.578750E-15	1.446608E-15	1.727576E-13	99.811758	3.764036
0.82	1.729277E+16	95.666667	1.234286E-06	1.635112E-15	1.464452E-15	1.770205E-13	99.807114	3.764027
0.83	1.729196E+16	96.833333	1.234286E-06	1.692797E-15	1.482295E-15	1.813352E-13	99.802412	3.764019
0.84	1.729113E+16	98.000000	1.234286E-06	1.751819E-15	1.500138E-15	1.857018E-13	99.797654	3.764010
0.85	1.729030E+16	99.166667	1.234286E-06	1.812195E-15	1.517980E-15	1.901202E-13	99.792838	3.764001
0.86	1.728945E+16	100.333333	1.234286E-06	1.873939E-15	1.535822E-15	1.945904E-13	99.787966	3.763992
0.87	1.728860E+16	101.500000	1.234286E-06	1.937066E-15	1.553662E-15	1.991125E-13	99.783037	3.763982
0.88	1.728774E+16	102.666667	1.234286E-06	2.001593E-15	1.571503E-15	2.036864E-13	99.778051	3.763973
0.89	1.728686E+16	103.833333	1.234286E-06	2.067533E-15	1.589342E-15	2.083122E-13	99.773007	3.763964
0.90	1.728598E+16	105.000000	1.234286E-06	2.134903E-15	1.607181E-15	2.129897E-13	99.767907	3.763954
0.91	1.728508E+16	106.166667	1.234286E-06	2.203718E-15	1.625020E-15	2.177191E-13	99.762750	3.763944
0.92	1.728418E+16	107.333333	1.234286E-06	2.273993E-15	1.642858E-15	2.225003E-13	99.757535	3.763935
0.93	1.728327E+16	108.500000	1.234286E-06	2.345744E-15	1.660695E-15	2.273333E-13	99.752264	3.763925
0.94	1.728234E+16	109.666667	1.234286E-06	2.418985E-15	1.678531E-15	2.322180E-13	99.746935	3.763915
0.95	1.728141E+16	110.833333	1.234286E-06	2.493731E-15	1.696367E-15	2.371546E-13	99.741550	3.763905
0.96	1.728047E+16	112.000000	1.234286E-06	2.569999E-15	1.714202E-15	2.421429E-13	99.736107	3.763894
0.97	1.727952E+16	113.166667	1.234286E-06	2.647804E-15	1.732037E-15	2.471831E-13	99.730607	3.763884
0.98	1.727855E+16	114.333333	1.234286E-06	2.727160E-15	1.749870E-15	2.522749E-13	99.725050	3.763874
0.99	1.727758E+16	115.500000	1.234286E-06	2.808083E-15	1.767704E-15	2.574186E-13	99.719436	3.763863
1.00	1.727660E+16	116.666667	1.234286E-06	2.890588E-15	1.785536E-15	2.626140E-13	99.713765	3.763853



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732618E+16	1.166667	3.509922E-07	1.730792E-20	1.147573E-17	3.383696E-17	99.999951	3.769611
0.02	1.732617E+16	2.333333	4.963775E-07	7.640088E-20	2.295147E-17	1.015108E-16	99.999867	3.769611
0.03	1.732615E+16	3.500000	6.079351E-07	1.950185E-19	3.442719E-17	2.030215E-16	99.999746	3.769610
0.04	1.732612E+16	4.666667	7.019819E-07	3.877913E-19	4.590290E-17	3.383690E-16	99.999588	3.769610
0.05	1.732609E+16	5.833333	7.848381E-07	6.674591E-19	5.737860E-17	5.075530E-16	99.999394	3.769609
0.06	1.732605E+16	7.000000	8.597451E-07	1.045456E-18	6.885428E-17	7.105735E-16	99.999164	3.769609
0.07	1.732600E+16	8.166667	9.286283E-07	1.532245E-18	8.032994E-17	9.474304E-16	99.998898	3.769609
0.08	1.732595E+16	9.333333	9.927424E-07	2.137530E-18	9.180558E-17	1.218123E-15	99.998595	3.769608
0.09	1.732589E+16	10.500000	1.052959E-06	2.870400E-18	1.032812E-16	1.522652E-15	99.998256	3.769607
0.10	1.732582E+16	11.666667	1.109912E-06	3.739432E-18	1.147568E-16	1.861017E-15	99.997880	3.769607
0.11	1.732575E+16	12.833333	1.164081E-06	4.752772E-18	1.262323E-16	2.233217E-15	99.997468	3.769606
0.12	1.732567E+16	14.000000	1.215837E-06	5.918191E-18	1.377078E-16	2.639253E-15	99.997020	3.769606
0.13	1.732559E+16	15.166667	1.234286E-06	7.244710E-18	1.491833E-16	3.079124E-15	99.996535	3.769605
0.14	1.732550E+16	16.333333	1.234286E-06	8.742173E-18	1.606587E-16	3.552829E-15	99.996014	3.769604
0.15	1.732540E+16	17.500000	1.234286E-06	1.042042E-17	1.721341E-16	4.060368E-15	99.995456	3.769603
0.16	1.732530E+16	18.666667	1.234286E-06	1.228930E-17	1.836094E-16	4.601741E-15	99.994862	3.769602
0.17	1.732519E+16	19.833333	1.234286E-06	1.435866E-17	1.950847E-16	5.176947E-15	99.994232	3.769600
0.18	1.732508E+16	21.000000	1.234286E-06	1.663832E-17	2.065599E-16	5.785986E-15	99.993565	3.769599
0.19	1.732495E+16	22.166667	1.234286E-06	1.913815E-17	2.180351E-16	6.428858E-15	99.992862	3.769598
0.20	1.732483E+16	23.333333	1.234286E-06	2.186798E-17	2.295102E-16	7.105561E-15	99.992122	3.769596
0.21	1.732469E+16	24.500000	1.234286E-06	2.483765E-17	2.409853E-16	7.816096E-15	99.991345	3.769595
0.22	1.732455E+16	25.666667	1.234286E-06	2.805701E-17	2.524603E-16	8.560462E-15	99.990532	3.769593
0.23	1.732440E+16	26.833333	1.234286E-06	3.153589E-17	2.639352E-16	9.338658E-15	99.989683	3.769592
0.24	1.732425E+16	28.000000	1.234286E-06	3.528415E-17	2.754101E-16	1.015068E-14	99.988797	3.769590
0.25	1.732409E+16	29.166667	1.234286E-06	3.931162E-17	2.868849E-16	1.099654E-14	99.987875	3.769588
0.26	1.732392E+16	30.333333	1.234286E-06	4.362815E-17	2.983596E-16	1.187622E-14	99.986916	3.769587
0.27	1.732375E+16	31.500000	1.234286E-06	4.824357E-17	3.098342E-16	1.278973E-14	99.985920	3.769585
0.28	1.732357E+16	32.666667	1.234286E-06	5.316773E-17	3.213088E-16	1.373707E-14	99.984888	3.769583
0.29	1.732339E+16	33.833333	1.234286E-06	5.841047E-17	3.327833E-16	1.471824E-14	99.983820	3.769581
0.30	1.732320E+16	35.000000	1.234286E-06	6.398164E-17	3.442577E-16	1.573323E-14	99.982714	3.769579
0.31	1.732300E+16	36.166667	1.234286E-06	6.989107E-17	3.557320E-16	1.678205E-14	99.981573	3.769576
0.32	1.732279E+16	37.333333	1.234286E-06	7.614860E-17	3.672062E-16	1.786469E-14	99.980394	3.769574
0.33	1.732258E+16	38.500000	1.234286E-06	8.276407E-17	3.786803E-16	1.898115E-14	99.979179	3.769572
0.34	1.732237E+16	39.666667	1.234286E-06	8.974734E-17	3.901543E-16	2.013144E-14	99.977928	3.769569
0.35	1.732214E+16	40.833333	1.234286E-06	9.710823E-17	4.016283E-16	2.131554E-14	99.976640	3.769567
0.36	1.732191E+16	42.000000	1.234286E-06	1.048566E-16	4.131021E-16	2.253347E-14	99.975315	3.769564
0.37	1.732168E+16	43.166667	1.234286E-06	1.130023E-16	4.245758E-16	2.378522E-14	99.973953	3.769562
0.38	1.732144E+16	44.333333	1.234286E-06	1.215551E-16	4.360494E-16	2.507079E-14	99.972555	3.769559
0.39	1.732119E+16	45.500000	1.234286E-06	1.305249E-16	4.475229E-16	2.639017E-14	99.971120	3.769556
0.40	1.732093E+16	46.666667	1.234286E-06	1.399215E-16	4.589963E-16	2.774338E-14	99.969649	3.769554
0.41	1.732067E+16	47.833333	1.234286E-06	1.497548E-16	4.704696E-16	2.913040E-14	99.968141	3.769551
0.42	1.732040E+16	49.000000	1.234286E-06	1.600346E-16	4.819427E-16	3.055123E-14	99.966596	3.769548
0.43	1.732013E+16	50.166667	1.234286E-06	1.707707E-16	4.934158E-16	3.200588E-14	99.965014	3.769545
0.44	1.731985E+16	51.333333	1.234286E-06	1.819731E-16	5.048887E-16	3.349434E-14	99.963396	3.769542
0.45	1.731956E+16	52.500000	1.234286E-06	1.936514E-16	5.163614E-16	3.501661E-14	99.961741	3.769539

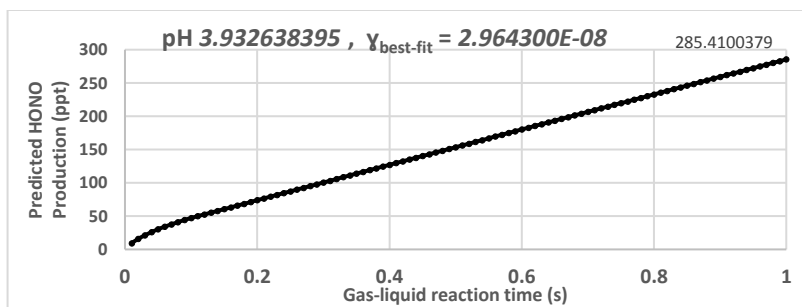


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0.47	1.731897E+16	54.833333	1.234286E-06	2.184756E-16	5.393066E-16	3.816259E-14	99.958321	3.769532
0.48	1.731866E+16	56.000000	1.234286E-06	2.316410E-16	5.507790E-16	3.978629E-14	99.956556	3.769529
0.49	1.731835E+16	57.166667	1.234286E-06	2.453219E-16	5.622512E-16	4.144380E-14	99.954754	3.769525
0.50	1.731803E+16	58.333333	1.234286E-06	2.595279E-16	5.737233E-16	4.313511E-14	99.952915	3.769522
0.51	1.731771E+16	59.500000	1.234286E-06	2.742690E-16	5.851952E-16	4.486023E-14	99.951040	3.769518
0.52	1.731738E+16	60.666667	1.234286E-06	2.895550E-16	5.966670E-16	4.661915E-14	99.949128	3.769515
0.53	1.731704E+16	61.833333	1.234286E-06	3.053957E-16	6.081387E-16	4.841188E-14	99.947179	3.769511
0.54	1.731670E+16	63.000000	1.234286E-06	3.218010E-16	6.196102E-16	5.023840E-14	99.945193	3.769507
0.55	1.731634E+16	64.166667	1.234286E-06	3.387807E-16	6.310815E-16	5.209873E-14	99.943170	3.769503
0.56	1.731599E+16	65.333333	1.234286E-06	3.563446E-16	6.425527E-16	5.399285E-14	99.941111	3.769499
0.57	1.731562E+16	66.500000	1.234286E-06	3.745026E-16	6.540237E-16	5.592077E-14	99.939014	3.769495
0.58	1.731526E+16	67.666667	1.234286E-06	3.932645E-16	6.654946E-16	5.788248E-14	99.936881	3.769491
0.59	1.731488E+16	68.833333	1.234286E-06	4.126401E-16	6.769653E-16	5.987799E-14	99.934711	3.769487
0.60	1.731450E+16	70.000000	1.234286E-06	4.326393E-16	6.884358E-16	6.190729E-14	99.932504	3.769483
0.61	1.731411E+16	71.166667	1.234286E-06	4.532719E-16	6.999061E-16	6.397038E-14	99.930261	3.769479
0.62	1.731371E+16	72.333333	1.234286E-06	4.745478E-16	7.113763E-16	6.606726E-14	99.927980	3.769474
0.63	1.731331E+16	73.500000	1.234286E-06	4.964767E-16	7.228463E-16	6.819793E-14	99.925663	3.769470
0.64	1.731290E+16	74.666667	1.234286E-06	5.190686E-16	7.343161E-16	7.036239E-14	99.923308	3.769465
0.65	1.731249E+16	75.833333	1.234286E-06	5.423332E-16	7.457857E-16	7.256063E-14	99.920917	3.769461
0.66	1.731207E+16	77.000000	1.234286E-06	5.662804E-16	7.572551E-16	7.479265E-14	99.918489	3.769456
0.67	1.731164E+16	78.166667	1.234286E-06	5.909200E-16	7.687244E-16	7.705845E-14	99.916024	3.769452
0.68	1.731121E+16	79.333333	1.234286E-06	6.162618E-16	7.801934E-16	7.935804E-14	99.913522	3.769447
0.69	1.731077E+16	80.500000	1.234286E-06	6.423157E-16	7.916623E-16	8.169140E-14	99.910983	3.769442
0.70	1.731032E+16	81.666667	1.234286E-06	6.690915E-16	8.031309E-16	8.405854E-14	99.908407	3.769437
0.71	1.730987E+16	82.833333	1.234286E-06	6.965991E-16	8.145994E-16	8.645945E-14	99.905794	3.769432
0.72	1.730941E+16	84.000000	1.234286E-06	7.248482E-16	8.260676E-16	8.889413E-14	99.903144	3.769427
0.73	1.730894E+16	85.166667	1.234286E-06	7.538488E-16	8.375357E-16	9.136259E-14	99.900458	3.769422
0.74	1.730847E+16	86.333333	1.234286E-06	7.836105E-16	8.490035E-16	9.386481E-14	99.897734	3.769417
0.75	1.730799E+16	87.500000	1.234286E-06	8.141434E-16	8.604711E-16	9.640081E-14	99.894973	3.769412
0.76	1.730751E+16	88.666667	1.234286E-06	8.454571E-16	8.719385E-16	9.897056E-14	99.892176	3.769406
0.77	1.730702E+16	89.833333	1.234286E-06	8.775615E-16	8.834057E-16	1.015741E-13	99.889341	3.769401
0.78	1.730652E+16	91.000000	1.234286E-06	9.104665E-16	8.948727E-16	1.042114E-13	99.886469	3.769395
0.79	1.730602E+16	92.166667	1.234286E-06	9.441819E-16	9.063394E-16	1.068824E-13	99.883560	3.769390
0.80	1.730551E+16	93.333333	1.234286E-06	9.787175E-16	9.178059E-16	1.095872E-13	99.880615	3.769384
0.81	1.730499E+16	94.500000	1.234286E-06	1.014083E-15	9.292722E-16	1.123258E-13	99.877632	3.769379
0.82	1.730447E+16	95.666667	1.234286E-06	1.050289E-15	9.407382E-16	1.150981E-13	99.874612	3.769373
0.83	1.730394E+16	96.833333	1.234286E-06	1.087344E-15	9.522040E-16	1.179041E-13	99.871555	3.769367
0.84	1.730340E+16	98.000000	1.234286E-06	1.125258E-15	9.636696E-16	1.207439E-13	99.868461	3.769361
0.85	1.730286E+16	99.166667	1.234286E-06	1.164042E-15	9.751349E-16	1.236175E-13	99.865330	3.769355
0.86	1.730231E+16	100.333333	1.234286E-06	1.203706E-15	9.866000E-16	1.265248E-13	99.862162	3.769349
0.87	1.730175E+16	101.500000	1.234286E-06	1.244258E-15	9.980648E-16	1.294659E-13	99.858957	3.769343
0.88	1.730119E+16	102.666667	1.234286E-06	1.285709E-15	1.009529E-15	1.324406E-13	99.855714	3.769337
0.89	1.730062E+16	103.833333	1.234286E-06	1.328068E-15	1.020994E-15	1.354492E-13	99.852435	3.769331
0.90	1.730005E+16	105.000000	1.234286E-06	1.371347E-15	1.032458E-15	1.384914E-13	99.849119	3.769325
0.91	1.729947E+16	106.166667	1.234286E-06	1.415553E-15	1.043922E-15	1.415674E-13	99.845765	3.769318
0.92	1.729888E+16	107.333333	1.234286E-06	1.460697E-15	1.055385E-15	1.446772E-13	99.842374	3.769312
0.93	1.729829E+16	108.500000	1.234286E-06	1.506790E-15	1.066848E-15	1.478206E-13	99.838946	3.769305
0.94	1.729769E+16	109.666667	1.234286E-06	1.553840E-15	1.078311E-15	1.509978E-13	99.835481	3.769299
0.95	1.729708E+16	110.833333	1.234286E-06	1.601858E-15	1.089774E-15	1.542087E-13	99.831979	3.769292
0.96	1.729647E+16	112.000000	1.234286E-06	1.650853E-15	1.101237E-15	1.574534E-13	99.828440	3.769285
0.97	1.729585E+16	113.166667	1.234286E-06	1.700835E-15	1.112699E-15	1.607317E-13	99.824863	3.769279
0.98	1.729522E+16	114.333333	1.234286E-06	1.751815E-15	1.124161E-15	1.640438E-13	99.821249	3.769272
0.99	1.729459E+16	115.500000	1.234286E-06	1.803801E-15	1.135622E-15	1.673896E-13	99.817599	3.769265
1.00	1.729395E+16	116.666667	1.234286E-06	1.856804E-15	1.147084E-15	1.707691E-13	99.813911	3.769258



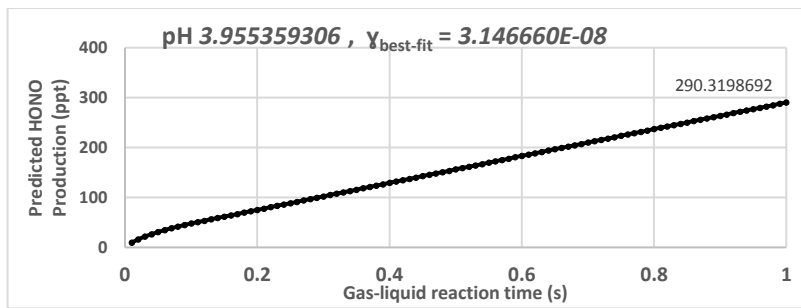
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO2}}$ (mol)	$\Phi_{\text{NO2}}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732604E+16	1.166667	3.509892E-07	2.478699E-19	1.643447E-16	6.732930E-16	99.999103	3.912448
0.02	1.732576E+16	2.333333	4.963657E-07	1.094155E-18	3.286890E-16	2.019854E-15	99.997484	3.912441
0.03	1.732535E+16	3.500000	6.079071E-07	2.792920E-18	4.930323E-16	4.039648E-15	99.995143	3.912432
0.04	1.732482E+16	4.666667	7.019292E-07	5.553705E-18	6.573737E-16	6.732630E-15	99.992080	3.912421
0.05	1.732416E+16	5.833333	7.847510E-07	9.558980E-18	8.217124E-16	1.009875E-14	99.988295	3.912410
0.06	1.732338E+16	7.000000	8.596129E-07	1.497252E-17	9.860476E-16	1.413794E-14	99.983788	3.912397
0.07	1.732248E+16	8.166667	9.284394E-07	2.194420E-17	1.150378E-15	1.885015E-14	99.978558	3.912383
0.08	1.732144E+16	9.333333	9.924844E-07	3.061302E-17	1.314704E-15	2.423528E-14	99.972606	3.912369
0.09	1.732029E+16	10.500000	1.052618E-06	4.110919E-17	1.479023E-15	3.029326E-14	99.965932	3.912353
0.10	1.731901E+16	11.666667	1.109475E-06	5.355558E-17	1.643335E-15	3.702400E-14	99.958535	3.912337
0.11	1.731760E+16	12.833333	1.163533E-06	6.806891E-17	1.807639E-15	4.442741E-14	99.950415	3.912320
0.12	1.731607E+16	14.000000	1.215163E-06	8.476051E-17	1.971933E-15	5.250337E-14	99.941573	3.912302
0.13	1.731441E+16	15.166667	1.234286E-06	1.037591E-16	2.136219E-15	6.125169E-14	99.932008	3.912279
0.14	1.731263E+16	16.333333	1.234286E-06	1.252054E-16	2.300496E-15	7.067219E-14	99.921721	3.912252
0.15	1.731072E+16	17.500000	1.234286E-06	1.492405E-16	2.464764E-15	8.076468E-14	99.910712	3.912223
0.16	1.730869E+16	18.666667	1.234286E-06	1.760051E-16	2.629022E-15	9.152899E-14	99.898980	3.912192
0.17	1.730653E+16	19.833333	1.234286E-06	2.056400E-16	2.793270E-15	1.029649E-13	99.886526	3.912159
0.18	1.730425E+16	21.000000	1.234286E-06	2.382860E-16	2.957506E-15	1.150723E-13	99.873349	3.912124
0.19	1.730184E+16	22.166667	1.234286E-06	2.740840E-16	3.121731E-15	1.278509E-13	99.859451	3.912088
0.20	1.729931E+16	23.333333	1.234286E-06	3.131746E-16	3.285944E-15	1.413005E-13	99.844830	3.912049
0.21	1.729665E+16	24.500000	1.234286E-06	3.556987E-16	3.450143E-15	1.554209E-13	99.829488	3.912008
0.22	1.729386E+16	25.666667	1.234286E-06	4.017970E-16	3.614329E-15	1.702117E-13	99.813423	3.911966
0.23	1.729096E+16	26.833333	1.234286E-06	4.516100E-16	3.778501E-15	1.856729E-13	99.796637	3.911922
0.24	1.728792E+16	28.000000	1.234286E-06	5.052786E-16	3.942658E-15	2.018040E-13	99.779130	3.911875
0.25	1.728476E+16	29.166667	1.234286E-06	5.629434E-16	4.106800E-15	2.186048E-13	99.760900	3.911827
0.26	1.728148E+16	30.333333	1.234286E-06	6.247449E-16	4.270926E-15	2.360750E-13	99.741950	3.911777
0.27	1.727807E+16	31.500000	1.234286E-06	6.908238E-16	4.435035E-15	2.542144E-13	99.722279	3.911725
0.28	1.727454E+16	32.666667	1.234286E-06	7.613207E-16	4.599128E-15	2.730226E-13	99.701886	3.911671
0.29	1.727088E+16	33.833333	1.234286E-06	8.363760E-16	4.763202E-15	2.924992E-13	99.680773	3.911615
0.30	1.726710E+16	35.000000	1.234286E-06	9.161303E-16	4.927258E-15	3.126440E-13	99.658939	3.911557
0.31	1.726319E+16	36.166667	1.234286E-06	1.000724E-15	5.091295E-15	3.334565E-13	99.636385	3.911497
0.32	1.725916E+16	37.333333	1.234286E-06	1.090298E-15	5.255313E-15	3.549365E-13	99.613111	3.911436
0.33	1.725500E+16	38.500000	1.234286E-06	1.184992E-15	5.419310E-15	3.770836E-13	99.589118	3.911372
0.34	1.725072E+16	39.666667	1.234286E-06	1.284946E-15	5.583286E-15	3.998973E-13	99.564404	3.911307
0.35	1.724631E+16	40.833333	1.234286E-06	1.390302E-15	5.747241E-15	4.233773E-13	99.538972	3.911239
0.36	1.724178E+16	42.000000	1.234286E-06	1.501199E-15	5.911174E-15	4.475233E-13	99.512820	3.911170
0.37	1.723713E+16	43.166667	1.234286E-06	1.617777E-15	6.075084E-15	4.723346E-13	99.485950	3.911099
0.38	1.723235E+16	44.333333	1.234286E-06	1.740177E-15	6.238971E-15	4.978111E-13	99.458361	3.911026
0.39	1.722744E+16	45.500000	1.234286E-06	1.868539E-15	6.402834E-15	5.239521E-13	99.430054	3.910951
0.40	1.722241E+16	46.666667	1.234286E-06	2.003004E-15	6.566672E-15	5.507574E-13	99.401030	3.910874
0.41	1.721726E+16	47.833333	1.234286E-06	2.143710E-15	6.730485E-15	5.782263E-13	99.371288	3.910795
0.42	1.721198E+16	49.000000	1.234286E-06	2.290799E-15	6.894272E-15	6.063585E-13	99.340829	3.910715
0.43	1.720658E+16	50.166667	1.234286E-06	2.444409E-15	7.058033E-15	6.351534E-13	99.309653	3.910632
0.44	1.720105E+16	51.333333	1.234286E-06	2.604682E-15	7.221767E-15	6.646106E-13	99.277761	3.910548
0.45	1.719540E+16	52.500000	1.234286E-06	2.771758E-15	7.385473E-15	6.947295E-13	99.245153	3.910462

0.46	1.718963E+16	53.666667	1.234286E-06	2.945775E-15	7.549151E-15	7.255098E-13	99.211830	3.910374
0.47	1.718373E+16	54.833333	1.234286E-06	3.126874E-15	7.712800E-15	7.569507E-13	99.177791	3.910284
0.48	1.717771E+16	56.000000	1.234286E-06	3.315194E-15	7.876420E-15	7.890519E-13	99.143038	3.910192
0.49	1.717157E+16	57.166667	1.234286E-06	3.510876E-15	8.040009E-15	8.218127E-13	99.107570	3.910098
0.50	1.716530E+16	58.333333	1.234286E-06	3.714059E-15	8.203567E-15	8.552326E-13	99.071389	3.910002
0.51	1.715891E+16	59.500000	1.234286E-06	3.924882E-15	8.367094E-15	8.893110E-13	99.034494	3.909905
0.52	1.715239E+16	60.666667	1.234286E-06	4.143485E-15	8.530589E-15	9.240474E-13	98.996887	3.909806
0.53	1.714575E+16	61.833333	1.234286E-06	4.370008E-15	8.694051E-15	9.594411E-13	98.958567	3.909704
0.54	1.713899E+16	63.000000	1.234286E-06	4.604590E-15	8.857480E-15	9.954917E-13	98.919535	3.909601
0.55	1.713210E+16	64.166667	1.234286E-06	4.847371E-15	9.020875E-15	1.032198E-12	98.879792	3.909497
0.56	1.712509E+16	65.333333	1.234286E-06	5.098489E-15	9.184235E-15	1.069561E-12	98.839337	3.909390
0.57	1.711796E+16	66.500000	1.234286E-06	5.358084E-15	9.347560E-15	1.107578E-12	98.798173	3.909281
0.58	1.711071E+16	67.666667	1.234286E-06	5.626295E-15	9.510849E-15	1.146249E-12	98.756298	3.909171
0.59	1.710333E+16	68.833333	1.234286E-06	5.903262E-15	9.674101E-15	1.185574E-12	98.713715	3.909059
0.60	1.709583E+16	70.000000	1.234286E-06	6.189123E-15	9.837317E-15	1.225552E-12	98.670422	3.908945
0.61	1.708820E+16	71.166667	1.234286E-06	6.484018E-15	1.000049E-14	1.266183E-12	98.626422	3.908829
0.62	1.708046E+16	72.333333	1.234286E-06	6.788085E-15	1.016363E-14	1.307464E-12	98.581713	3.908711
0.63	1.707259E+16	73.500000	1.234286E-06	7.101463E-15	1.032673E-14	1.349397E-12	98.536298	3.908591
0.64	1.706460E+16	74.666667	1.234286E-06	7.424291E-15	1.048979E-14	1.391980E-12	98.490177	3.908470
0.65	1.705648E+16	75.833333	1.234286E-06	7.756709E-15	1.065281E-14	1.435213E-12	98.443349	3.908347
0.66	1.704825E+16	77.000000	1.234286E-06	8.098853E-15	1.081579E-14	1.479094E-12	98.395817	3.908222
0.67	1.703989E+16	78.166667	1.234286E-06	8.450864E-15	1.097873E-14	1.523624E-12	98.347580	3.908095
0.68	1.703141E+16	79.333333	1.234286E-06	8.812880E-15	1.114162E-14	1.568800E-12	98.298639	3.907966
0.69	1.702281E+16	80.500000	1.234286E-06	9.185038E-15	1.130447E-14	1.614624E-12	98.248995	3.907836
0.70	1.701409E+16	81.666667	1.234286E-06	9.567478E-15	1.146728E-14	1.661093E-12	98.198649	3.907704
0.71	1.700524E+16	82.833333	1.234286E-06	9.960338E-15	1.163004E-14	1.708207E-12	98.147600	3.907570
0.72	1.699627E+16	84.000000	1.234286E-06	1.036376E-14	1.179276E-14	1.755965E-12	98.095851	3.907434
0.73	1.698719E+16	85.166667	1.234286E-06	1.077787E-14	1.195544E-14	1.804367E-12	98.043401	3.907296
0.74	1.697798E+16	86.333333	1.234286E-06	1.120282E-14	1.211806E-14	1.853412E-12	97.990251	3.907157
0.75	1.696865E+16	87.500000	1.234286E-06	1.163874E-14	1.228064E-14	1.903098E-12	97.936402	3.907016
0.76	1.695920E+16	88.666667	1.234286E-06	1.208577E-14	1.244317E-14	1.953425E-12	97.881855	3.906873
0.77	1.694963E+16	89.833333	1.234286E-06	1.254405E-14	1.260566E-14	2.004393E-12	97.826610	3.906728
0.78	1.693993E+16	91.000000	1.234286E-06	1.301371E-14	1.276809E-14	2.056000E-12	97.770669	3.906582
0.79	1.693012E+16	92.166667	1.234286E-06	1.349490E-14	1.293047E-14	2.108245E-12	97.714031	3.906433
0.80	1.692019E+16	93.333333	1.234286E-06	1.398775E-14	1.309281E-14	2.161128E-12	97.656698	3.906283
0.81	1.691013E+16	94.500000	1.234286E-06	1.449239E-14	1.325509E-14	2.214648E-12	97.598671	3.906132
0.82	1.689996E+16	95.666667	1.234286E-06	1.500898E-14	1.341732E-14	2.268803E-12	97.539950	3.905978
0.83	1.688966E+16	96.833333	1.234286E-06	1.553763E-14	1.357950E-14	2.323594E-12	97.480536	3.905823
0.84	1.687925E+16	98.000000	1.234286E-06	1.607850E-14	1.374163E-14	2.379019E-12	97.420430	3.905666
0.85	1.686872E+16	99.166667	1.234286E-06	1.663171E-14	1.390370E-14	2.435077E-12	97.359633	3.905507
0.86	1.685806E+16	100.333333	1.234286E-06	1.719741E-14	1.406572E-14	2.491767E-12	97.298145	3.905347
0.87	1.684729E+16	101.500000	1.234286E-06	1.777572E-14	1.422768E-14	2.549089E-12	97.235968	3.905185
0.88	1.683640E+16	102.666667	1.234286E-06	1.836680E-14	1.438959E-14	2.607041E-12	97.173102	3.905021
0.89	1.682539E+16	103.833333	1.234286E-06	1.897077E-14	1.455144E-14	2.665623E-12	97.109548	3.904855
0.90	1.681426E+16	105.000000	1.234286E-06	1.958777E-14	1.471323E-14	2.724833E-12	97.045308	3.904688
0.91	1.680301E+16	106.166667	1.234286E-06	2.021795E-14	1.487497E-14	2.784671E-12	96.980381	3.904519
0.92	1.679164E+16	107.333333	1.234286E-06	2.086142E-14	1.503665E-14	2.845135E-12	96.914769	3.904348
0.93	1.678015E+16	108.500000	1.234286E-06	2.151834E-14	1.519826E-14	2.906225E-12	96.848472	3.904176
0.94	1.676855E+16	109.666667	1.234286E-06	2.218883E-14	1.535982E-14	2.967939E-12	96.781493	3.904002
0.95	1.675682E+16	110.833333	1.234286E-06	2.287303E-14	1.552132E-14	3.030278E-12	96.713830	3.903826
0.96	1.674498E+16	112.000000	1.234286E-06	2.357109E-14	1.568275E-14	3.093238E-12	96.645487	3.903648
0.97	1.673302E+16	113.166667	1.234286E-06	2.428313E-14	1.584413E-14	3.156821E-12	96.576462	3.903469
0.98	1.672095E+16	114.333333	1.234286E-06	2.500929E-14	1.600544E-14	3.221024E-12	96.506758	3.903288
0.99	1.670875E+16	115.500000	1.234286E-06	2.574971E-14	1.616669E-14	3.285847E-12	96.436376	3.903106
1.00	1.669644E+16	116.666667	1.234286E-06	2.650452E-14	1.632787E-14	3.351288E-12	96.365315	3.902922



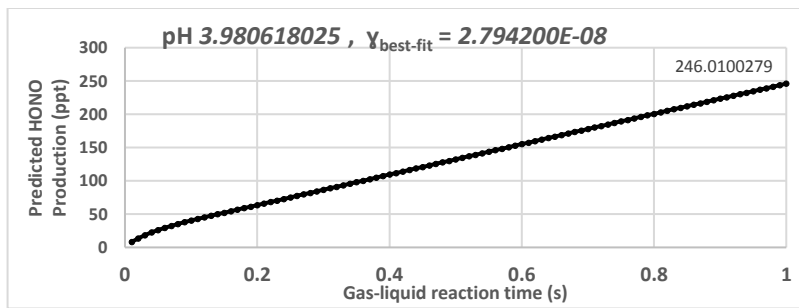
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732603E+16	1.166667	3.509892E-07	2.430760E-19	1.611662E-16	6.916795E-16	99.999086	3.932631
0.02	1.732575E+16	2.333333	4.963654E-07	1.072994E-18	3.223321E-16	2.075011E-15	99.997432	3.932623
0.03	1.732533E+16	3.500000	6.079065E-07	2.738906E-18	4.834972E-16	4.149958E-15	99.995035	3.932613
0.04	1.732479E+16	4.666667	7.019279E-07	5.446301E-18	6.446606E-16	6.916472E-15	99.991897	3.932602
0.05	1.732412E+16	5.833333	7.847488E-07	9.374121E-18	8.058215E-16	1.037450E-14	99.988017	3.932589
0.06	1.732331E+16	7.000000	8.596095E-07	1.468298E-17	9.669790E-16	1.452397E-14	99.983395	3.932576
0.07	1.732238E+16	8.166667	9.284346E-07	2.151985E-17	1.128132E-15	1.936481E-14	99.978032	3.932561
0.08	1.732133E+16	9.333333	9.924777E-07	3.002105E-17	1.289281E-15	2.489694E-14	99.971926	3.932545
0.09	1.732014E+16	10.500000	1.052609E-06	4.031426E-17	1.450423E-15	3.112027E-14	99.965078	3.932528
0.10	1.731883E+16	11.666667	1.109464E-06	5.252002E-17	1.611558E-15	3.803471E-14	99.957487	3.932511
0.11	1.731738E+16	12.833333	1.163518E-06	6.675275E-17	1.772685E-15	4.564015E-14	99.949155	3.932493
0.12	1.731581E+16	14.000000	1.215145E-06	8.312165E-17	1.933804E-15	5.393648E-14	99.940081	3.932473
0.13	1.731411E+16	15.166667	1.234286E-06	1.017529E-16	2.094914E-15	6.292348E-14	99.930264	3.932449
0.14	1.731228E+16	16.333333	1.234286E-06	1.227847E-16	2.256016E-15	7.260095E-14	99.919706	3.932420
0.15	1.731032E+16	17.500000	1.234286E-06	1.463551E-16	2.417109E-15	8.296871E-14	99.908406	3.932388
0.16	1.730823E+16	18.666667	1.234286E-06	1.726022E-16	2.578192E-15	9.402655E-14	99.896363	3.932355
0.17	1.730602E+16	19.833333	1.234286E-06	2.016642E-16	2.739266E-15	1.057743E-13	99.883579	3.932320
0.18	1.730368E+16	21.000000	1.234286E-06	2.336792E-16	2.900329E-15	1.182117E-13	99.870054	3.932282
0.19	1.730120E+16	22.166667	1.234286E-06	2.687851E-16	3.061381E-15	1.313385E-13	99.855786	3.932243
0.20	1.729860E+16	23.333333	1.234286E-06	3.071201E-16	3.222421E-15	1.451546E-13	99.840778	3.932201
0.21	1.729588E+16	24.500000	1.234286E-06	3.488222E-16	3.383449E-15	1.596595E-13	99.825027	3.932158
0.22	1.729302E+16	25.666667	1.234286E-06	3.940294E-16	3.544464E-15	1.748532E-13	99.808536	3.932112
0.23	1.729003E+16	26.833333	1.234286E-06	4.428796E-16	3.705466E-15	1.907353E-13	99.791304	3.932064
0.24	1.728692E+16	28.000000	1.234286E-06	4.955109E-16	3.866453E-15	2.073054E-13	99.773330	3.932014
0.25	1.728368E+16	29.166667	1.234286E-06	5.520612E-16	4.027426E-15	2.245634E-13	99.754616	3.931962
0.26	1.728030E+16	30.333333	1.234286E-06	6.126683E-16	4.188384E-15	2.425089E-13	99.735162	3.931908
0.27	1.727681E+16	31.500000	1.234286E-06	6.774701E-16	4.349326E-15	2.611415E-13	99.714967	3.931852
0.28	1.727318E+16	32.666667	1.234286E-06	7.466046E-16	4.510252E-15	2.804610E-13	99.694031	3.931794
0.29	1.726942E+16	33.833333	1.234286E-06	8.202095E-16	4.671161E-15	3.004669E-13	99.672356	3.931734
0.30	1.726554E+16	35.000000	1.234286E-06	8.984227E-16	4.832052E-15	3.211590E-13	99.649942	3.931672
0.31	1.726153E+16	36.166667	1.234286E-06	9.813819E-16	4.992925E-15	3.425367E-13	99.626788	3.931608
0.32	1.725739E+16	37.333333	1.234286E-06	1.069225E-15	5.153780E-15	3.645999E-13	99.602894	3.931541
0.33	1.725312E+16	38.500000	1.234286E-06	1.162089E-15	5.314615E-15	3.873479E-13	99.578262	3.931473
0.34	1.724872E+16	39.666667	1.234286E-06	1.260113E-15	5.475431E-15	4.107806E-13	99.552892	3.931402
0.35	1.724420E+16	40.833333	1.234286E-06	1.363433E-15	5.636226E-15	4.348973E-13	99.526783	3.931330
0.36	1.723955E+16	42.000000	1.234286E-06	1.472188E-15	5.797000E-15	4.596977E-13	99.499936	3.931256
0.37	1.723477E+16	43.166667	1.234286E-06	1.586514E-15	5.957752E-15	4.851813E-13	99.472352	3.931179
0.38	1.722986E+16	44.333333	1.234286E-06	1.706550E-15	6.118483E-15	5.113477E-13	99.444030	3.931100
0.39	1.722483E+16	45.500000	1.234286E-06	1.832433E-15	6.279190E-15	5.381965E-13	99.414971	3.931020
0.40	1.721967E+16	46.666667	1.234286E-06	1.964301E-15	6.439874E-15	5.657270E-13	99.385176	3.930937
0.41	1.721438E+16	47.833333	1.234286E-06	2.102290E-15	6.600534E-15	5.939388E-13	99.354645	3.930853
0.42	1.720896E+16	49.000000	1.234286E-06	2.246538E-15	6.761170E-15	6.228315E-13	99.323378	3.930766
0.43	1.720341E+16	50.166667	1.234286E-06	2.397183E-15	6.921780E-15	6.524045E-13	99.291376	3.930677
0.44	1.719774E+16	51.333333	1.234286E-06	2.554362E-15	7.082364E-15	6.826572E-13	99.258638	3.930586
0.45	1.719194E+16	52.500000	1.234286E-06	2.718211E-15	7.242923E-15	7.135892E-13	99.225167	3.930494

0.46	1.718602E+16	53.666667	1.234286E-06	2.888869E-15	7.403454E-15	7.451998E-13	99.190961	3.930399
0.47	1.717996E+16	54.833333	1.234286E-06	3.066473E-15	7.563957E-15	7.774885E-13	99.156022	3.930302
0.48	1.717378E+16	56.000000	1.234286E-06	3.251158E-15	7.724433E-15	8.104548E-13	99.120349	3.930203
0.49	1.716747E+16	57.166667	1.234286E-06	3.443064E-15	7.884879E-15	8.440980E-13	99.083944	3.930102
0.50	1.716104E+16	58.333333	1.234286E-06	3.642325E-15	8.045297E-15	8.784176E-13	99.046807	3.930000
0.51	1.715448E+16	59.500000	1.234286E-06	3.849081E-15	8.205684E-15	9.134129E-13	99.008938	3.929895
0.52	1.714779E+16	60.666667	1.234286E-06	4.063466E-15	8.366041E-15	9.490833E-13	98.970338	3.929788
0.53	1.714098E+16	61.833333	1.234286E-06	4.285619E-15	8.526366E-15	9.854282E-13	98.931008	3.929679
0.54	1.713403E+16	63.000000	1.234286E-06	4.515676E-15	8.686660E-15	1.022447E-12	98.890947	3.929569
0.55	1.712697E+16	64.166667	1.234286E-06	4.753773E-15	8.846921E-15	1.060139E-12	98.850157	3.929456
0.56	1.711977E+16	65.333333	1.234286E-06	5.000048E-15	9.007149E-15	1.098503E-12	98.808638	3.929341
0.57	1.711245E+16	66.500000	1.234286E-06	5.254637E-15	9.167344E-15	1.137539E-12	98.766391	3.929224
0.58	1.710501E+16	67.666667	1.234286E-06	5.517676E-15	9.327504E-15	1.177247E-12	98.723416	3.929106
0.59	1.709744E+16	68.833333	1.234286E-06	5.789302E-15	9.487630E-15	1.217625E-12	98.679714	3.928985
0.60	1.708974E+16	70.000000	1.234286E-06	6.069652E-15	9.647720E-15	1.258672E-12	98.635286	3.928862
0.61	1.708191E+16	71.166667	1.234286E-06	6.358862E-15	9.807774E-15	1.300389E-12	98.590131	3.928738
0.62	1.707397E+16	72.333333	1.234286E-06	6.657068E-15	9.967791E-15	1.342774E-12	98.544252	3.928611
0.63	1.706589E+16	73.500000	1.234286E-06	6.964406E-15	1.012777E-14	1.385826E-12	98.497648	3.928483
0.64	1.705769E+16	74.666667	1.234286E-06	7.281014E-15	1.028771E-14	1.429545E-12	98.450320	3.928352
0.65	1.704937E+16	75.833333	1.234286E-06	7.607025E-15	1.044762E-14	1.473930E-12	98.402268	3.928220
0.66	1.704091E+16	77.000000	1.234286E-06	7.942578E-15	1.060748E-14	1.518980E-12	98.353494	3.928086
0.67	1.703234E+16	78.166667	1.234286E-06	8.287807E-15	1.076730E-14	1.564695E-12	98.303999	3.927949
0.68	1.702364E+16	79.333333	1.234286E-06	8.642849E-15	1.092709E-14	1.611073E-12	98.253782	3.927811
0.69	1.701481E+16	80.500000	1.234286E-06	9.007840E-15	1.108683E-14	1.658115E-12	98.202845	3.927671
0.70	1.700586E+16	81.666667	1.234286E-06	9.382915E-15	1.124653E-14	1.705818E-12	98.151188	3.927529
0.71	1.699679E+16	82.833333	1.234286E-06	9.768210E-15	1.140619E-14	1.754182E-12	98.098812	3.927385
0.72	1.698759E+16	84.000000	1.234286E-06	1.016386E-14	1.156580E-14	1.803207E-12	98.045718	3.927239
0.73	1.697827E+16	85.166667	1.234286E-06	1.057000E-14	1.172538E-14	1.852891E-12	97.991906	3.927091
0.74	1.696882E+16	86.333333	1.234286E-06	1.098677E-14	1.188490E-14	1.903234E-12	97.937378	3.926941
0.75	1.695925E+16	87.500000	1.234286E-06	1.141430E-14	1.204438E-14	1.954234E-12	97.882135	3.926790
0.76	1.694955E+16	88.666667	1.234286E-06	1.185273E-14	1.220382E-14	2.005892E-12	97.826176	3.926636
0.77	1.693973E+16	89.833333	1.234286E-06	1.230219E-14	1.236321E-14	2.058205E-12	97.769503	3.926481
0.78	1.692979E+16	91.000000	1.234286E-06	1.276282E-14	1.252256E-14	2.111173E-12	97.712116	3.926323
0.79	1.691972E+16	92.166667	1.234286E-06	1.323475E-14	1.268185E-14	2.164796E-12	97.654017	3.926164
0.80	1.690953E+16	93.333333	1.234286E-06	1.371812E-14	1.284110E-14	2.219071E-12	97.595206	3.926003
0.81	1.689922E+16	94.500000	1.234286E-06	1.421306E-14	1.300030E-14	2.273999E-12	97.535685	3.925840
0.82	1.688878E+16	95.666667	1.234286E-06	1.471971E-14	1.315945E-14	2.329579E-12	97.475453	3.925675
0.83	1.687822E+16	96.833333	1.234286E-06	1.523820E-14	1.331855E-14	2.385808E-12	97.414512	3.925509
0.84	1.686754E+16	98.000000	1.234286E-06	1.576867E-14	1.347760E-14	2.442687E-12	97.352864	3.925340
0.85	1.685674E+16	99.166667	1.234286E-06	1.631125E-14	1.363659E-14	2.500215E-12	97.290507	3.925170
0.86	1.684581E+16	100.333333	1.234286E-06	1.686607E-14	1.379554E-14	2.558390E-12	97.227445	3.924997
0.87	1.683476E+16	101.500000	1.234286E-06	1.743328E-14	1.395443E-14	2.617211E-12	97.163677	3.924823
0.88	1.682359E+16	102.666667	1.234286E-06	1.801300E-14	1.411327E-14	2.676678E-12	97.099204	3.924647
0.89	1.681230E+16	103.833333	1.234286E-06	1.860537E-14	1.427206E-14	2.736790E-12	97.034028	3.924470
0.90	1.680089E+16	105.000000	1.234286E-06	1.921052E-14	1.443079E-14	2.797544E-12	96.968149	3.924290
0.91	1.678935E+16	106.166667	1.234286E-06	1.982859E-14	1.458946E-14	2.858941E-12	96.901569	3.924109
0.92	1.677769E+16	107.333333	1.234286E-06	2.045971E-14	1.474808E-14	2.920980E-12	96.834287	3.923925
0.93	1.676592E+16	108.500000	1.234286E-06	2.110401E-14	1.490664E-14	2.983658E-12	96.766306	3.923740
0.94	1.675402E+16	109.666667	1.234286E-06	2.176163E-14	1.506515E-14	3.046976E-12	96.697627	3.923553
0.95	1.674200E+16	110.833333	1.234286E-06	2.243271E-14	1.522359E-14	3.110932E-12	96.628249	3.923365
0.96	1.672985E+16	112.000000	1.234286E-06	2.311736E-14	1.538198E-14	3.175526E-12	96.558175	3.923174
0.97	1.671759E+16	113.166667	1.234286E-06	2.381574E-14	1.554031E-14	3.240755E-12	96.487405	3.922982
0.98	1.670521E+16	114.333333	1.234286E-06	2.452797E-14	1.569858E-14	3.306619E-12	96.415941	3.922788
0.99	1.669271E+16	115.500000	1.234286E-06	2.525419E-14	1.585678E-14	3.373117E-12	96.343783	3.922592
1.00	1.668009E+16	116.666667	1.234286E-06	2.599452E-14	1.601493E-14	3.440247E-12	96.270932	3.922395



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732602E+16	1.166667	3.509890E-07	2.472596E-19	1.639399E-16	7.413712E-16	99.999030	3.955351
0.02	1.732572E+16	2.333333	4.963646E-07	1.091463E-18	3.278798E-16	2.224082E-15	99.997266	3.955342
0.03	1.732527E+16	3.500000	6.079045E-07	2.786050E-18	4.918189E-16	4.448087E-15	99.994707	3.955331
0.04	1.732469E+16	4.666667	7.019241E-07	5.540050E-18	6.557565E-16	7.413332E-15	99.991353	3.955318
0.05	1.732397E+16	5.833333	7.847424E-07	9.535488E-18	8.196916E-16	1.111975E-14	99.987204	3.955304
0.06	1.732312E+16	7.000000	8.595997E-07	1.493575E-17	9.836234E-16	1.556726E-14	99.982260	3.955288
0.07	1.732212E+16	8.166667	9.284205E-07	2.189033E-17	1.147551E-15	2.075578E-14	99.976521	3.955272
0.08	1.732099E+16	9.333333	9.924584E-07	3.053791E-17	1.311473E-15	2.668522E-14	99.969986	3.955254
0.09	1.731972E+16	10.500000	1.052584E-06	4.100838E-17	1.475389E-15	3.335546E-14	99.962657	3.955235
0.10	1.731831E+16	11.666667	1.109431E-06	5.342434E-17	1.639298E-15	4.076640E-14	99.954532	3.955215
0.11	1.731677E+16	12.833333	1.163477E-06	6.790220E-17	1.803199E-15	4.891792E-14	99.945611	3.955195
0.12	1.731508E+16	14.000000	1.215094E-06	8.455306E-17	1.967090E-15	5.780987E-14	99.935896	3.955173
0.13	1.731326E+16	15.166667	1.234286E-06	1.035052E-16	2.130973E-15	6.744202E-14	99.925385	3.955145
0.14	1.731130E+16	16.333333	1.234286E-06	1.248992E-16	2.294847E-15	7.781411E-14	99.914079	3.955112
0.15	1.730921E+16	17.500000	1.234286E-06	1.488756E-16	2.458713E-15	8.892592E-14	99.901979	3.955077
0.16	1.730697E+16	18.666667	1.234286E-06	1.755748E-16	2.622569E-15	1.007772E-13	99.889084	3.955039
0.17	1.730460E+16	19.833333	1.234286E-06	2.051373E-16	2.786415E-15	1.133678E-13	99.875393	3.955000
0.18	1.730209E+16	21.000000	1.234286E-06	2.377036E-16	2.950250E-15	1.266974E-13	99.860909	3.954957
0.19	1.729944E+16	22.166667	1.234286E-06	2.734141E-16	3.114073E-15	1.407657E-13	99.845630	3.954913
0.20	1.729666E+16	23.333333	1.234286E-06	3.124093E-16	3.277885E-15	1.555724E-13	99.829556	3.954866
0.21	1.729374E+16	24.500000	1.234286E-06	3.548295E-16	3.441685E-15	1.711173E-13	99.812689	3.954816
0.22	1.729068E+16	25.666667	1.234286E-06	4.008151E-16	3.605471E-15	1.874000E-13	99.795027	3.954765
0.23	1.728748E+16	26.833333	1.234286E-06	4.505066E-16	3.769244E-15	2.044202E-13	99.776572	3.954711
0.24	1.728414E+16	28.000000	1.234286E-06	5.040441E-16	3.933003E-15	2.221776E-13	99.757324	3.954654
0.25	1.728067E+16	29.166667	1.234286E-06	5.615681E-16	4.096746E-15	2.406718E-13	99.737282	3.954596
0.26	1.727706E+16	30.333333	1.234286E-06	6.232188E-16	4.260475E-15	2.599024E-13	99.716447	3.954535
0.27	1.727331E+16	31.500000	1.234286E-06	6.891365E-16	4.424187E-15	2.798690E-13	99.694819	3.954472
0.28	1.726943E+16	32.666667	1.234286E-06	7.594614E-16	4.587883E-15	3.005713E-13	99.672399	3.954406
0.29	1.726541E+16	33.833333	1.234286E-06	8.343337E-16	4.751561E-15	3.220088E-13	99.649186	3.954338
0.30	1.726125E+16	35.000000	1.234286E-06	9.138936E-16	4.915222E-15	3.441811E-13	99.625182	3.954268
0.31	1.725695E+16	36.166667	1.234286E-06	9.982812E-16	5.078865E-15	3.670878E-13	99.600386	3.954195
0.32	1.725252E+16	37.333333	1.234286E-06	1.087637E-15	5.242488E-15	3.907284E-13	99.574799	3.954121
0.33	1.724795E+16	38.500000	1.234286E-06	1.182100E-15	5.406092E-15	4.151024E-13	99.548421	3.954043
0.34	1.724324E+16	39.666667	1.234286E-06	1.281811E-15	5.569676E-15	4.402093E-13	99.521253	3.953964
0.35	1.723840E+16	40.833333	1.234286E-06	1.386911E-15	5.733239E-15	4.660487E-13	99.493294	3.953882
0.36	1.723342E+16	42.000000	1.234286E-06	1.497538E-15	5.896781E-15	4.926200E-13	99.464546	3.953798
0.37	1.722830E+16	43.166667	1.234286E-06	1.613833E-15	6.060301E-15	5.199228E-13	99.435009	3.953712
0.38	1.722305E+16	44.333333	1.234286E-06	1.735936E-15	6.223798E-15	5.479563E-13	99.404682	3.953623
0.39	1.721765E+16	45.500000	1.234286E-06	1.863986E-15	6.387272E-15	5.767202E-13	99.373568	3.953532
0.40	1.721213E+16	46.666667	1.234286E-06	1.998124E-15	6.550722E-15	6.062138E-13	99.341665	3.953439
0.41	1.720646E+16	47.833333	1.234286E-06	2.138489E-15	6.714148E-15	6.364366E-13	99.308975	3.953343
0.42	1.720066E+16	49.000000	1.234286E-06	2.285221E-15	6.877549E-15	6.673879E-13	99.275498	3.953246
0.43	1.719473E+16	50.166667	1.234286E-06	2.438459E-15	7.040924E-15	6.990672E-13	99.241234	3.953146
0.44	1.718865E+16	51.333333	1.234286E-06	2.598344E-15	7.204273E-15	7.314738E-13	99.206184	3.953043
0.45	1.718244E+16	52.500000	1.234286E-06	2.765015E-15	7.367595E-15	7.646071E-13	99.170349	3.952939

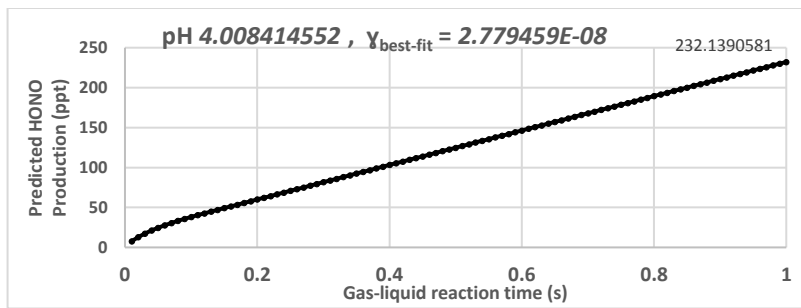
0.46	1.717610E+16	53.666667	1.234286E-06	2.938611E-15	7.530890E-15	7.984664E-13	99.133729	3.952832
0.47	1.716962E+16	54.833333	1.234286E-06	3.119273E-15	7.694157E-15	8.330510E-13	99.096325	3.952722
0.48	1.716300E+16	56.000000	1.234286E-06	3.307138E-15	7.857395E-15	8.683604E-13	99.058137	3.952611
0.49	1.715625E+16	57.166667	1.234286E-06	3.502347E-15	8.020604E-15	9.043937E-13	99.019166	3.952497
0.50	1.714936E+16	58.333333	1.234286E-06	3.705040E-15	8.183783E-15	9.411503E-13	98.979412	3.952381
0.51	1.714234E+16	59.500000	1.234286E-06	3.915355E-15	8.346931E-15	9.786295E-13	98.938877	3.952263
0.52	1.713518E+16	60.666667	1.234286E-06	4.133432E-15	8.510049E-15	1.016831E-12	98.897560	3.952143
0.53	1.712789E+16	61.833333	1.234286E-06	4.359409E-15	8.673134E-15	1.055753E-12	98.855463	3.952020
0.54	1.712046E+16	63.000000	1.234286E-06	4.593427E-15	8.836187E-15	1.095395E-12	98.812585	3.951895
0.55	1.711289E+16	64.166667	1.234286E-06	4.835624E-15	8.999207E-15	1.135757E-12	98.768929	3.951768
0.56	1.710519E+16	65.333333	1.234286E-06	5.086139E-15	9.162193E-15	1.176838E-12	98.724493	3.951639
0.57	1.709736E+16	66.500000	1.234286E-06	5.345111E-15	9.325146E-15	1.218637E-12	98.679280	3.951507
0.58	1.708939E+16	67.666667	1.234286E-06	5.612679E-15	9.488063E-15	1.261152E-12	98.633290	3.951374
0.59	1.708129E+16	68.833333	1.234286E-06	5.888982E-15	9.650944E-15	1.304385E-12	98.586523	3.951238
0.60	1.707305E+16	70.000000	1.234286E-06	6.174158E-15	9.813790E-15	1.348332E-12	98.538981	3.951099
0.61	1.706468E+16	71.166667	1.234286E-06	6.468347E-15	9.976598E-15	1.392995E-12	98.490664	3.950959
0.62	1.705618E+16	72.333333	1.234286E-06	6.771687E-15	1.013937E-14	1.438371E-12	98.441572	3.950816
0.63	1.704754E+16	73.500000	1.234286E-06	7.084317E-15	1.030210E-14	1.484460E-12	98.391708	3.950672
0.64	1.703876E+16	74.666667	1.234286E-06	7.406375E-15	1.046480E-14	1.531261E-12	98.341070	3.950525
0.65	1.702985E+16	75.833333	1.234286E-06	7.738000E-15	1.062745E-14	1.578773E-12	98.289661	3.950376
0.66	1.702081E+16	77.000000	1.234286E-06	8.079329E-15	1.079007E-14	1.626995E-12	98.237482	3.950224
0.67	1.701164E+16	78.166667	1.234286E-06	8.430502E-15	1.095264E-14	1.675927E-12	98.184532	3.950071
0.68	1.700233E+16	79.333333	1.234286E-06	8.791656E-15	1.111517E-14	1.725567E-12	98.130813	3.949915
0.69	1.699289E+16	80.500000	1.234286E-06	9.162931E-15	1.127766E-14	1.775914E-12	98.076325	3.949757
0.70	1.698332E+16	81.666667	1.234286E-06	9.544463E-15	1.144011E-14	1.826968E-12	98.021070	3.949597
0.71	1.697361E+16	82.833333	1.234286E-06	9.936391E-15	1.160252E-14	1.878727E-12	97.965049	3.949435
0.72	1.696377E+16	84.000000	1.234286E-06	1.033885E-14	1.176488E-14	1.931191E-12	97.908262	3.949271
0.73	1.695380E+16	85.166667	1.234286E-06	1.075199E-14	1.192719E-14	1.984358E-12	97.850711	3.949104
0.74	1.694370E+16	86.333333	1.234286E-06	1.117593E-14	1.208946E-14	2.038227E-12	97.792395	3.948936
0.75	1.693346E+16	87.500000	1.234286E-06	1.161082E-14	1.225169E-14	2.092798E-12	97.733317	3.948765
0.76	1.692309E+16	88.666667	1.234286E-06	1.205679E-14	1.241387E-14	2.148070E-12	97.673477	3.948592
0.77	1.691259E+16	89.833333	1.234286E-06	1.251399E-14	1.257600E-14	2.204040E-12	97.612876	3.948418
0.78	1.690196E+16	91.000000	1.234286E-06	1.298255E-14	1.273808E-14	2.260709E-12	97.551515	3.948240
0.79	1.689120E+16	92.166667	1.234286E-06	1.346260E-14	1.290012E-14	2.318075E-12	97.489396	3.948061
0.80	1.688030E+16	93.333333	1.234286E-06	1.395429E-14	1.306210E-14	2.376137E-12	97.426518	3.947880
0.81	1.686928E+16	94.500000	1.234286E-06	1.445775E-14	1.322404E-14	2.434894E-12	97.362884	3.947697
0.82	1.685812E+16	95.666667	1.234286E-06	1.497312E-14	1.338592E-14	2.494345E-12	97.298494	3.947511
0.83	1.684684E+16	96.833333	1.234286E-06	1.550054E-14	1.354775E-14	2.554489E-12	97.233349	3.947324
0.84	1.683542E+16	98.000000	1.234286E-06	1.604014E-14	1.370953E-14	2.615325E-12	97.167451	3.947134
0.85	1.682387E+16	99.166667	1.234286E-06	1.659205E-14	1.387126E-14	2.676851E-12	97.100800	3.946943
0.86	1.681219E+16	100.333333	1.234286E-06	1.715643E-14	1.403294E-14	2.739066E-12	97.033398	3.946749
0.87	1.680038E+16	101.500000	1.234286E-06	1.773340E-14	1.419456E-14	2.801970E-12	96.965245	3.946553
0.88	1.678845E+16	102.666667	1.234286E-06	1.832309E-14	1.435612E-14	2.865560E-12	96.896343	3.946355
0.89	1.677638E+16	103.833333	1.234286E-06	1.892566E-14	1.451763E-14	2.929837E-12	96.826692	3.946156
0.90	1.676418E+16	105.000000	1.234286E-06	1.954122E-14	1.467909E-14	2.994798E-12	96.756295	3.945954
0.91	1.675185E+16	106.166667	1.234286E-06	2.016993E-14	1.484048E-14	3.060442E-12	96.685152	3.945750
0.92	1.673940E+16	107.333333	1.234286E-06	2.081191E-14	1.500182E-14	3.126769E-12	96.613264	3.945544
0.93	1.672681E+16	108.500000	1.234286E-06	2.146730E-14	1.516310E-14	3.193776E-12	96.540632	3.945336
0.94	1.671410E+16	109.666667	1.234286E-06	2.213624E-14	1.532432E-14	3.261464E-12	96.467259	3.945126
0.95	1.670126E+16	110.833333	1.234286E-06	2.281886E-14	1.548549E-14	3.329829E-12	96.393144	3.944914
0.96	1.668829E+16	112.000000	1.234286E-06	2.351530E-14	1.564659E-14	3.398872E-12	96.318289	3.944700
0.97	1.667519E+16	113.166667	1.234286E-06	2.422569E-14	1.580763E-14	3.468591E-12	96.242695	3.944484
0.98	1.666197E+16	114.333333	1.234286E-06	2.495017E-14	1.596861E-14	3.538985E-12	96.166364	3.944266
0.99	1.664862E+16	115.500000	1.234286E-06	2.568888E-14	1.612952E-14	3.610052E-12	96.089297	3.944046
1.00	1.663514E+16	116.666667	1.234286E-06	2.644195E-14	1.629038E-14	3.681791E-12	96.011494	3.943825



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732604E+16	1.166667	3.509894E-07	2.092995E-19	1.387715E-16	6.651359E-16	99.999139	3.980610
0.02	1.732577E+16	2.333333	4.963661E-07	9.238976E-19	2.775431E-16	1.995381E-15	99.997565	3.980601
0.03	1.732537E+16	3.500000	6.079079E-07	2.358326E-18	4.163144E-16	3.990699E-15	99.995278	3.980591
0.04	1.732485E+16	4.666667	7.019306E-07	4.689520E-18	5.550846E-16	6.651044E-15	99.992278	3.980579
0.05	1.732421E+16	5.833333	7.847531E-07	8.071562E-18	6.938533E-16	9.976360E-15	99.988565	3.980565
0.06	1.732344E+16	7.000000	8.596159E-07	1.264275E-17	8.326197E-16	1.396658E-14	99.984138	3.980551
0.07	1.732255E+16	8.166667	9.284435E-07	1.852963E-17	9.713832E-16	1.862164E-14	99.978998	3.980535
0.08	1.732154E+16	9.333333	9.924898E-07	2.584959E-17	1.110143E-15	2.394146E-14	99.973145	3.980518
0.09	1.732040E+16	10.500000	1.052625E-06	3.471257E-17	1.248898E-15	2.992595E-14	99.966578	3.980500
0.10	1.731914E+16	11.666667	1.109484E-06	4.522236E-17	1.387649E-15	3.657502E-14	99.959298	3.980481
0.11	1.731775E+16	12.833333	1.163543E-06	5.747749E-17	1.526393E-15	4.388856E-14	99.951305	3.980461
0.12	1.731625E+16	14.000000	1.215175E-06	7.157199E-17	1.665131E-15	5.186647E-14	99.942598	3.980441
0.13	1.731461E+16	15.166667	1.234286E-06	8.761454E-17	1.803863E-15	6.050854E-14	99.933177	3.980414
0.14	1.731286E+16	16.333333	1.234286E-06	1.057241E-16	1.942588E-15	6.981456E-14	99.923044	3.980383
0.15	1.731098E+16	17.500000	1.234286E-06	1.260196E-16	2.081308E-15	7.978435E-14	99.912197	3.980350
0.16	1.730898E+16	18.666667	1.234286E-06	1.486201E-16	2.220021E-15	9.041772E-14	99.900637	3.980314
0.17	1.730685E+16	19.833333	1.234286E-06	1.736444E-16	2.358727E-15	1.017145E-13	99.888364	3.980276
0.18	1.730460E+16	21.000000	1.234286E-06	2.012115E-16	2.497426E-15	1.136744E-13	99.875379	3.980236
0.19	1.730223E+16	22.166667	1.234286E-06	2.314403E-16	2.636117E-15	1.262973E-13	99.861680	3.980193
0.20	1.729973E+16	23.333333	1.234286E-06	2.644496E-16	2.774799E-15	1.395828E-13	99.847269	3.980149
0.21	1.729711E+16	24.500000	1.234286E-06	3.003584E-16	2.913473E-15	1.535309E-13	99.832146	3.980102
0.22	1.729436E+16	25.666667	1.234286E-06	3.392856E-16	3.052138E-15	1.681411E-13	99.816310	3.980053
0.23	1.729150E+16	26.833333	1.234286E-06	3.813499E-16	3.190794E-15	1.834132E-13	99.799762	3.980001
0.24	1.728851E+16	28.000000	1.234286E-06	4.266702E-16	3.329439E-15	1.993470E-13	99.782502	3.979948
0.25	1.728539E+16	29.166667	1.234286E-06	4.753654E-16	3.468075E-15	2.159421E-13	99.764530	3.979892
0.26	1.728216E+16	30.333333	1.234286E-06	5.275542E-16	3.606700E-15	2.331983E-13	99.745846	3.979834
0.27	1.727880E+16	31.500000	1.234286E-06	5.833554E-16	3.745313E-15	2.511151E-13	99.726451	3.979774
0.28	1.727531E+16	32.666667	1.234286E-06	6.428878E-16	3.883916E-15	2.696924E-13	99.706345	3.979711
0.29	1.727171E+16	33.833333	1.234286E-06	7.062701E-16	4.022506E-15	2.889297E-13	99.685528	3.979647
0.30	1.726798E+16	35.000000	1.234286E-06	7.736211E-16	4.161084E-15	3.088266E-13	99.664000	3.979580
0.31	1.726412E+16	36.166667	1.234286E-06	8.450594E-16	4.299649E-15	3.293829E-13	99.641762	3.979511
0.32	1.726015E+16	37.333333	1.234286E-06	9.207037E-16	4.438201E-15	3.505981E-13	99.618814	3.979440
0.33	1.725605E+16	38.500000	1.234286E-06	1.000673E-15	4.576740E-15	3.724718E-13	99.595156	3.979366
0.34	1.725183E+16	39.666667	1.234286E-06	1.085085E-15	4.715265E-15	3.950036E-13	99.570788	3.979291
0.35	1.724748E+16	40.833333	1.234286E-06	1.174059E-15	4.853775E-15	4.181932E-13	99.545712	3.979213
0.36	1.724301E+16	42.000000	1.234286E-06	1.267714E-15	4.992271E-15	4.420401E-13	99.519926	3.979133
0.37	1.723842E+16	43.166667	1.234286E-06	1.366168E-15	5.130751E-15	4.665438E-13	99.493432	3.979051
0.38	1.723371E+16	44.333333	1.234286E-06	1.469539E-15	5.269216E-15	4.917039E-13	99.466229	3.978967
0.39	1.722887E+16	45.500000	1.234286E-06	1.577946E-15	5.407664E-15	5.175199E-13	99.438319	3.978880
0.40	1.722391E+16	46.666667	1.234286E-06	1.691508E-15	5.546096E-15	5.439914E-13	99.409702	3.978791
0.41	1.721883E+16	47.833333	1.234286E-06	1.810343E-15	5.684512E-15	5.711179E-13	99.380377	3.978700
0.42	1.721363E+16	49.000000	1.234286E-06	1.934570E-15	5.822910E-15	5.988989E-13	99.350346	3.978607
0.43	1.720831E+16	50.166667	1.234286E-06	2.064306E-15	5.961290E-15	6.273339E-13	99.319608	3.978512
0.44	1.720286E+16	51.333333	1.234286E-06	2.199671E-15	6.099652E-15	6.564222E-13	99.288165	3.978415
0.45	1.719729E+16	52.500000	1.234286E-06	2.340782E-15	6.237995E-15	6.861636E-13	99.256017	3.978315

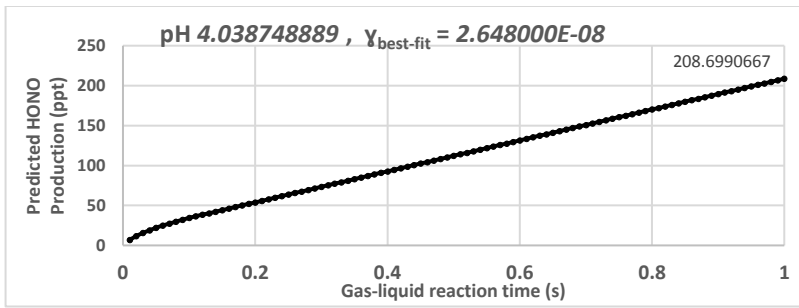


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0.47	1.718578E+16	54.833333	1.234286E-06	2.640716E-15	6.514625E-15	7.476028E-13	99.189605	3.978110
0.48	1.717984E+16	56.000000	1.234286E-06	2.799776E-15	6.652910E-15	7.792996E-13	99.155343	3.978004
0.49	1.717379E+16	57.166667	1.234286E-06	2.965056E-15	6.791175E-15	8.116470E-13	99.120378	3.977895
0.50	1.716761E+16	58.333333	1.234286E-06	3.136673E-15	6.929419E-15	8.446446E-13	99.084710	3.977785
0.51	1.716130E+16	59.500000	1.234286E-06	3.314746E-15	7.067642E-15	8.782917E-13	99.048340	3.977673
0.52	1.715488E+16	60.666667	1.234286E-06	3.499393E-15	7.205843E-15	9.125876E-13	99.011267	3.977558
0.53	1.714834E+16	61.833333	1.234286E-06	3.690731E-15	7.344023E-15	9.475318E-13	98.973493	3.977441
0.54	1.714167E+16	63.000000	1.234286E-06	3.888880E-15	7.482180E-15	9.831237E-13	98.935019	3.977322
0.55	1.713488E+16	64.166667	1.234286E-06	4.093956E-15	7.620314E-15	1.019363E-12	98.895844	3.977201
0.56	1.712797E+16	65.333333	1.234286E-06	4.306078E-15	7.758424E-15	1.056248E-12	98.855969	3.977078
0.57	1.712094E+16	66.500000	1.234286E-06	4.525364E-15	7.896511E-15	1.093779E-12	98.815396	3.976953
0.58	1.711379E+16	67.666667	1.234286E-06	4.751932E-15	8.034574E-15	1.131954E-12	98.774124	3.976826
0.59	1.710652E+16	68.833333	1.234286E-06	4.985898E-15	8.172612E-15	1.170774E-12	98.732154	3.976696
0.60	1.709913E+16	70.000000	1.234286E-06	5.227382E-15	8.310624E-15	1.210238E-12	98.689486	3.976565
0.61	1.709162E+16	71.166667	1.234286E-06	5.476501E-15	8.448612E-15	1.250345E-12	98.646123	3.976431
0.62	1.708398E+16	72.333333	1.234286E-06	5.733372E-15	8.586573E-15	1.291094E-12	98.602063	3.976295
0.63	1.707623E+16	73.500000	1.234286E-06	5.998113E-15	8.724508E-15	1.332484E-12	98.557308	3.976157
0.64	1.706835E+16	74.666667	1.234286E-06	6.270841E-15	8.862416E-15	1.374515E-12	98.511858	3.976017
0.65	1.706036E+16	75.833333	1.234286E-06	6.551675E-15	9.000296E-15	1.417186E-12	98.465714	3.975875
0.66	1.705224E+16	77.000000	1.234286E-06	6.840732E-15	9.138149E-15	1.460496E-12	98.418877	3.975731
0.67	1.704401E+16	78.166667	1.234286E-06	7.138129E-15	9.275973E-15	1.504444E-12	98.371348	3.975585
0.68	1.703565E+16	79.333333	1.234286E-06	7.443983E-15	9.413769E-15	1.549031E-12	98.323127	3.975437
0.69	1.702718E+16	80.500000	1.234286E-06	7.758412E-15	9.551536E-15	1.594254E-12	98.274214	3.975286
0.70	1.701858E+16	81.666667	1.234286E-06	8.081534E-15	9.689273E-15	1.640113E-12	98.224611	3.975134
0.71	1.700987E+16	82.833333	1.234286E-06	8.413464E-15	9.826979E-15	1.686607E-12	98.174319	3.974979
0.72	1.700104E+16	84.000000	1.234286E-06	8.754321E-15	9.964656E-15	1.733736E-12	98.123337	3.974823
0.73	1.699208E+16	85.166667	1.234286E-06	9.104222E-15	1.010230E-14	1.781498E-12	98.071668	3.974664
0.74	1.698301E+16	86.333333	1.234286E-06	9.463284E-15	1.023991E-14	1.829893E-12	98.019311	3.974504
0.75	1.697382E+16	87.500000	1.234286E-06	9.831623E-15	1.037750E-14	1.878920E-12	97.966267	3.974341
0.76	1.696451E+16	88.666667	1.234286E-06	1.020936E-14	1.051505E-14	1.928577E-12	97.912538	3.974176
0.77	1.695509E+16	89.833333	1.234286E-06	1.059660E-14	1.065256E-14	1.978865E-12	97.858124	3.974010
0.78	1.694554E+16	91.000000	1.234286E-06	1.099348E-14	1.079005E-14	2.029782E-12	97.803026	3.973841
0.79	1.693587E+16	92.166667	1.234286E-06	1.140010E-14	1.092749E-14	2.081328E-12	97.747244	3.973670
0.80	1.692609E+16	93.333333	1.234286E-06	1.181658E-14	1.106491E-14	2.133501E-12	97.690780	3.973497
0.81	1.691619E+16	94.500000	1.234286E-06	1.224304E-14	1.120229E-14	2.186300E-12	97.633635	3.973323
0.82	1.690617E+16	95.666667	1.234286E-06	1.267959E-14	1.133963E-14	2.239725E-12	97.575808	3.973146
0.83	1.689603E+16	96.833333	1.234286E-06	1.312636E-14	1.147694E-14	2.293775E-12	97.517302	3.972967
0.84	1.688578E+16	98.000000	1.234286E-06	1.358345E-14	1.161422E-14	2.348449E-12	97.458117	3.972787
0.85	1.687541E+16	99.166667	1.234286E-06	1.405099E-14	1.175145E-14	2.403745E-12	97.398254	3.972604
0.86	1.686492E+16	100.333333	1.234286E-06	1.452909E-14	1.188865E-14	2.459663E-12	97.337714	3.972419
0.87	1.685431E+16	101.500000	1.234286E-06	1.501787E-14	1.202581E-14	2.516202E-12	97.276498	3.972232
0.88	1.684359E+16	102.666667	1.234286E-06	1.551744E-14	1.216294E-14	2.573360E-12	97.214606	3.972044
0.89	1.683275E+16	103.833333	1.234286E-06	1.602792E-14	1.230002E-14	2.631138E-12	97.152040	3.971853
0.90	1.682179E+16	105.000000	1.234286E-06	1.654943E-14	1.243707E-14	2.689533E-12	97.088800	3.971661
0.91	1.681072E+16	106.166667	1.234286E-06	1.708208E-14	1.257407E-14	2.748546E-12	97.024888	3.971466
0.92	1.679953E+16	107.333333	1.234286E-06	1.762599E-14	1.271104E-14	2.808174E-12	96.960305	3.971270
0.93	1.678822E+16	108.500000	1.234286E-06	1.818127E-14	1.284796E-14	2.868416E-12	96.895051	3.971071
0.94	1.677680E+16	109.666667	1.234286E-06	1.874804E-14	1.298485E-14	2.929273E-12	96.829127	3.970871
0.95	1.676526E+16	110.833333	1.234286E-06	1.932641E-14	1.312169E-14	2.990743E-12	96.762535	3.970669
0.96	1.675361E+16	112.000000	1.234286E-06	1.991650E-14	1.325849E-14	3.052824E-12	96.695276	3.970465
0.97	1.674184E+16	113.166667	1.234286E-06	2.051843E-14	1.339525E-14	3.115515E-12	96.627350	3.970259
0.98	1.672996E+16	114.333333	1.234286E-06	2.113232E-14	1.353196E-14	3.178816E-12	96.558758	3.970051
0.99	1.671796E+16	115.500000	1.234286E-06	2.175827E-14	1.366863E-14	3.242726E-12	96.489502	3.969841
1.00	1.670584E+16	116.666667	1.234286E-06	2.239640E-14	1.380526E-14	3.307243E-12	96.419583	3.969629



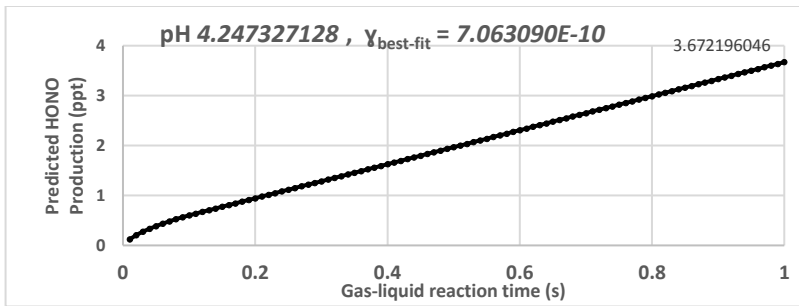
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732604E+16	1.166667	3.509894E-07	1.974003E-19	1.308820E-16	6.687843E-16	99.999143	4.008406
0.02	1.732577E+16	2.333333	4.963661E-07	8.713723E-19	2.617643E-16	2.006325E-15	99.997570	4.008397
0.03	1.732537E+16	3.500000	6.079079E-07	2.224251E-18	3.926465E-16	4.012585E-15	99.995280	4.008385
0.04	1.732485E+16	4.666667	7.019305E-07	4.422917E-18	5.235281E-16	6.687514E-15	99.992273	4.008372
0.05	1.732421E+16	5.833333	7.847530E-07	7.612690E-18	6.544084E-16	1.003106E-14	99.988549	4.008358
0.06	1.732344E+16	7.000000	8.596156E-07	1.192401E-17	7.852868E-16	1.404315E-14	99.984108	4.008342
0.07	1.732254E+16	8.166667	9.284431E-07	1.747623E-17	9.161627E-16	1.872371E-14	99.978949	4.008325
0.08	1.732153E+16	9.333333	9.924891E-07	2.438007E-17	1.047036E-15	2.407266E-14	99.973074	4.008307
0.09	1.732038E+16	10.500000	1.052624E-06	3.273922E-17	1.177905E-15	3.008991E-14	99.966481	4.008288
0.10	1.731912E+16	11.666667	1.109482E-06	4.265157E-17	1.308769E-15	3.677536E-14	99.959171	4.008268
0.11	1.731773E+16	12.833333	1.163541E-06	5.421005E-17	1.439629E-15	4.412891E-14	99.951144	4.008247
0.12	1.731621E+16	14.000000	1.215173E-06	6.750337E-17	1.570482E-15	5.215045E-14	99.942399	4.008225
0.13	1.731457E+16	15.166667	1.234286E-06	8.263401E-17	1.701330E-15	6.083975E-14	99.932938	4.008196
0.14	1.731281E+16	16.333333	1.234286E-06	9.971419E-17	1.832174E-15	7.019659E-14	99.922759	4.008163
0.15	1.731092E+16	17.500000	1.234286E-06	1.188561E-16	1.963012E-15	8.022079E-14	99.911864	4.008127
0.16	1.730891E+16	18.666667	1.234286E-06	1.401720E-16	2.093844E-15	9.091215E-14	99.900252	4.008089
0.17	1.730677E+16	19.833333	1.234286E-06	1.637739E-16	2.224671E-15	1.022705E-13	99.887923	4.008048
0.18	1.730451E+16	21.000000	1.234286E-06	1.897742E-16	2.355491E-15	1.142955E-13	99.874878	4.008005
0.19	1.730213E+16	22.166667	1.234286E-06	2.182849E-16	2.486305E-15	1.269870E-13	99.861116	4.007959
0.20	1.729962E+16	23.333333	1.234286E-06	2.494182E-16	2.617112E-15	1.403448E-13	99.846638	4.007911
0.21	1.729699E+16	24.500000	1.234286E-06	2.832863E-16	2.747912E-15	1.543685E-13	99.831444	4.007861
0.22	1.729423E+16	25.666667	1.234286E-06	3.200012E-16	2.878704E-15	1.690580E-13	99.815534	4.007808
0.23	1.729135E+16	26.833333	1.234286E-06	3.596751E-16	3.009488E-15	1.844128E-13	99.798909	4.007753
0.24	1.728835E+16	28.000000	1.234286E-06	4.024200E-16	3.140264E-15	2.004328E-13	99.781567	4.007696
0.25	1.728522E+16	29.166667	1.234286E-06	4.483482E-16	3.271031E-15	2.171176E-13	99.763511	4.007636
0.26	1.728196E+16	30.333333	1.234286E-06	4.975715E-16	3.401790E-15	2.344669E-13	99.744739	4.007574
0.27	1.727859E+16	31.500000	1.234286E-06	5.502022E-16	3.532539E-15	2.524804E-13	99.725253	4.007510
0.28	1.727509E+16	32.666667	1.234286E-06	6.063521E-16	3.663278E-15	2.711576E-13	99.705051	4.007443
0.29	1.727146E+16	33.833333	1.234286E-06	6.661334E-16	3.794007E-15	2.904983E-13	99.684136	4.007374
0.30	1.726772E+16	35.000000	1.234286E-06	7.296581E-16	3.924726E-15	3.105020E-13	99.662506	4.007302
0.31	1.726385E+16	36.166667	1.234286E-06	7.970381E-16	4.055435E-15	3.311685E-13	99.640163	4.007228
0.32	1.725985E+16	37.333333	1.234286E-06	8.683854E-16	4.186132E-15	3.524972E-13	99.617106	4.007152
0.33	1.725573E+16	38.500000	1.234286E-06	9.438119E-16	4.316818E-15	3.744878E-13	99.593336	4.007073
0.34	1.725149E+16	39.666667	1.234286E-06	1.023430E-15	4.447492E-15	3.971398E-13	99.568853	4.006992
0.35	1.724712E+16	40.833333	1.234286E-06	1.107350E-15	4.578154E-15	4.204529E-13	99.543658	4.006909
0.36	1.724264E+16	42.000000	1.234286E-06	1.195686E-15	4.708803E-15	4.444265E-13	99.517751	4.006823
0.37	1.723802E+16	43.166667	1.234286E-06	1.288549E-15	4.839440E-15	4.690602E-13	99.491132	4.006735
0.38	1.723329E+16	44.333333	1.234286E-06	1.386050E-15	4.970063E-15	4.943536E-13	99.463802	4.006645
0.39	1.722843E+16	45.500000	1.234286E-06	1.488302E-15	5.100673E-15	5.203061E-13	99.435760	4.006552
0.40	1.722345E+16	46.666667	1.234286E-06	1.595416E-15	5.231269E-15	5.469173E-13	99.407008	4.006457
0.41	1.721834E+16	47.833333	1.234286E-06	1.707504E-15	5.361851E-15	5.741866E-13	99.377546	4.006360
0.42	1.721312E+16	49.000000	1.234286E-06	1.824678E-15	5.492419E-15	6.021135E-13	99.347375	4.006260
0.43	1.720777E+16	50.166667	1.234286E-06	1.947050E-15	5.622971E-15	6.306976E-13	99.316494	4.006158
0.44	1.720229E+16	51.333333	1.234286E-06	2.074730E-15	5.753508E-15	6.599382E-13	99.284904	4.006054
0.45	1.719670E+16	52.500000	1.234286E-06	2.207832E-15	5.884029E-15	6.898348E-13	99.252607	4.005947

0.46	1.719098E+16	53.666667	1.234286E-06	2.346466E-15	6.014534E-15	7.203868E-13	99.219601	4.005838
0.47	1.718514E+16	54.833333	1.234286E-06	2.490745E-15	6.145023E-15	7.515937E-13	99.185888	4.005727
0.48	1.717917E+16	56.000000	1.234286E-06	2.640779E-15	6.275495E-15	7.834548E-13	99.151468	4.005613
0.49	1.717309E+16	57.166667	1.234286E-06	2.796680E-15	6.405950E-15	8.159696E-13	99.116342	4.005497
0.50	1.716688E+16	58.333333	1.234286E-06	2.958560E-15	6.536388E-15	8.491374E-13	99.080511	4.005379
0.51	1.716055E+16	59.500000	1.234286E-06	3.126531E-15	6.666807E-15	8.829576E-13	99.043974	4.005259
0.52	1.715410E+16	60.666667	1.234286E-06	3.300703E-15	6.797208E-15	9.174296E-13	99.006732	4.005136
0.53	1.714752E+16	61.833333	1.234286E-06	3.481189E-15	6.927591E-15	9.525527E-13	98.968787	4.005011
0.54	1.714082E+16	63.000000	1.234286E-06	3.668099E-15	7.057955E-15	9.883262E-13	98.930138	4.004883
0.55	1.713401E+16	64.166667	1.234286E-06	3.861545E-15	7.188299E-15	1.024750E-12	98.890786	4.004754
0.56	1.712707E+16	65.333333	1.234286E-06	4.061639E-15	7.318624E-15	1.061822E-12	98.850733	4.004622
0.57	1.712001E+16	66.500000	1.234286E-06	4.268491E-15	7.448928E-15	1.099543E-12	98.809977	4.004488
0.58	1.711282E+16	67.666667	1.234286E-06	4.482213E-15	7.579212E-15	1.137911E-12	98.768521	4.004351
0.59	1.710552E+16	68.833333	1.234286E-06	4.702916E-15	7.709475E-15	1.176927E-12	98.726364	4.004213
0.60	1.709809E+16	70.000000	1.234286E-06	4.930711E-15	7.839716E-15	1.216589E-12	98.683508	4.004072
0.61	1.709055E+16	71.166667	1.234286E-06	5.165710E-15	7.969937E-15	1.256896E-12	98.639952	4.003929
0.62	1.708288E+16	72.333333	1.234286E-06	5.408023E-15	8.100135E-15	1.297848E-12	98.595699	4.003783
0.63	1.707509E+16	73.500000	1.234286E-06	5.657762E-15	8.230310E-15	1.339444E-12	98.550748	4.003636
0.64	1.706718E+16	74.666667	1.234286E-06	5.915038E-15	8.360463E-15	1.381683E-12	98.505100	4.003486
0.65	1.705915E+16	75.833333	1.234286E-06	6.179962E-15	8.490593E-15	1.424565E-12	98.458756	4.003334
0.66	1.705100E+16	77.000000	1.234286E-06	6.452644E-15	8.620699E-15	1.468088E-12	98.411716	4.003180
0.67	1.704273E+16	78.166667	1.234286E-06	6.733195E-15	8.750781E-15	1.512253E-12	98.363982	4.003023
0.68	1.703434E+16	79.333333	1.234286E-06	7.021727E-15	8.880838E-15	1.557057E-12	98.315554	4.002864
0.69	1.702583E+16	80.500000	1.234286E-06	7.318350E-15	9.010871E-15	1.602500E-12	98.266433	4.002703
0.70	1.701720E+16	81.666667	1.234286E-06	7.623175E-15	9.140879E-15	1.648582E-12	98.216620	4.002540
0.71	1.700845E+16	82.833333	1.234286E-06	7.936313E-15	9.270861E-15	1.695301E-12	98.166115	4.002375
0.72	1.699958E+16	84.000000	1.234286E-06	8.257875E-15	9.400817E-15	1.742657E-12	98.114919	4.002207
0.73	1.699059E+16	85.166667	1.234286E-06	8.587970E-15	9.530747E-15	1.790648E-12	98.063033	4.002038
0.74	1.698148E+16	86.333333	1.234286E-06	8.926710E-15	9.660650E-15	1.839275E-12	98.010459	4.001866
0.75	1.697225E+16	87.500000	1.234286E-06	9.274206E-15	9.790525E-15	1.888535E-12	97.957196	4.001692
0.76	1.696290E+16	88.666667	1.234286E-06	9.630567E-15	9.920374E-15	1.938429E-12	97.903245	4.001516
0.77	1.695344E+16	89.833333	1.234286E-06	9.995905E-15	1.005019E-14	1.988954E-12	97.848608	4.001337
0.78	1.694385E+16	91.000000	1.234286E-06	1.037033E-14	1.017999E-14	2.040111E-12	97.793286	4.001157
0.79	1.693415E+16	92.166667	1.234286E-06	1.075395E-14	1.030975E-14	2.091898E-12	97.737278	4.000974
0.80	1.692433E+16	93.333333	1.234286E-06	1.114688E-14	1.043948E-14	2.144315E-12	97.680587	4.000789
0.81	1.691438E+16	94.500000	1.234286E-06	1.154922E-14	1.056919E-14	2.197360E-12	97.623212	4.000602
0.82	1.690433E+16	95.666667	1.234286E-06	1.196110E-14	1.069886E-14	2.251032E-12	97.565156	4.000413
0.83	1.689415E+16	96.833333	1.234286E-06	1.238261E-14	1.082850E-14	2.305331E-12	97.506418	4.000222
0.84	1.688385E+16	98.000000	1.234286E-06	1.281387E-14	1.095812E-14	2.360255E-12	97.447001	4.000029
0.85	1.687344E+16	99.166667	1.234286E-06	1.325499E-14	1.108770E-14	2.415804E-12	97.386903	3.999833
0.86	1.686291E+16	100.333333	1.234286E-06	1.370607E-14	1.121725E-14	2.471976E-12	97.326128	3.999636
0.87	1.685226E+16	101.500000	1.234286E-06	1.416723E-14	1.134676E-14	2.528771E-12	97.264675	3.999436
0.88	1.684150E+16	102.666667	1.234286E-06	1.463859E-14	1.147625E-14	2.586187E-12	97.202546	3.999235
0.89	1.683062E+16	103.833333	1.234286E-06	1.512023E-14	1.160570E-14	2.644224E-12	97.139742	3.999031
0.90	1.681962E+16	105.000000	1.234286E-06	1.561229E-14	1.173512E-14	2.702880E-12	97.076263	3.998825
0.91	1.680850E+16	106.166667	1.234286E-06	1.611486E-14	1.186450E-14	2.762154E-12	97.012111	3.998617
0.92	1.679727E+16	107.333333	1.234286E-06	1.662806E-14	1.199385E-14	2.822046E-12	96.947286	3.998407
0.93	1.678592E+16	108.500000	1.234286E-06	1.715200E-14	1.212317E-14	2.882553E-12	96.881790	3.998195
0.94	1.677446E+16	109.666667	1.234286E-06	1.768678E-14	1.225245E-14	2.943676E-12	96.815624	3.997981
0.95	1.676288E+16	110.833333	1.234286E-06	1.823252E-14	1.238169E-14	3.005413E-12	96.748789	3.997765
0.96	1.675118E+16	112.000000	1.234286E-06	1.878932E-14	1.251090E-14	3.067763E-12	96.681285	3.997546
0.97	1.673937E+16	113.166667	1.234286E-06	1.935730E-14	1.264007E-14	3.130725E-12	96.613114	3.997326
0.98	1.672745E+16	114.333333	1.234286E-06	1.993655E-14	1.276921E-14	3.194297E-12	96.544278	3.997104
0.99	1.671540E+16	115.500000	1.234286E-06	2.052720E-14	1.289830E-14	3.258479E-12	96.474776	3.996880
1.00	1.670325E+16	116.666667	1.234286E-06	2.112936E-14	1.302736E-14	3.323269E-12	96.404611	3.996653



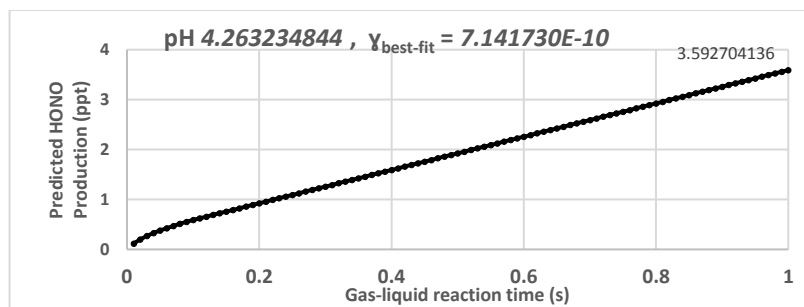
$t_{\text{react}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi\text{HONO}$ (mol)	$\Phi\text{HNO}_2$ (mol)	$\Phi\text{NO}_2$ - (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732605E+16	1.166667	3.509895E-07	1.773346E-19	1.175779E-16	6.442672E-16	99.999184	4.038740
0.02	1.732579E+16	2.333333	4.963667E-07	7.827978E-19	2.351563E-16	1.932775E-15	99.997678	4.038730
0.03	1.732541E+16	3.500000	6.079092E-07	1.998158E-18	3.527348E-16	3.865487E-15	99.995481	4.038719
0.04	1.732491E+16	4.666667	7.019328E-07	3.973332E-18	4.703130E-16	6.442356E-15	99.992593	4.038705
0.05	1.732429E+16	5.833333	7.847566E-07	6.838869E-18	5.878904E-16	9.663326E-15	99.989015	4.038690
0.06	1.732355E+16	7.000000	8.596211E-07	1.071195E-17	7.054665E-16	1.352834E-14	99.984746	4.038674
0.07	1.732269E+16	8.166667	9.284508E-07	1.569980E-17	8.230407E-16	1.803731E-14	99.979786	4.038657
0.08	1.732171E+16	9.333333	9.924996E-07	2.190189E-17	9.406126E-16	2.319018E-14	99.974135	4.038638
0.09	1.732061E+16	10.500000	1.052638E-06	2.941136E-17	1.058182E-15	2.898684E-14	99.967794	4.038618
0.10	1.731939E+16	11.666667	1.109500E-06	3.831615E-17	1.175747E-15	3.542722E-14	99.960762	4.038597
0.11	1.731805E+16	12.833333	1.163563E-06	4.869977E-17	1.293308E-15	4.251120E-14	99.953039	4.038575
0.12	1.731660E+16	14.000000	1.215200E-06	6.064188E-17	1.410865E-15	5.023869E-14	99.944625	4.038553
0.13	1.731502E+16	15.166667	1.234286E-06	7.423459E-17	1.528418E-15	5.860946E-14	99.935520	4.038523
0.14	1.731332E+16	16.333333	1.234286E-06	8.957872E-17	1.645967E-15	6.762330E-14	99.925725	4.038489
0.15	1.731151E+16	17.500000	1.234286E-06	1.067751E-16	1.763512E-15	7.728003E-14	99.915240	4.038452
0.16	1.730957E+16	18.666667	1.234286E-06	1.259244E-16	1.881053E-15	8.757946E-14	99.904064	4.038412
0.17	1.730751E+16	19.833333	1.234286E-06	1.471276E-16	1.998590E-15	9.852139E-14	99.892198	4.038370
0.18	1.730534E+16	21.000000	1.234286E-06	1.704854E-16	2.116122E-15	1.101056E-13	99.879642	4.038326
0.19	1.730304E+16	22.166667	1.234286E-06	1.960985E-16	2.233650E-15	1.223319E-13	99.866396	4.038279
0.20	1.730063E+16	23.333333	1.234286E-06	2.240678E-16	2.351172E-15	1.351999E-13	99.852460	4.038229
0.21	1.729809E+16	24.500000	1.234286E-06	2.544940E-16	2.468689E-15	1.487096E-13	99.837834	4.038177
0.22	1.729544E+16	25.666667	1.234286E-06	2.874778E-16	2.586200E-15	1.628605E-13	99.822519	4.038123
0.23	1.729267E+16	26.833333	1.234286E-06	3.231201E-16	2.703706E-15	1.776524E-13	99.806515	4.038066
0.24	1.728978E+16	28.000000	1.234286E-06	3.615215E-16	2.821205E-15	1.930851E-13	99.789821	4.038007
0.25	1.728676E+16	29.166667	1.234286E-06	4.027827E-16	2.938698E-15	2.091582E-13	99.772439	4.037945
0.26	1.728363E+16	30.333333	1.234286E-06	4.470045E-16	3.056185E-15	2.258715E-13	99.754368	4.037881
0.27	1.728038E+16	31.500000	1.234286E-06	4.942875E-16	3.173665E-15	2.432245E-13	99.735609	4.037814
0.28	1.727701E+16	32.666667	1.234286E-06	5.447325E-16	3.291137E-15	2.612170E-13	99.716161	4.037745
0.29	1.727352E+16	33.833333	1.234286E-06	5.984401E-16	3.408602E-15	2.798486E-13	99.696026	4.037674
0.30	1.726992E+16	35.000000	1.234286E-06	6.555109E-16	3.526060E-15	2.991189E-13	99.675203	4.037600
0.31	1.726619E+16	36.166667	1.234286E-06	7.160457E-16	3.643509E-15	3.190276E-13	99.653692	4.037523
0.32	1.726234E+16	37.333333	1.234286E-06	7.801451E-16	3.760951E-15	3.395743E-13	99.631495	4.037445
0.33	1.725838E+16	38.500000	1.234286E-06	8.479096E-16	3.878384E-15	3.607586E-13	99.608611	4.037363
0.34	1.725429E+16	39.666667	1.234286E-06	9.194399E-16	3.995808E-15	3.825801E-13	99.585040	4.037280
0.35	1.725009E+16	40.833333	1.234286E-06	9.948366E-16	4.113224E-15	4.050384E-13	99.560784	4.037194
0.36	1.724577E+16	42.000000	1.234286E-06	1.074200E-15	4.230630E-15	4.281329E-13	99.535842	4.037105
0.37	1.724133E+16	43.166667	1.234286E-06	1.157631E-15	4.348027E-15	4.518634E-13	99.510214	4.037014
0.38	1.723677E+16	44.333333	1.234286E-06	1.245231E-15	4.465414E-15	4.762293E-13	99.483902	4.036921
0.39	1.723209E+16	45.500000	1.234286E-06	1.337098E-15	4.582791E-15	5.012302E-13	99.456905	4.036825
0.40	1.722730E+16	46.666667	1.234286E-06	1.433335E-15	4.700158E-15	5.268655E-13	99.429224	4.036727
0.41	1.722238E+16	47.833333	1.234286E-06	1.534042E-15	4.817514E-15	5.531349E-13	99.400859	4.036626
0.42	1.721735E+16	49.000000	1.234286E-06	1.639318E-15	4.934860E-15	5.800377E-13	99.371811	4.036523
0.43	1.721220E+16	50.166667	1.234286E-06	1.749265E-15	5.052194E-15	6.075735E-13	99.342080	4.036418
0.44	1.720693E+16	51.333333	1.234286E-06	1.863983E-15	5.169517E-15	6.357418E-13	99.311667	4.036310
0.45	1.720154E+16	52.500000	1.234286E-06	1.983572E-15	5.286829E-15	6.645419E-13	99.280572	4.036200

0.46	1.719604E+16	53.666667	1.234286E-06	2.108133E-15	5.404129E-15	6.939735E-13	99.248795	4.036087
0.47	1.719041E+16	54.833333	1.234286E-06	2.237766E-15	5.521416E-15	7.240358E-13	99.216338	4.035972
0.48	1.718467E+16	56.000000	1.234286E-06	2.372572E-15	5.638691E-15	7.547284E-13	99.183200	4.035855
0.49	1.717881E+16	57.166667	1.234286E-06	2.512650E-15	5.755954E-15	7.860507E-13	99.149382	4.035735
0.50	1.717283E+16	58.333333	1.234286E-06	2.658102E-15	5.873203E-15	8.180020E-13	99.114885	4.035613
0.51	1.716674E+16	59.500000	1.234286E-06	2.809027E-15	5.990440E-15	8.505817E-13	99.079709	4.035489
0.52	1.716053E+16	60.666667	1.234286E-06	2.965525E-15	6.107662E-15	8.837893E-13	99.043854	4.035362
0.53	1.715420E+16	61.833333	1.234286E-06	3.127698E-15	6.224871E-15	9.176241E-13	99.007322	4.035233
0.54	1.714775E+16	63.000000	1.234286E-06	3.295644E-15	6.342066E-15	9.520854E-13	98.970113	4.035102
0.55	1.714119E+16	64.166667	1.234286E-06	3.469465E-15	6.459247E-15	9.871727E-13	98.932227	4.034968
0.56	1.713451E+16	65.333333	1.234286E-06	3.649260E-15	6.576412E-15	1.022885E-12	98.893665	4.034832
0.57	1.712771E+16	66.500000	1.234286E-06	3.835130E-15	6.693563E-15	1.059222E-12	98.854428	4.034693
0.58	1.712079E+16	67.666667	1.234286E-06	4.027174E-15	6.810699E-15	1.096183E-12	98.814517	4.034552
0.59	1.711376E+16	68.833333	1.234286E-06	4.225494E-15	6.927819E-15	1.133768E-12	98.773931	4.034409
0.60	1.710661E+16	70.000000	1.234286E-06	4.430188E-15	7.044923E-15	1.171974E-12	98.732671	4.034264
0.61	1.709935E+16	71.166667	1.234286E-06	4.641357E-15	7.162012E-15	1.210803E-12	98.690739	4.034116
0.62	1.709196E+16	72.333333	1.234286E-06	4.859101E-15	7.279083E-15	1.250252E-12	98.648135	4.033966
0.63	1.708447E+16	73.500000	1.234286E-06	5.083519E-15	7.396139E-15	1.290322E-12	98.604860	4.033813
0.64	1.707685E+16	74.666667	1.234286E-06	5.314713E-15	7.513177E-15	1.331012E-12	98.560913	4.033658
0.65	1.706912E+16	75.833333	1.234286E-06	5.552781E-15	7.630198E-15	1.372320E-12	98.516297	4.033501
0.66	1.706128E+16	77.000000	1.234286E-06	5.797824E-15	7.747201E-15	1.414246E-12	98.471011	4.033342
0.67	1.705331E+16	78.166667	1.234286E-06	6.049941E-15	7.864187E-15	1.456790E-12	98.425057	4.033181
0.68	1.704524E+16	79.333333	1.234286E-06	6.309232E-15	7.981154E-15	1.499950E-12	98.378435	4.033017
0.69	1.703704E+16	80.500000	1.234286E-06	6.575798E-15	8.098103E-15	1.543726E-12	98.331146	4.032850
0.70	1.702873E+16	81.666667	1.234286E-06	6.849737E-15	8.215033E-15	1.588117E-12	98.283190	4.032682
0.71	1.702031E+16	82.833333	1.234286E-06	7.131150E-15	8.331944E-15	1.633121E-12	98.234569	4.032511
0.72	1.701177E+16	84.000000	1.234286E-06	7.420136E-15	8.448835E-15	1.678739E-12	98.185284	4.032338
0.73	1.700312E+16	85.166667	1.234286E-06	7.716794E-15	8.565707E-15	1.724969E-12	98.135334	4.032163
0.74	1.699435E+16	86.333333	1.234286E-06	8.021226E-15	8.682559E-15	1.771811E-12	98.084721	4.031986
0.75	1.698546E+16	87.500000	1.234286E-06	8.333529E-15	8.799391E-15	1.819264E-12	98.033446	4.031806
0.76	1.697646E+16	88.666667	1.234286E-06	8.653804E-15	8.916202E-15	1.867326E-12	97.981509	4.031624
0.77	1.696735E+16	89.833333	1.234286E-06	8.982149E-15	9.032992E-15	1.915997E-12	97.928911	4.031440
0.78	1.695812E+16	91.000000	1.234286E-06	9.318666E-15	9.149761E-15	1.965276E-12	97.875654	4.031254
0.79	1.694878E+16	92.166667	1.234286E-06	9.663452E-15	9.266508E-15	2.015162E-12	97.821738	4.031065
0.80	1.693933E+16	93.333333	1.234286E-06	1.001661E-14	9.383233E-15	2.065655E-12	97.767163	4.030874
0.81	1.692976E+16	94.500000	1.234286E-06	1.037823E-14	9.499936E-15	2.116753E-12	97.711932	4.030681
0.82	1.692007E+16	95.666667	1.234286E-06	1.074843E-14	9.616617E-15	2.168455E-12	97.656044	4.030486
0.83	1.691028E+16	96.833333	1.234286E-06	1.112728E-14	9.733275E-15	2.220760E-12	97.599500	4.030289
0.84	1.690037E+16	98.000000	1.234286E-06	1.151491E-14	9.849909E-15	2.273668E-12	97.542302	4.030089
0.85	1.689034E+16	99.166667	1.234286E-06	1.191140E-14	9.966520E-15	2.327178E-12	97.484451	4.029887
0.86	1.688021E+16	100.333333	1.234286E-06	1.231686E-14	1.008311E-14	2.381288E-12	97.425946	4.029683
0.87	1.686996E+16	101.500000	1.234286E-06	1.273138E-14	1.019967E-14	2.435997E-12	97.366790	4.029477
0.88	1.685959E+16	102.666667	1.234286E-06	1.315507E-14	1.031621E-14	2.491306E-12	97.306984	4.029269
0.89	1.684912E+16	103.833333	1.234286E-06	1.358801E-14	1.043272E-14	2.547211E-12	97.246527	4.029059
0.90	1.683853E+16	105.000000	1.234286E-06	1.403032E-14	1.054921E-14	2.603714E-12	97.185422	4.028846
0.91	1.682783E+16	106.166667	1.234286E-06	1.448209E-14	1.066567E-14	2.660812E-12	97.123668	4.028632
0.92	1.681702E+16	107.333333	1.234286E-06	1.494341E-14	1.078211E-14	2.718504E-12	97.061268	4.028415
0.93	1.680610E+16	108.500000	1.234286E-06	1.541440E-14	1.089852E-14	2.776790E-12	96.998222	4.028196
0.94	1.679506E+16	109.666667	1.234286E-06	1.589514E-14	1.101491E-14	2.835668E-12	96.934531	4.027975
0.95	1.678392E+16	110.833333	1.234286E-06	1.638573E-14	1.113126E-14	2.895138E-12	96.870197	4.027752
0.96	1.677266E+16	112.000000	1.234286E-06	1.688628E-14	1.124759E-14	2.955198E-12	96.805219	4.027527
0.97	1.676129E+16	113.166667	1.234286E-06	1.739688E-14	1.136390E-14	3.015848E-12	96.739600	4.027299
0.98	1.674981E+16	114.333333	1.234286E-06	1.791763E-14	1.148017E-14	3.077085E-12	96.673339	4.027070
0.99	1.673822E+16	115.500000	1.234286E-06	1.844864E-14	1.159642E-14	3.138910E-12	96.606440	4.026838
1.00	1.672651E+16	116.666667	1.234286E-06	1.898999E-14	1.171263E-14	3.201321E-12	96.538901	4.026605



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732619E+16	1.166667	3.509923E-07	3.109070E-21	2.061418E-18	1.825967E-17	99.999978	4.247327
0.02	1.732618E+16	2.333333	4.963779E-07	1.372410E-20	4.122838E-18	5.477897E-17	99.999937	4.247326
0.03	1.732617E+16	3.500000	6.079359E-07	3.503173E-20	6.184258E-18	1.095579E-16	99.999876	4.247326
0.04	1.732616E+16	4.666667	7.019833E-07	6.966005E-20	8.245679E-18	1.825963E-16	99.999796	4.247325
0.05	1.732614E+16	5.833333	7.848404E-07	1.198976E-19	1.030710E-17	2.738943E-16	99.999696	4.247324
0.06	1.732612E+16	7.000000	8.597486E-07	1.877983E-19	1.236852E-17	3.834516E-16	99.999576	4.247324
0.07	1.732609E+16	8.166667	9.286333E-07	2.752417E-19	1.442995E-17	5.112684E-16	99.999437	4.247323
0.08	1.732607E+16	9.333333	9.927492E-07	3.839709E-19	1.649137E-17	6.573444E-16	99.999278	4.247322
0.09	1.732604E+16	10.500000	1.052968E-06	5.156185E-19	1.855280E-17	8.216795E-16	99.999100	4.247321
0.10	1.732600E+16	11.666667	1.109923E-06	6.717255E-19	2.061422E-17	1.004274E-15	99.998902	4.247320
0.11	1.732596E+16	12.833333	1.164095E-06	8.537550E-19	2.267564E-17	1.205127E-15	99.998684	4.247319
0.12	1.732592E+16	14.000000	1.215854E-06	1.063103E-18	2.473707E-17	1.424239E-15	99.998447	4.247318
0.13	1.732588E+16	15.166667	1.234286E-06	1.301390E-18	2.679849E-17	1.661610E-15	99.998191	4.247317
0.14	1.732583E+16	16.333333	1.234286E-06	1.570385E-18	2.885992E-17	1.917239E-15	99.997914	4.247315
0.15	1.732578E+16	17.500000	1.234286E-06	1.871856E-18	3.092134E-17	2.191126E-15	99.997618	4.247314
0.16	1.732572E+16	18.666667	1.234286E-06	2.207570E-18	3.298277E-17	2.483271E-15	99.997303	4.247312
0.17	1.732567E+16	19.833333	1.234286E-06	2.579297E-18	3.504420E-17	2.793674E-15	99.996968	4.247310
0.18	1.732560E+16	21.000000	1.234286E-06	2.988805E-18	3.710563E-17	3.122335E-15	99.996613	4.247308
0.19	1.732554E+16	22.166667	1.234286E-06	3.437861E-18	3.916706E-17	3.469253E-15	99.996239	4.247306
0.20	1.732547E+16	23.333333	1.234286E-06	3.928235E-18	4.122849E-17	3.834427E-15	99.995845	4.247303
0.21	1.732540E+16	24.500000	1.234286E-06	4.461694E-18	4.328993E-17	4.217859E-15	99.995432	4.247301
0.22	1.732532E+16	25.666667	1.234286E-06	5.040006E-18	4.535136E-17	4.619547E-15	99.994999	4.247298
0.23	1.732525E+16	26.833333	1.234286E-06	5.664941E-18	4.741280E-17	5.039491E-15	99.994546	4.247296
0.24	1.732516E+16	28.000000	1.234286E-06	6.338265E-18	4.947424E-17	5.477691E-15	99.994074	4.247293
0.25	1.732508E+16	29.166667	1.234286E-06	7.061749E-18	5.153568E-17	5.934146E-15	99.993583	4.247290
0.26	1.732499E+16	30.333333	1.234286E-06	7.837159E-18	5.359713E-17	6.408856E-15	99.993071	4.247287
0.27	1.732490E+16	31.500000	1.234286E-06	8.666264E-18	5.565857E-17	6.901822E-15	99.992540	4.247284
0.28	1.732480E+16	32.666667	1.234286E-06	9.550832E-18	5.772002E-17	7.413041E-15	99.991990	4.247281
0.29	1.732470E+16	33.833333	1.234286E-06	1.049263E-17	5.978147E-17	7.942515E-15	99.991419	4.247278
0.30	1.732460E+16	35.000000	1.234286E-06	1.149343E-17	6.184293E-17	8.490242E-15	99.990829	4.247274
0.31	1.732450E+16	36.166667	1.234286E-06	1.255500E-17	6.390438E-17	9.056223E-15	99.990220	4.247271
0.32	1.732439E+16	37.333333	1.234286E-06	1.367911E-17	6.596584E-17	9.640456E-15	99.989591	4.247267
0.33	1.732428E+16	38.500000	1.234286E-06	1.486752E-17	6.802730E-17	1.024294E-14	99.988942	4.247263
0.34	1.732416E+16	39.666667	1.234286E-06	1.612200E-17	7.008876E-17	1.086368E-14	99.988274	4.247260
0.35	1.732404E+16	40.833333	1.234286E-06	1.744432E-17	7.215023E-17	1.150267E-14	99.987586	4.247256
0.36	1.732392E+16	42.000000	1.234286E-06	1.883626E-17	7.421170E-17	1.215991E-14	99.986879	4.247252
0.37	1.732379E+16	43.166667	1.234286E-06	2.029957E-17	7.627317E-17	1.283540E-14	99.986151	4.247247
0.38	1.732366E+16	44.333333	1.234286E-06	2.183603E-17	7.833465E-17	1.352914E-14	99.985405	4.247243
0.39	1.732353E+16	45.500000	1.234286E-06	2.344741E-17	8.039613E-17	1.424113E-14	99.984638	4.247239
0.40	1.732339E+16	46.666667	1.234286E-06	2.513546E-17	8.245761E-17	1.497137E-14	99.983852	4.247234
0.41	1.732325E+16	47.833333	1.234286E-06	2.690197E-17	8.451909E-17	1.571985E-14	99.983047	4.247229
0.42	1.732311E+16	49.000000	1.234286E-06	2.874870E-17	8.658058E-17	1.648659E-14	99.982221	4.247225
0.43	1.732296E+16	50.166667	1.234286E-06	3.067742E-17	8.864207E-17	1.727157E-14	99.981376	4.247220
0.44	1.732281E+16	51.333333	1.234286E-06	3.268989E-17	9.070356E-17	1.807480E-14	99.980512	4.247215
0.45	1.732266E+16	52.500000	1.234286E-06	3.478789E-17	9.276506E-17	1.889627E-14	99.979628	4.247210

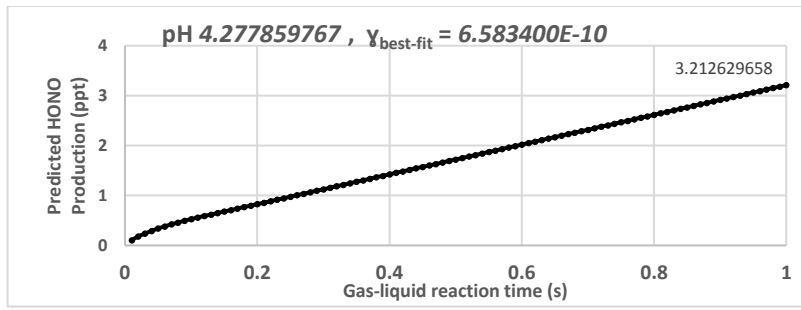
0.46	1.732250E+16	53.666667	1.234286E-06	3.697319E-17	9.482656E-17	1.973599E-14	99.978724	4.247204
0.47	1.732234E+16	54.833333	1.234286E-06	3.924754E-17	9.688807E-17	2.059396E-14	99.977801	4.247199
0.48	1.732218E+16	56.000000	1.234286E-06	4.161273E-17	9.894958E-17	2.147017E-14	99.976858	4.247194
0.49	1.732201E+16	57.166667	1.234286E-06	4.407051E-17	1.010111E-16	2.236462E-14	99.975895	4.247188
0.50	1.732184E+16	58.333333	1.234286E-06	4.662266E-17	1.030726E-16	2.327731E-14	99.974913	4.247182
0.51	1.732167E+16	59.500000	1.234286E-06	4.927095E-17	1.051341E-16	2.420825E-14	99.973911	4.247177
0.52	1.732149E+16	60.666667	1.234286E-06	5.201714E-17	1.071957E-16	2.515743E-14	99.972889	4.247171
0.53	1.732131E+16	61.833333	1.234286E-06	5.486300E-17	1.092572E-16	2.612485E-14	99.971848	4.247165
0.54	1.732113E+16	63.000000	1.234286E-06	5.781030E-17	1.113187E-16	2.711051E-14	99.970787	4.247159
0.55	1.732094E+16	64.166667	1.234286E-06	6.086082E-17	1.133803E-16	2.811441E-14	99.969706	4.247152
0.56	1.732075E+16	65.333333	1.234286E-06	6.401631E-17	1.154418E-16	2.913654E-14	99.968606	4.247146
0.57	1.732056E+16	66.500000	1.234286E-06	6.727854E-17	1.175033E-16	3.017692E-14	99.967486	4.247140
0.58	1.732036E+16	67.666667	1.234286E-06	7.064929E-17	1.195649E-16	3.123553E-14	99.966347	4.247133
0.59	1.732016E+16	68.833333	1.234286E-06	7.413033E-17	1.216265E-16	3.231238E-14	99.965188	4.247126
0.60	1.731996E+16	70.000000	1.234286E-06	7.772341E-17	1.236880E-16	3.340746E-14	99.964009	4.247119
0.61	1.731975E+16	71.166667	1.234286E-06	8.143032E-17	1.257496E-16	3.452078E-14	99.962811	4.247113
0.62	1.731954E+16	72.333333	1.234286E-06	8.525281E-17	1.278112E-16	3.565233E-14	99.961593	4.247105
0.63	1.731932E+16	73.500000	1.234286E-06	8.919267E-17	1.298727E-16	3.680211E-14	99.960355	4.247098
0.64	1.731910E+16	74.666667	1.234286E-06	9.325164E-17	1.319343E-16	3.797013E-14	99.959098	4.247091
0.65	1.731888E+16	75.833333	1.234286E-06	9.743151E-17	1.339959E-16	3.915638E-14	99.957821	4.247084
0.66	1.731866E+16	77.000000	1.234286E-06	1.017340E-16	1.360575E-16	4.036085E-14	99.956524	4.247076
0.67	1.731843E+16	78.166667	1.234286E-06	1.061610E-16	1.381191E-16	4.158356E-14	99.955208	4.247069
0.68	1.731820E+16	79.333333	1.234286E-06	1.107142E-16	1.401807E-16	4.282449E-14	99.953872	4.247061
0.69	1.731796E+16	80.500000	1.234286E-06	1.153953E-16	1.422423E-16	4.408366E-14	99.952516	4.247053
0.70	1.731773E+16	81.666667	1.234286E-06	1.202062E-16	1.443039E-16	4.536105E-14	99.951141	4.247045
0.71	1.731748E+16	82.833333	1.234286E-06	1.251486E-16	1.463655E-16	4.665666E-14	99.949746	4.247037
0.72	1.731724E+16	84.000000	1.234286E-06	1.302242E-16	1.484271E-16	4.797050E-14	99.948331	4.247029
0.73	1.731699E+16	85.166667	1.234286E-06	1.354349E-16	1.504888E-16	4.930256E-14	99.946897	4.247021
0.74	1.731674E+16	86.333333	1.234286E-06	1.407824E-16	1.525504E-16	5.065285E-14	99.945443	4.247012
0.75	1.731648E+16	87.500000	1.234286E-06	1.462685E-16	1.546120E-16	5.202136E-14	99.943969	4.247004
0.76	1.731622E+16	88.666667	1.234286E-06	1.518949E-16	1.566737E-16	5.340808E-14	99.942476	4.246995
0.77	1.731596E+16	89.833333	1.234286E-06	1.576635E-16	1.587353E-16	5.481303E-14	99.940963	4.246986
0.78	1.731570E+16	91.000000	1.234286E-06	1.635759E-16	1.607970E-16	5.623620E-14	99.939431	4.246978
0.79	1.731543E+16	92.166667	1.234286E-06	1.696340E-16	1.628587E-16	5.767758E-14	99.937878	4.246969
0.80	1.731516E+16	93.333333	1.234286E-06	1.758395E-16	1.649203E-16	5.913718E-14	99.936306	4.246960
0.81	1.731488E+16	94.500000	1.234286E-06	1.821942E-16	1.669820E-16	6.061499E-14	99.934715	4.246950
0.82	1.731460E+16	95.666667	1.234286E-06	1.886999E-16	1.690437E-16	6.211102E-14	99.933104	4.246941
0.83	1.731432E+16	96.833333	1.234286E-06	1.953583E-16	1.711054E-16	6.362527E-14	99.931473	4.246932
0.84	1.731403E+16	98.000000	1.234286E-06	2.021712E-16	1.731671E-16	6.515772E-14	99.929822	4.246922
0.85	1.731374E+16	99.166667	1.234286E-06	2.091403E-16	1.752288E-16	6.670838E-14	99.928152	4.246912
0.86	1.731345E+16	100.333333	1.234286E-06	2.162675E-16	1.772905E-16	6.827726E-14	99.926462	4.246903
0.87	1.731315E+16	101.500000	1.234286E-06	2.235545E-16	1.793522E-16	6.986434E-14	99.924752	4.246893
0.88	1.731285E+16	102.666667	1.234286E-06	2.310031E-16	1.814139E-16	7.146963E-14	99.923023	4.246883
0.89	1.731255E+16	103.833333	1.234286E-06	2.386150E-16	1.834757E-16	7.309313E-14	99.921274	4.246873
0.90	1.731224E+16	105.000000	1.234286E-06	2.463920E-16	1.855374E-16	7.473483E-14	99.919506	4.246863
0.91	1.731193E+16	106.166667	1.234286E-06	2.543359E-16	1.875992E-16	7.639474E-14	99.917717	4.246852
0.92	1.731162E+16	107.333333	1.234286E-06	2.624485E-16	1.896609E-16	7.807284E-14	99.915909	4.246842
0.93	1.731130E+16	108.500000	1.234286E-06	2.707314E-16	1.917227E-16	7.976915E-14	99.914082	4.246831
0.94	1.731098E+16	109.666667	1.234286E-06	2.791866E-16	1.937844E-16	8.148366E-14	99.912235	4.246821
0.95	1.731066E+16	110.833333	1.234286E-06	2.878157E-16	1.958462E-16	8.321637E-14	99.910368	4.246810
0.96	1.731033E+16	112.000000	1.234286E-06	2.966205E-16	1.979080E-16	8.496727E-14	99.908481	4.246799
0.97	1.731000E+16	113.166667	1.234286E-06	3.056029E-16	1.999698E-16	8.673637E-14	99.906575	4.246788
0.98	1.730967E+16	114.333333	1.234286E-06	3.147644E-16	2.020316E-16	8.852367E-14	99.904649	4.246777
0.99	1.730933E+16	115.500000	1.234286E-06	3.241071E-16	2.040934E-16	9.032915E-14	99.902703	4.246766
1.00	1.730899E+16	116.666667	1.234286E-06	3.336325E-16	2.061552E-16	9.215283E-14	99.900738	4.246754



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO2}}$ (mol)	$\Phi_{\text{NO2}}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732619E+16	1.166667	3.509923E-07	3.041717E-21	2.016761E-18	1.853058E-17	99.999978	4.263234
0.02	1.732618E+16	2.333333	4.963779E-07	1.342679E-20	4.033524E-18	5.559170E-17	99.999936	4.263234
0.03	1.732617E+16	3.500000	6.079359E-07	3.427283E-20	6.050288E-18	1.111833E-16	99.999874	4.263233
0.04	1.732616E+16	4.666667	7.019833E-07	6.815100E-20	8.067052E-18	1.853054E-16	99.999793	4.263233
0.05	1.732614E+16	5.833333	7.848404E-07	1.173002E-19	1.008382E-17	2.779579E-16	99.999691	4.263232
0.06	1.732612E+16	7.000000	8.597485E-07	1.837300E-19	1.210058E-17	3.891407E-16	99.999570	4.263231
0.07	1.732609E+16	8.166667	9.286333E-07	2.692791E-19	1.411735E-17	5.188537E-16	99.999429	4.263230
0.08	1.732606E+16	9.333333	9.927491E-07	3.756529E-19	1.613412E-17	6.670969E-16	99.999268	4.263229
0.09	1.732603E+16	10.500000	1.052968E-06	5.044486E-19	1.815089E-17	8.338702E-16	99.999087	4.263229
0.10	1.732600E+16	11.666667	1.109923E-06	6.571739E-19	2.016766E-17	1.019173E-15	99.998886	4.263228
0.11	1.732596E+16	12.833333	1.164095E-06	8.352602E-19	2.218442E-17	1.223006E-15	99.998666	4.263226
0.12	1.732592E+16	14.000000	1.215854E-06	1.040073E-18	2.420119E-17	1.445369E-15	99.998425	4.263225
0.13	1.732587E+16	15.166667	1.234286E-06	1.273198E-18	2.621796E-17	1.686262E-15	99.998165	4.263224
0.14	1.732582E+16	16.333333	1.234286E-06	1.536366E-18	2.823473E-17	1.945683E-15	99.997885	4.263222
0.15	1.732577E+16	17.500000	1.234286E-06	1.831306E-18	3.025150E-17	2.223634E-15	99.997584	4.263221
0.16	1.732572E+16	18.666667	1.234286E-06	2.159748E-18	3.226828E-17	2.520113E-15	99.997264	4.263219
0.17	1.732566E+16	19.833333	1.234286E-06	2.523422E-18	3.428505E-17	2.835121E-15	99.996925	4.263217
0.18	1.732560E+16	21.000000	1.234286E-06	2.924059E-18	3.630183E-17	3.168657E-15	99.996565	4.263214
0.19	1.732553E+16	22.166667	1.234286E-06	3.363388E-18	3.831861E-17	3.520721E-15	99.996185	4.263212
0.20	1.732546E+16	23.333333	1.234286E-06	3.843138E-18	4.033539E-17	3.891313E-15	99.995786	4.263210
0.21	1.732539E+16	24.500000	1.234286E-06	4.365041E-18	4.235217E-17	4.280432E-15	99.995366	4.263207
0.22	1.732531E+16	25.666667	1.234286E-06	4.930826E-18	4.436895E-17	4.688079E-15	99.994927	4.263205
0.23	1.732523E+16	26.833333	1.234286E-06	5.542223E-18	4.638574E-17	5.114252E-15	99.994468	4.263202
0.24	1.732515E+16	28.000000	1.234286E-06	6.200962E-18	4.840253E-17	5.558952E-15	99.993989	4.263199
0.25	1.732506E+16	29.166667	1.234286E-06	6.908773E-18	5.041932E-17	6.022178E-15	99.993490	4.263196
0.26	1.732497E+16	30.333333	1.234286E-06	7.667386E-18	5.243611E-17	6.503930E-15	99.992971	4.263193
0.27	1.732488E+16	31.500000	1.234286E-06	8.478531E-18	5.445291E-17	7.004207E-15	99.992432	4.263190
0.28	1.732478E+16	32.666667	1.234286E-06	9.343938E-18	5.646971E-17	7.523010E-15	99.991873	4.263186
0.29	1.732468E+16	33.833333	1.234286E-06	1.026534E-17	5.848651E-17	8.060336E-15	99.991295	4.263183
0.30	1.732458E+16	35.000000	1.234286E-06	1.124446E-17	6.050332E-17	8.616188E-15	99.990696	4.263179
0.31	1.732447E+16	36.166667	1.234286E-06	1.228303E-17	6.252013E-17	9.190562E-15	99.990078	4.263176
0.32	1.732436E+16	37.333333	1.234286E-06	1.338279E-17	6.453694E-17	9.783461E-15	99.989440	4.263172
0.33	1.732425E+16	38.500000	1.234286E-06	1.454545E-17	6.655375E-17	1.039488E-14	99.988782	4.263168
0.34	1.732413E+16	39.666667	1.234286E-06	1.577276E-17	6.857057E-17	1.102482E-14	99.988103	4.263164
0.35	1.732401E+16	40.833333	1.234286E-06	1.706644E-17	7.058739E-17	1.167329E-14	99.987405	4.263160
0.36	1.732388E+16	42.000000	1.234286E-06	1.842823E-17	7.260422E-17	1.234028E-14	99.986688	4.263155
0.37	1.732376E+16	43.166667	1.234286E-06	1.985984E-17	7.462104E-17	1.302578E-14	99.985950	4.263151
0.38	1.732363E+16	44.333333	1.234286E-06	2.136302E-17	7.663788E-17	1.372981E-14	99.985192	4.263146
0.39	1.732349E+16	45.500000	1.234286E-06	2.293949E-17	7.865471E-17	1.445236E-14	99.984415	4.263142
0.40	1.732335E+16	46.666667	1.234286E-06	2.459099E-17	8.067155E-17	1.519343E-14	99.983617	4.263137
0.41	1.732321E+16	47.833333	1.234286E-06	2.631923E-17	8.268840E-17	1.595301E-14	99.982800	4.263132
0.42	1.732307E+16	49.000000	1.234286E-06	2.812596E-17	8.470525E-17	1.673111E-14	99.981962	4.263127
0.43	1.732292E+16	50.166667	1.234286E-06	3.001290E-17	8.672210E-17	1.752774E-14	99.981105	4.263122
0.44	1.732277E+16	51.333333	1.234286E-06	3.198179E-17	8.873895E-17	1.834287E-14	99.980228	4.263117
0.45	1.732261E+16	52.500000	1.234286E-06	3.403434E-17	9.075582E-17	1.917653E-14	99.979331	4.263111

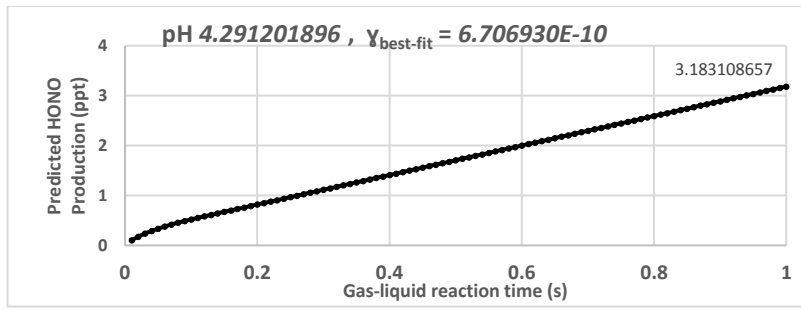






$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi\text{HONO}$ (mol)	$\Phi\text{HNO}_2$ (mol)	$\Phi\text{NO}_2$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732619E+16	1.166667	3.509923E-07	2.719910E-21	1.803393E-18	1.713759E-17	99.999980	4.277859
0.02	1.732618E+16	2.333333	4.963779E-07	1.200627E-20	3.606786E-18	5.141273E-17	99.999941	4.277859
0.03	1.732617E+16	3.500000	6.079359E-07	3.064684E-20	5.410181E-18	1.028254E-16	99.999884	4.277858
0.04	1.732616E+16	4.666667	7.019834E-07	6.094077E-20	7.213576E-18	1.713755E-16	99.999809	4.277858
0.05	1.732614E+16	5.833333	7.848406E-07	1.048901E-19	9.016973E-18	2.570631E-16	99.999715	4.277857
0.06	1.732612E+16	7.000000	8.597488E-07	1.642918E-19	1.082037E-17	3.598880E-16	99.999603	4.277856
0.07	1.732610E+16	8.166667	9.286337E-07	2.407900E-19	1.262377E-17	4.798503E-16	99.999472	4.277856
0.08	1.732607E+16	9.333333	9.927497E-07	3.359096E-19	1.442717E-17	6.169497E-16	99.999324	4.277855
0.09	1.732604E+16	10.500000	1.052968E-06	4.510790E-19	1.623057E-17	7.711863E-16	99.999156	4.277854
0.10	1.732601E+16	11.666667	1.109924E-06	5.876463E-19	1.803396E-17	9.425599E-16	99.998971	4.277853
0.11	1.732598E+16	12.833333	1.164096E-06	7.468914E-19	1.983736E-17	1.131070E-15	99.998767	4.277852
0.12	1.732594E+16	14.000000	1.215856E-06	9.300355E-19	2.164076E-17	1.336718E-15	99.998544	4.277851
0.13	1.732590E+16	15.166667	1.234286E-06	1.138497E-18	2.344416E-17	1.559502E-15	99.998304	4.277849
0.14	1.732585E+16	16.333333	1.234286E-06	1.373822E-18	2.524756E-17	1.799422E-15	99.998045	4.277848
0.15	1.732580E+16	17.500000	1.234286E-06	1.637557E-18	2.705097E-17	2.056479E-15	99.997767	4.277846
0.16	1.732575E+16	18.666667	1.234286E-06	1.931251E-18	2.885437E-17	2.330672E-15	99.997471	4.277844
0.17	1.732570E+16	19.833333	1.234286E-06	2.256450E-18	3.065778E-17	2.622000E-15	99.997157	4.277842
0.18	1.732564E+16	21.000000	1.234286E-06	2.614700E-18	3.246118E-17	2.930464E-15	99.996824	4.277840
0.19	1.732558E+16	22.166667	1.234286E-06	3.007548E-18	3.426459E-17	3.256064E-15	99.996473	4.277838
0.20	1.732552E+16	23.333333	1.234286E-06	3.436542E-18	3.606801E-17	3.598798E-15	99.996104	4.277836
0.21	1.732545E+16	24.500000	1.234286E-06	3.903229E-18	3.787142E-17	3.958668E-15	99.995716	4.277833
0.22	1.732538E+16	25.666667	1.234286E-06	4.409155E-18	3.967483E-17	4.335672E-15	99.995310	4.277831
0.23	1.732530E+16	26.833333	1.234286E-06	4.955868E-18	4.147825E-17	4.729810E-15	99.994885	4.277828
0.24	1.732523E+16	28.000000	1.234286E-06	5.544914E-18	4.328167E-17	5.141082E-15	99.994442	4.277825
0.25	1.732515E+16	29.166667	1.234286E-06	6.177840E-18	4.508509E-17	5.569488E-15	99.993981	4.277823
0.26	1.732507E+16	30.333333	1.234286E-06	6.856194E-18	4.688852E-17	6.015028E-15	99.993501	4.277820
0.27	1.732498E+16	31.500000	1.234286E-06	7.581522E-18	4.869195E-17	6.477700E-15	99.993003	4.277817
0.28	1.732489E+16	32.666667	1.234286E-06	8.355371E-18	5.049538E-17	6.957506E-15	99.992486	4.277813
0.29	1.732480E+16	33.833333	1.234286E-06	9.179289E-18	5.229881E-17	7.454443E-15	99.991951	4.277810
0.30	1.732470E+16	35.000000	1.234286E-06	1.005482E-17	5.410225E-17	7.968513E-15	99.991398	4.277807
0.31	1.732460E+16	36.166667	1.234286E-06	1.098352E-17	5.590569E-17	8.499714E-15	99.990826	4.277803
0.32	1.732450E+16	37.333333	1.234286E-06	1.196692E-17	5.770913E-17	9.048046E-15	99.990236	4.277799
0.33	1.732439E+16	38.500000	1.234286E-06	1.300658E-17	5.951257E-17	9.613510E-15	99.989627	4.277796
0.34	1.732429E+16	39.666667	1.234286E-06	1.410404E-17	6.131602E-17	1.019610E-14	99.989000	4.277792
0.35	1.732417E+16	40.833333	1.234286E-06	1.526086E-17	6.311947E-17	1.079583E-14	99.988355	4.277788
0.36	1.732406E+16	42.000000	1.234286E-06	1.647857E-17	6.492293E-17	1.141268E-14	99.987691	4.277784
0.37	1.732394E+16	43.166667	1.234286E-06	1.775872E-17	6.672639E-17	1.204666E-14	99.987009	4.277779
0.38	1.732382E+16	44.333333	1.234286E-06	1.910287E-17	6.852985E-17	1.269777E-14	99.986308	4.277775
0.39	1.732369E+16	45.500000	1.234286E-06	2.051256E-17	7.033332E-17	1.336601E-14	99.985589	4.277771
0.40	1.732357E+16	46.666667	1.234286E-06	2.198933E-17	7.213679E-17	1.405138E-14	99.984852	4.277766
0.41	1.732344E+16	47.833333	1.234286E-06	2.353473E-17	7.394026E-17	1.475387E-14	99.984096	4.277761
0.42	1.732330E+16	49.000000	1.234286E-06	2.515031E-17	7.574374E-17	1.547349E-14	99.983322	4.277757
0.43	1.732316E+16	50.166667	1.234286E-06	2.683762E-17	7.754722E-17	1.621024E-14	99.982529	4.277752
0.44	1.732302E+16	51.333333	1.234286E-06	2.859820E-17	7.935071E-17	1.696411E-14	99.981718	4.277747
0.45	1.732288E+16	52.500000	1.234286E-06	3.043361E-17	8.115420E-17	1.773511E-14	99.980888	4.277741





$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO2}}$ (mol)	$\Phi_{\text{NO2}}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732619E+16	1.166667	3.509923E-07	2.694876E-21	1.786794E-18	1.750959E-17	99.999979	4.291201
0.02	1.732618E+16	2.333333	4.963779E-07	1.189576E-20	3.573589E-18	5.252874E-17	99.999940	4.291201
0.03	1.732617E+16	3.500000	6.079359E-07	3.036476E-20	5.360385E-18	1.050574E-16	99.999882	4.291200
0.04	1.732616E+16	4.666667	7.019834E-07	6.037987E-20	7.147183E-18	1.750956E-16	99.999805	4.291200
0.05	1.732614E+16	5.833333	7.848405E-07	1.039247E-19	8.933981E-18	2.626431E-16	99.999709	4.291199
0.06	1.732612E+16	7.000000	8.597488E-07	1.627796E-19	1.072078E-17	3.677001E-16	99.999595	4.291198
0.07	1.732610E+16	8.166667	9.286336E-07	2.385738E-19	1.250758E-17	4.902663E-16	99.999461	4.291197
0.08	1.732607E+16	9.333333	9.927495E-07	3.328179E-19	1.429438E-17	6.303416E-16	99.999309	4.291197
0.09	1.732604E+16	10.500000	1.052968E-06	4.469274E-19	1.608118E-17	7.879262E-16	99.999139	4.291196
0.10	1.732601E+16	11.666667	1.109924E-06	5.822377E-19	1.786798E-17	9.630197E-16	99.998949	4.291195
0.11	1.732597E+16	12.833333	1.164095E-06	7.400171E-19	1.965479E-17	1.155622E-15	99.998741	4.291193
0.12	1.732593E+16	14.000000	1.215855E-06	9.214756E-19	2.144159E-17	1.365733E-15	99.998514	4.291192
0.13	1.732589E+16	15.166667	1.234286E-06	1.128018E-18	2.322839E-17	1.593353E-15	99.998268	4.291191
0.14	1.732585E+16	16.333333	1.234286E-06	1.361177E-18	2.501519E-17	1.838481E-15	99.998003	4.291189
0.15	1.732580E+16	17.500000	1.234286E-06	1.622486E-18	2.680200E-17	2.101118E-15	99.997720	4.291187
0.16	1.732574E+16	18.666667	1.234286E-06	1.913476E-18	2.858881E-17	2.381262E-15	99.997417	4.291186
0.17	1.732569E+16	19.833333	1.234286E-06	2.235682E-18	3.037562E-17	2.678914E-15	99.997096	4.291183
0.18	1.732563E+16	21.000000	1.234286E-06	2.590635E-18	3.216243E-17	2.994073E-15	99.996757	4.291181
0.19	1.732557E+16	22.166667	1.234286E-06	2.979868E-18	3.394924E-17	3.326739E-15	99.996398	4.291179
0.20	1.732550E+16	23.333333	1.234286E-06	3.404914E-18	3.573606E-17	3.676913E-15	99.996021	4.291177
0.21	1.732543E+16	24.500000	1.234286E-06	3.867306E-18	3.752288E-17	4.044593E-15	99.995624	4.291174
0.22	1.732536E+16	25.666667	1.234286E-06	4.368576E-18	3.930970E-17	4.429780E-15	99.995209	4.291171
0.23	1.732529E+16	26.833333	1.234286E-06	4.910257E-18	4.109652E-17	4.832472E-15	99.994776	4.291169
0.24	1.732521E+16	28.000000	1.234286E-06	5.493882E-18	4.288335E-17	5.252671E-15	99.994323	4.291166
0.25	1.732513E+16	29.166667	1.234286E-06	6.120983E-18	4.467018E-17	5.690375E-15	99.993852	4.291163
0.26	1.732504E+16	30.333333	1.234286E-06	6.793094E-18	4.645701E-17	6.145584E-15	99.993362	4.291160
0.27	1.732495E+16	31.500000	1.234286E-06	7.511747E-18	4.824385E-17	6.618298E-15	99.992853	4.291156
0.28	1.732486E+16	32.666667	1.234286E-06	8.278474E-18	5.003068E-17	7.108516E-15	99.992325	4.291153
0.29	1.732477E+16	33.833333	1.234286E-06	9.094809E-18	5.181753E-17	7.616238E-15	99.991779	4.291150
0.30	1.732467E+16	35.000000	1.234286E-06	9.962285E-18	5.360437E-17	8.141464E-15	99.991213	4.291146
0.31	1.732457E+16	36.166667	1.234286E-06	1.088243E-17	5.539122E-17	8.684193E-15	99.990629	4.291142
0.32	1.732446E+16	37.333333	1.234286E-06	1.185679E-17	5.717807E-17	9.244425E-15	99.990026	4.291138
0.33	1.732436E+16	38.500000	1.234286E-06	1.288688E-17	5.896493E-17	9.822159E-15	99.989405	4.291134
0.34	1.732424E+16	39.666667	1.234286E-06	1.397424E-17	6.075179E-17	1.041740E-14	99.988764	4.291130
0.35	1.732413E+16	40.833333	1.234286E-06	1.512041E-17	6.253865E-17	1.103013E-14	99.988105	4.291126
0.36	1.732401E+16	42.000000	1.234286E-06	1.632692E-17	6.432552E-17	1.166037E-14	99.987427	4.291122
0.37	1.732389E+16	43.166667	1.234286E-06	1.759529E-17	6.611239E-17	1.230811E-14	99.986730	4.291117
0.38	1.732377E+16	44.333333	1.234286E-06	1.892707E-17	6.789927E-17	1.297335E-14	99.986014	4.291113
0.39	1.732364E+16	45.500000	1.234286E-06	2.032379E-17	6.968615E-17	1.365609E-14	99.985280	4.291108
0.40	1.732351E+16	46.666667	1.234286E-06	2.178697E-17	7.147303E-17	1.435633E-14	99.984526	4.291103
0.41	1.732338E+16	47.833333	1.234286E-06	2.331815E-17	7.325992E-17	1.507406E-14	99.983754	4.291098
0.42	1.732324E+16	49.000000	1.234286E-06	2.491887E-17	7.504682E-17	1.580930E-14	99.982963	4.291093
0.43	1.732310E+16	50.166667	1.234286E-06	2.659065E-17	7.683372E-17	1.656203E-14	99.982153	4.291088
0.44	1.732296E+16	51.333333	1.234286E-06	2.833503E-17	7.862062E-17	1.733225E-14	99.981325	4.291083
0.45	1.732281E+16	52.500000	1.234286E-06	3.015355E-17	8.040753E-17	1.811998E-14	99.980477	4.291077



## APPENDIX C1-2: DEPENDENCE OF $\gamma_{\text{best-fit}}$ ON HA STANDARD

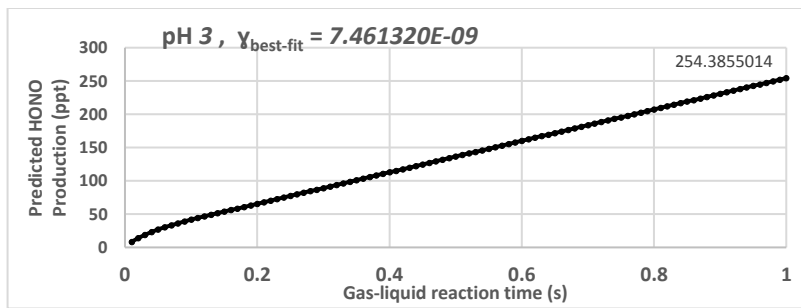
( $[\text{HA}]_{\text{solution}} (\text{pH } 3) = 0.76 \text{ g L}^{-1}$ ;  $[\text{NO}_2]_0 = 36 \text{ ppbv}$ ; 4 lamps;  $t_{\text{reac}}$  of 1 s)

## COMMERCIAL HA STANDARD



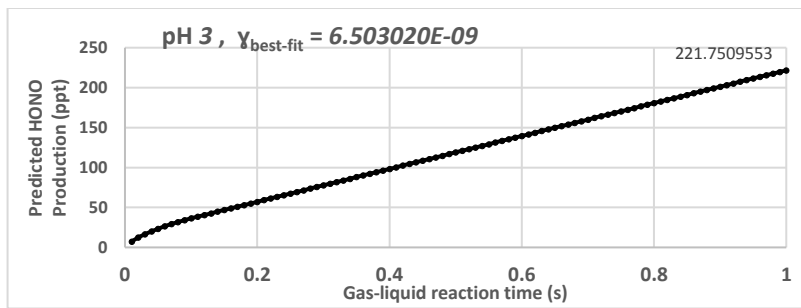


0.46	1.731197E+16	53.666667	1.234286E-06	2.268881E-15	5.818188E-15	6.853320E-14	99.917949	2.999976
0.47	1.731137E+16	54.833333	1.234286E-06	2.408432E-15	5.944601E-15	7.151238E-14	99.914474	2.999975
0.48	1.731076E+16	56.000000	1.234286E-06	2.553554E-15	6.071009E-15	7.455491E-14	99.910925	2.999974
0.49	1.731013E+16	57.166667	1.234286E-06	2.704356E-15	6.197413E-15	7.766078E-14	99.907302	2.999973
0.50	1.730949E+16	58.333333	1.234286E-06	2.860946E-15	6.323813E-15	8.082999E-14	99.903605	2.999972
0.51	1.730884E+16	59.500000	1.234286E-06	3.023433E-15	6.450208E-15	8.406253E-14	99.899834	2.999970
0.52	1.730817E+16	60.666667	1.234286E-06	3.191924E-15	6.576598E-15	8.735840E-14	99.895989	2.999969
0.53	1.730749E+16	61.833333	1.234286E-06	3.366529E-15	6.702983E-15	9.071760E-14	99.892069	2.999968
0.54	1.730680E+16	63.000000	1.234286E-06	3.547355E-15	6.829363E-15	9.414013E-14	99.888075	2.999967
0.55	1.730609E+16	64.166667	1.234286E-06	3.734510E-15	6.955739E-15	9.762599E-14	99.884007	2.999966
0.56	1.730538E+16	65.333333	1.234286E-06	3.928104E-15	7.082109E-15	1.011752E-13	99.879863	2.999964
0.57	1.730465E+16	66.500000	1.234286E-06	4.128244E-15	7.208474E-15	1.047876E-13	99.875645	2.999963
0.58	1.730390E+16	67.666667	1.234286E-06	4.335038E-15	7.334834E-15	1.084634E-13	99.871352	2.999962
0.59	1.730314E+16	68.833333	1.234286E-06	4.548595E-15	7.461188E-15	1.122026E-13	99.866984	2.999961
0.60	1.730237E+16	70.000000	1.234286E-06	4.769023E-15	7.587537E-15	1.160050E-13	99.862541	2.999959
0.61	1.730159E+16	71.166667	1.234286E-06	4.996431E-15	7.713880E-15	1.198707E-13	99.858022	2.999958
0.62	1.730080E+16	72.333333	1.234286E-06	5.230926E-15	7.840217E-15	1.237997E-13	99.853428	2.999956
0.63	1.729999E+16	73.500000	1.234286E-06	5.472616E-15	7.966549E-15	1.277920E-13	99.848759	2.999955
0.64	1.729916E+16	74.666667	1.234286E-06	5.721611E-15	8.092875E-15	1.318477E-13	99.844014	2.999954
0.65	1.729833E+16	75.833333	1.234286E-06	5.978017E-15	8.219195E-15	1.359666E-13	99.839193	2.999952
0.66	1.729748E+16	77.000000	1.234286E-06	6.241944E-15	8.345509E-15	1.401487E-13	99.834297	2.999951
0.67	1.729662E+16	78.166667	1.234286E-06	6.513499E-15	8.471816E-15	1.443942E-13	99.829324	2.999949
0.68	1.729574E+16	79.333333	1.234286E-06	6.792790E-15	8.598118E-15	1.487030E-13	99.824276	2.999948
0.69	1.729486E+16	80.500000	1.234286E-06	7.079927E-15	8.724413E-15	1.530750E-13	99.819151	2.999946
0.70	1.729396E+16	81.666667	1.234286E-06	7.375016E-15	8.850702E-15	1.575103E-13	99.813950	2.999945
0.71	1.729304E+16	82.833333	1.234286E-06	7.678167E-15	8.976984E-15	1.620088E-13	99.808673	2.999943
0.72	1.729211E+16	84.000000	1.234286E-06	7.989486E-15	9.103259E-15	1.665707E-13	99.803319	2.999941
0.73	1.729117E+16	85.166667	1.234286E-06	8.309083E-15	9.229528E-15	1.711957E-13	99.797889	2.999940
0.74	1.729022E+16	86.333333	1.234286E-06	8.637065E-15	9.355790E-15	1.758841E-13	99.792382	2.999938
0.75	1.728925E+16	87.500000	1.234286E-06	8.973540E-15	9.482045E-15	1.806357E-13	99.786798	2.999936
0.76	1.728827E+16	88.666667	1.234286E-06	9.318617E-15	9.608293E-15	1.854505E-13	99.781137	2.999935
0.77	1.728728E+16	89.833333	1.234286E-06	9.672403E-15	9.734535E-15	1.903286E-13	99.775399	2.999933
0.78	1.728627E+16	91.000000	1.234286E-06	1.003501E-14	9.860768E-15	1.952699E-13	99.769584	2.999931
0.79	1.728525E+16	92.166667	1.234286E-06	1.040654E-14	9.986995E-15	2.002744E-13	99.763692	2.999930
0.80	1.728421E+16	93.333333	1.234286E-06	1.078710E-14	1.011321E-14	2.053422E-13	99.757722	2.999928
0.81	1.728317E+16	94.500000	1.234286E-06	1.117681E-14	1.023943E-14	2.104732E-13	99.751675	2.999926
0.82	1.728210E+16	95.666667	1.234286E-06	1.157576E-14	1.036563E-14	2.156674E-13	99.745550	2.999924
0.83	1.728103E+16	96.833333	1.234286E-06	1.198407E-14	1.049183E-14	2.209248E-13	99.739348	2.999922
0.84	1.727994E+16	98.000000	1.234286E-06	1.240185E-14	1.061802E-14	2.262455E-13	99.733068	2.999920
0.85	1.727884E+16	99.166667	1.234286E-06	1.282920E-14	1.074420E-14	2.316293E-13	99.726709	2.999919
0.86	1.727773E+16	100.333333	1.234286E-06	1.326623E-14	1.087037E-14	2.370763E-13	99.720273	2.999917
0.87	1.727660E+16	101.500000	1.234286E-06	1.371306E-14	1.099653E-14	2.425866E-13	99.713759	2.999915
0.88	1.727545E+16	102.666667	1.234286E-06	1.416978E-14	1.112269E-14	2.481600E-13	99.707166	2.999913
0.89	1.727430E+16	103.833333	1.234286E-06	1.463650E-14	1.124884E-14	2.537966E-13	99.700495	2.999911
0.90	1.727313E+16	105.000000	1.234286E-06	1.511334E-14	1.137498E-14	2.594964E-13	99.693746	2.999909
0.91	1.727195E+16	106.166667	1.234286E-06	1.560040E-14	1.150111E-14	2.652594E-13	99.686917	2.999907
0.92	1.727075E+16	107.333333	1.234286E-06	1.609779E-14	1.162723E-14	2.710855E-13	99.680011	2.999905
0.93	1.726954E+16	108.500000	1.234286E-06	1.660561E-14	1.175335E-14	2.769748E-13	99.673025	2.999903
0.94	1.726831E+16	109.666667	1.234286E-06	1.712398E-14	1.187945E-14	2.829273E-13	99.665961	2.999900
0.95	1.726708E+16	110.833333	1.234286E-06	1.765300E-14	1.200555E-14	2.889429E-13	99.658817	2.999898
0.96	1.726583E+16	112.000000	1.234286E-06	1.819278E-14	1.213164E-14	2.950217E-13	99.651594	2.999896
0.97	1.726456E+16	113.166667	1.234286E-06	1.874343E-14	1.225772E-14	3.011636E-13	99.644292	2.999894
0.98	1.726328E+16	114.333333	1.234286E-06	1.930506E-14	1.238379E-14	3.073687E-13	99.636911	2.999892
0.99	1.726199E+16	115.500000	1.234286E-06	1.987776E-14	1.250985E-14	3.136368E-13	99.629450	2.999890
1.00	1.726068E+16	116.666667	1.234286E-06	2.046166E-14	1.263590E-14	3.199682E-13	99.621910	2.999887



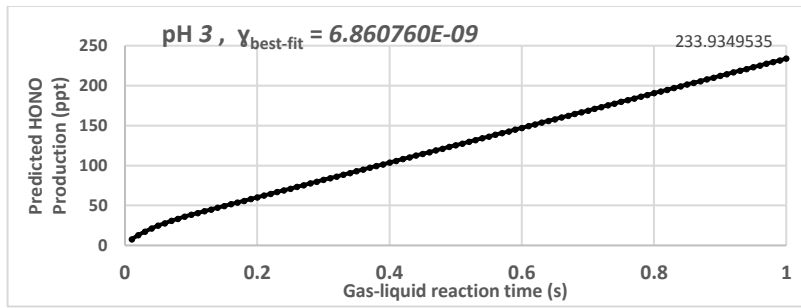
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732615E+16	1.166667	3.509916E-07	2.156738E-19	1.429987E-16	7.166911E-17	99.999770	3.000000
0.02	1.732610E+16	2.333333	4.963755E-07	9.520300E-19	2.859970E-16	2.150071E-16	99.999462	3.000000
0.03	1.732603E+16	3.500000	6.079310E-07	2.430122E-18	4.289947E-16	4.300136E-16	99.999078	3.000000
0.04	1.732595E+16	4.666667	7.019750E-07	4.832260E-18	5.719918E-16	7.166883E-16	99.998615	3.000000
0.05	1.732586E+16	5.833333	7.848277E-07	8.317193E-18	7.149881E-16	1.075031E-15	99.998074	2.999999
0.06	1.732575E+16	7.000000	8.597304E-07	1.302740E-17	8.579836E-16	1.505040E-15	99.997456	2.999999
0.07	1.732563E+16	8.166667	9.286085E-07	1.909327E-17	1.000978E-15	2.006717E-15	99.996759	2.999999
0.08	1.732550E+16	9.333333	9.927165E-07	2.663570E-17	1.143971E-15	2.580059E-15	99.995983	2.999999
0.09	1.732535E+16	10.500000	1.052926E-06	3.576797E-17	1.286964E-15	3.225067E-15	99.995130	2.999999
0.10	1.732519E+16	11.666667	1.109871E-06	4.659695E-17	1.429955E-15	3.941739E-15	99.994198	2.999998
0.11	1.732501E+16	12.833333	1.164031E-06	5.922413E-17	1.572944E-15	4.730076E-15	99.993187	2.999998
0.12	1.732482E+16	14.000000	1.215777E-06	7.374636E-17	1.715932E-15	5.590075E-15	99.992097	2.999998
0.13	1.732462E+16	15.166667	1.234286E-06	9.027601E-17	1.858918E-15	6.521736E-15	99.990929	2.999998
0.14	1.732440E+16	16.333333	1.234286E-06	1.089357E-16	2.001903E-15	7.525058E-15	99.989681	2.999997
0.15	1.732417E+16	17.500000	1.234286E-06	1.298481E-16	2.144886E-15	8.600040E-15	99.988354	2.999997
0.16	1.732393E+16	18.666667	1.234286E-06	1.531358E-16	2.287866E-15	9.746680E-15	99.986948	2.999997
0.17	1.732367E+16	19.833333	1.234286E-06	1.789215E-16	2.430845E-15	1.096498E-14	99.985463	2.999996
0.18	1.732340E+16	21.000000	1.234286E-06	2.073278E-16	2.573821E-15	1.225493E-14	99.983898	2.999996
0.19	1.732312E+16	22.166667	1.234286E-06	2.384773E-16	2.716796E-15	1.361654E-14	99.982254	2.999995
0.20	1.732282E+16	23.333333	1.234286E-06	2.724926E-16	2.859767E-15	1.504980E-14	99.980529	2.999995
0.21	1.732251E+16	24.500000	1.234286E-06	3.094963E-16	3.002737E-15	1.655471E-14	99.978725	2.999994
0.22	1.732218E+16	25.666667	1.234286E-06	3.496112E-16	3.145703E-15	1.813128E-14	99.976841	2.999994
0.23	1.732184E+16	26.833333	1.234286E-06	3.929596E-16	3.288667E-15	1.977949E-14	99.974876	2.999993
0.24	1.732148E+16	28.000000	1.234286E-06	4.396644E-16	3.431628E-15	2.149935E-14	99.972831	2.999992
0.25	1.732112E+16	29.166667	1.234286E-06	4.898480E-16	3.574586E-15	2.329085E-14	99.970706	2.999992
0.26	1.732073E+16	30.333333	1.234286E-06	5.436331E-16	3.717541E-15	2.515400E-14	99.968500	2.999991
0.27	1.732034E+16	31.500000	1.234286E-06	6.011422E-16	3.860493E-15	2.708878E-14	99.966213	2.999990
0.28	1.731993E+16	32.666667	1.234286E-06	6.624979E-16	4.003441E-15	2.909521E-14	99.963846	2.999990
0.29	1.731950E+16	33.833333	1.234286E-06	7.278228E-16	4.146386E-15	3.117327E-14	99.961398	2.999989
0.30	1.731906E+16	35.000000	1.234286E-06	7.972396E-16	4.289328E-15	3.332297E-14	99.958868	2.999988
0.31	1.731861E+16	36.166667	1.234286E-06	8.708706E-16	4.432266E-15	3.554430E-14	99.956257	2.999987
0.32	1.731815E+16	37.333333	1.234286E-06	9.488385E-16	4.575200E-15	3.783726E-14	99.953565	2.999987
0.33	1.731767E+16	38.500000	1.234286E-06	1.031266E-15	4.718130E-15	4.020185E-14	99.950792	2.999986
0.34	1.731717E+16	39.666667	1.234286E-06	1.118275E-15	4.861056E-15	4.263807E-14	99.947937	2.999985
0.35	1.731666E+16	40.833333	1.234286E-06	1.209989E-15	5.003978E-15	4.514591E-14	99.945000	2.999984
0.36	1.731614E+16	42.000000	1.234286E-06	1.306530E-15	5.146896E-15	4.772536E-14	99.941981	2.999983
0.37	1.731560E+16	43.166667	1.234286E-06	1.408021E-15	5.289810E-15	5.037644E-14	99.938880	2.999982
0.38	1.731505E+16	44.333333	1.234286E-06	1.514583E-15	5.432719E-15	5.309913E-14	99.935698	2.999981
0.39	1.731448E+16	45.500000	1.234286E-06	1.626340E-15	5.575623E-15	5.589344E-14	99.932433	2.999980
0.40	1.731390E+16	46.666667	1.234286E-06	1.743415E-15	5.718523E-15	5.875935E-14	99.929085	2.999979
0.41	1.731331E+16	47.833333	1.234286E-06	1.865929E-15	5.861418E-15	6.169687E-14	99.925655	2.999978
0.42	1.731270E+16	49.000000	1.234286E-06	1.994005E-15	6.004308E-15	6.470600E-14	99.922143	2.999977
0.43	1.731208E+16	50.166667	1.234286E-06	2.127765E-15	6.147194E-15	6.778672E-14	99.918547	2.999976
0.44	1.731144E+16	51.333333	1.234286E-06	2.267333E-15	6.290074E-15	7.093905E-14	99.914869	2.999975
0.45	1.731079E+16	52.500000	1.234286E-06	2.412830E-15	6.432948E-15	7.416297E-14	99.911108	2.999974

0.46	1.731012E+16	53.666667	1.234286E-06	2.564379E-15	6.575818E-15	7.745848E-14	99.907263	2.999973
0.47	1.730944E+16	54.833333	1.234286E-06	2.722102E-15	6.718682E-15	8.082557E-14	99.903336	2.999972
0.48	1.730875E+16	56.000000	1.234286E-06	2.886123E-15	6.861540E-15	8.426425E-14	99.899325	2.999970
0.49	1.730804E+16	57.166667	1.234286E-06	3.056562E-15	7.004393E-15	8.777452E-14	99.895230	2.999969
0.50	1.730731E+16	58.333333	1.234286E-06	3.233543E-15	7.147239E-15	9.135636E-14	99.891052	2.999968
0.51	1.730658E+16	59.500000	1.234286E-06	3.417188E-15	7.290080E-15	9.500977E-14	99.886790	2.999967
0.52	1.730582E+16	60.666667	1.234286E-06	3.607620E-15	7.432915E-15	9.873475E-14	99.882444	2.999965
0.53	1.730506E+16	61.833333	1.234286E-06	3.804960E-15	7.575743E-15	1.025313E-13	99.878014	2.999964
0.54	1.730427E+16	63.000000	1.234286E-06	4.009331E-15	7.718566E-15	1.063994E-13	99.873500	2.999963
0.55	1.730348E+16	64.166667	1.234286E-06	4.220856E-15	7.861381E-15	1.103391E-13	99.868902	2.999961
0.56	1.730267E+16	65.333333	1.234286E-06	4.439657E-15	8.004191E-15	1.143503E-13	99.864219	2.999960
0.57	1.730184E+16	66.500000	1.234286E-06	4.665856E-15	8.146993E-15	1.184331E-13	99.859452	2.999958
0.58	1.730100E+16	67.666667	1.234286E-06	4.899576E-15	8.289789E-15	1.225874E-13	99.854600	2.999957
0.59	1.730014E+16	68.833333	1.234286E-06	5.140938E-15	8.432578E-15	1.268133E-13	99.849663	2.999955
0.60	1.729927E+16	70.000000	1.234286E-06	5.390066E-15	8.575360E-15	1.311107E-13	99.844641	2.999954
0.61	1.729839E+16	71.166667	1.234286E-06	5.647081E-15	8.718135E-15	1.354796E-13	99.839535	2.999952
0.62	1.729749E+16	72.333333	1.234286E-06	5.912106E-15	8.860902E-15	1.399201E-13	99.834343	2.999951
0.63	1.729657E+16	73.500000	1.234286E-06	6.185263E-15	9.003663E-15	1.444321E-13	99.829066	2.999949
0.64	1.729565E+16	74.666667	1.234286E-06	6.466674E-15	9.146415E-15	1.490156E-13	99.823703	2.999948
0.65	1.729470E+16	75.833333	1.234286E-06	6.756462E-15	9.289160E-15	1.536706E-13	99.818255	2.999946
0.66	1.729374E+16	77.000000	1.234286E-06	7.054748E-15	9.431898E-15	1.583972E-13	99.812721	2.999944
0.67	1.729277E+16	78.166667	1.234286E-06	7.361655E-15	9.574627E-15	1.631952E-13	99.807101	2.999943
0.68	1.729178E+16	79.333333	1.234286E-06	7.677305E-15	9.717349E-15	1.680648E-13	99.801396	2.999941
0.69	1.729078E+16	80.500000	1.234286E-06	8.001821E-15	9.860062E-15	1.730058E-13	99.795604	2.999939
0.70	1.728976E+16	81.666667	1.234286E-06	8.335324E-15	1.000277E-14	1.780183E-13	99.789726	2.999937
0.71	1.728873E+16	82.833333	1.234286E-06	8.677936E-15	1.014546E-14	1.831024E-13	99.783762	2.999936
0.72	1.728768E+16	84.000000	1.234286E-06	9.029781E-15	1.028815E-14	1.882579E-13	99.777712	2.999934
0.73	1.728661E+16	85.166667	1.234286E-06	9.390979E-15	1.043083E-14	1.934849E-13	99.771575	2.999932
0.74	1.728554E+16	86.333333	1.234286E-06	9.761653E-15	1.057350E-14	1.987833E-13	99.765351	2.999930
0.75	1.728444E+16	87.500000	1.234286E-06	1.014193E-14	1.071617E-14	2.041532E-13	99.759041	2.999928
0.76	1.728333E+16	88.666667	1.234286E-06	1.053192E-14	1.085882E-14	2.095946E-13	99.752643	2.999926
0.77	1.728221E+16	89.833333	1.234286E-06	1.093175E-14	1.100146E-14	2.151074E-13	99.746159	2.999924
0.78	1.728107E+16	91.000000	1.234286E-06	1.134155E-14	1.114410E-14	2.206917E-13	99.739587	2.999922
0.79	1.727992E+16	92.166667	1.234286E-06	1.176144E-14	1.128672E-14	2.263474E-13	99.732928	2.999920
0.80	1.727875E+16	93.333333	1.234286E-06	1.219153E-14	1.142934E-14	2.320746E-13	99.726182	2.999918
0.81	1.727756E+16	94.500000	1.234286E-06	1.263196E-14	1.157195E-14	2.378732E-13	99.719348	2.999916
0.82	1.727637E+16	95.666667	1.234286E-06	1.308283E-14	1.171454E-14	2.437432E-13	99.712426	2.999914
0.83	1.727515E+16	96.833333	1.234286E-06	1.354428E-14	1.185713E-14	2.496847E-13	99.705417	2.999912
0.84	1.727392E+16	98.000000	1.234286E-06	1.401643E-14	1.199971E-14	2.556975E-13	99.698319	2.999910
0.85	1.727268E+16	99.166667	1.234286E-06	1.449940E-14	1.214228E-14	2.617818E-13	99.691134	2.999908
0.86	1.727142E+16	100.333333	1.234286E-06	1.499330E-14	1.228483E-14	2.679374E-13	99.683860	2.999906
0.87	1.727014E+16	101.500000	1.234286E-06	1.549827E-14	1.242738E-14	2.741645E-13	99.676499	2.999904
0.88	1.726885E+16	102.666667	1.234286E-06	1.601442E-14	1.256992E-14	2.804630E-13	99.669048	2.999901
0.89	1.726754E+16	103.833333	1.234286E-06	1.654188E-14	1.271244E-14	2.868328E-13	99.661510	2.999899
0.90	1.726622E+16	105.000000	1.234286E-06	1.708076E-14	1.285496E-14	2.932740E-13	99.653882	2.999897
0.91	1.726489E+16	106.166667	1.234286E-06	1.763119E-14	1.299746E-14	2.997866E-13	99.646166	2.999895
0.92	1.726353E+16	107.333333	1.234286E-06	1.819330E-14	1.313996E-14	3.063705E-13	99.638361	2.999892
0.93	1.726217E+16	108.500000	1.234286E-06	1.876720E-14	1.328244E-14	3.130258E-13	99.630467	2.999890
0.94	1.726078E+16	109.666667	1.234286E-06	1.935301E-14	1.342491E-14	3.197525E-13	99.622483	2.999888
0.95	1.725938E+16	110.833333	1.234286E-06	1.995086E-14	1.356737E-14	3.265505E-13	99.614411	2.999885
0.96	1.725797E+16	112.000000	1.234286E-06	2.056087E-14	1.370982E-14	3.334198E-13	99.606249	2.999883
0.97	1.725654E+16	113.166667	1.234286E-06	2.118316E-14	1.385226E-14	3.403605E-13	99.597997	2.999880
0.98	1.725509E+16	114.333333	1.234286E-06	2.181785E-14	1.399468E-14	3.473725E-13	99.589656	2.999878
0.99	1.725363E+16	115.500000	1.234286E-06	2.246506E-14	1.413710E-14	3.544558E-13	99.581225	2.999875
1.00	1.725216E+16	116.666667	1.234286E-06	2.312492E-14	1.427950E-14	3.616104E-13	99.572704	2.999873



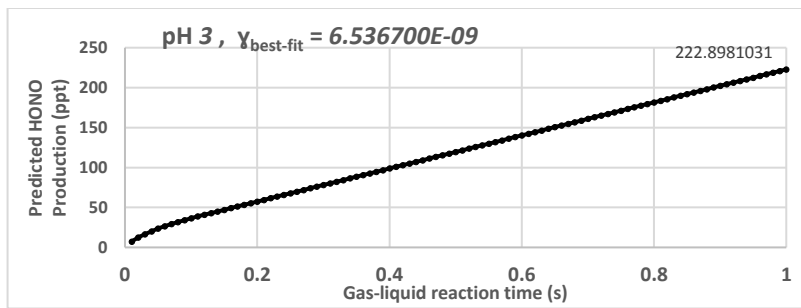
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO2}}$ (mol)	$\Phi_{\text{NO2}}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732616E+16	1.166667	3.509917E-07	1.879735E-19	1.246326E-16	6.246425E-17	99.999799	3.000000
0.02	1.732611E+16	2.333333	4.963759E-07	8.297554E-19	2.492649E-16	1.873926E-16	99.999532	3.000000
0.03	1.732605E+16	3.500000	6.079318E-07	2.118008E-18	3.738967E-16	3.747847E-16	99.999196	3.000000
0.04	1.732598E+16	4.666667	7.019763E-07	4.211625E-18	4.985281E-16	6.246404E-16	99.998793	3.000000
0.05	1.732590E+16	5.833333	7.848297E-07	7.248968E-18	6.231589E-16	9.369593E-16	99.998322	2.999999
0.06	1.732581E+16	7.000000	8.597332E-07	1.135422E-17	7.477890E-16	1.311741E-15	99.997782	2.999999
0.07	1.732570E+16	8.166667	9.286123E-07	1.664101E-17	8.724184E-16	1.748985E-15	99.997175	2.999999
0.08	1.732558E+16	9.333333	9.927216E-07	2.321473E-17	9.970470E-16	2.248691E-15	99.996499	2.999999
0.09	1.732546E+16	10.500000	1.052932E-06	3.117408E-17	1.121675E-15	2.810859E-15	99.995755	2.999999
0.10	1.732531E+16	11.666667	1.109879E-06	4.061223E-17	1.246301E-15	3.435487E-15	99.994943	2.999999
0.11	1.732516E+16	12.833333	1.164041E-06	5.161764E-17	1.370927E-15	4.122576E-15	99.994062	2.999998
0.12	1.732500E+16	14.000000	1.215790E-06	6.427469E-17	1.495551E-15	4.872124E-15	99.993112	2.999998
0.13	1.732482E+16	15.166667	1.234286E-06	7.868135E-17	1.620174E-15	5.684131E-15	99.992094	2.999998
0.14	1.732463E+16	16.333333	1.234286E-06	9.494449E-17	1.744796E-15	6.558596E-15	99.991006	2.999998
0.15	1.732443E+16	17.500000	1.234286E-06	1.131710E-16	1.869417E-15	7.495518E-15	99.989850	2.999997
0.16	1.732422E+16	18.666667	1.234286E-06	1.334678E-16	1.994036E-15	8.494897E-15	99.988625	2.999997
0.17	1.732400E+16	19.833333	1.234286E-06	1.559418E-16	2.118653E-15	9.556730E-15	99.987330	2.999997
0.18	1.732376E+16	21.000000	1.234286E-06	1.806997E-16	2.243269E-15	1.068102E-14	99.985966	2.999996
0.19	1.732351E+16	22.166667	1.234286E-06	2.078486E-16	2.367883E-15	1.186776E-14	99.984533	2.999996
0.20	1.732325E+16	23.333333	1.234286E-06	2.374953E-16	2.492495E-15	1.311695E-14	99.983030	2.999995
0.21	1.732298E+16	24.500000	1.234286E-06	2.697467E-16	2.617105E-15	1.442860E-14	99.981457	2.999995
0.22	1.732269E+16	25.666667	1.234286E-06	3.047095E-16	2.741713E-15	1.580269E-14	99.979815	2.999994
0.23	1.732240E+16	26.833333	1.234286E-06	3.424908E-16	2.866319E-15	1.723923E-14	99.978103	2.999994
0.24	1.732209E+16	28.000000	1.234286E-06	3.831973E-16	2.990923E-15	1.873822E-14	99.976320	2.999993
0.25	1.732177E+16	29.166667	1.234286E-06	4.269360E-16	3.115525E-15	2.029966E-14	99.974468	2.999993
0.26	1.732143E+16	30.333333	1.234286E-06	4.738136E-16	3.240124E-15	2.192354E-14	99.972545	2.999992
0.27	1.732109E+16	31.500000	1.234286E-06	5.239370E-16	3.364721E-15	2.360986E-14	99.970552	2.999992
0.28	1.732073E+16	32.666667	1.234286E-06	5.774131E-16	3.489316E-15	2.535863E-14	99.968489	2.999991
0.29	1.732036E+16	33.833333	1.234286E-06	6.343487E-16	3.613908E-15	2.716983E-14	99.966355	2.999990
0.30	1.731998E+16	35.000000	1.234286E-06	6.948507E-16	3.738497E-15	2.904347E-14	99.964150	2.999990
0.31	1.731959E+16	36.166667	1.234286E-06	7.590258E-16	3.863083E-15	3.097955E-14	99.961875	2.999989
0.32	1.731918E+16	37.333333	1.234286E-06	8.269810E-16	3.987667E-15	3.297807E-14	99.959529	2.999988
0.33	1.731876E+16	38.500000	1.234286E-06	8.988230E-16	4.112247E-15	3.503902E-14	99.957111	2.999988
0.34	1.731833E+16	39.666667	1.234286E-06	9.746586E-16	4.236825E-15	3.716239E-14	99.954623	2.999987
0.35	1.731789E+16	40.833333	1.234286E-06	1.054595E-15	4.361399E-15	3.934820E-14	99.952063	2.999986
0.36	1.731743E+16	42.000000	1.234286E-06	1.138738E-15	4.485970E-15	4.159644E-14	99.949432	2.999985
0.37	1.731696E+16	43.166667	1.234286E-06	1.227196E-15	4.610538E-15	4.390710E-14	99.946729	2.999985
0.38	1.731648E+16	44.333333	1.234286E-06	1.320074E-15	4.735103E-15	4.628018E-14	99.943955	2.999984
0.39	1.731599E+16	45.500000	1.234286E-06	1.417480E-15	4.859664E-15	4.871569E-14	99.941109	2.999983
0.40	1.731548E+16	46.666667	1.234286E-06	1.519520E-15	4.984221E-15	5.121361E-14	99.938192	2.999982
0.41	1.731496E+16	47.833333	1.234286E-06	1.626302E-15	5.108775E-15	5.377395E-14	99.935202	2.999981
0.42	1.731443E+16	49.000000	1.234286E-06	1.737932E-15	5.233325E-15	5.639671E-14	99.932141	2.999980
0.43	1.731389E+16	50.166667	1.234286E-06	1.854516E-15	5.357872E-15	5.908188E-14	99.929007	2.999979
0.44	1.731334E+16	51.333333	1.234286E-06	1.976162E-15	5.482414E-15	6.182946E-14	99.925801	2.999978
0.45	1.731277E+16	52.500000	1.234286E-06	2.102976E-15	5.606953E-15	6.463944E-14	99.922523	2.999977

0.46	1.731219E+16	53.666667	1.234286E-06	2.235066E-15	5.731487E-15	6.751183E-14	99.919172	2.999976
0.47	1.731159E+16	54.833333	1.234286E-06	2.372537E-15	5.856017E-15	7.044663E-14	99.915749	2.999975
0.48	1.731099E+16	56.000000	1.234286E-06	2.515496E-15	5.980543E-15	7.344382E-14	99.912253	2.999974
0.49	1.731037E+16	57.166667	1.234286E-06	2.664051E-15	6.105065E-15	7.650341E-14	99.908684	2.999973
0.50	1.730974E+16	58.333333	1.234286E-06	2.818308E-15	6.229582E-15	7.962540E-14	99.905042	2.999972
0.51	1.730909E+16	59.500000	1.234286E-06	2.978373E-15	6.354095E-15	8.280977E-14	99.901327	2.999971
0.52	1.730844E+16	60.666667	1.234286E-06	3.144354E-15	6.478603E-15	8.605654E-14	99.897539	2.999970
0.53	1.730777E+16	61.833333	1.234286E-06	3.316357E-15	6.603106E-15	8.936569E-14	99.893678	2.999969
0.54	1.730709E+16	63.000000	1.234286E-06	3.494488E-15	6.727605E-15	9.273723E-14	99.889743	2.999967
0.55	1.730639E+16	64.166667	1.234286E-06	3.678855E-15	6.852098E-15	9.617115E-14	99.885735	2.999966
0.56	1.730569E+16	65.333333	1.234286E-06	3.869564E-15	6.976587E-15	9.966744E-14	99.881654	2.999965
0.57	1.730497E+16	66.500000	1.234286E-06	4.066722E-15	7.101071E-15	1.032261E-13	99.877498	2.999964
0.58	1.730423E+16	67.666667	1.234286E-06	4.270435E-15	7.225549E-15	1.068471E-13	99.873269	2.999962
0.59	1.730349E+16	68.833333	1.234286E-06	4.480810E-15	7.350022E-15	1.105306E-13	99.868966	2.999961
0.60	1.730273E+16	70.000000	1.234286E-06	4.697954E-15	7.474490E-15	1.142763E-13	99.864589	2.999960
0.61	1.730196E+16	71.166667	1.234286E-06	4.921973E-15	7.598953E-15	1.180845E-13	99.860138	2.999958
0.62	1.730117E+16	72.333333	1.234286E-06	5.152974E-15	7.723410E-15	1.219550E-13	99.855612	2.999957
0.63	1.730038E+16	73.500000	1.234286E-06	5.391063E-15	7.847861E-15	1.258878E-13	99.851012	2.999956
0.64	1.729957E+16	74.666667	1.234286E-06	5.636348E-15	7.972307E-15	1.298830E-13	99.846338	2.999954
0.65	1.729874E+16	75.833333	1.234286E-06	5.888934E-15	8.096747E-15	1.339405E-13	99.841589	2.999953
0.66	1.729791E+16	77.000000	1.234286E-06	6.148929E-15	8.221181E-15	1.380604E-13	99.836766	2.999951
0.67	1.729706E+16	78.166667	1.234286E-06	6.416438E-15	8.345609E-15	1.422427E-13	99.831867	2.999950
0.68	1.729620E+16	79.333333	1.234286E-06	6.691569E-15	8.470031E-15	1.464872E-13	99.826894	2.999948
0.69	1.729532E+16	80.500000	1.234286E-06	6.974428E-15	8.594447E-15	1.507941E-13	99.821846	2.999947
0.70	1.729444E+16	81.666667	1.234286E-06	7.265121E-15	8.718856E-15	1.551634E-13	99.816722	2.999945
0.71	1.729354E+16	82.833333	1.234286E-06	7.563755E-15	8.843260E-15	1.595949E-13	99.811524	2.999944
0.72	1.729262E+16	84.000000	1.234286E-06	7.870437E-15	8.967657E-15	1.640888E-13	99.806250	2.999942
0.73	1.729169E+16	85.166667	1.234286E-06	8.185273E-15	9.092047E-15	1.686450E-13	99.800900	2.999941
0.74	1.729075E+16	86.333333	1.234286E-06	8.508369E-15	9.216431E-15	1.732635E-13	99.795475	2.999939
0.75	1.728980E+16	87.500000	1.234286E-06	8.839832E-15	9.340808E-15	1.779443E-13	99.789974	2.999937
0.76	1.728884E+16	88.666667	1.234286E-06	9.179769E-15	9.465178E-15	1.826874E-13	99.784398	2.999936
0.77	1.728786E+16	89.833333	1.234286E-06	9.528285E-15	9.589541E-15	1.874929E-13	99.778745	2.999934
0.78	1.728686E+16	91.000000	1.234286E-06	9.885488E-15	9.713898E-15	1.923606E-13	99.773017	2.999932
0.79	1.728586E+16	92.166667	1.234286E-06	1.025148E-14	9.838247E-15	1.972906E-13	99.767212	2.999931
0.80	1.728484E+16	93.333333	1.234286E-06	1.062638E-14	9.962589E-15	2.022829E-13	99.761332	2.999929
0.81	1.728381E+16	94.500000	1.234286E-06	1.101028E-14	1.008692E-14	2.073375E-13	99.755375	2.999927
0.82	1.728276E+16	95.666667	1.234286E-06	1.140329E-14	1.021125E-14	2.124544E-13	99.749341	2.999925
0.83	1.728170E+16	96.833333	1.234286E-06	1.180552E-14	1.033557E-14	2.176335E-13	99.743231	2.999923
0.84	1.728063E+16	98.000000	1.234286E-06	1.221708E-14	1.045988E-14	2.228749E-13	99.737044	2.999922
0.85	1.727955E+16	99.166667	1.234286E-06	1.263806E-14	1.058419E-14	2.281786E-13	99.730781	2.999920
0.86	1.727845E+16	100.333333	1.234286E-06	1.306859E-14	1.070849E-14	2.335446E-13	99.724440	2.999918
0.87	1.727734E+16	101.500000	1.234286E-06	1.350876E-14	1.083278E-14	2.389727E-13	99.718023	2.999916
0.88	1.727621E+16	102.666667	1.234286E-06	1.395867E-14	1.095706E-14	2.444632E-13	99.711528	2.999914
0.89	1.727507E+16	103.833333	1.234286E-06	1.441845E-14	1.108133E-14	2.500159E-13	99.704957	2.999912
0.90	1.727392E+16	105.000000	1.234286E-06	1.488818E-14	1.120560E-14	2.556308E-13	99.698308	2.999910
0.91	1.727275E+16	106.166667	1.234286E-06	1.536799E-14	1.132985E-14	2.613080E-13	99.691581	2.999908
0.92	1.727158E+16	107.333333	1.234286E-06	1.585797E-14	1.145410E-14	2.670474E-13	99.684777	2.999906
0.93	1.727038E+16	108.500000	1.234286E-06	1.635823E-14	1.157834E-14	2.728491E-13	99.677896	2.999904
0.94	1.726918E+16	109.666667	1.234286E-06	1.686888E-14	1.170258E-14	2.787129E-13	99.670936	2.999902
0.95	1.726796E+16	110.833333	1.234286E-06	1.739003E-14	1.182680E-14	2.846390E-13	99.663899	2.999900
0.96	1.726672E+16	112.000000	1.234286E-06	1.792177E-14	1.195101E-14	2.906273E-13	99.656784	2.999898
0.97	1.726548E+16	113.166667	1.234286E-06	1.846422E-14	1.207522E-14	2.966778E-13	99.649591	2.999896
0.98	1.726422E+16	114.333333	1.234286E-06	1.901749E-14	1.219942E-14	3.027905E-13	99.642319	2.999893
0.99	1.726295E+16	115.500000	1.234286E-06	1.958167E-14	1.232361E-14	3.089653E-13	99.634970	2.999891
1.00	1.726166E+16	116.666667	1.234286E-06	2.015687E-14	1.244778E-14	3.152024E-13	99.627541	2.999889



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732615E+16	1.166667	3.509916E-07	1.983142E-19	1.314888E-16	6.590049E-17	99.999788	3.000000
0.02	1.732611E+16	2.333333	4.963757E-07	8.754013E-19	2.629772E-16	1.977013E-16	99.999506	3.000000
0.03	1.732604E+16	3.500000	6.079315E-07	2.234522E-18	3.944652E-16	3.954020E-16	99.999152	3.000000
0.04	1.732597E+16	4.666667	7.019758E-07	4.443312E-18	5.259526E-16	6.590025E-16	99.998726	3.000000
0.05	1.732588E+16	5.833333	7.848289E-07	7.647744E-18	6.574394E-16	9.885024E-16	99.998229	2.999999
0.06	1.732579E+16	7.000000	8.597321E-07	1.197883E-17	7.889255E-16	1.383901E-15	99.997660	2.999999
0.07	1.732567E+16	8.166667	9.286109E-07	1.755646E-17	9.204107E-16	1.845198E-15	99.997020	2.999999
0.08	1.732555E+16	9.333333	9.927197E-07	2.449180E-17	1.051895E-15	2.372393E-15	99.996307	2.999999
0.09	1.732542E+16	10.500000	1.052930E-06	3.288901E-17	1.183378E-15	2.965486E-15	99.995522	2.999999
0.10	1.732527E+16	11.666667	1.109876E-06	4.284637E-17	1.314860E-15	3.624475E-15	99.994665	2.999999
0.11	1.732511E+16	12.833333	1.164037E-06	5.445719E-17	1.446341E-15	4.349360E-15	99.993735	2.999998
0.12	1.732493E+16	14.000000	1.215785E-06	6.781053E-17	1.577821E-15	5.140141E-15	99.992733	2.999998
0.13	1.732475E+16	15.166667	1.234286E-06	8.300971E-17	1.709299E-15	5.996815E-15	99.991659	2.999998
0.14	1.732455E+16	16.333333	1.234286E-06	1.001675E-16	1.840776E-15	6.919384E-15	99.990512	2.999998
0.15	1.732434E+16	17.500000	1.234286E-06	1.193967E-16	1.972252E-15	7.907845E-15	99.989292	2.999997
0.16	1.732411E+16	18.666667	1.234286E-06	1.408100E-16	2.103725E-15	8.962197E-15	99.987999	2.999997
0.17	1.732388E+16	19.833333	1.234286E-06	1.645203E-16	2.235197E-15	1.008244E-14	99.986633	2.999996
0.18	1.732363E+16	21.000000	1.234286E-06	1.906402E-16	2.366667E-15	1.126857E-14	99.985194	2.999996
0.19	1.732336E+16	22.166667	1.234286E-06	2.192825E-16	2.498135E-15	1.252059E-14	99.983682	2.999996
0.20	1.732309E+16	23.333333	1.234286E-06	2.505601E-16	2.629601E-15	1.383850E-14	99.982096	2.999995
0.21	1.732280E+16	24.500000	1.234286E-06	2.845855E-16	2.761065E-15	1.522229E-14	99.980437	2.999995
0.22	1.732250E+16	25.666667	1.234286E-06	3.214717E-16	2.892527E-15	1.667197E-14	99.978705	2.999994
0.23	1.732219E+16	26.833333	1.234286E-06	3.613312E-16	3.023986E-15	1.818753E-14	99.976898	2.999994
0.24	1.732186E+16	28.000000	1.234286E-06	4.042769E-16	3.155443E-15	1.976898E-14	99.975018	2.999993
0.25	1.732152E+16	29.166667	1.234286E-06	4.504215E-16	3.286897E-15	2.141630E-14	99.973064	2.999992
0.26	1.732117E+16	30.333333	1.234286E-06	4.998778E-16	3.418349E-15	2.312950E-14	99.971035	2.999992
0.27	1.732081E+16	31.500000	1.234286E-06	5.527583E-16	3.549798E-15	2.490858E-14	99.968933	2.999991
0.28	1.732043E+16	32.666667	1.234286E-06	6.091760E-16	3.681244E-15	2.675353E-14	99.966756	2.999991
0.29	1.732004E+16	33.833333	1.234286E-06	6.692434E-16	3.812688E-15	2.866436E-14	99.964504	2.999990
0.30	1.731964E+16	35.000000	1.234286E-06	7.330733E-16	3.944128E-15	3.064105E-14	99.962179	2.999989
0.31	1.731922E+16	36.166667	1.234286E-06	8.007785E-16	4.075566E-15	3.268362E-14	99.959778	2.999989
0.32	1.731879E+16	37.333333	1.234286E-06	8.724715E-16	4.207000E-15	3.479206E-14	99.957303	2.999988
0.33	1.731835E+16	38.500000	1.234286E-06	9.482651E-16	4.338431E-15	3.696636E-14	99.954752	2.999987
0.34	1.731790E+16	39.666667	1.234286E-06	1.028272E-15	4.469858E-15	3.920652E-14	99.952127	2.999986
0.35	1.731743E+16	40.833333	1.234286E-06	1.112605E-15	4.601282E-15	4.151255E-14	99.949426	2.999985
0.36	1.731695E+16	42.000000	1.234286E-06	1.201376E-15	4.732703E-15	4.388443E-14	99.946651	2.999985
0.37	1.731645E+16	43.166667	1.234286E-06	1.294699E-15	4.864119E-15	4.632218E-14	99.943799	2.999984
0.38	1.731595E+16	44.333333	1.234286E-06	1.392686E-15	4.995532E-15	4.882577E-14	99.940873	2.999983
0.39	1.731543E+16	45.500000	1.234286E-06	1.495450E-15	5.126942E-15	5.139522E-14	99.937870	2.999982
0.40	1.731489E+16	46.666667	1.234286E-06	1.603102E-15	5.258347E-15	5.403053E-14	99.934792	2.999981
0.41	1.731435E+16	47.833333	1.234286E-06	1.715757E-15	5.389748E-15	5.673167E-14	99.931638	2.999980
0.42	1.731379E+16	49.000000	1.234286E-06	1.833527E-15	5.521145E-15	5.949867E-14	99.928408	2.999979
0.43	1.731321E+16	50.166667	1.234286E-06	1.956523E-15	5.652538E-15	6.233151E-14	99.925102	2.999978
0.44	1.731263E+16	51.333333	1.234286E-06	2.084859E-15	5.783926E-15	6.523018E-14	99.921720	2.999977
0.45	1.731203E+16	52.500000	1.234286E-06	2.218648E-15	5.915310E-15	6.819470E-14	99.918261	2.999976

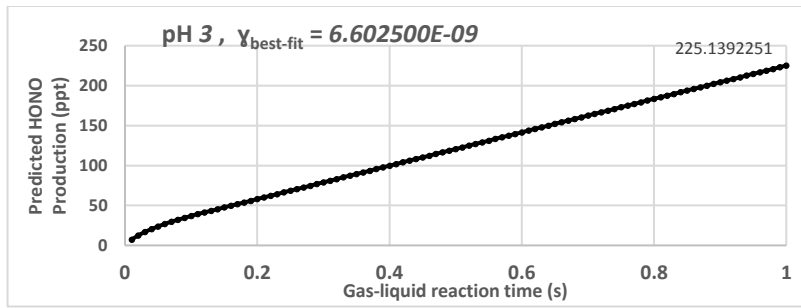
0.46	1.731142E+16	53.666667	1.234286E-06	2.358002E-15	6.046690E-15	7.122505E-14	99.914726	2.999975
0.47	1.731079E+16	54.833333	1.234286E-06	2.503034E-15	6.178065E-15	7.432123E-14	99.911115	2.999974
0.48	1.731015E+16	56.000000	1.234286E-06	2.653856E-15	6.309435E-15	7.748324E-14	99.907426	2.999973
0.49	1.730950E+16	57.166667	1.234286E-06	2.810580E-15	6.440800E-15	8.071107E-14	99.903661	2.999972
0.50	1.730883E+16	58.333333	1.234286E-06	2.973320E-15	6.572160E-15	8.400473E-14	99.899819	2.999970
0.51	1.730815E+16	59.500000	1.234286E-06	3.142188E-15	6.703516E-15	8.736421E-14	99.895900	2.999969
0.52	1.730746E+16	60.666667	1.234286E-06	3.317297E-15	6.834866E-15	9.078950E-14	99.891904	2.999968
0.53	1.730676E+16	61.833333	1.234286E-06	3.498759E-15	6.966211E-15	9.428061E-14	99.887830	2.999967
0.54	1.730604E+16	63.000000	1.234286E-06	3.686686E-15	7.097550E-15	9.783753E-14	99.883679	2.999966
0.55	1.730530E+16	64.166667	1.234286E-06	3.881192E-15	7.228884E-15	1.014603E-13	99.879451	2.999964
0.56	1.730456E+16	65.333333	1.234286E-06	4.082388E-15	7.360213E-15	1.051488E-13	99.875145	2.999963
0.57	1.730380E+16	66.500000	1.234286E-06	4.290387E-15	7.491536E-15	1.089031E-13	99.870761	2.999962
0.58	1.730303E+16	67.666667	1.234286E-06	4.505302E-15	7.622853E-15	1.127232E-13	99.866300	2.999960
0.59	1.730224E+16	68.833333	1.234286E-06	4.727246E-15	7.754165E-15	1.166092E-13	99.861760	2.999959
0.60	1.730144E+16	70.000000	1.234286E-06	4.956330E-15	7.885470E-15	1.205609E-13	99.857142	2.999958
0.61	1.730063E+16	71.166667	1.234286E-06	5.192667E-15	8.016770E-15	1.245784E-13	99.852446	2.999956
0.62	1.729980E+16	72.333333	1.234286E-06	5.436370E-15	8.148063E-15	1.286617E-13	99.847672	2.999955
0.63	1.729896E+16	73.500000	1.234286E-06	5.687551E-15	8.279350E-15	1.328107E-13	99.842819	2.999953
0.64	1.729810E+16	74.666667	1.234286E-06	5.946322E-15	8.410631E-15	1.370255E-13	99.837888	2.999952
0.65	1.729724E+16	75.833333	1.234286E-06	6.212797E-15	8.541905E-15	1.413062E-13	99.832878	2.999950
0.66	1.729635E+16	77.000000	1.234286E-06	6.487086E-15	8.673173E-15	1.456525E-13	99.827789	2.999949
0.67	1.729546E+16	78.166667	1.234286E-06	6.769304E-15	8.804434E-15	1.500647E-13	99.822622	2.999947
0.68	1.729455E+16	79.333333	1.234286E-06	7.059562E-15	8.935689E-15	1.545425E-13	99.817375	2.999946
0.69	1.729363E+16	80.500000	1.234286E-06	7.357972E-15	9.066936E-15	1.590862E-13	99.812049	2.999944
0.70	1.729269E+16	81.666667	1.234286E-06	7.664647E-15	9.198177E-15	1.636956E-13	99.806644	2.999942
0.71	1.729174E+16	82.833333	1.234286E-06	7.979700E-15	9.329410E-15	1.683707E-13	99.801160	2.999941
0.72	1.729078E+16	84.000000	1.234286E-06	8.303242E-15	9.460637E-15	1.731116E-13	99.795596	2.999939
0.73	1.728980E+16	85.166667	1.234286E-06	8.635386E-15	9.591856E-15	1.779182E-13	99.789952	2.999937
0.74	1.728881E+16	86.333333	1.234286E-06	8.976244E-15	9.723068E-15	1.827906E-13	99.784229	2.999936
0.75	1.728780E+16	87.500000	1.234286E-06	9.325930E-15	9.854272E-15	1.877287E-13	99.778426	2.999934
0.76	1.728678E+16	88.666667	1.234286E-06	9.684554E-15	9.985469E-15	1.927325E-13	99.772543	2.999932
0.77	1.728575E+16	89.833333	1.234286E-06	1.005223E-14	1.011666E-14	1.978020E-13	99.766580	2.999930
0.78	1.728470E+16	91.000000	1.234286E-06	1.042907E-14	1.024784E-14	2.029373E-13	99.760537	2.999929
0.79	1.728364E+16	92.166667	1.234286E-06	1.081518E-14	1.037901E-14	2.081382E-13	99.754413	2.999927
0.80	1.728257E+16	93.333333	1.234286E-06	1.121068E-14	1.051018E-14	2.134049E-13	99.748209	2.999925
0.81	1.728148E+16	94.500000	1.234286E-06	1.161569E-14	1.064134E-14	2.187372E-13	99.741925	2.999923
0.82	1.728037E+16	95.666667	1.234286E-06	1.203030E-14	1.077249E-14	2.241353E-13	99.735560	2.999921
0.83	1.727926E+16	96.833333	1.234286E-06	1.245464E-14	1.090363E-14	2.295990E-13	99.729114	2.999919
0.84	1.727813E+16	98.000000	1.234286E-06	1.288882E-14	1.103476E-14	2.351285E-13	99.722587	2.999917
0.85	1.727698E+16	99.166667	1.234286E-06	1.333294E-14	1.116588E-14	2.407236E-13	99.715980	2.999915
0.86	1.727582E+16	100.333333	1.234286E-06	1.378713E-14	1.129700E-14	2.463843E-13	99.709291	2.999913
0.87	1.727465E+16	101.500000	1.234286E-06	1.425149E-14	1.142811E-14	2.521108E-13	99.702521	2.999911
0.88	1.727346E+16	102.666667	1.234286E-06	1.472613E-14	1.155920E-14	2.579029E-13	99.695669	2.999909
0.89	1.727226E+16	103.833333	1.234286E-06	1.521118E-14	1.169029E-14	2.637607E-13	99.688737	2.999907
0.90	1.727105E+16	105.000000	1.234286E-06	1.570673E-14	1.182137E-14	2.696841E-13	99.681722	2.999905
0.91	1.726982E+16	106.166667	1.234286E-06	1.621290E-14	1.195244E-14	2.756732E-13	99.674626	2.999903
0.92	1.726857E+16	107.333333	1.234286E-06	1.672981E-14	1.208351E-14	2.817279E-13	99.667449	2.999901
0.93	1.726731E+16	108.500000	1.234286E-06	1.725757E-14	1.221456E-14	2.878482E-13	99.660189	2.999899
0.94	1.726604E+16	109.666667	1.234286E-06	1.779628E-14	1.234560E-14	2.940342E-13	99.652847	2.999897
0.95	1.726476E+16	110.833333	1.234286E-06	1.834606E-14	1.247663E-14	3.002858E-13	99.645424	2.999894
0.96	1.726346E+16	112.000000	1.234286E-06	1.890702E-14	1.260766E-14	3.066031E-13	99.637918	2.999892
0.97	1.726214E+16	113.166667	1.234286E-06	1.947928E-14	1.273867E-14	3.129859E-13	99.630329	2.999890
0.98	1.726081E+16	114.333333	1.234286E-06	2.006294E-14	1.286968E-14	3.194344E-13	99.622658	2.999888
0.99	1.725947E+16	115.500000	1.234286E-06	2.065812E-14	1.300067E-14	3.259484E-13	99.614905	2.999885
1.00	1.725811E+16	116.666667	1.234286E-06	2.126493E-14	1.313166E-14	3.325281E-13	99.607069	2.999883



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732616E+16	1.166667	3.509917E-07	1.889471E-19	1.252781E-16	6.278776E-17	99.999798	3.000000
0.02	1.732611E+16	2.333333	4.963759E-07	8.340528E-19	2.505558E-16	1.883631E-16	99.999529	3.000000
0.03	1.732605E+16	3.500000	6.079317E-07	2.128977E-18	3.758332E-16	3.767258E-16	99.999192	3.000000
0.04	1.732598E+16	4.666667	7.019762E-07	4.233438E-18	5.011100E-16	6.278755E-16	99.998786	3.000000
0.05	1.732590E+16	5.833333	7.848296E-07	7.286512E-18	6.263863E-16	9.418119E-16	99.998313	2.999999
0.06	1.732580E+16	7.000000	8.597331E-07	1.141302E-17	7.516619E-16	1.318535E-15	99.997771	2.999999
0.07	1.732570E+16	8.166667	9.286122E-07	1.672720E-17	8.769367E-16	1.758043E-15	99.997160	2.999999
0.08	1.732558E+16	9.333333	9.927214E-07	2.333496E-17	1.002211E-15	2.260337E-15	99.996481	2.999999
0.09	1.732545E+16	10.500000	1.052932E-06	3.133554E-17	1.127484E-15	2.825416E-15	99.995733	2.999999
0.10	1.732531E+16	11.666667	1.109879E-06	4.082257E-17	1.252756E-15	3.453280E-15	99.994917	2.999999
0.11	1.732516E+16	12.833333	1.164041E-06	5.188497E-17	1.378027E-15	4.143927E-15	99.994031	2.999998
0.12	1.732499E+16	14.000000	1.215789E-06	6.460758E-17	1.503297E-15	4.897357E-15	99.993077	2.999998
0.13	1.732481E+16	15.166667	1.234286E-06	7.908885E-17	1.628565E-15	5.713569E-15	99.992053	2.999998
0.14	1.732462E+16	16.333333	1.234286E-06	9.543622E-17	1.753833E-15	6.592563E-15	99.990960	2.999998
0.15	1.732442E+16	17.500000	1.234286E-06	1.137571E-16	1.879098E-15	7.534337E-15	99.989798	2.999997
0.16	1.732421E+16	18.666667	1.234286E-06	1.341591E-16	2.004363E-15	8.538891E-15	99.988566	2.999997
0.17	1.732398E+16	19.833333	1.234286E-06	1.567494E-16	2.129625E-15	9.606224E-15	99.987264	2.999997
0.18	1.732375E+16	21.000000	1.234286E-06	1.816356E-16	2.254886E-15	1.073633E-14	99.985893	2.999996
0.19	1.732350E+16	22.166667	1.234286E-06	2.089251E-16	2.380146E-15	1.192922E-14	99.984453	2.999996
0.20	1.732324E+16	23.333333	1.234286E-06	2.387253E-16	2.505403E-15	1.318488E-14	99.982942	2.999995
0.21	1.732296E+16	24.500000	1.234286E-06	2.711437E-16	2.630658E-15	1.450332E-14	99.981361	2.999995
0.22	1.732268E+16	25.666667	1.234286E-06	3.062876E-16	2.755912E-15	1.588453E-14	99.979710	2.999994
0.23	1.732238E+16	26.833333	1.234286E-06	3.442646E-16	2.881163E-15	1.732851E-14	99.977989	2.999994
0.24	1.732207E+16	28.000000	1.234286E-06	3.851819E-16	3.006412E-15	1.883527E-14	99.976198	2.999993
0.25	1.732174E+16	29.166667	1.234286E-06	4.291471E-16	3.131659E-15	2.040479E-14	99.974336	2.999993
0.26	1.732141E+16	30.333333	1.234286E-06	4.762674E-16	3.256904E-15	2.203708E-14	99.972403	2.999992
0.27	1.732106E+16	31.500000	1.234286E-06	5.266504E-16	3.382146E-15	2.373213E-14	99.970400	2.999992
0.28	1.732070E+16	32.666667	1.234286E-06	5.804035E-16	3.507385E-15	2.548995E-14	99.968326	2.999991
0.29	1.732033E+16	33.833333	1.234286E-06	6.376340E-16	3.632622E-15	2.731054E-14	99.966181	2.999990
0.30	1.731995E+16	35.000000	1.234286E-06	6.984492E-16	3.757856E-15	2.919388E-14	99.963965	2.999990
0.31	1.731955E+16	36.166667	1.234286E-06	7.629567E-16	3.883088E-15	3.113999E-14	99.961678	2.999989
0.32	1.731914E+16	37.333333	1.234286E-06	8.312638E-16	4.008316E-15	3.314885E-14	99.959319	2.999988
0.33	1.731872E+16	38.500000	1.234286E-06	9.034778E-16	4.133542E-15	3.522047E-14	99.956889	2.999988
0.34	1.731829E+16	39.666667	1.234286E-06	9.797062E-16	4.258764E-15	3.735484E-14	99.954388	2.999987
0.35	1.731784E+16	40.833333	1.234286E-06	1.060056E-15	4.383984E-15	3.955197E-14	99.951815	2.999986
0.36	1.731738E+16	42.000000	1.234286E-06	1.144635E-15	4.509200E-15	4.181185E-14	99.949170	2.999985
0.37	1.731691E+16	43.166667	1.234286E-06	1.233551E-15	4.634412E-15	4.413447E-14	99.946454	2.999984
0.38	1.731643E+16	44.333333	1.234286E-06	1.326910E-15	4.759622E-15	4.651984E-14	99.943665	2.999984
0.39	1.731593E+16	45.500000	1.234286E-06	1.424821E-15	4.884827E-15	4.896796E-14	99.940804	2.999983
0.40	1.731543E+16	46.666667	1.234286E-06	1.527389E-15	5.010030E-15	5.147882E-14	99.937872	2.999982
0.41	1.731491E+16	47.833333	1.234286E-06	1.634724E-15	5.135228E-15	5.405241E-14	99.934867	2.999981
0.42	1.731437E+16	49.000000	1.234286E-06	1.746932E-15	5.260423E-15	5.668875E-14	99.931789	2.999980
0.43	1.731383E+16	50.166667	1.234286E-06	1.864120E-15	5.385614E-15	5.938782E-14	99.928639	2.999979
0.44	1.731327E+16	51.333333	1.234286E-06	1.986396E-15	5.510801E-15	6.214963E-14	99.925417	2.999978
0.45	1.731270E+16	52.500000	1.234286E-06	2.113867E-15	5.635984E-15	6.497416E-14	99.922122	2.999977

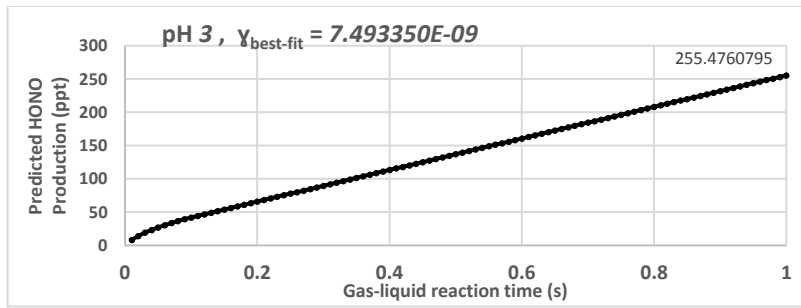


0.46	1.731211E+16	53.666667	1.234286E-06	2.246640E-15	5.761163E-15	6.786142E-14	99.918753	2.999976
0.47	1.731152E+16	54.833333	1.234286E-06	2.384823E-15	5.886337E-15	7.081141E-14	99.915312	2.999975
0.48	1.731091E+16	56.000000	1.234286E-06	2.528522E-15	6.011508E-15	7.382412E-14	99.911798	2.999974
0.49	1.731029E+16	57.166667	1.234286E-06	2.677846E-15	6.136674E-15	7.689955E-14	99.908211	2.999973
0.50	1.730965E+16	58.333333	1.234286E-06	2.832902E-15	6.261835E-15	8.003770E-14	99.904550	2.999972
0.51	1.730901E+16	59.500000	1.234286E-06	2.993796E-15	6.386992E-15	8.323856E-14	99.900816	2.999971
0.52	1.730835E+16	60.666667	1.234286E-06	3.160636E-15	6.512144E-15	8.650214E-14	99.897009	2.999970
0.53	1.730767E+16	61.833333	1.234286E-06	3.333529E-15	6.637292E-15	8.982842E-14	99.893127	2.999968
0.54	1.730699E+16	63.000000	1.234286E-06	3.512583E-15	6.762434E-15	9.321741E-14	99.889172	2.999967
0.55	1.730629E+16	64.166667	1.234286E-06	3.697905E-15	6.887572E-15	9.666910E-14	99.885144	2.999966
0.56	1.730558E+16	65.333333	1.234286E-06	3.889601E-15	7.012705E-15	1.001835E-13	99.881041	2.999965
0.57	1.730486E+16	66.500000	1.234286E-06	4.087779E-15	7.137832E-15	1.037606E-13	99.876864	2.999963
0.58	1.730412E+16	67.666667	1.234286E-06	4.292547E-15	7.262955E-15	1.074004E-13	99.872613	2.999962
0.59	1.730337E+16	68.833333	1.234286E-06	4.504011E-15	7.388072E-15	1.111028E-13	99.868288	2.999961
0.60	1.730261E+16	70.000000	1.234286E-06	4.722279E-15	7.513184E-15	1.148680E-13	99.863888	2.999960
0.61	1.730183E+16	71.166667	1.234286E-06	4.947458E-15	7.638290E-15	1.186959E-13	99.859414	2.999958
0.62	1.730104E+16	72.333333	1.234286E-06	5.179655E-15	7.763390E-15	1.225864E-13	99.854865	2.999957
0.63	1.730024E+16	73.500000	1.234286E-06	5.418977E-15	7.888485E-15	1.265396E-13	99.850241	2.999955
0.64	1.729943E+16	74.666667	1.234286E-06	5.665531E-15	8.013575E-15	1.305555E-13	99.845543	2.999954
0.65	1.729860E+16	75.833333	1.234286E-06	5.919425E-15	8.138658E-15	1.346340E-13	99.840769	2.999953
0.66	1.729776E+16	77.000000	1.234286E-06	6.180766E-15	8.263735E-15	1.387752E-13	99.835921	2.999951
0.67	1.729691E+16	78.166667	1.234286E-06	6.449660E-15	8.388807E-15	1.429791E-13	99.830997	2.999950
0.68	1.729604E+16	79.333333	1.234286E-06	6.726215E-15	8.513872E-15	1.472456E-13	99.825998	2.999948
0.69	1.729516E+16	80.500000	1.234286E-06	7.010538E-15	8.638931E-15	1.515748E-13	99.820923	2.999947
0.70	1.729427E+16	81.666667	1.234286E-06	7.302736E-15	8.763984E-15	1.559667E-13	99.815773	2.999945
0.71	1.729337E+16	82.833333	1.234286E-06	7.602916E-15	8.889031E-15	1.604211E-13	99.810548	2.999944
0.72	1.729245E+16	84.000000	1.234286E-06	7.911185E-15	9.014070E-15	1.649383E-13	99.805247	2.999942
0.73	1.729152E+16	85.166667	1.234286E-06	8.227650E-15	9.139104E-15	1.695181E-13	99.799869	2.999940
0.74	1.729057E+16	86.333333	1.234286E-06	8.552419E-15	9.264130E-15	1.741605E-13	99.794416	2.999939
0.75	1.728961E+16	87.500000	1.234286E-06	8.885597E-15	9.389150E-15	1.788655E-13	99.788887	2.999937
0.76	1.728864E+16	88.666667	1.234286E-06	9.227293E-15	9.514163E-15	1.836332E-13	99.783282	2.999935
0.77	1.728766E+16	89.833333	1.234286E-06	9.577614E-15	9.639169E-15	1.884635E-13	99.777600	2.999934
0.78	1.728666E+16	91.000000	1.234286E-06	9.936665E-15	9.764169E-15	1.933564E-13	99.771842	2.999932
0.79	1.728565E+16	92.166667	1.234286E-06	1.030455E-14	9.889160E-15	1.983119E-13	99.766007	2.999930
0.80	1.728462E+16	93.333333	1.234286E-06	1.068139E-14	1.001415E-14	2.033300E-13	99.760096	2.999928
0.81	1.728359E+16	94.500000	1.234286E-06	1.106728E-14	1.013912E-14	2.084108E-13	99.754108	2.999927
0.82	1.728254E+16	95.666667	1.234286E-06	1.146232E-14	1.026409E-14	2.135541E-13	99.748044	2.999925
0.83	1.728147E+16	96.833333	1.234286E-06	1.186664E-14	1.038905E-14	2.187601E-13	99.741902	2.999923
0.84	1.728040E+16	98.000000	1.234286E-06	1.228032E-14	1.051401E-14	2.240286E-13	99.735683	2.999921
0.85	1.727930E+16	99.166667	1.234286E-06	1.270349E-14	1.063896E-14	2.293597E-13	99.729387	2.999919
0.86	1.727820E+16	100.333333	1.234286E-06	1.313624E-14	1.076390E-14	2.347534E-13	99.723014	2.999917
0.87	1.727708E+16	101.500000	1.234286E-06	1.357868E-14	1.088883E-14	2.402097E-13	99.716563	2.999915
0.88	1.727595E+16	102.666667	1.234286E-06	1.403093E-14	1.101375E-14	2.457285E-13	99.710035	2.999914
0.89	1.727481E+16	103.833333	1.234286E-06	1.449308E-14	1.113867E-14	2.513100E-13	99.703430	2.999912
0.90	1.727365E+16	105.000000	1.234286E-06	1.496525E-14	1.126357E-14	2.569539E-13	99.696746	2.999910
0.91	1.727248E+16	106.166667	1.234286E-06	1.544754E-14	1.138847E-14	2.626605E-13	99.689985	2.999908
0.92	1.727129E+16	107.333333	1.234286E-06	1.594005E-14	1.151336E-14	2.684296E-13	99.683146	2.999906
0.93	1.727009E+16	108.500000	1.234286E-06	1.644291E-14	1.163824E-14	2.742612E-13	99.676229	2.999904
0.94	1.726888E+16	109.666667	1.234286E-06	1.695620E-14	1.176312E-14	2.801554E-13	99.669233	2.999901
0.95	1.726766E+16	110.833333	1.234286E-06	1.748004E-14	1.188798E-14	2.861121E-13	99.662160	2.999899
0.96	1.726642E+16	112.000000	1.234286E-06	1.801453E-14	1.201284E-14	2.921314E-13	99.655008	2.999897
0.97	1.726516E+16	113.166667	1.234286E-06	1.855979E-14	1.213769E-14	2.982132E-13	99.647777	2.999895
0.98	1.726390E+16	114.333333	1.234286E-06	1.911591E-14	1.226252E-14	3.043575E-13	99.640468	2.999893
0.99	1.726262E+16	115.500000	1.234286E-06	1.968301E-14	1.238735E-14	3.105643E-13	99.633080	2.999891
1.00	1.726132E+16	116.666667	1.234286E-06	2.026120E-14	1.251217E-14	3.168336E-13	99.625614	2.999889



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732616E+16	1.166667	3.509917E-07	1.908491E-19	1.265392E-16	6.341980E-17	99.999796	3.000000
0.02	1.732611E+16	2.333333	4.963758E-07	8.424486E-19	2.530780E-16	1.902592E-16	99.999524	3.000000
0.03	1.732605E+16	3.500000	6.079317E-07	2.150408E-18	3.796164E-16	3.805180E-16	99.999184	3.000000
0.04	1.732598E+16	4.666667	7.019762E-07	4.276052E-18	5.061543E-16	6.341958E-16	99.998774	3.000000
0.05	1.732590E+16	5.833333	7.848295E-07	7.359859E-18	6.326916E-16	9.512924E-16	99.998296	2.999999
0.06	1.732580E+16	7.000000	8.597329E-07	1.152791E-17	7.592282E-16	1.331807E-15	99.997748	2.999999
0.07	1.732569E+16	8.166667	9.286119E-07	1.689558E-17	8.857641E-16	1.775740E-15	99.997132	2.999999
0.08	1.732558E+16	9.333333	9.927211E-07	2.356986E-17	1.012299E-15	2.283090E-15	99.996446	2.999999
0.09	1.732544E+16	10.500000	1.052932E-06	3.165097E-17	1.138833E-15	2.853857E-15	99.995690	2.999999
0.10	1.732530E+16	11.666667	1.109878E-06	4.123350E-17	1.265366E-15	3.488041E-15	99.994866	2.999999
0.11	1.732515E+16	12.833333	1.164040E-06	5.240726E-17	1.391898E-15	4.185640E-15	99.993971	2.999998
0.12	1.732498E+16	14.000000	1.215788E-06	6.525793E-17	1.518429E-15	4.946654E-15	99.993007	2.999998
0.13	1.732480E+16	15.166667	1.234286E-06	7.988498E-17	1.644958E-15	5.771082E-15	99.991973	2.999998
0.14	1.732461E+16	16.333333	1.234286E-06	9.639691E-17	1.771486E-15	6.658924E-15	99.990869	2.999998
0.15	1.732441E+16	17.500000	1.234286E-06	1.149023E-16	1.898013E-15	7.610178E-15	99.989695	2.999997
0.16	1.732419E+16	18.666667	1.234286E-06	1.355095E-16	2.024538E-15	8.624843E-15	99.988451	2.999997
0.17	1.732396E+16	19.833333	1.234286E-06	1.583273E-16	2.151062E-15	9.702919E-15	99.987136	2.999997
0.18	1.732372E+16	21.000000	1.234286E-06	1.834640E-16	2.277583E-15	1.084441E-14	99.985751	2.999996
0.19	1.732347E+16	22.166667	1.234286E-06	2.110282E-16	2.404103E-15	1.204930E-14	99.984296	2.999996
0.20	1.732321E+16	23.333333	1.234286E-06	2.411284E-16	2.530621E-15	1.331760E-14	99.982770	2.999995
0.21	1.732293E+16	24.500000	1.234286E-06	2.738730E-16	2.657137E-15	1.464931E-14	99.981174	2.999995
0.22	1.732264E+16	25.666667	1.234286E-06	3.093707E-16	2.783651E-15	1.604442E-14	99.979506	2.999994
0.23	1.732234E+16	26.833333	1.234286E-06	3.477299E-16	2.910163E-15	1.750294E-14	99.977768	2.999994
0.24	1.732203E+16	28.000000	1.234286E-06	3.890591E-16	3.036673E-15	1.902485E-14	99.975958	2.999993
0.25	1.732170E+16	29.166667	1.234286E-06	4.334668E-16	3.163180E-15	2.061017E-14	99.974077	2.999993
0.26	1.732136E+16	30.333333	1.234286E-06	4.810615E-16	3.289685E-15	2.225889E-14	99.972125	2.999992
0.27	1.732101E+16	31.500000	1.234286E-06	5.319516E-16	3.416188E-15	2.397101E-14	99.970102	2.999992
0.28	1.732065E+16	32.666667	1.234286E-06	5.862457E-16	3.542687E-15	2.574652E-14	99.968007	2.999991
0.29	1.732027E+16	33.833333	1.234286E-06	6.440522E-16	3.669184E-15	2.758543E-14	99.965840	2.999990
0.30	1.731988E+16	35.000000	1.234286E-06	7.054796E-16	3.795679E-15	2.948773E-14	99.963602	2.999990
0.31	1.731948E+16	36.166667	1.234286E-06	7.706364E-16	3.922170E-15	3.145342E-14	99.961292	2.999989
0.32	1.731907E+16	37.333333	1.234286E-06	8.396310E-16	4.048659E-15	3.348250E-14	99.958910	2.999988
0.33	1.731865E+16	38.500000	1.234286E-06	9.125718E-16	4.175144E-15	3.557497E-14	99.956455	2.999987
0.34	1.731821E+16	39.666667	1.234286E-06	9.895674E-16	4.301627E-15	3.773083E-14	99.953929	2.999987
0.35	1.731776E+16	40.833333	1.234286E-06	1.070726E-15	4.428106E-15	3.995006E-14	99.951330	2.999986
0.36	1.731730E+16	42.000000	1.234286E-06	1.156157E-15	4.554582E-15	4.223268E-14	99.948659	2.999985
0.37	1.731682E+16	43.166667	1.234286E-06	1.245967E-15	4.681054E-15	4.457868E-14	99.945915	2.999984
0.38	1.731633E+16	44.333333	1.234286E-06	1.340266E-15	4.807523E-15	4.698806E-14	99.943098	2.999983
0.39	1.731583E+16	45.500000	1.234286E-06	1.439162E-15	4.933989E-15	4.946081E-14	99.940209	2.999983
0.40	1.731532E+16	46.666667	1.234286E-06	1.542763E-15	5.060451E-15	5.199694E-14	99.937246	2.999982
0.41	1.731479E+16	47.833333	1.234286E-06	1.651178E-15	5.186909E-15	5.459644E-14	99.934211	2.999981
0.42	1.731425E+16	49.000000	1.234286E-06	1.764515E-15	5.313363E-15	5.725930E-14	99.931103	2.999980
0.43	1.731370E+16	50.166667	1.234286E-06	1.882882E-15	5.439813E-15	5.998554E-14	99.927921	2.999979
0.44	1.731314E+16	51.333333	1.234286E-06	2.006389E-15	5.566259E-15	6.277513E-14	99.924666	2.999978
0.45	1.731256E+16	52.500000	1.234286E-06	2.135143E-15	5.692701E-15	6.562809E-14	99.921338	2.999977

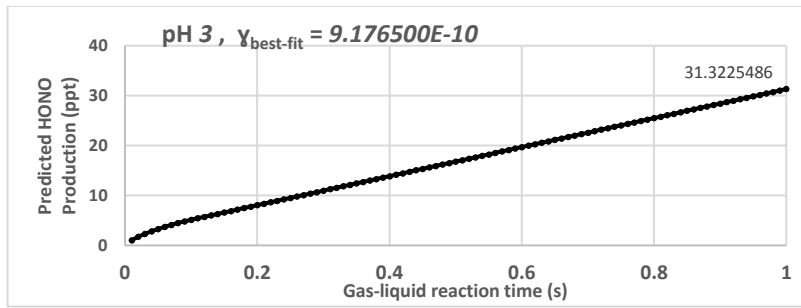
0.46	1.731197E+16	53.666667	1.234286E-06	2.269252E-15	5.819139E-15	6.854441E-14	99.917936	2.999976
0.47	1.731137E+16	54.833333	1.234286E-06	2.408825E-15	5.945573E-15	7.152408E-14	99.914460	2.999975
0.48	1.731076E+16	56.000000	1.234286E-06	2.553971E-15	6.072002E-15	7.456711E-14	99.910910	2.999974
0.49	1.731013E+16	57.166667	1.234286E-06	2.704798E-15	6.198427E-15	7.767348E-14	99.907287	2.999973
0.50	1.730949E+16	58.333333	1.234286E-06	2.861414E-15	6.324847E-15	8.084321E-14	99.903590	2.999972
0.51	1.730883E+16	59.500000	1.234286E-06	3.023927E-15	6.451263E-15	8.407628E-14	99.899818	2.999970
0.52	1.730817E+16	60.666667	1.234286E-06	3.192446E-15	6.577673E-15	8.737269E-14	99.895972	2.999969
0.53	1.730749E+16	61.833333	1.234286E-06	3.367079E-15	6.704079E-15	9.073244E-14	99.892052	2.999968
0.54	1.730680E+16	63.000000	1.234286E-06	3.547935E-15	6.830480E-15	9.415553E-14	99.888057	2.999967
0.55	1.730609E+16	64.166667	1.234286E-06	3.735121E-15	6.956876E-15	9.764195E-14	99.883988	2.999966
0.56	1.730537E+16	65.333333	1.234286E-06	3.928746E-15	7.083267E-15	1.011917E-13	99.879844	2.999964
0.57	1.730464E+16	66.500000	1.234286E-06	4.128919E-15	7.209653E-15	1.048048E-13	99.875625	2.999963
0.58	1.730390E+16	67.666667	1.234286E-06	4.335747E-15	7.336033E-15	1.084812E-13	99.871331	2.999962
0.59	1.730314E+16	68.833333	1.234286E-06	4.549339E-15	7.462408E-15	1.122209E-13	99.866962	2.999961
0.60	1.730237E+16	70.000000	1.234286E-06	4.769803E-15	7.588777E-15	1.160240E-13	99.862518	2.999959
0.61	1.730159E+16	71.166667	1.234286E-06	4.997248E-15	7.715141E-15	1.198903E-13	99.857999	2.999958
0.62	1.730079E+16	72.333333	1.234286E-06	5.231781E-15	7.841499E-15	1.238200E-13	99.853404	2.999956
0.63	1.729998E+16	73.500000	1.234286E-06	5.473511E-15	7.967852E-15	1.278129E-13	99.848734	2.999955
0.64	1.729916E+16	74.666667	1.234286E-06	5.722546E-15	8.094198E-15	1.318692E-13	99.843988	2.999954
0.65	1.729832E+16	75.833333	1.234286E-06	5.978995E-15	8.220539E-15	1.359888E-13	99.839167	2.999952
0.66	1.729748E+16	77.000000	1.234286E-06	6.242965E-15	8.346873E-15	1.401717E-13	99.834269	2.999951
0.67	1.729661E+16	78.166667	1.234286E-06	6.514564E-15	8.473201E-15	1.444178E-13	99.829296	2.999949
0.68	1.729574E+16	79.333333	1.234286E-06	6.793901E-15	8.599524E-15	1.487273E-13	99.824247	2.999948
0.69	1.729485E+16	80.500000	1.234286E-06	7.081085E-15	8.725839E-15	1.531000E-13	99.819121	2.999946
0.70	1.729395E+16	81.666667	1.234286E-06	7.376222E-15	8.852149E-15	1.575360E-13	99.813920	2.999945
0.71	1.729304E+16	82.833333	1.234286E-06	7.679422E-15	8.978451E-15	1.620353E-13	99.808642	2.999943
0.72	1.729211E+16	84.000000	1.234286E-06	7.990793E-15	9.104748E-15	1.665979E-13	99.803287	2.999941
0.73	1.729117E+16	85.166667	1.234286E-06	8.310442E-15	9.231037E-15	1.712237E-13	99.797856	2.999940
0.74	1.729021E+16	86.333333	1.234286E-06	8.638477E-15	9.357320E-15	1.759128E-13	99.792348	2.999938
0.75	1.728925E+16	87.500000	1.234286E-06	8.975008E-15	9.483595E-15	1.806652E-13	99.786763	2.999936
0.76	1.728826E+16	88.666667	1.234286E-06	9.320141E-15	9.609864E-15	1.854808E-13	99.781101	2.999935
0.77	1.728727E+16	89.833333	1.234286E-06	9.673985E-15	9.736126E-15	1.903597E-13	99.775362	2.999933
0.78	1.728626E+16	91.000000	1.234286E-06	1.003665E-14	9.862380E-15	1.953018E-13	99.769546	2.999931
0.79	1.728524E+16	92.166667	1.234286E-06	1.040824E-14	9.988628E-15	2.003072E-13	99.763653	2.999930
0.80	1.728421E+16	93.333333	1.234286E-06	1.078886E-14	1.011487E-14	2.053758E-13	99.757683	2.999928
0.81	1.728316E+16	94.500000	1.234286E-06	1.117863E-14	1.024110E-14	2.105076E-13	99.751634	2.999926
0.82	1.728210E+16	95.666667	1.234286E-06	1.157765E-14	1.036732E-14	2.157027E-13	99.745509	2.999924
0.83	1.728102E+16	96.833333	1.234286E-06	1.198603E-14	1.049354E-14	2.209609E-13	99.739305	2.999922
0.84	1.727993E+16	98.000000	1.234286E-06	1.240388E-14	1.061975E-14	2.262825E-13	99.733024	2.999920
0.85	1.727883E+16	99.166667	1.234286E-06	1.283130E-14	1.074595E-14	2.316672E-13	99.726665	2.999918
0.86	1.727772E+16	100.333333	1.234286E-06	1.326840E-14	1.087215E-14	2.371151E-13	99.720227	2.999917
0.87	1.727659E+16	101.500000	1.234286E-06	1.371530E-14	1.099833E-14	2.426262E-13	99.713712	2.999915
0.88	1.727545E+16	102.666667	1.234286E-06	1.417209E-14	1.112451E-14	2.482006E-13	99.707118	2.999913
0.89	1.727429E+16	103.833333	1.234286E-06	1.463889E-14	1.125068E-14	2.538381E-13	99.700446	2.999911
0.90	1.727312E+16	105.000000	1.234286E-06	1.511581E-14	1.137684E-14	2.595389E-13	99.693695	2.999909
0.91	1.727194E+16	106.166667	1.234286E-06	1.560295E-14	1.150299E-14	2.653028E-13	99.686866	2.999907
0.92	1.727074E+16	107.333333	1.234286E-06	1.610042E-14	1.162913E-14	2.711299E-13	99.679958	2.999905
0.93	1.726953E+16	108.500000	1.234286E-06	1.660833E-14	1.175527E-14	2.770201E-13	99.672972	2.999903
0.94	1.726831E+16	109.666667	1.234286E-06	1.712678E-14	1.188140E-14	2.829736E-13	99.665906	2.999900
0.95	1.726707E+16	110.833333	1.234286E-06	1.765589E-14	1.200751E-14	2.889902E-13	99.658761	2.999898
0.96	1.726582E+16	112.000000	1.234286E-06	1.819576E-14	1.213362E-14	2.950699E-13	99.651537	2.999896
0.97	1.726455E+16	113.166667	1.234286E-06	1.874650E-14	1.225972E-14	3.012128E-13	99.644234	2.999894
0.98	1.726327E+16	114.333333	1.234286E-06	1.930821E-14	1.238581E-14	3.074189E-13	99.636852	2.999892
0.99	1.726198E+16	115.500000	1.234286E-06	1.988101E-14	1.251189E-14	3.136881E-13	99.629390	2.999890
1.00	1.726067E+16	116.666667	1.234286E-06	2.046501E-14	1.263796E-14	3.200205E-13	99.621848	2.999887



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732615E+16	1.166667	3.509916E-07	2.165996E-19	1.436126E-16	7.197677E-17	99.999769	3.000000
0.02	1.732610E+16	2.333333	4.963755E-07	9.561169E-19	2.872247E-16	2.159301E-16	99.999460	3.000000
0.03	1.732603E+16	3.500000	6.079310E-07	2.440554E-18	4.308363E-16	4.318595E-16	99.999074	3.000000
0.04	1.732595E+16	4.666667	7.019750E-07	4.853004E-18	5.744472E-16	7.197649E-16	99.998609	3.000000
0.05	1.732586E+16	5.833333	7.848277E-07	8.352897E-18	7.180574E-16	1.079646E-15	99.998066	2.999999
0.06	1.732575E+16	7.000000	8.597303E-07	1.308333E-17	8.616667E-16	1.511501E-15	99.997445	2.999999
0.07	1.732563E+16	8.166667	9.286083E-07	1.917523E-17	1.005275E-15	2.015331E-15	99.996745	2.999999
0.08	1.732549E+16	9.333333	9.927163E-07	2.675005E-17	1.148882E-15	2.591135E-15	99.995966	2.999999
0.09	1.732534E+16	10.500000	1.052926E-06	3.592151E-17	1.292488E-15	3.238911E-15	99.995109	2.999999
0.10	1.732518E+16	11.666667	1.109871E-06	4.679698E-17	1.436093E-15	3.958660E-15	99.994173	2.999998
0.11	1.732501E+16	12.833333	1.164030E-06	5.947837E-17	1.579696E-15	4.750380E-15	99.993158	2.999998
0.12	1.732482E+16	14.000000	1.215777E-06	7.406294E-17	1.723298E-15	5.614071E-15	99.992063	2.999998
0.13	1.732461E+16	15.166667	1.234286E-06	9.066354E-17	1.866898E-15	6.549732E-15	99.990890	2.999998
0.14	1.732440E+16	16.333333	1.234286E-06	1.094033E-16	2.010496E-15	7.557361E-15	99.989637	2.999997
0.15	1.732416E+16	17.500000	1.234286E-06	1.304055E-16	2.154093E-15	8.636957E-15	99.988304	2.999997
0.16	1.732392E+16	18.666667	1.234286E-06	1.537932E-16	2.297687E-15	9.788519E-15	99.986892	2.999997
0.17	1.732366E+16	19.833333	1.234286E-06	1.796896E-16	2.441279E-15	1.101205E-14	99.985401	2.999996
0.18	1.732339E+16	21.000000	1.234286E-06	2.082178E-16	2.584870E-15	1.230754E-14	99.983829	2.999996
0.19	1.732310E+16	22.166667	1.234286E-06	2.395010E-16	2.728457E-15	1.367499E-14	99.982177	2.999995
0.20	1.732280E+16	23.333333	1.234286E-06	2.736623E-16	2.872043E-15	1.511440E-14	99.980446	2.999995
0.21	1.732249E+16	24.500000	1.234286E-06	3.108249E-16	3.015626E-15	1.662578E-14	99.978634	2.999994
0.22	1.732216E+16	25.666667	1.234286E-06	3.511119E-16	3.159206E-15	1.820911E-14	99.976741	2.999994
0.23	1.732182E+16	26.833333	1.234286E-06	3.946465E-16	3.302783E-15	1.986439E-14	99.974768	2.999993
0.24	1.732146E+16	28.000000	1.234286E-06	4.415517E-16	3.446358E-15	2.159163E-14	99.972715	2.999992
0.25	1.732109E+16	29.166667	1.234286E-06	4.919507E-16	3.589929E-15	2.339083E-14	99.970580	2.999992
0.26	1.732071E+16	30.333333	1.234286E-06	5.459667E-16	3.733498E-15	2.526197E-14	99.968365	2.999991
0.27	1.732031E+16	31.500000	1.234286E-06	6.037226E-16	3.877063E-15	2.720506E-14	99.966068	2.999990
0.28	1.731990E+16	32.666667	1.234286E-06	6.653417E-16	4.020625E-15	2.922010E-14	99.963691	2.999990
0.29	1.731947E+16	33.833333	1.234286E-06	7.309471E-16	4.164183E-15	3.130708E-14	99.961232	2.999989
0.30	1.731903E+16	35.000000	1.234286E-06	8.006617E-16	4.307738E-15	3.346601E-14	99.958692	2.999988
0.31	1.731858E+16	36.166667	1.234286E-06	8.746088E-16	4.451289E-15	3.569687E-14	99.956070	2.999987
0.32	1.731811E+16	37.333333	1.234286E-06	9.529114E-16	4.594837E-15	3.799967E-14	99.953366	2.999987
0.33	1.731763E+16	38.500000	1.234286E-06	1.035693E-15	4.738380E-15	4.037441E-14	99.950581	2.999986
0.34	1.731713E+16	39.666667	1.234286E-06	1.123075E-15	4.881920E-15	4.282108E-14	99.947713	2.999985
0.35	1.731662E+16	40.833333	1.234286E-06	1.215183E-15	5.025455E-15	4.533968E-14	99.944764	2.999984
0.36	1.731610E+16	42.000000	1.234286E-06	1.312138E-15	5.168986E-15	4.793021E-14	99.941732	2.999983
0.37	1.731556E+16	43.166667	1.234286E-06	1.414064E-15	5.312513E-15	5.059267E-14	99.938618	2.999982
0.38	1.731500E+16	44.333333	1.234286E-06	1.521084E-15	5.456035E-15	5.332704E-14	99.935422	2.999981
0.39	1.731443E+16	45.500000	1.234286E-06	1.633321E-15	5.599553E-15	5.613334E-14	99.932143	2.999980
0.40	1.731385E+16	46.666667	1.234286E-06	1.750898E-15	5.743065E-15	5.901155E-14	99.928781	2.999979
0.41	1.731325E+16	47.833333	1.234286E-06	1.873938E-15	5.886574E-15	6.196168E-14	99.925336	2.999978
0.42	1.731264E+16	49.000000	1.234286E-06	2.002564E-15	6.030077E-15	6.498372E-14	99.921808	2.999977
0.43	1.731202E+16	50.166667	1.234286E-06	2.136898E-15	6.173575E-15	6.807767E-14	99.918198	2.999976
0.44	1.731138E+16	51.333333	1.234286E-06	2.277065E-15	6.317068E-15	7.124352E-14	99.914504	2.999975
0.45	1.731072E+16	52.500000	1.234286E-06	2.423186E-15	6.460555E-15	7.448127E-14	99.910726	2.999974

0.46	1.731005E+16	53.666667	1.234286E-06	2.575386E-15	6.604037E-15	7.779092E-14	99.906865	2.999973
0.47	1.730937E+16	54.833333	1.234286E-06	2.733786E-15	6.747514E-15	8.117247E-14	99.902921	2.999971
0.48	1.730867E+16	56.000000	1.234286E-06	2.898510E-15	6.890985E-15	8.462590E-14	99.898893	2.999970
0.49	1.730796E+16	57.166667	1.234286E-06	3.069681E-15	7.034450E-15	8.815123E-14	99.894781	2.999969
0.50	1.730723E+16	58.333333	1.234286E-06	3.247421E-15	7.177909E-15	9.174844E-14	99.890584	2.999968
0.51	1.730649E+16	59.500000	1.234286E-06	3.431854E-15	7.321363E-15	9.541753E-14	99.886304	2.999966
0.52	1.730574E+16	60.666667	1.234286E-06	3.623103E-15	7.464810E-15	9.915849E-14	99.881940	2.999965
0.53	1.730496E+16	61.833333	1.234286E-06	3.821290E-15	7.608251E-15	1.029713E-13	99.877491	2.999964
0.54	1.730418E+16	63.000000	1.234286E-06	4.026539E-15	7.751685E-15	1.068560E-13	99.872957	2.999962
0.55	1.730338E+16	64.166667	1.234286E-06	4.238971E-15	7.895114E-15	1.108126E-13	99.868339	2.999961
0.56	1.730256E+16	65.333333	1.234286E-06	4.458711E-15	8.038535E-15	1.148411E-13	99.863636	2.999960
0.57	1.730174E+16	66.500000	1.234286E-06	4.685881E-15	8.181950E-15	1.189413E-13	99.858849	2.999958
0.58	1.730089E+16	67.666667	1.234286E-06	4.920604E-15	8.325358E-15	1.231135E-13	99.853976	2.999957
0.59	1.730003E+16	68.833333	1.234286E-06	5.163002E-15	8.468759E-15	1.273575E-13	99.849018	2.999955
0.60	1.729916E+16	70.000000	1.234286E-06	5.413198E-15	8.612153E-15	1.316733E-13	99.843975	2.999954
0.61	1.729827E+16	71.166667	1.234286E-06	5.671316E-15	8.755539E-15	1.360610E-13	99.838846	2.999952
0.62	1.729737E+16	72.333333	1.234286E-06	5.937478E-15	8.898919E-15	1.405205E-13	99.833632	2.999951
0.63	1.729645E+16	73.500000	1.234286E-06	6.211807E-15	9.042291E-15	1.450519E-13	99.828332	2.999949
0.64	1.729551E+16	74.666667	1.234286E-06	6.494425E-15	9.185655E-15	1.496551E-13	99.822946	2.999947
0.65	1.729457E+16	75.833333	1.234286E-06	6.785456E-15	9.329012E-15	1.543300E-13	99.817475	2.999946
0.66	1.729360E+16	77.000000	1.234286E-06	7.085022E-15	9.472361E-15	1.590769E-13	99.811917	2.999944
0.67	1.729263E+16	78.166667	1.234286E-06	7.393246E-15	9.615702E-15	1.638955E-13	99.806274	2.999942
0.68	1.729163E+16	79.333333	1.234286E-06	7.710251E-15	9.759035E-15	1.687859E-13	99.800544	2.999941
0.69	1.729063E+16	80.500000	1.234286E-06	8.036158E-15	9.902360E-15	1.737482E-13	99.794727	2.999939
0.70	1.728960E+16	81.666667	1.234286E-06	8.371092E-15	1.004568E-14	1.787822E-13	99.788824	2.999937
0.71	1.728856E+16	82.833333	1.234286E-06	8.715175E-15	1.018898E-14	1.838880E-13	99.782835	2.999935
0.72	1.728751E+16	84.000000	1.234286E-06	9.068528E-15	1.033228E-14	1.890656E-13	99.776758	2.999933
0.73	1.728644E+16	85.166667	1.234286E-06	9.431276E-15	1.047557E-14	1.943150E-13	99.770595	2.999932
0.74	1.728536E+16	86.333333	1.234286E-06	9.803541E-15	1.061886E-14	1.996362E-13	99.764344	2.999930
0.75	1.728426E+16	87.500000	1.234286E-06	1.018544E-14	1.076213E-14	2.050292E-13	99.758007	2.999928
0.76	1.728315E+16	88.666667	1.234286E-06	1.057711E-14	1.090539E-14	2.104939E-13	99.751582	2.999926
0.77	1.728202E+16	89.833333	1.234286E-06	1.097866E-14	1.104865E-14	2.160303E-13	99.745070	2.999924
0.78	1.728088E+16	91.000000	1.234286E-06	1.139022E-14	1.119190E-14	2.216386E-13	99.738470	2.999922
0.79	1.727972E+16	92.166667	1.234286E-06	1.181190E-14	1.133513E-14	2.273186E-13	99.731782	2.999920
0.80	1.727855E+16	93.333333	1.234286E-06	1.224384E-14	1.147836E-14	2.330703E-13	99.725007	2.999918
0.81	1.727736E+16	94.500000	1.234286E-06	1.268615E-14	1.162158E-14	2.388937E-13	99.718144	2.999916
0.82	1.727615E+16	95.666667	1.234286E-06	1.313896E-14	1.176478E-14	2.447889E-13	99.711192	2.999914
0.83	1.727493E+16	96.833333	1.234286E-06	1.360239E-14	1.190798E-14	2.507558E-13	99.704153	2.999912
0.84	1.727370E+16	98.000000	1.234286E-06	1.407657E-14	1.205117E-14	2.567945E-13	99.697025	2.999910
0.85	1.727245E+16	99.166667	1.234286E-06	1.456160E-14	1.219435E-14	2.629048E-13	99.689809	2.999908
0.86	1.727118E+16	100.333333	1.234286E-06	1.505763E-14	1.233751E-14	2.690869E-13	99.682504	2.999905
0.87	1.726990E+16	101.500000	1.234286E-06	1.556476E-14	1.248067E-14	2.753406E-13	99.675111	2.999903
0.88	1.726860E+16	102.666667	1.234286E-06	1.608312E-14	1.262382E-14	2.816661E-13	99.667629	2.999901
0.89	1.726729E+16	103.833333	1.234286E-06	1.661284E-14	1.276695E-14	2.880632E-13	99.660058	2.999899
0.90	1.726596E+16	105.000000	1.234286E-06	1.715404E-14	1.291008E-14	2.945321E-13	99.652397	2.999896
0.91	1.726462E+16	106.166667	1.234286E-06	1.770683E-14	1.305319E-14	3.010726E-13	99.644648	2.999894
0.92	1.726326E+16	107.333333	1.234286E-06	1.827135E-14	1.319630E-14	3.076847E-13	99.636810	2.999892
0.93	1.726189E+16	108.500000	1.234286E-06	1.884771E-14	1.333939E-14	3.143686E-13	99.628882	2.999889
0.94	1.726050E+16	109.666667	1.234286E-06	1.943603E-14	1.348247E-14	3.211240E-13	99.620864	2.999887
0.95	1.725910E+16	110.833333	1.234286E-06	2.003645E-14	1.362554E-14	3.279512E-13	99.612757	2.999885
0.96	1.725768E+16	112.000000	1.234286E-06	2.064907E-14	1.376860E-14	3.348499E-13	99.604560	2.999882
0.97	1.725624E+16	113.166667	1.234286E-06	2.127402E-14	1.391164E-14	3.418203E-13	99.596273	2.999880
0.98	1.725479E+16	114.333333	1.234286E-06	2.191144E-14	1.405468E-14	3.488624E-13	99.587896	2.999877
0.99	1.725332E+16	115.500000	1.234286E-06	2.256142E-14	1.419770E-14	3.559760E-13	99.579429	2.999875
1.00	1.725184E+16	116.666667	1.234286E-06	2.322411E-14	1.434071E-14	3.631613E-13	99.570872	2.999872

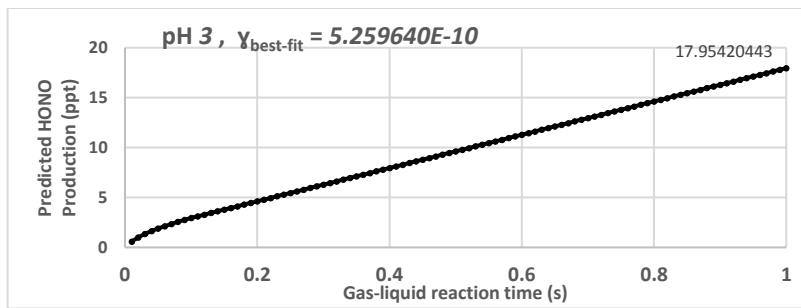
## ELLIOTT SOIL HA STANDARD



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732619E+16	1.166667	3.509923E-07	2.652520E-20	1.758710E-17	8.814432E-18	99.999972	3.000000
0.02	1.732618E+16	2.333333	4.963779E-07	1.170879E-19	3.517420E-17	2.644329E-17	99.999934	3.000000
0.03	1.732617E+16	3.500000	6.079360E-07	2.988749E-19	5.276129E-17	5.288658E-17	99.999887	3.000000
0.04	1.732616E+16	4.666667	7.019836E-07	5.943081E-19	7.034837E-17	8.814428E-17	99.999830	3.000000
0.05	1.732615E+16	5.833333	7.848410E-07	1.022912E-18	8.793544E-17	1.322164E-16	99.999763	3.000000
0.06	1.732614E+16	7.000000	8.597496E-07	1.602209E-18	1.055225E-16	1.851029E-16	99.999687	3.000000
0.07	1.732612E+16	8.166667	9.286349E-07	2.348235E-18	1.231095E-16	2.468038E-16	99.999601	3.000000
0.08	1.732611E+16	9.333333	9.927515E-07	3.275861E-18	1.406966E-16	3.173191E-16	99.999506	3.000000
0.09	1.732609E+16	10.500000	1.052971E-06	4.399016E-18	1.582836E-16	3.966488E-16	99.999401	3.000000
0.10	1.732607E+16	11.666667	1.109927E-06	5.730846E-18	1.758706E-16	4.847928E-16	99.999286	3.000000
0.11	1.732605E+16	12.833333	1.164100E-06	7.283833E-18	1.934575E-16	5.817512E-16	99.999162	3.000000
0.12	1.732602E+16	14.000000	1.215861E-06	9.069886E-18	2.110445E-16	6.875239E-16	99.999028	3.000000
0.13	1.732600E+16	15.166667	1.234286E-06	1.110283E-17	2.286314E-16	8.021110E-16	99.998884	3.000000
0.14	1.732597E+16	16.333333	1.234286E-06	1.339776E-17	2.462183E-16	9.255124E-16	99.998731	3.000000
0.15	1.732594E+16	17.500000	1.234286E-06	1.596976E-17	2.638051E-16	1.057728E-15	99.998568	3.000000
0.16	1.732591E+16	18.666667	1.234286E-06	1.883391E-17	2.813920E-16	1.198758E-15	99.998395	3.000000
0.17	1.732588E+16	19.833333	1.234286E-06	2.200529E-17	2.989788E-16	1.348602E-15	99.998212	3.000000
0.18	1.732585E+16	21.000000	1.234286E-06	2.549899E-17	3.165655E-16	1.507261E-15	99.998020	2.999999
0.19	1.732581E+16	22.166667	1.234286E-06	2.933011E-17	3.341523E-16	1.674733E-15	99.997817	2.999999
0.20	1.732578E+16	23.333333	1.234286E-06	3.351371E-17	3.517390E-16	1.851020E-15	99.997605	2.999999
0.21	1.732574E+16	24.500000	1.234286E-06	3.806490E-17	3.693256E-16	2.036121E-15	99.997383	2.999999
0.22	1.732570E+16	25.666667	1.234286E-06	4.299875E-17	3.869122E-16	2.230036E-15	99.997152	2.999999
0.23	1.732566E+16	26.833333	1.234286E-06	4.833034E-17	4.044988E-16	2.432765E-15	99.996910	2.999999
0.24	1.732561E+16	28.000000	1.234286E-06	5.407477E-17	4.220854E-16	2.644309E-15	99.996658	2.999999
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0.26	1.732552E+16	30.333333	1.234286E-06	6.686247E-17	4.572583E-16	3.093837E-15	99.996126	2.999999
0.27	1.732547E+16	31.500000	1.234286E-06	7.393590E-17	4.748447E-16	3.331823E-15	99.995844	2.999999
0.28	1.732542E+16	32.666667	1.234286E-06	8.148251E-17	4.924310E-16	3.578622E-15	99.995553	2.999999
0.29	1.732537E+16	33.833333	1.234286E-06	8.951738E-17	5.100173E-16	3.834236E-15	99.995252	2.999999
0.30	1.732531E+16	35.000000	1.234286E-06	9.805558E-17	5.276036E-16	4.098663E-15	99.994941	2.999999
0.31	1.732526E+16	36.166667	1.234286E-06	1.071122E-16	5.451897E-16	4.371904E-15	99.994620	2.999998
0.32	1.732520E+16	37.333333	1.234286E-06	1.167024E-16	5.627759E-16	4.653959E-15	99.994289	2.999998
0.33	1.732514E+16	38.500000	1.234286E-06	1.268411E-16	5.803619E-16	4.944828E-15	99.993947	2.999998
0.34	1.732508E+16	39.666667	1.234286E-06	1.375435E-16	5.979479E-16	5.244511E-15	99.993596	2.999998
0.35	1.732502E+16	40.833333	1.234286E-06	1.488247E-16	6.155339E-16	5.553007E-15	99.993235	2.999998
0.36	1.732495E+16	42.000000	1.234286E-06	1.606997E-16	6.331198E-16	5.870317E-15	99.992864	2.999998
0.37	1.732489E+16	43.166667	1.234286E-06	1.731837E-16	6.507056E-16	6.196441E-15	99.992482	2.999998
0.38	1.732482E+16	44.333333	1.234286E-06	1.862916E-16	6.682913E-16	6.531378E-15	99.992091	2.999998
0.39	1.732475E+16	45.500000	1.234286E-06	2.000387E-16	6.858770E-16	6.875129E-15	99.991689	2.999998
0.40	1.732468E+16	46.666667	1.234286E-06	2.144400E-16	7.034626E-16	7.227693E-15	99.991277	2.999997
0.41	1.732461E+16	47.833333	1.234286E-06	2.295105E-16	7.210482E-16	7.589071E-15	99.990855	2.999997
0.42	1.732453E+16	49.000000	1.234286E-06	2.452653E-16	7.386336E-16	7.959263E-15	99.990423	2.999997
0.43	1.732446E+16	50.166667	1.234286E-06	2.617196E-16	7.562190E-16	8.338267E-15	99.989981	2.999997
0.44	1.732438E+16	51.333333	1.234286E-06	2.788884E-16	7.738043E-16	8.726085E-15	99.989528	2.999997
0.45	1.732430E+16	52.500000	1.234286E-06	2.967868E-16	7.913895E-16	9.122717E-15	99.989065	2.999997

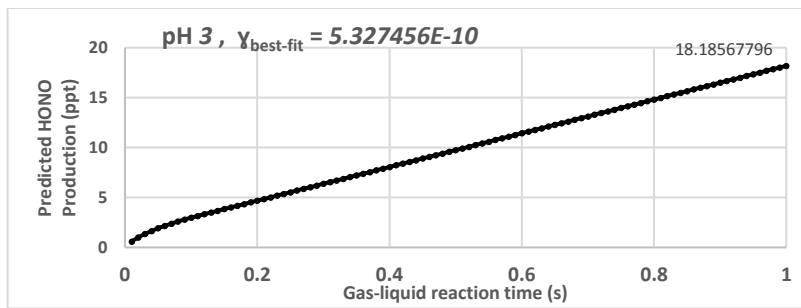
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0.47	1.732413E+16	54.833333	1.234286E-06	3.348327E-16	8.265598E-16	9.942419E-15	99.988109	2.999997
0.48	1.732405E+16	56.000000	1.234286E-06	3.550104E-16	8.441447E-16	1.036549E-14	99.987616	2.999996
0.49	1.732396E+16	57.166667	1.234286E-06	3.759780E-16	8.617296E-16	1.079737E-14	99.987112	2.999996
0.50	1.732387E+16	58.333333	1.234286E-06	3.977506E-16	8.793144E-16	1.123807E-14	99.986598	2.999996
0.51	1.732378E+16	59.500000	1.234286E-06	4.203433E-16	8.968992E-16	1.168758E-14	99.986073	2.999996
0.52	1.732369E+16	60.666667	1.234286E-06	4.437712E-16	9.144838E-16	1.214590E-14	99.985539	2.999996
0.53	1.732359E+16	61.833333	1.234286E-06	4.680493E-16	9.320683E-16	1.261304E-14	99.984994	2.999996
0.54	1.732349E+16	63.000000	1.234286E-06	4.931928E-16	9.496527E-16	1.308899E-14	99.984438	2.999995
0.55	1.732340E+16	64.166667	1.234286E-06	5.192167E-16	9.672371E-16	1.357375E-14	99.983872	2.999995
0.56	1.732330E+16	65.333333	1.234286E-06	5.461361E-16	9.848213E-16	1.406733E-14	99.983296	2.999995
0.57	1.732320E+16	66.500000	1.234286E-06	5.739660E-16	1.002405E-15	1.456971E-14	99.982710	2.999995
0.58	1.732309E+16	67.666667	1.234286E-06	6.027216E-16	1.019989E-15	1.508091E-14	99.982112	2.999995
0.59	1.732299E+16	68.833333	1.234286E-06	6.324180E-16	1.037573E-15	1.560092E-14	99.981505	2.999995
0.60	1.732288E+16	70.000000	1.234286E-06	6.630702E-16	1.055157E-15	1.612975E-14	99.980887	2.999994
0.61	1.732277E+16	71.166667	1.234286E-06	6.946932E-16	1.072741E-15	1.666738E-14	99.980259	2.999994
0.62	1.732266E+16	72.333333	1.234286E-06	7.273023E-16	1.090325E-15	1.721383E-14	99.979620	2.999994
0.63	1.732255E+16	73.500000	1.234286E-06	7.609124E-16	1.107908E-15	1.776910E-14	99.978970	2.999994
0.64	1.732243E+16	74.666667	1.234286E-06	7.955387E-16	1.125491E-15	1.833317E-14	99.978310	2.999994
0.65	1.732232E+16	75.833333	1.234286E-06	8.311961E-16	1.143075E-15	1.890605E-14	99.977640	2.999993
0.66	1.732220E+16	77.000000	1.234286E-06	8.678999E-16	1.160658E-15	1.948775E-14	99.976959	2.999993
0.67	1.732208E+16	78.166667	1.234286E-06	9.056651E-16	1.178241E-15	2.007826E-14	99.976267	2.999993
0.68	1.732196E+16	79.333333	1.234286E-06	9.445067E-16	1.195824E-15	2.067758E-14	99.975565	2.999993
0.69	1.732183E+16	80.500000	1.234286E-06	9.844398E-16	1.213407E-15	2.128572E-14	99.974852	2.999993
0.70	1.732171E+16	81.666667	1.234286E-06	1.025480E-15	1.230989E-15	2.190266E-14	99.974129	2.999992
0.71	1.732158E+16	82.833333	1.234286E-06	1.067641E-15	1.248572E-15	2.252842E-14	99.973394	2.999992
0.72	1.732145E+16	84.000000	1.234286E-06	1.110939E-15	1.266154E-15	2.316299E-14	99.972650	2.999992
0.73	1.732132E+16	85.166667	1.234286E-06	1.155389E-15	1.283736E-15	2.380637E-14	99.971894	2.999992
0.74	1.732119E+16	86.333333	1.234286E-06	1.201006E-15	1.301319E-15	2.445856E-14	99.971128	2.999991
0.75	1.732105E+16	87.500000	1.234286E-06	1.247805E-15	1.318901E-15	2.511956E-14	99.970351	2.999991
0.76	1.732092E+16	88.666667	1.234286E-06	1.295801E-15	1.336483E-15	2.578938E-14	99.969564	2.999991
0.77	1.732078E+16	89.833333	1.234286E-06	1.345010E-15	1.354064E-15	2.646800E-14	99.968766	2.999991
0.78	1.732064E+16	91.000000	1.234286E-06	1.395445E-15	1.371646E-15	2.715544E-14	99.967957	2.999990
0.79	1.732050E+16	92.166667	1.234286E-06	1.447123E-15	1.389227E-15	2.785168E-14	99.967137	2.999990
0.80	1.732035E+16	93.333333	1.234286E-06	1.500058E-15	1.406809E-15	2.855674E-14	99.966306	2.999990
0.81	1.732021E+16	94.500000	1.234286E-06	1.554266E-15	1.424390E-15	2.927061E-14	99.965465	2.999990
0.82	1.732006E+16	95.666667	1.234286E-06	1.609761E-15	1.441971E-15	2.999329E-14	99.964613	2.999989
0.83	1.731991E+16	96.833333	1.234286E-06	1.666558E-15	1.459552E-15	3.072478E-14	99.963750	2.999989
0.84	1.731976E+16	98.000000	1.234286E-06	1.724674E-15	1.477132E-15	3.146508E-14	99.962876	2.999989
0.85	1.731961E+16	99.166667	1.234286E-06	1.784122E-15	1.494713E-15	3.221419E-14	99.961991	2.999989
0.86	1.731945E+16	100.333333	1.234286E-06	1.844918E-15	1.512293E-15	3.297212E-14	99.961096	2.999988
0.87	1.731929E+16	101.500000	1.234286E-06	1.907077E-15	1.529874E-15	3.373885E-14	99.960189	2.999988
0.88	1.731913E+16	102.666667	1.234286E-06	1.970614E-15	1.547454E-15	3.451439E-14	99.959272	2.999988
0.89	1.731897E+16	103.833333	1.234286E-06	2.035544E-15	1.565034E-15	3.529874E-14	99.958344	2.999988
0.90	1.731881E+16	105.000000	1.234286E-06	2.101882E-15	1.582614E-15	3.609191E-14	99.957404	2.999987
0.91	1.731865E+16	106.166667	1.234286E-06	2.169644E-15	1.600193E-15	3.689388E-14	99.956454	2.999987
0.92	1.731848E+16	107.333333	1.234286E-06	2.238843E-15	1.617773E-15	3.770466E-14	99.955493	2.999987
0.93	1.731831E+16	108.500000	1.234286E-06	2.309496E-15	1.635352E-15	3.852425E-14	99.954521	2.999986
0.94	1.731814E+16	109.666667	1.234286E-06	2.381618E-15	1.652931E-15	3.935265E-14	99.953538	2.999986
0.95	1.731797E+16	110.833333	1.234286E-06	2.455223E-15	1.670510E-15	4.018987E-14	99.952543	2.999986
0.96	1.731779E+16	112.000000	1.234286E-06	2.530326E-15	1.688089E-15	4.103589E-14	99.951538	2.999986
0.97	1.731762E+16	113.166667	1.234286E-06	2.606943E-15	1.705667E-15	4.189072E-14	99.950522	2.999985
0.98	1.731744E+16	114.333333	1.234286E-06	2.685089E-15	1.723246E-15	4.275435E-14	99.949495	2.999985
0.99	1.731726E+16	115.500000	1.234286E-06	2.764778E-15	1.740824E-15	4.362680E-14	99.948456	2.999985
1.00	1.731708E+16	116.666667	1.234286E-06	2.846027E-15	1.758402E-15	4.450806E-14	99.947407	2.999984





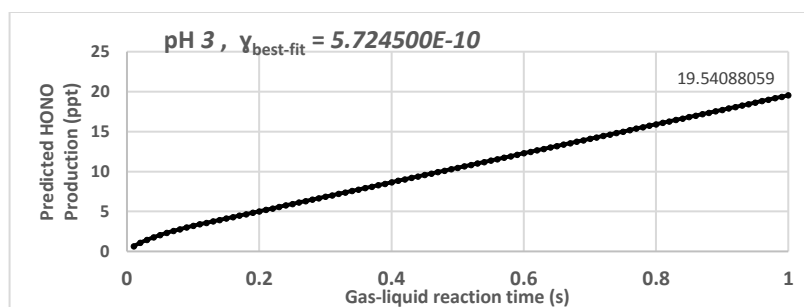
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732619E+16	1.166667	3.509923E-07	1.520329E-20	1.008030E-17	5.052116E-18	99.999984	3.000000
0.02	1.732618E+16	2.333333	4.963780E-07	6.711058E-20	2.016059E-17	1.515635E-17	99.999962	3.000000
0.03	1.732618E+16	3.500000	6.079362E-07	1.713044E-19	3.024089E-17	3.031269E-17	99.999935	3.000000
0.04	1.732617E+16	4.666667	7.019841E-07	3.406360E-19	4.032117E-17	5.052115E-17	99.999902	3.000000
0.05	1.732617E+16	5.833333	7.848418E-07	5.862962E-19	5.040146E-17	7.578171E-17	99.999864	3.000000
0.06	1.732616E+16	7.000000	8.597507E-07	9.183287E-19	6.048174E-17	1.060944E-16	99.999821	3.000000
0.07	1.732615E+16	8.166667	9.286364E-07	1.345924E-18	7.056202E-17	1.414592E-16	99.999772	3.000000
0.08	1.732614E+16	9.333333	9.927536E-07	1.877606E-18	8.064229E-17	1.818760E-16	99.999717	3.000000
0.09	1.732613E+16	10.500000	1.052974E-06	2.521358E-18	9.072255E-17	2.273450E-16	99.999657	3.000000
0.10	1.732612E+16	11.666667	1.109931E-06	3.284715E-18	1.008028E-16	2.778661E-16	99.999591	3.000000
0.11	1.732611E+16	12.833333	1.164104E-06	4.174831E-18	1.108831E-16	3.334392E-16	99.999520	3.000000
0.12	1.732609E+16	14.000000	1.215867E-06	5.198533E-18	1.209633E-16	3.940645E-16	99.999443	3.000000
0.13	1.732608E+16	15.166667	1.234286E-06	6.363746E-18	1.310435E-16	4.597418E-16	99.999361	3.000000
0.14	1.732607E+16	16.333333	1.234286E-06	7.679118E-18	1.411238E-16	5.304712E-16	99.999273	3.000000
0.15	1.732605E+16	17.500000	1.234286E-06	9.153294E-18	1.512040E-16	6.062527E-16	99.999179	3.000000
0.16	1.732603E+16	18.666667	1.234286E-06	1.079492E-17	1.612842E-16	6.870862E-16	99.999080	3.000000
0.17	1.732601E+16	19.833333	1.234286E-06	1.261265E-17	1.713644E-16	7.729718E-16	99.998975	3.000000
0.18	1.732599E+16	21.000000	1.234286E-06	1.461512E-17	1.814446E-16	8.639095E-16	99.998865	3.000000
0.19	1.732597E+16	22.166667	1.234286E-06	1.681098E-17	1.915248E-16	9.598992E-16	99.998749	3.000000
0.20	1.732595E+16	23.333333	1.234286E-06	1.920887E-17	2.016049E-16	1.060941E-15	99.998627	3.000000
0.21	1.732593E+16	24.500000	1.234286E-06	2.181745E-17	2.116851E-16	1.167035E-15	99.998500	3.000000
0.22	1.732591E+16	25.666667	1.234286E-06	2.464537E-17	2.217652E-16	1.278180E-15	99.998367	3.000000
0.23	1.732588E+16	26.833333	1.234286E-06	2.770125E-17	2.318453E-16	1.394378E-15	99.998229	3.000000
0.24	1.732586E+16	28.000000	1.234286E-06	3.099377E-17	2.419254E-16	1.515628E-15	99.998085	2.999999
0.25	1.732583E+16	29.166667	1.234286E-06	3.453155E-17	2.520055E-16	1.641930E-15	99.997935	2.999999
0.26	1.732581E+16	30.333333	1.234286E-06	3.832324E-17	2.620856E-16	1.773284E-15	99.997779	2.999999
0.27	1.732578E+16	31.500000	1.234286E-06	4.237750E-17	2.721657E-16	1.909689E-15	99.997618	2.999999
0.28	1.732575E+16	32.666667	1.234286E-06	4.670297E-17	2.822457E-16	2.051147E-15	99.997451	2.999999
0.29	1.732572E+16	33.833333	1.234286E-06	5.130829E-17	2.923258E-16	2.197657E-15	99.997279	2.999999
0.30	1.732569E+16	35.000000	1.234286E-06	5.620211E-17	3.024058E-16	2.349218E-15	99.997100	2.999999
0.31	1.732566E+16	36.166667	1.234286E-06	6.139308E-17	3.124858E-16	2.505832E-15	99.996916	2.999999
0.32	1.732562E+16	37.333333	1.234286E-06	6.688984E-17	3.225657E-16	2.667497E-15	99.996726	2.999999
0.33	1.732559E+16	38.500000	1.234286E-06	7.270104E-17	3.326457E-16	2.834215E-15	99.996531	2.999999
0.34	1.732556E+16	39.666667	1.234286E-06	7.883533E-17	3.427256E-16	3.005984E-15	99.996330	2.999999
0.35	1.732552E+16	40.833333	1.234286E-06	8.530134E-17	3.528056E-16	3.182805E-15	99.996122	2.999999
0.36	1.732548E+16	42.000000	1.234286E-06	9.210774E-17	3.628855E-16	3.364678E-15	99.995910	2.999999
0.37	1.732544E+16	43.166667	1.234286E-06	9.926316E-17	3.729653E-16	3.551603E-15	99.995691	2.999999
0.38	1.732541E+16	44.333333	1.234286E-06	1.067762E-16	3.830452E-16	3.743580E-15	99.995467	2.999999
0.39	1.732537E+16	45.500000	1.234286E-06	1.146556E-16	3.931250E-16	3.940609E-15	99.995236	2.999999
0.40	1.732532E+16	46.666667	1.234286E-06	1.229100E-16	4.032048E-16	4.142689E-15	99.995000	2.999999
0.41	1.732528E+16	47.833333	1.234286E-06	1.315480E-16	4.132846E-16	4.349821E-15	99.994758	2.999998
0.42	1.732524E+16	49.000000	1.234286E-06	1.405782E-16	4.233644E-16	4.562005E-15	99.994511	2.999998
0.43	1.732520E+16	50.166667	1.234286E-06	1.500093E-16	4.334441E-16	4.779241E-15	99.994257	2.999998
0.44	1.732515E+16	51.333333	1.234286E-06	1.598500E-16	4.435238E-16	5.001529E-15	99.993998	2.999998
0.45	1.732511E+16	52.500000	1.234286E-06	1.701089E-16	4.536035E-16	5.228868E-15	99.993733	2.999998

0.46	1.732506E+16	53.666667	1.234286E-06	1.807945E-16	4.636831E-16	5.461259E-15	99.993462	2.999998
0.47	1.732501E+16	54.833333	1.234286E-06	1.919157E-16	4.737628E-16	5.698702E-15	99.993185	2.999998
0.48	1.732496E+16	56.000000	1.234286E-06	2.034810E-16	4.838424E-16	5.941196E-15	99.992902	2.999998
0.49	1.732491E+16	57.166667	1.234286E-06	2.154991E-16	4.939219E-16	6.188742E-15	99.992613	2.999998
0.50	1.732486E+16	58.333333	1.234286E-06	2.279786E-16	5.040015E-16	6.441340E-15	99.992318	2.999998
0.51	1.732481E+16	59.500000	1.234286E-06	2.409281E-16	5.140810E-16	6.698990E-15	99.992018	2.999998
0.52	1.732476E+16	60.666667	1.234286E-06	2.543564E-16	5.241605E-16	6.961691E-15	99.991711	2.999998
0.53	1.732470E+16	61.833333	1.234286E-06	2.682720E-16	5.342399E-16	7.229443E-15	99.991399	2.999997
0.54	1.732465E+16	63.000000	1.234286E-06	2.826836E-16	5.443193E-16	7.502247E-15	99.991080	2.999997
0.55	1.732459E+16	64.166667	1.234286E-06	2.975999E-16	5.543987E-16	7.780103E-15	99.990756	2.999997
0.56	1.732453E+16	65.333333	1.234286E-06	3.130294E-16	5.644781E-16	8.063011E-15	99.990426	2.999997
0.57	1.732447E+16	66.500000	1.234286E-06	3.289809E-16	5.745574E-16	8.350970E-15	99.990090	2.999997
0.58	1.732441E+16	67.666667	1.234286E-06	3.454630E-16	5.846367E-16	8.643980E-15	99.989747	2.999997
0.59	1.732435E+16	68.833333	1.234286E-06	3.624843E-16	5.947159E-16	8.942042E-15	99.989399	2.999997
0.60	1.732429E+16	70.000000	1.234286E-06	3.800534E-16	6.047952E-16	9.245155E-15	99.989045	2.999997
0.61	1.732423E+16	71.166667	1.234286E-06	3.981791E-16	6.148744E-16	9.553320E-15	99.988685	2.999997
0.62	1.732417E+16	72.333333	1.234286E-06	4.168699E-16	6.249535E-16	9.866536E-15	99.988318	2.999997
0.63	1.732410E+16	73.500000	1.234286E-06	4.361346E-16	6.350326E-16	1.018480E-14	99.987946	2.999996
0.64	1.732404E+16	74.666667	1.234286E-06	4.559816E-16	6.451117E-16	1.050812E-14	99.987568	2.999996
0.65	1.732397E+16	75.833333	1.234286E-06	4.764198E-16	6.551907E-16	1.083649E-14	99.987184	2.999996
0.66	1.732390E+16	77.000000	1.234286E-06	4.974577E-16	6.652697E-16	1.116991E-14	99.986793	2.999996
0.67	1.732383E+16	78.166667	1.234286E-06	5.191040E-16	6.753487E-16	1.150839E-14	99.986397	2.999996
0.68	1.732376E+16	79.333333	1.234286E-06	5.413673E-16	6.854276E-16	1.185191E-14	99.985994	2.999996
0.69	1.732369E+16	80.500000	1.234286E-06	5.642563E-16	6.955065E-16	1.220049E-14	99.985586	2.999996
0.70	1.732362E+16	81.666667	1.234286E-06	5.877796E-16	7.055853E-16	1.255411E-14	99.985171	2.999996
0.71	1.732355E+16	82.833333	1.234286E-06	6.119459E-16	7.156641E-16	1.291279E-14	99.984750	2.999995
0.72	1.732348E+16	84.000000	1.234286E-06	6.367637E-16	7.257429E-16	1.327652E-14	99.984323	2.999995
0.73	1.732340E+16	85.166667	1.234286E-06	6.622419E-16	7.358216E-16	1.364530E-14	99.983890	2.999995
0.74	1.732332E+16	86.333333	1.234286E-06	6.883889E-16	7.459003E-16	1.401913E-14	99.983451	2.999995
0.75	1.732325E+16	87.500000	1.234286E-06	7.152134E-16	7.559789E-16	1.439802E-14	99.983006	2.999995
0.76	1.732317E+16	88.666667	1.234286E-06	7.427241E-16	7.660575E-16	1.478195E-14	99.982555	2.999995
0.77	1.732309E+16	89.833333	1.234286E-06	7.709296E-16	7.761360E-16	1.517093E-14	99.982097	2.999995
0.78	1.732301E+16	91.000000	1.234286E-06	7.998386E-16	7.862145E-16	1.556497E-14	99.981633	2.999995
0.79	1.732293E+16	92.166667	1.234286E-06	8.294598E-16	7.962929E-16	1.596406E-14	99.981163	2.999994
0.80	1.732285E+16	93.333333	1.234286E-06	8.598016E-16	8.063713E-16	1.636819E-14	99.980687	2.999994
0.81	1.732276E+16	94.500000	1.234286E-06	8.908729E-16	8.164497E-16	1.677738E-14	99.980205	2.999994
0.82	1.732268E+16	95.666667	1.234286E-06	9.226822E-16	8.265280E-16	1.719162E-14	99.979717	2.999994
0.83	1.732259E+16	96.833333	1.234286E-06	9.552382E-16	8.366062E-16	1.761091E-14	99.979222	2.999994
0.84	1.732250E+16	98.000000	1.234286E-06	9.885495E-16	8.466844E-16	1.803525E-14	99.978721	2.999994
0.85	1.732242E+16	99.166667	1.234286E-06	1.022625E-15	8.567626E-16	1.846465E-14	99.978214	2.999994
0.86	1.732233E+16	100.333333	1.234286E-06	1.057473E-15	8.668407E-16	1.889909E-14	99.977701	2.999993
0.87	1.732224E+16	101.500000	1.234286E-06	1.093102E-15	8.769187E-16	1.933858E-14	99.977181	2.999993
0.88	1.732215E+16	102.666667	1.234286E-06	1.129521E-15	8.869967E-16	1.978313E-14	99.976655	2.999993
0.89	1.732205E+16	103.833333	1.234286E-06	1.166738E-15	8.970747E-16	2.023272E-14	99.976123	2.999993
0.90	1.732196E+16	105.000000	1.234286E-06	1.204763E-15	9.071526E-16	2.068737E-14	99.975585	2.999993
0.91	1.732187E+16	106.166667	1.234286E-06	1.243604E-15	9.172304E-16	2.114706E-14	99.975040	2.999993
0.92	1.732177E+16	107.333333	1.234286E-06	1.283269E-15	9.273082E-16	2.161181E-14	99.974489	2.999992
0.93	1.732167E+16	108.500000	1.234286E-06	1.323767E-15	9.373859E-16	2.208161E-14	99.973932	2.999992
0.94	1.732158E+16	109.666667	1.234286E-06	1.365107E-15	9.474636E-16	2.255646E-14	99.973368	2.999992
0.95	1.732148E+16	110.833333	1.234286E-06	1.407297E-15	9.575412E-16	2.303635E-14	99.972798	2.999992
0.96	1.732138E+16	112.000000	1.234286E-06	1.450347E-15	9.676188E-16	2.352130E-14	99.972222	2.999992
0.97	1.732128E+16	113.166667	1.234286E-06	1.494264E-15	9.776963E-16	2.401130E-14	99.971640	2.999992
0.98	1.732118E+16	114.333333	1.234286E-06	1.539057E-15	9.877737E-16	2.450635E-14	99.971051	2.999991
0.99	1.732107E+16	115.500000	1.234286E-06	1.584735E-15	9.978511E-16	2.500645E-14	99.970456	2.999991
1.00	1.732097E+16	116.666667	1.234286E-06	1.631307E-15	1.007928E-15	2.551160E-14	99.969854	2.999991



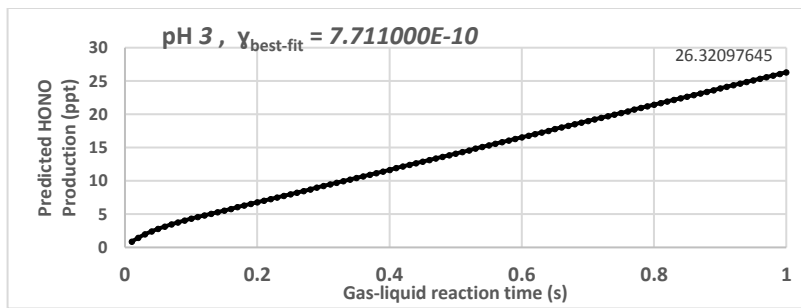
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732619E+16	1.166667	3.509923E-07	1.539932E-20	1.021027E-17	5.117257E-18	99.999984	3.000000
0.02	1.732618E+16	2.333333	4.963780E-07	6.797588E-20	2.042054E-17	1.535177E-17	99.999962	3.000000
0.03	1.732618E+16	3.500000	6.079362E-07	1.735131E-19	3.063080E-17	3.070353E-17	99.999934	3.000000
0.04	1.732617E+16	4.666667	7.019841E-07	3.450281E-19	4.084106E-17	5.117255E-17	99.999901	3.000000
0.05	1.732617E+16	5.833333	7.848418E-07	5.938557E-19	5.105132E-17	7.675882E-17	99.999862	3.000000
0.06	1.732616E+16	7.000000	8.597507E-07	9.301693E-19	6.126157E-17	1.074623E-16	99.999818	3.000000
0.07	1.732615E+16	8.166667	9.286364E-07	1.363278E-18	7.147182E-17	1.432831E-16	99.999769	3.000000
0.08	1.732614E+16	9.333333	9.927535E-07	1.901815E-18	8.168206E-17	1.842211E-16	99.999713	3.000000
0.09	1.732613E+16	10.500000	1.052973E-06	2.553867E-18	9.189230E-17	2.302763E-16	99.999652	3.000000
0.10	1.732612E+16	11.666667	1.109931E-06	3.327067E-18	1.021025E-16	2.814488E-16	99.999586	3.000000
0.11	1.732611E+16	12.833333	1.164104E-06	4.228660E-18	1.123127E-16	3.377385E-16	99.999514	3.000000
0.12	1.732609E+16	14.000000	1.215866E-06	5.265561E-18	1.225230E-16	3.991454E-16	99.999436	3.000000
0.13	1.732608E+16	15.166667	1.234286E-06	6.445798E-18	1.327332E-16	4.656696E-16	99.999352	3.000000
0.14	1.732606E+16	16.333333	1.234286E-06	7.778129E-18	1.429434E-16	5.373109E-16	99.999263	3.000000
0.15	1.732605E+16	17.500000	1.234286E-06	9.271313E-18	1.531536E-16	6.140695E-16	99.999168	3.000000
0.16	1.732603E+16	18.666667	1.234286E-06	1.093411E-17	1.633637E-16	6.959453E-16	99.999068	3.000000
0.17	1.732601E+16	19.833333	1.234286E-06	1.277527E-17	1.735739E-16	7.829382E-16	99.998962	3.000000
0.18	1.732599E+16	21.000000	1.234286E-06	1.480356E-17	1.837841E-16	8.750484E-16	99.998850	3.000000
0.19	1.732597E+16	22.166667	1.234286E-06	1.702773E-17	1.939942E-16	9.722757E-16	99.998733	3.000000
0.20	1.732595E+16	23.333333	1.234286E-06	1.945655E-17	2.042043E-16	1.074620E-15	99.998610	3.000000
0.21	1.732593E+16	24.500000	1.234286E-06	2.209876E-17	2.144144E-16	1.182082E-15	99.998481	3.000000
0.22	1.732590E+16	25.666667	1.234286E-06	2.496313E-17	2.246246E-16	1.294661E-15	99.998346	3.000000
0.23	1.732588E+16	26.833333	1.234286E-06	2.805842E-17	2.348346E-16	1.412357E-15	99.998206	3.000000
0.24	1.732586E+16	28.000000	1.234286E-06	3.139339E-17	2.450447E-16	1.535170E-15	99.998060	2.999999
0.25	1.732583E+16	29.166667	1.234286E-06	3.497678E-17	2.552548E-16	1.663100E-15	99.997908	2.999999
0.26	1.732580E+16	30.333333	1.234286E-06	3.881737E-17	2.654648E-16	1.796148E-15	99.997751	2.999999
0.27	1.732577E+16	31.500000	1.234286E-06	4.292390E-17	2.756749E-16	1.934312E-15	99.997587	2.999999
0.28	1.732574E+16	32.666667	1.234286E-06	4.730514E-17	2.858849E-16	2.077594E-15	99.997418	2.999999
0.29	1.732571E+16	33.833333	1.234286E-06	5.196984E-17	2.960949E-16	2.225992E-15	99.997244	2.999999
0.30	1.732568E+16	35.000000	1.234286E-06	5.692676E-17	3.063048E-16	2.379508E-15	99.997063	2.999999
0.31	1.732565E+16	36.166667	1.234286E-06	6.218465E-17	3.165148E-16	2.538141E-15	99.996876	2.999999
0.32	1.732562E+16	37.333333	1.234286E-06	6.775229E-17	3.267247E-16	2.701891E-15	99.996684	2.999999
0.33	1.732558E+16	38.500000	1.234286E-06	7.363842E-17	3.369347E-16	2.870758E-15	99.996486	2.999999
0.34	1.732555E+16	39.666667	1.234286E-06	7.985180E-17	3.471446E-16	3.044742E-15	99.996282	2.999999
0.35	1.732551E+16	40.833333	1.234286E-06	8.640118E-17	3.573544E-16	3.223843E-15	99.996072	2.999999
0.36	1.732547E+16	42.000000	1.234286E-06	9.329534E-17	3.675643E-16	3.408061E-15	99.995857	2.999999
0.37	1.732543E+16	43.166667	1.234286E-06	1.005430E-16	3.777741E-16	3.597396E-15	99.995635	2.999999
0.38	1.732540E+16	44.333333	1.234286E-06	1.081530E-16	3.879840E-16	3.791848E-15	99.995408	2.999999
0.39	1.732536E+16	45.500000	1.234286E-06	1.161340E-16	3.981937E-16	3.991417E-15	99.995175	2.999999
0.40	1.732531E+16	46.666667	1.234286E-06	1.244948E-16	4.084035E-16	4.196103E-15	99.994936	2.999999
0.41	1.732527E+16	47.833333	1.234286E-06	1.332441E-16	4.186132E-16	4.405906E-15	99.994691	2.999998
0.42	1.732523E+16	49.000000	1.234286E-06	1.423908E-16	4.288230E-16	4.620826E-15	99.994440	2.999998
0.43	1.732518E+16	50.166667	1.234286E-06	1.519435E-16	4.390327E-16	4.840862E-15	99.994183	2.999998
0.44	1.732514E+16	51.333333	1.234286E-06	1.619110E-16	4.492423E-16	5.066016E-15	99.993920	2.999998
0.45	1.732509E+16	52.500000	1.234286E-06	1.723022E-16	4.594520E-16	5.296286E-15	99.993652	2.999998

0.46	1.732504E+16	53.666667	1.234286E-06	1.831256E-16	4.696616E-16	5.531674E-15	99.993377	2.999998
0.47	1.732500E+16	54.833333	1.234286E-06	1.943902E-16	4.798711E-16	5.772178E-15	99.993097	2.999998
0.48	1.732495E+16	56.000000	1.234286E-06	2.061046E-16	4.900807E-16	6.017799E-15	99.992810	2.999998
0.49	1.732489E+16	57.166667	1.234286E-06	2.182776E-16	5.002902E-16	6.268537E-15	99.992518	2.999998
0.50	1.732484E+16	58.333333	1.234286E-06	2.309180E-16	5.104997E-16	6.524391E-15	99.992219	2.999998
0.51	1.732479E+16	59.500000	1.234286E-06	2.440345E-16	5.207092E-16	6.785362E-15	99.991915	2.999998
0.52	1.732474E+16	60.666667	1.234286E-06	2.576359E-16	5.309186E-16	7.051451E-15	99.991604	2.999998
0.53	1.732468E+16	61.833333	1.234286E-06	2.717310E-16	5.411280E-16	7.322655E-15	99.991288	2.999997
0.54	1.732463E+16	63.000000	1.234286E-06	2.863284E-16	5.513374E-16	7.598977E-15	99.990965	2.999997
0.55	1.732457E+16	64.166667	1.234286E-06	3.014370E-16	5.615467E-16	7.880415E-15	99.990637	2.999997
0.56	1.732451E+16	65.333333	1.234286E-06	3.170655E-16	5.717560E-16	8.166970E-15	99.990302	2.999997
0.57	1.732445E+16	66.500000	1.234286E-06	3.332226E-16	5.819653E-16	8.458642E-15	99.989962	2.999997
0.58	1.732439E+16	67.666667	1.234286E-06	3.499172E-16	5.921745E-16	8.755430E-15	99.989615	2.999997
0.59	1.732433E+16	68.833333	1.234286E-06	3.671579E-16	6.023837E-16	9.057335E-15	99.989262	2.999997
0.60	1.732427E+16	70.000000	1.234286E-06	3.849536E-16	6.125929E-16	9.364356E-15	99.988904	2.999997
0.61	1.732421E+16	71.166667	1.234286E-06	4.033130E-16	6.228020E-16	9.676494E-15	99.988539	2.999997
0.62	1.732414E+16	72.333333	1.234286E-06	4.222448E-16	6.330111E-16	9.993749E-15	99.988168	2.999996
0.63	1.732408E+16	73.500000	1.234286E-06	4.417578E-16	6.432202E-16	1.031612E-14	99.987791	2.999996
0.64	1.732401E+16	74.666667	1.234286E-06	4.618608E-16	6.534292E-16	1.064361E-14	99.987408	2.999996
0.65	1.732394E+16	75.833333	1.234286E-06	4.825625E-16	6.636382E-16	1.097621E-14	99.987018	2.999996
0.66	1.732387E+16	77.000000	1.234286E-06	5.038716E-16	6.738471E-16	1.131393E-14	99.986623	2.999996
0.67	1.732380E+16	78.166667	1.234286E-06	5.257970E-16	6.840560E-16	1.165677E-14	99.986221	2.999996
0.68	1.732373E+16	79.333333	1.234286E-06	5.483474E-16	6.942648E-16	1.200472E-14	99.985814	2.999996
0.69	1.732366E+16	80.500000	1.234286E-06	5.715315E-16	7.044737E-16	1.235779E-14	99.985400	2.999996
0.70	1.732359E+16	81.666667	1.234286E-06	5.953580E-16	7.146824E-16	1.271598E-14	99.984980	2.999996
0.71	1.732351E+16	82.833333	1.234286E-06	6.198359E-16	7.248912E-16	1.307928E-14	99.984554	2.999995
0.72	1.732344E+16	84.000000	1.234286E-06	6.449737E-16	7.350998E-16	1.344770E-14	99.984121	2.999995
0.73	1.732336E+16	85.166667	1.234286E-06	6.707803E-16	7.453085E-16	1.382123E-14	99.983683	2.999995
0.74	1.732329E+16	86.333333	1.234286E-06	6.972644E-16	7.555171E-16	1.419988E-14	99.983238	2.999995
0.75	1.732321E+16	87.500000	1.234286E-06	7.244348E-16	7.657256E-16	1.458365E-14	99.982787	2.999995
0.76	1.732313E+16	88.666667	1.234286E-06	7.523002E-16	7.759341E-16	1.497254E-14	99.982330	2.999995
0.77	1.732305E+16	89.833333	1.234286E-06	7.808694E-16	7.861426E-16	1.536654E-14	99.981866	2.999995
0.78	1.732297E+16	91.000000	1.234286E-06	8.101511E-16	7.963510E-16	1.576565E-14	99.981397	2.999994
0.79	1.732289E+16	92.166667	1.234286E-06	8.401542E-16	8.065594E-16	1.616988E-14	99.980921	2.999994
0.80	1.732280E+16	93.333333	1.234286E-06	8.708872E-16	8.167677E-16	1.657923E-14	99.980438	2.999994
0.81	1.732272E+16	94.500000	1.234286E-06	9.023591E-16	8.269760E-16	1.699370E-14	99.979950	2.999994
0.82	1.732263E+16	95.666667	1.234286E-06	9.345785E-16	8.371842E-16	1.741328E-14	99.979455	2.999994
0.83	1.732254E+16	96.833333	1.234286E-06	9.675542E-16	8.473924E-16	1.783797E-14	99.978954	2.999994
0.84	1.732246E+16	98.000000	1.234286E-06	1.001295E-15	8.576005E-16	1.826778E-14	99.978447	2.999994
0.85	1.732237E+16	99.166667	1.234286E-06	1.035810E-15	8.678086E-16	1.870271E-14	99.977933	2.999993
0.86	1.732228E+16	100.333333	1.234286E-06	1.071107E-15	8.780166E-16	1.914276E-14	99.977413	2.999993
0.87	1.732219E+16	101.500000	1.234286E-06	1.107195E-15	8.882245E-16	1.958792E-14	99.976887	2.999993
0.88	1.732209E+16	102.666667	1.234286E-06	1.144084E-15	8.984325E-16	2.003819E-14	99.976354	2.999993
0.89	1.732200E+16	103.833333	1.234286E-06	1.181781E-15	9.086403E-16	2.049358E-14	99.975815	2.999993
0.90	1.732191E+16	105.000000	1.234286E-06	1.220296E-15	9.188481E-16	2.095409E-14	99.975270	2.999993
0.91	1.732181E+16	106.166667	1.234286E-06	1.259638E-15	9.290559E-16	2.141971E-14	99.974718	2.999992
0.92	1.732171E+16	107.333333	1.234286E-06	1.299814E-15	9.392636E-16	2.189045E-14	99.974160	2.999992
0.93	1.732162E+16	108.500000	1.234286E-06	1.340834E-15	9.494712E-16	2.236630E-14	99.973596	2.999992
0.94	1.732152E+16	109.666667	1.234286E-06	1.382707E-15	9.596788E-16	2.284727E-14	99.973025	2.999992
0.95	1.732142E+16	110.833333	1.234286E-06	1.425442E-15	9.698863E-16	2.333336E-14	99.972448	2.999992
0.96	1.732132E+16	112.000000	1.234286E-06	1.469046E-15	9.800938E-16	2.382456E-14	99.971864	2.999992
0.97	1.732121E+16	113.166667	1.234286E-06	1.513529E-15	9.903012E-16	2.432088E-14	99.971274	2.999991
0.98	1.732111E+16	114.333333	1.234286E-06	1.558900E-15	1.000509E-15	2.482231E-14	99.970678	2.999991
0.99	1.732101E+16	115.500000	1.234286E-06	1.605167E-15	1.010716E-15	2.532886E-14	99.970075	2.999991
1.00	1.732090E+16	116.666667	1.234286E-06	1.652340E-15	1.020923E-15	2.584052E-14	99.969465	2.999991



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732619E+16	1.166667	3.509923E-07	1.654700E-20	1.097122E-17	5.498635E-18	99.999982	3.000000
0.02	1.732618E+16	2.333333	4.963780E-07	7.304197E-20	2.194244E-17	1.649590E-17	99.999959	3.000000
0.03	1.732618E+16	3.500000	6.079362E-07	1.864447E-19	3.291365E-17	3.299180E-17	99.999929	3.000000
0.04	1.732617E+16	4.666667	7.019840E-07	3.707423E-19	4.388486E-17	5.498633E-17	99.999894	3.000000
0.05	1.732617E+16	5.833333	7.848417E-07	6.381145E-19	5.485606E-17	8.247949E-17	99.999852	3.000000
0.06	1.732616E+16	7.000000	8.597506E-07	9.994928E-19	6.582726E-17	1.154713E-16	99.999805	3.000000
0.07	1.732615E+16	8.166667	9.286363E-07	1.464880E-18	7.679846E-17	1.539617E-16	99.999751	3.000000
0.08	1.732614E+16	9.333333	9.927533E-07	2.043553E-18	8.776964E-17	1.979507E-16	99.999692	3.000000
0.09	1.732613E+16	10.500000	1.052973E-06	2.744202E-18	9.874082E-17	2.474383E-16	99.999626	3.000000
0.10	1.732611E+16	11.666667	1.109930E-06	3.575026E-18	1.097120E-16	3.024245E-16	99.999555	3.000000
0.11	1.732610E+16	12.833333	1.164104E-06	4.543813E-18	1.206832E-16	3.629094E-16	99.999477	3.000000
0.12	1.732609E+16	14.000000	1.215866E-06	5.657992E-18	1.316543E-16	4.288928E-16	99.999394	3.000000
0.13	1.732607E+16	15.166667	1.234286E-06	6.926190E-18	1.426255E-16	5.003749E-16	99.999304	3.000000
0.14	1.732605E+16	16.333333	1.234286E-06	8.357817E-18	1.535966E-16	5.773555E-16	99.999208	3.000000
0.15	1.732604E+16	17.500000	1.234286E-06	9.962284E-18	1.645677E-16	6.598347E-16	99.999106	3.000000
0.16	1.732602E+16	18.666667	1.234286E-06	1.174900E-17	1.755388E-16	7.478124E-16	99.998999	3.000000
0.17	1.732600E+16	19.833333	1.234286E-06	1.372738E-17	1.865099E-16	8.412888E-16	99.998885	3.000000
0.18	1.732598E+16	21.000000	1.234286E-06	1.590683E-17	1.974810E-16	9.402637E-16	99.998765	3.000000
0.19	1.732596E+16	22.166667	1.234286E-06	1.829677E-17	2.084521E-16	1.044737E-15	99.998638	3.000000
0.20	1.732593E+16	23.333333	1.234286E-06	2.090660E-17	2.194232E-16	1.154709E-15	99.998506	3.000000
0.21	1.732591E+16	24.500000	1.234286E-06	2.374573E-17	2.303942E-16	1.270180E-15	99.998368	3.000000
0.22	1.732588E+16	25.666667	1.234286E-06	2.682358E-17	2.413652E-16	1.391149E-15	99.998223	3.000000
0.23	1.732586E+16	26.833333	1.234286E-06	3.014955E-17	2.523362E-16	1.517616E-15	99.998072	2.999999
0.24	1.732583E+16	28.000000	1.234286E-06	3.373306E-17	2.633072E-16	1.649582E-15	99.997915	2.999999
0.25	1.732580E+16	29.166667	1.234286E-06	3.758352E-17	2.742782E-16	1.787047E-15	99.997752	2.999999
0.26	1.732577E+16	30.333333	1.234286E-06	4.171033E-17	2.852492E-16	1.930010E-15	99.997583	2.999999
0.27	1.732574E+16	31.500000	1.234286E-06	4.612292E-17	2.962201E-16	2.078471E-15	99.997408	2.999999
0.28	1.732571E+16	32.666667	1.234286E-06	5.083067E-17	3.071911E-16	2.232431E-15	99.997226	2.999999
0.29	1.732568E+16	33.833333	1.234286E-06	5.584302E-17	3.181620E-16	2.391890E-15	99.997038	2.999999
0.30	1.732564E+16	35.000000	1.234286E-06	6.116937E-17	3.291328E-16	2.556847E-15	99.996844	2.999999
0.31	1.732561E+16	36.166667	1.234286E-06	6.681912E-17	3.401037E-16	2.727302E-15	99.996644	2.999999
0.32	1.732557E+16	37.333333	1.234286E-06	7.280170E-17	3.510745E-16	2.903255E-15	99.996437	2.999999
0.33	1.732554E+16	38.500000	1.234286E-06	7.912650E-17	3.620454E-16	3.084707E-15	99.996224	2.999999
0.34	1.732550E+16	39.666667	1.234286E-06	8.580294E-17	3.730161E-16	3.271658E-15	99.996005	2.999999
0.35	1.732546E+16	40.833333	1.234286E-06	9.284044E-17	3.839869E-16	3.464107E-15	99.995780	2.999999
0.36	1.732542E+16	42.000000	1.234286E-06	1.002484E-16	3.949577E-16	3.662054E-15	99.995548	2.999999
0.37	1.732538E+16	43.166667	1.234286E-06	1.080362E-16	4.059284E-16	3.865499E-15	99.995310	2.999999
0.38	1.732534E+16	44.333333	1.234286E-06	1.162133E-16	4.168991E-16	4.074443E-15	99.995066	2.999999
0.39	1.732529E+16	45.500000	1.234286E-06	1.247891E-16	4.278697E-16	4.288885E-15	99.994815	2.999998
0.40	1.732525E+16	46.666667	1.234286E-06	1.337730E-16	4.388404E-16	4.508826E-15	99.994558	2.999998
0.41	1.732520E+16	47.833333	1.234286E-06	1.431744E-16	4.498110E-16	4.734264E-15	99.994295	2.999998
0.42	1.732516E+16	49.000000	1.234286E-06	1.530027E-16	4.607816E-16	4.965201E-15	99.994026	2.999998
0.43	1.732511E+16	50.166667	1.234286E-06	1.632674E-16	4.717521E-16	5.201636E-15	99.993750	2.999998
0.44	1.732506E+16	51.333333	1.234286E-06	1.739778E-16	4.827226E-16	5.443570E-15	99.993467	2.999998
0.45	1.732501E+16	52.500000	1.234286E-06	1.851433E-16	4.936931E-16	5.691001E-15	99.993179	2.999998

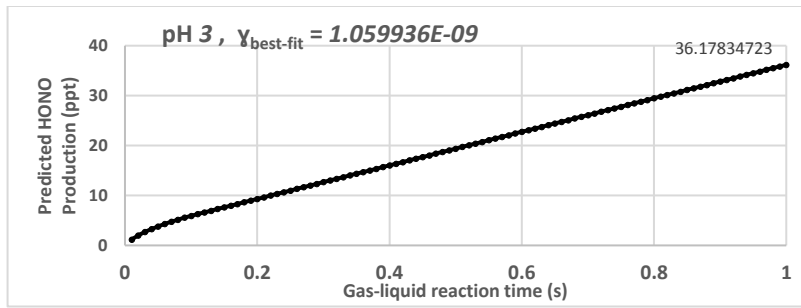
0.46	1.732496E+16	53.666667	1.234286E-06	1.967734E-16	5.046636E-16	5.943931E-15	99.992884	2.999998
0.47	1.732491E+16	54.833333	1.234286E-06	2.088775E-16	5.156340E-16	6.202359E-15	99.992582	2.999998
0.48	1.732485E+16	56.000000	1.234286E-06	2.214649E-16	5.266044E-16	6.466285E-15	99.992274	2.999998
0.49	1.732480E+16	57.166667	1.234286E-06	2.345452E-16	5.375747E-16	6.735709E-15	99.991960	2.999998
0.50	1.732474E+16	58.333333	1.234286E-06	2.481276E-16	5.485451E-16	7.010631E-15	99.991639	2.999998
0.51	1.732469E+16	59.500000	1.234286E-06	2.622217E-16	5.595154E-16	7.291051E-15	99.991312	2.999997
0.52	1.732463E+16	60.666667	1.234286E-06	2.768367E-16	5.704856E-16	7.576970E-15	99.990979	2.999997
0.53	1.732457E+16	61.833333	1.234286E-06	2.919822E-16	5.814558E-16	7.868386E-15	99.990639	2.999997
0.54	1.732451E+16	63.000000	1.234286E-06	3.076675E-16	5.924260E-16	8.165301E-15	99.990292	2.999997
0.55	1.732445E+16	64.166667	1.234286E-06	3.239021E-16	6.033962E-16	8.467713E-15	99.989939	2.999997
0.56	1.732439E+16	65.333333	1.234286E-06	3.406953E-16	6.143663E-16	8.775623E-15	99.989580	2.999997
0.57	1.732432E+16	66.500000	1.234286E-06	3.580565E-16	6.253363E-16	9.089032E-15	99.989214	2.999997
0.58	1.732426E+16	67.666667	1.234286E-06	3.759953E-16	6.363063E-16	9.407938E-15	99.988841	2.999997
0.59	1.732419E+16	68.833333	1.234286E-06	3.945209E-16	6.472763E-16	9.732342E-15	99.988462	2.999997
0.60	1.732413E+16	70.000000	1.234286E-06	4.136428E-16	6.582463E-16	1.006224E-14	99.988077	2.999996
0.61	1.732406E+16	71.166667	1.234286E-06	4.333704E-16	6.692162E-16	1.039764E-14	99.987685	2.999996
0.62	1.732399E+16	72.333333	1.234286E-06	4.537131E-16	6.801860E-16	1.073854E-14	99.987286	2.999996
0.63	1.732392E+16	73.500000	1.234286E-06	4.746803E-16	6.911558E-16	1.108494E-14	99.986881	2.999996
0.64	1.732385E+16	74.666667	1.234286E-06	4.962815E-16	7.021256E-16	1.143683E-14	99.986469	2.999996
0.65	1.732377E+16	75.833333	1.234286E-06	5.185259E-16	7.130953E-16	1.179422E-14	99.986051	2.999996
0.66	1.732370E+16	77.000000	1.234286E-06	5.414231E-16	7.240650E-16	1.215711E-14	99.985626	2.999996
0.67	1.732363E+16	78.166667	1.234286E-06	5.649825E-16	7.350347E-16	1.252550E-14	99.985195	2.999996
0.68	1.732355E+16	79.333333	1.234286E-06	5.892134E-16	7.460042E-16	1.289938E-14	99.984757	2.999995
0.69	1.732347E+16	80.500000	1.234286E-06	6.141253E-16	7.569738E-16	1.327876E-14	99.984312	2.999995
0.70	1.732339E+16	81.666667	1.234286E-06	6.397275E-16	7.679433E-16	1.366364E-14	99.983860	2.999995
0.71	1.732332E+16	82.833333	1.234286E-06	6.660296E-16	7.789127E-16	1.405402E-14	99.983403	2.999995
0.72	1.732323E+16	84.000000	1.234286E-06	6.930408E-16	7.898821E-16	1.444989E-14	99.982938	2.999995
0.73	1.732315E+16	85.166667	1.234286E-06	7.207706E-16	8.008514E-16	1.485126E-14	99.982467	2.999995
0.74	1.732307E+16	86.333333	1.234286E-06	7.492284E-16	8.118207E-16	1.525813E-14	99.981989	2.999995
0.75	1.732299E+16	87.500000	1.234286E-06	7.784236E-16	8.227900E-16	1.567050E-14	99.981504	2.999994
0.76	1.732290E+16	88.666667	1.234286E-06	8.083657E-16	8.337592E-16	1.608836E-14	99.981013	2.999994
0.77	1.732282E+16	89.833333	1.234286E-06	8.390639E-16	8.447283E-16	1.651172E-14	99.980515	2.999994
0.78	1.732273E+16	91.000000	1.234286E-06	8.705278E-16	8.556974E-16	1.694058E-14	99.980010	2.999994
0.79	1.732264E+16	92.166667	1.234286E-06	9.027668E-16	8.666664E-16	1.737494E-14	99.979499	2.999994
0.80	1.732255E+16	93.333333	1.234286E-06	9.357901E-16	8.776354E-16	1.781479E-14	99.978981	2.999994
0.81	1.732246E+16	94.500000	1.234286E-06	9.696074E-16	8.886043E-16	1.826014E-14	99.978456	2.999994
0.82	1.732237E+16	95.666667	1.234286E-06	1.004228E-15	8.995731E-16	1.871099E-14	99.977924	2.999993
0.83	1.732227E+16	96.833333	1.234286E-06	1.039661E-15	9.105419E-16	1.916733E-14	99.977386	2.999993
0.84	1.732218E+16	98.000000	1.234286E-06	1.075916E-15	9.215107E-16	1.962918E-14	99.976841	2.999993
0.85	1.732208E+16	99.166667	1.234286E-06	1.113003E-15	9.324793E-16	2.009652E-14	99.976289	2.999993
0.86	1.732199E+16	100.333333	1.234286E-06	1.150931E-15	9.434480E-16	2.056935E-14	99.975730	2.999993
0.87	1.732189E+16	101.500000	1.234286E-06	1.189708E-15	9.544165E-16	2.104769E-14	99.975164	2.999993
0.88	1.732179E+16	102.666667	1.234286E-06	1.229346E-15	9.653850E-16	2.153152E-14	99.974592	2.999992
0.89	1.732169E+16	103.833333	1.234286E-06	1.269853E-15	9.763534E-16	2.202084E-14	99.974013	2.999992
0.90	1.732159E+16	105.000000	1.234286E-06	1.311238E-15	9.873218E-16	2.251567E-14	99.973427	2.999992
0.91	1.732148E+16	106.166667	1.234286E-06	1.353511E-15	9.982901E-16	2.301599E-14	99.972834	2.999992
0.92	1.732138E+16	107.333333	1.234286E-06	1.396682E-15	1.009258E-15	2.352181E-14	99.972235	2.999992
0.93	1.732128E+16	108.500000	1.234286E-06	1.440759E-15	1.020227E-15	2.403312E-14	99.971628	2.999992
0.94	1.732117E+16	109.666667	1.234286E-06	1.485752E-15	1.031195E-15	2.454993E-14	99.971015	2.999991
0.95	1.732106E+16	110.833333	1.234286E-06	1.531671E-15	1.042163E-15	2.507224E-14	99.970394	2.999991
0.96	1.732095E+16	112.000000	1.234286E-06	1.578525E-15	1.053131E-15	2.560004E-14	99.969767	2.999991
0.97	1.732084E+16	113.166667	1.234286E-06	1.626323E-15	1.064099E-15	2.613335E-14	99.969133	2.999991
0.98	1.732073E+16	114.333333	1.234286E-06	1.675075E-15	1.075066E-15	2.667214E-14	99.968492	2.999991
0.99	1.732062E+16	115.500000	1.234286E-06	1.724790E-15	1.086034E-15	2.721644E-14	99.967845	2.999990
1.00	1.732051E+16	116.666667	1.234286E-06	1.775478E-15	1.097002E-15	2.776623E-14	99.967190	2.999990



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732619E+16	1.166667	3.509923E-07	2.228909E-20	1.477842E-17	7.406755E-18	99.999976	3.000000
0.02	1.732618E+16	2.333333	4.963779E-07	9.838880E-20	2.955683E-17	2.222026E-17	99.999944	3.000000
0.03	1.732617E+16	3.500000	6.079361E-07	2.511442E-19	4.433524E-17	4.444052E-17	99.999905	3.000000
0.04	1.732617E+16	4.666667	7.019838E-07	4.993962E-19	5.911365E-17	7.406752E-17	99.999857	3.000000
0.05	1.732616E+16	5.833333	7.848413E-07	8.595512E-19	7.389204E-17	1.111013E-16	99.999801	3.000000
0.06	1.732615E+16	7.000000	8.597500E-07	1.346334E-18	8.867043E-17	1.555417E-16	99.999737	3.000000
0.07	1.732613E+16	8.166667	9.286354E-07	1.973219E-18	1.034488E-16	2.073889E-16	99.999665	3.000000
0.08	1.732612E+16	9.333333	9.927523E-07	2.752702E-18	1.182272E-16	2.666429E-16	99.999585	3.000000
0.09	1.732610E+16	10.500000	1.052972E-06	3.696487E-18	1.330055E-16	3.333035E-16	99.999497	3.000000
0.10	1.732609E+16	11.666667	1.109929E-06	4.815622E-18	1.477839E-16	4.073709E-16	99.999400	3.000000
0.11	1.732607E+16	12.833333	1.164102E-06	6.120594E-18	1.625622E-16	4.888449E-16	99.999296	3.000000
0.12	1.732605E+16	14.000000	1.215863E-06	7.621413E-18	1.773405E-16	5.777257E-16	99.999183	3.000000
0.13	1.732603E+16	15.166667	1.234286E-06	9.329697E-18	1.921188E-16	6.740131E-16	99.999062	3.000000
0.14	1.732601E+16	16.333333	1.234286E-06	1.125812E-17	2.068970E-16	7.777072E-16	99.998934	3.000000
0.15	1.732598E+16	17.500000	1.234286E-06	1.341937E-17	2.216753E-16	8.888079E-16	99.998796	3.000000
0.16	1.732596E+16	18.666667	1.234286E-06	1.582611E-17	2.364535E-16	1.007315E-15	99.998651	3.000000
0.17	1.732593E+16	19.833333	1.234286E-06	1.849102E-17	2.512317E-16	1.133229E-15	99.998498	3.000000
0.18	1.732590E+16	21.000000	1.234286E-06	2.142677E-17	2.660099E-16	1.266550E-15	99.998336	3.000000
0.19	1.732587E+16	22.166667	1.234286E-06	2.464606E-17	2.807881E-16	1.407277E-15	99.998166	3.000000
0.20	1.732584E+16	23.333333	1.234286E-06	2.816154E-17	2.955662E-16	1.555411E-15	99.997988	2.999999
0.21	1.732581E+16	24.500000	1.234286E-06	3.198589E-17	3.103443E-16	1.710951E-15	99.997801	2.999999
0.22	1.732578E+16	25.666667	1.234286E-06	3.613180E-17	3.251224E-16	1.873898E-15	99.997606	2.999999
0.23	1.732574E+16	26.833333	1.234286E-06	4.061194E-17	3.399004E-16	2.044252E-15	99.997403	2.999999
0.24	1.732570E+16	28.000000	1.234286E-06	4.543898E-17	3.546784E-16	2.222012E-15	99.997192	2.999999
0.25	1.732567E+16	29.166667	1.234286E-06	5.062560E-17	3.694564E-16	2.407178E-15	99.996972	2.999999
0.26	1.732563E+16	30.333333	1.234286E-06	5.618448E-17	3.842344E-16	2.599751E-15	99.996744	2.999999
0.27	1.732559E+16	31.500000	1.234286E-06	6.212829E-17	3.990123E-16	2.799731E-15	99.996508	2.999999
0.28	1.732554E+16	32.666667	1.234286E-06	6.846970E-17	4.137902E-16	3.007116E-15	99.996263	2.999999
0.29	1.732550E+16	33.833333	1.234286E-06	7.522140E-17	4.285680E-16	3.221909E-15	99.996010	2.999999
0.30	1.732545E+16	35.000000	1.234286E-06	8.239606E-17	4.433458E-16	3.444107E-15	99.995749	2.999999
0.31	1.732541E+16	36.166667	1.234286E-06	9.000636E-17	4.581236E-16	3.673712E-15	99.995479	2.999999
0.32	1.732536E+16	37.333333	1.234286E-06	9.806496E-17	4.729013E-16	3.910724E-15	99.995201	2.999999
0.33	1.732531E+16	38.500000	1.234286E-06	1.065846E-16	4.876790E-16	4.155141E-15	99.994914	2.999999
0.34	1.732526E+16	39.666667	1.234286E-06	1.155778E-16	5.024567E-16	4.406965E-15	99.994619	2.999998
0.35	1.732521E+16	40.833333	1.234286E-06	1.250574E-16	5.172343E-16	4.666196E-15	99.994315	2.999998
0.36	1.732515E+16	42.000000	1.234286E-06	1.350360E-16	5.320118E-16	4.932832E-15	99.994003	2.999998
0.37	1.732510E+16	43.166667	1.234286E-06	1.455263E-16	5.467893E-16	5.206875E-15	99.993683	2.999998
0.38	1.732504E+16	44.333333	1.234286E-06	1.565409E-16	5.615668E-16	5.488324E-15	99.993354	2.999998
0.39	1.732498E+16	45.500000	1.234286E-06	1.680926E-16	5.763442E-16	5.777179E-15	99.993016	2.999998
0.40	1.732492E+16	46.666667	1.234286E-06	1.801940E-16	5.911216E-16	6.073440E-15	99.992670	2.999998
0.41	1.732486E+16	47.833333	1.234286E-06	1.928578E-16	6.058989E-16	6.377107E-15	99.992316	2.999998
0.42	1.732480E+16	49.000000	1.234286E-06	2.060966E-16	6.206761E-16	6.688180E-15	99.991952	2.999998
0.43	1.732473E+16	50.166667	1.234286E-06	2.199232E-16	6.354533E-16	7.006659E-15	99.991581	2.999998
0.44	1.732467E+16	51.333333	1.234286E-06	2.343502E-16	6.502305E-16	7.332545E-15	99.991200	2.999997
0.45	1.732460E+16	52.500000	1.234286E-06	2.493903E-16	6.650076E-16	7.665836E-15	99.990812	2.999997

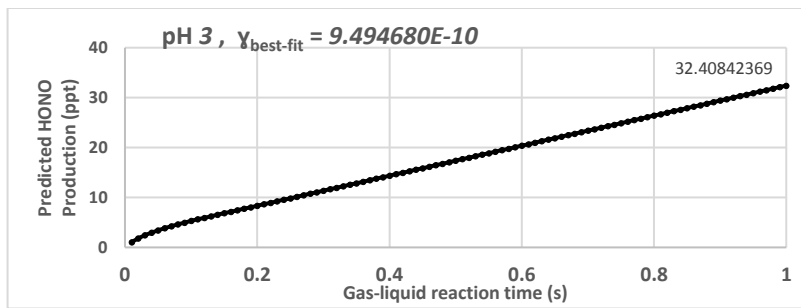
0.46	1.732453E+16	53.666667	1.234286E-06	2.650561E-16	6.797846E-16	8.006533E-15	99.990414	2.999997
0.47	1.732446E+16	54.833333	1.234286E-06	2.813604E-16	6.945616E-16	8.354636E-15	99.990008	2.999997
0.48	1.732439E+16	56.000000	1.234286E-06	2.983157E-16	7.093385E-16	8.710145E-15	99.989593	2.999997
0.49	1.732431E+16	57.166667	1.234286E-06	3.159349E-16	7.241154E-16	9.073060E-15	99.989170	2.999997
0.50	1.732424E+16	58.333333	1.234286E-06	3.342305E-16	7.388922E-16	9.443380E-15	99.988738	2.999997
0.51	1.732416E+16	59.500000	1.234286E-06	3.532153E-16	7.536689E-16	9.821107E-15	99.988297	2.999997
0.52	1.732409E+16	60.666667	1.234286E-06	3.729018E-16	7.684456E-16	1.020624E-14	99.987848	2.999996
0.53	1.732401E+16	61.833333	1.234286E-06	3.933028E-16	7.832222E-16	1.059878E-14	99.987390	2.999996
0.54	1.732393E+16	63.000000	1.234286E-06	4.144310E-16	7.979987E-16	1.099872E-14	99.986923	2.999996
0.55	1.732384E+16	64.166667	1.234286E-06	4.362990E-16	8.127752E-16	1.140607E-14	99.986448	2.999996
0.56	1.732376E+16	65.333333	1.234286E-06	4.589195E-16	8.275516E-16	1.182082E-14	99.985964	2.999996
0.57	1.732367E+16	66.500000	1.234286E-06	4.823052E-16	8.423279E-16	1.224298E-14	99.985471	2.999996
0.58	1.732359E+16	67.666667	1.234286E-06	5.064687E-16	8.571042E-16	1.267255E-14	99.984969	2.999996
0.59	1.732350E+16	68.833333	1.234286E-06	5.314227E-16	8.718803E-16	1.310952E-14	99.984459	2.999995
0.60	1.732341E+16	70.000000	1.234286E-06	5.571799E-16	8.866564E-16	1.355389E-14	99.983939	2.999995
0.61	1.732332E+16	71.166667	1.234286E-06	5.837530E-16	9.014325E-16	1.400568E-14	99.983411	2.999995
0.62	1.732322E+16	72.333333	1.234286E-06	6.111546E-16	9.162084E-16	1.446486E-14	99.982874	2.999995
0.63	1.732313E+16	73.500000	1.234286E-06	6.393974E-16	9.309843E-16	1.493145E-14	99.982329	2.999995
0.64	1.732303E+16	74.666667	1.234286E-06	6.684941E-16	9.457601E-16	1.540545E-14	99.981774	2.999995
0.65	1.732294E+16	75.833333	1.234286E-06	6.984574E-16	9.605358E-16	1.588685E-14	99.981211	2.999994
0.66	1.732284E+16	77.000000	1.234286E-06	7.292998E-16	9.753114E-16	1.637566E-14	99.980638	2.999994
0.67	1.732274E+16	78.166667	1.234286E-06	7.610342E-16	9.900870E-16	1.687187E-14	99.980057	2.999994
0.68	1.732263E+16	79.333333	1.234286E-06	7.936731E-16	1.004862E-15	1.737549E-14	99.979467	2.999994
0.69	1.732253E+16	80.500000	1.234286E-06	8.272293E-16	1.019638E-15	1.788651E-14	99.978868	2.999994
0.70	1.732242E+16	81.666667	1.234286E-06	8.617154E-16	1.034413E-15	1.840494E-14	99.978260	2.999994
0.71	1.732232E+16	82.833333	1.234286E-06	8.971440E-16	1.049188E-15	1.893077E-14	99.977643	2.999993
0.72	1.732221E+16	84.000000	1.234286E-06	9.335280E-16	1.063963E-15	1.946401E-14	99.977017	2.999993
0.73	1.732210E+16	85.166667	1.234286E-06	9.708798E-16	1.078738E-15	2.000465E-14	99.976383	2.999993
0.74	1.732199E+16	86.333333	1.234286E-06	1.009212E-15	1.093513E-15	2.055269E-14	99.975739	2.999993
0.75	1.732187E+16	87.500000	1.234286E-06	1.048538E-15	1.108288E-15	2.110814E-14	99.975086	2.999993
0.76	1.732176E+16	88.666667	1.234286E-06	1.088870E-15	1.123063E-15	2.167100E-14	99.974424	2.999992
0.77	1.732164E+16	89.833333	1.234286E-06	1.130220E-15	1.137838E-15	2.224126E-14	99.973754	2.999992
0.78	1.732153E+16	91.000000	1.234286E-06	1.172601E-15	1.152612E-15	2.281892E-14	99.973074	2.999992
0.79	1.732141E+16	92.166667	1.234286E-06	1.216027E-15	1.167386E-15	2.340399E-14	99.972385	2.999992
0.80	1.732129E+16	93.333333	1.234286E-06	1.260509E-15	1.182161E-15	2.399646E-14	99.971687	2.999992
0.81	1.732116E+16	94.500000	1.234286E-06	1.306060E-15	1.196935E-15	2.459634E-14	99.970980	2.999991
0.82	1.732104E+16	95.666667	1.234286E-06	1.352693E-15	1.211709E-15	2.520362E-14	99.970264	2.999991
0.83	1.732091E+16	96.833333	1.234286E-06	1.400421E-15	1.226483E-15	2.581830E-14	99.969539	2.999991
0.84	1.732079E+16	98.000000	1.234286E-06	1.449257E-15	1.241257E-15	2.644039E-14	99.968804	2.999991
0.85	1.732066E+16	99.166667	1.234286E-06	1.499212E-15	1.256031E-15	2.706989E-14	99.968061	2.999990
0.86	1.732053E+16	100.333333	1.234286E-06	1.550300E-15	1.270805E-15	2.770678E-14	99.967308	2.999990
0.87	1.732039E+16	101.500000	1.234286E-06	1.602533E-15	1.285578E-15	2.835108E-14	99.966547	2.999990
0.88	1.732026E+16	102.666667	1.234286E-06	1.655924E-15	1.300352E-15	2.900279E-14	99.965776	2.999990
0.89	1.732013E+16	103.833333	1.234286E-06	1.710486E-15	1.315125E-15	2.966190E-14	99.964996	2.999990
0.90	1.731999E+16	105.000000	1.234286E-06	1.766231E-15	1.329898E-15	3.032841E-14	99.964206	2.999989
0.91	1.731985E+16	106.166667	1.234286E-06	1.823172E-15	1.344671E-15	3.100232E-14	99.963408	2.999989
0.92	1.731971E+16	107.333333	1.234286E-06	1.881321E-15	1.359444E-15	3.168364E-14	99.962600	2.999989
0.93	1.731957E+16	108.500000	1.234286E-06	1.940692E-15	1.374217E-15	3.237236E-14	99.961783	2.999989
0.94	1.731943E+16	109.666667	1.234286E-06	2.001297E-15	1.388990E-15	3.306849E-14	99.960957	2.999988
0.95	1.731928E+16	110.833333	1.234286E-06	2.063149E-15	1.403763E-15	3.377202E-14	99.960122	2.999988
0.96	1.731914E+16	112.000000	1.234286E-06	2.126259E-15	1.418535E-15	3.448295E-14	99.959277	2.999988
0.97	1.731899E+16	113.166667	1.234286E-06	2.190642E-15	1.433308E-15	3.520129E-14	99.958423	2.999988
0.98	1.731884E+16	114.333333	1.234286E-06	2.256310E-15	1.448080E-15	3.592702E-14	99.957560	2.999987
0.99	1.731869E+16	115.500000	1.234286E-06	2.323274E-15	1.462852E-15	3.666016E-14	99.956687	2.999987
1.00	1.731853E+16	116.666667	1.234286E-06	2.391549E-15	1.477624E-15	3.740071E-14	99.955805	2.999987





$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732619E+16	1.166667	3.509923E-07	3.063806E-20	2.031407E-17	1.018115E-17	99.999967	3.000000
0.02	1.732618E+16	2.333333	4.963778E-07	1.352429E-19	4.062813E-17	3.054345E-17	99.999924	3.000000
0.03	1.732617E+16	3.500000	6.079358E-07	3.452169E-19	6.094218E-17	6.108689E-17	99.999869	3.000000
0.04	1.732616E+16	4.666667	7.019834E-07	6.864584E-19	8.125621E-17	1.018115E-16	99.999803	3.000000
0.05	1.732614E+16	5.833333	7.848407E-07	1.181519E-18	1.015702E-16	1.527171E-16	99.999726	3.000000
0.06	1.732613E+16	7.000000	8.597491E-07	1.850639E-18	1.218842E-16	2.138040E-16	99.999639	3.000000
0.07	1.732611E+16	8.166667	9.286343E-07	2.712340E-18	1.421982E-16	2.850719E-16	99.999540	3.000000
0.08	1.732609E+16	9.333333	9.927507E-07	3.783799E-18	1.625122E-16	3.665209E-16	99.999429	3.000000
0.09	1.732607E+16	10.500000	1.052970E-06	5.081104E-18	1.828261E-16	4.581509E-16	99.999308	3.000000
0.10	1.732605E+16	11.666667	1.109926E-06	6.619441E-18	2.031400E-16	5.599621E-16	99.999176	3.000000
0.11	1.732602E+16	12.833333	1.164099E-06	8.413226E-18	2.234539E-16	6.719542E-16	99.999032	3.000000
0.12	1.732600E+16	14.000000	1.215860E-06	1.047622E-17	2.437678E-16	7.941275E-16	99.998877	3.000000
0.13	1.732597E+16	15.166667	1.234286E-06	1.282438E-17	2.640816E-16	9.264817E-16	99.998711	3.000000
0.14	1.732594E+16	16.333333	1.234286E-06	1.547515E-17	2.843954E-16	1.069017E-15	99.998534	3.000000
0.15	1.732590E+16	17.500000	1.234286E-06	1.844594E-17	3.047091E-16	1.221733E-15	99.998346	3.000000
0.16	1.732587E+16	18.666667	1.234286E-06	2.175419E-17	3.250228E-16	1.384630E-15	99.998146	3.000000
0.17	1.732583E+16	19.833333	1.234286E-06	2.541731E-17	3.453365E-16	1.557708E-15	99.997935	2.999999
0.18	1.732579E+16	21.000000	1.234286E-06	2.945273E-17	3.656501E-16	1.740967E-15	99.997713	2.999999
0.19	1.732575E+16	22.166667	1.234286E-06	3.387787E-17	3.859637E-16	1.934407E-15	99.997479	2.999999
0.20	1.732571E+16	23.333333	1.234286E-06	3.871016E-17	4.062772E-16	2.138027E-15	99.997234	2.999999
0.21	1.732567E+16	24.500000	1.234286E-06	4.396702E-17	4.265907E-16	2.351829E-15	99.996978	2.999999
0.22	1.732562E+16	25.666667	1.234286E-06	4.966588E-17	4.469041E-16	2.575811E-15	99.996710	2.999999
0.23	1.732557E+16	26.833333	1.234286E-06	5.582416E-17	4.672174E-16	2.809974E-15	99.996431	2.999999
0.24	1.732552E+16	28.000000	1.234286E-06	6.245928E-17	4.875307E-16	3.054317E-15	99.996140	2.999999
0.25	1.732547E+16	29.166667	1.234286E-06	6.958867E-17	5.078440E-16	3.308842E-15	99.995838	2.999999
0.26	1.732542E+16	30.333333	1.234286E-06	7.722975E-17	5.281572E-16	3.573546E-15	99.995525	2.999999
0.27	1.732536E+16	31.500000	1.234286E-06	8.539994E-17	5.484703E-16	3.848432E-15	99.995200	2.999999
0.28	1.732530E+16	32.666667	1.234286E-06	9.411668E-17	5.687834E-16	4.133498E-15	99.994864	2.999999
0.29	1.732524E+16	33.833333	1.234286E-06	1.033974E-16	5.890963E-16	4.428744E-15	99.994516	2.999998
0.30	1.732518E+16	35.000000	1.234286E-06	1.132594E-16	6.094093E-16	4.734171E-15	99.994156	2.999998
0.31	1.732511E+16	36.166667	1.234286E-06	1.237203E-16	6.297221E-16	5.049779E-15	99.993785	2.999998
0.32	1.732505E+16	37.333333	1.234286E-06	1.347974E-16	6.500349E-16	5.375567E-15	99.993403	2.999998
0.33	1.732498E+16	38.500000	1.234286E-06	1.465082E-16	6.703475E-16	5.711535E-15	99.993009	2.999998
0.34	1.732491E+16	39.666667	1.234286E-06	1.588701E-16	6.906601E-16	6.057683E-15	99.992603	2.999998
0.35	1.732484E+16	40.833333	1.234286E-06	1.719004E-16	7.109727E-16	6.414012E-15	99.992186	2.999998
0.36	1.732476E+16	42.000000	1.234286E-06	1.856167E-16	7.312851E-16	6.780520E-15	99.991757	2.999998
0.37	1.732469E+16	43.166667	1.234286E-06	2.000363E-16	7.515975E-16	7.157209E-15	99.991316	2.999997
0.38	1.732461E+16	44.333333	1.234286E-06	2.151766E-16	7.719097E-16	7.544078E-15	99.990864	2.999997
0.39	1.732453E+16	45.500000	1.234286E-06	2.310552E-16	7.922219E-16	7.941127E-15	99.990400	2.999997
0.40	1.732445E+16	46.666667	1.234286E-06	2.476893E-16	8.125340E-16	8.348356E-15	99.989925	2.999997
0.41	1.732436E+16	47.833333	1.234286E-06	2.650965E-16	8.328459E-16	8.765765E-15	99.989437	2.999997
0.42	1.732427E+16	49.000000	1.234286E-06	2.832942E-16	8.531578E-16	9.193353E-15	99.988938	2.999997
0.43	1.732419E+16	50.166667	1.234286E-06	3.022997E-16	8.734696E-16	9.631122E-15	99.988427	2.999997
0.44	1.732410E+16	51.333333	1.234286E-06	3.221305E-16	8.937813E-16	1.007907E-14	99.987904	2.999996
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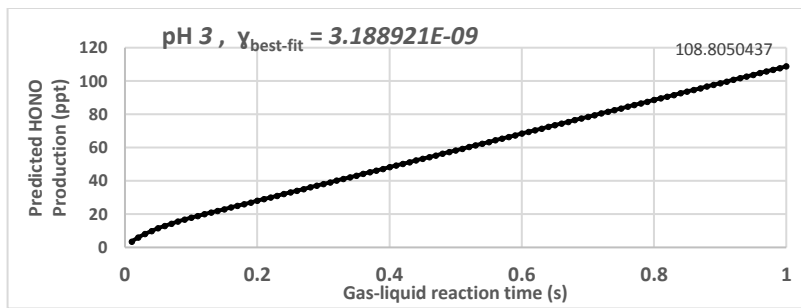
0.46	1.732391E+16	53.666667	1.234286E-06	3.643377E-16	9.344043E-16	1.100550E-14	99.986824	2.999996
0.47	1.732381E+16	54.833333	1.234286E-06	3.867489E-16	9.547156E-16	1.148399E-14	99.986266	2.999996
0.48	1.732371E+16	56.000000	1.234286E-06	4.100551E-16	9.750269E-16	1.197266E-14	99.985696	2.999996
0.49	1.732361E+16	57.166667	1.234286E-06	4.342737E-16	9.953380E-16	1.247150E-14	99.985114	2.999996
0.50	1.732351E+16	58.333333	1.234286E-06	4.594221E-16	1.015649E-15	1.298053E-14	99.984520	2.999995
0.51	1.732340E+16	59.500000	1.234286E-06	4.855178E-16	1.035960E-15	1.349973E-14	99.983914	2.999995
0.52	1.732330E+16	60.666667	1.234286E-06	5.125781E-16	1.056271E-15	1.402912E-14	99.983297	2.999995
0.53	1.732319E+16	61.833333	1.234286E-06	5.406204E-16	1.076581E-15	1.456868E-14	99.982667	2.999995
0.54	1.732308E+16	63.000000	1.234286E-06	5.696623E-16	1.096892E-15	1.511842E-14	99.982025	2.999995
0.55	1.732296E+16	64.166667	1.234286E-06	5.997211E-16	1.117202E-15	1.567834E-14	99.981372	2.999994
0.56	1.732285E+16	65.333333	1.234286E-06	6.308142E-16	1.137512E-15	1.624844E-14	99.980706	2.999994
0.57	1.732273E+16	66.500000	1.234286E-06	6.629591E-16	1.157822E-15	1.682872E-14	99.980029	2.999994
0.58	1.732261E+16	67.666667	1.234286E-06	6.961731E-16	1.178132E-15	1.741917E-14	99.979339	2.999994
0.59	1.732249E+16	68.833333	1.234286E-06	7.304737E-16	1.198442E-15	1.801981E-14	99.978637	2.999994
0.60	1.732237E+16	70.000000	1.234286E-06	7.658784E-16	1.218752E-15	1.863062E-14	99.977924	2.999993
0.61	1.732224E+16	71.166667	1.234286E-06	8.024044E-16	1.239062E-15	1.925162E-14	99.977198	2.999993
0.62	1.732211E+16	72.333333	1.234286E-06	8.400693E-16	1.259371E-15	1.988279E-14	99.976460	2.999993
0.63	1.732198E+16	73.500000	1.234286E-06	8.788904E-16	1.279680E-15	2.052413E-14	99.975710	2.999993
0.64	1.732185E+16	74.666667	1.234286E-06	9.188852E-16	1.299989E-15	2.117566E-14	99.974947	2.999993
0.65	1.732172E+16	75.833333	1.234286E-06	9.600711E-16	1.320298E-15	2.183737E-14	99.974173	2.999992
0.66	1.732158E+16	77.000000	1.234286E-06	1.002466E-15	1.340607E-15	2.250925E-14	99.973386	2.999992
0.67	1.732144E+16	78.166667	1.234286E-06	1.046086E-15	1.360916E-15	2.319131E-14	99.972587	2.999992
0.68	1.732130E+16	79.333333	1.234286E-06	1.090950E-15	1.381224E-15	2.388355E-14	99.971776	2.999992
0.69	1.732116E+16	80.500000	1.234286E-06	1.137074E-15	1.401532E-15	2.458596E-14	99.970953	2.999991
0.70	1.732101E+16	81.666667	1.234286E-06	1.184477E-15	1.421841E-15	2.529856E-14	99.970117	2.999991
0.71	1.732087E+16	82.833333	1.234286E-06	1.233175E-15	1.442149E-15	2.602133E-14	99.969269	2.999991
0.72	1.732072E+16	84.000000	1.234286E-06	1.283186E-15	1.462456E-15	2.675428E-14	99.968409	2.999991
0.73	1.732057E+16	85.166667	1.234286E-06	1.334527E-15	1.482764E-15	2.749740E-14	99.967537	2.999990
0.74	1.732041E+16	86.333333	1.234286E-06	1.387217E-15	1.503071E-15	2.825071E-14	99.966652	2.999990
0.75	1.732026E+16	87.500000	1.234286E-06	1.441271E-15	1.523379E-15	2.901419E-14	99.965755	2.999990
0.76	1.732010E+16	88.666667	1.234286E-06	1.496709E-15	1.543686E-15	2.978784E-14	99.964845	2.999990
0.77	1.731994E+16	89.833333	1.234286E-06	1.553546E-15	1.563993E-15	3.057168E-14	99.963923	2.999989
0.78	1.731978E+16	91.000000	1.234286E-06	1.611801E-15	1.584299E-15	3.136569E-14	99.962989	2.999989
0.79	1.731961E+16	92.166667	1.234286E-06	1.671491E-15	1.604606E-15	3.216987E-14	99.962042	2.999989
0.80	1.731945E+16	93.333333	1.234286E-06	1.732633E-15	1.624912E-15	3.298424E-14	99.961082	2.999988
0.81	1.731928E+16	94.500000	1.234286E-06	1.795244E-15	1.645219E-15	3.380878E-14	99.960111	2.999988
0.82	1.731911E+16	95.666667	1.234286E-06	1.859343E-15	1.665524E-15	3.464349E-14	99.959126	2.999988
0.83	1.731894E+16	96.833333	1.234286E-06	1.924947E-15	1.685830E-15	3.548839E-14	99.958130	2.999988
0.84	1.731876E+16	98.000000	1.234286E-06	1.992072E-15	1.706136E-15	3.634346E-14	99.957120	2.999987
0.85	1.731858E+16	99.166667	1.234286E-06	2.060737E-15	1.726441E-15	3.720870E-14	99.956098	2.999987
0.86	1.731841E+16	100.333333	1.234286E-06	2.130958E-15	1.746746E-15	3.808412E-14	99.955064	2.999987
0.87	1.731822E+16	101.500000	1.234286E-06	2.202754E-15	1.767051E-15	3.896971E-14	99.954017	2.999986
0.88	1.731804E+16	102.666667	1.234286E-06	2.276141E-15	1.787356E-15	3.986549E-14	99.952957	2.999986
0.89	1.731785E+16	103.833333	1.234286E-06	2.351137E-15	1.807661E-15	4.077143E-14	99.951885	2.999986
0.90	1.731767E+16	105.000000	1.234286E-06	2.427760E-15	1.827965E-15	4.168755E-14	99.950800	2.999985
0.91	1.731748E+16	106.166667	1.234286E-06	2.506026E-15	1.848269E-15	4.261385E-14	99.949703	2.999985
0.92	1.731728E+16	107.333333	1.234286E-06	2.585954E-15	1.868573E-15	4.355032E-14	99.948593	2.999985
0.93	1.731709E+16	108.500000	1.234286E-06	2.667560E-15	1.888876E-15	4.449697E-14	99.947470	2.999984
0.94	1.731689E+16	109.666667	1.234286E-06	2.750863E-15	1.909180E-15	4.545379E-14	99.946334	2.999984
0.95	1.731669E+16	110.833333	1.234286E-06	2.835878E-15	1.929483E-15	4.642079E-14	99.945186	2.999984
0.96	1.731649E+16	112.000000	1.234286E-06	2.922625E-15	1.949786E-15	4.739796E-14	99.944025	2.999983
0.97	1.731629E+16	113.166667	1.234286E-06	3.011120E-15	1.970089E-15	4.838530E-14	99.942851	2.999983
0.98	1.731608E+16	114.333333	1.234286E-06	3.101380E-15	1.990391E-15	4.938282E-14	99.941664	2.999983
0.99	1.731588E+16	115.500000	1.234286E-06	3.193424E-15	2.010694E-15	5.039051E-14	99.940465	2.999982
1.00	1.731567E+16	116.666667	1.234286E-06	3.287268E-15	2.030996E-15	5.140838E-14	99.939253	2.999982



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732619E+16	1.166667	3.509923E-07	2.744492E-20	1.819691E-17	9.120058E-18	99.999971	3.000000
0.02	1.732618E+16	2.333333	4.963779E-07	1.211477E-19	3.639381E-17	2.736017E-17	99.999932	3.000000
0.03	1.732617E+16	3.500000	6.079359E-07	3.092379E-19	5.459070E-17	5.472033E-17	99.999883	3.000000
0.04	1.732616E+16	4.666667	7.019835E-07	6.149147E-19	7.278758E-17	9.120053E-17	99.999824	3.000000
0.05	1.732615E+16	5.833333	7.848409E-07	1.058379E-18	9.098445E-17	1.368008E-16	99.999755	3.000000
0.06	1.732614E+16	7.000000	8.597495E-07	1.657763E-18	1.091813E-16	1.915210E-16	99.999676	3.000000
0.07	1.732612E+16	8.166667	9.286347E-07	2.429656E-18	1.273781E-16	2.553613E-16	99.999588	3.000000
0.08	1.732610E+16	9.333333	9.927513E-07	3.389446E-18	1.455750E-16	3.283216E-16	99.999489	3.000000
0.09	1.732608E+16	10.500000	1.052971E-06	4.551545E-18	1.637718E-16	4.104019E-16	99.999380	3.000000
0.10	1.732606E+16	11.666667	1.109927E-06	5.929553E-18	1.819686E-16	5.016022E-16	99.999262	3.000000
0.11	1.732604E+16	12.833333	1.164100E-06	7.536388E-18	2.001653E-16	6.019224E-16	99.999133	3.000000
0.12	1.732602E+16	14.000000	1.215861E-06	9.384370E-18	2.183620E-16	7.113626E-16	99.998994	3.000000
0.13	1.732599E+16	15.166667	1.234286E-06	1.148781E-17	2.365588E-16	8.299228E-16	99.998846	3.000000
0.14	1.732596E+16	16.333333	1.234286E-06	1.386231E-17	2.547554E-16	9.576029E-16	99.998687	3.000000
0.15	1.732593E+16	17.500000	1.234286E-06	1.652348E-17	2.729521E-16	1.094403E-15	99.998518	3.000000
0.16	1.732590E+16	18.666667	1.234286E-06	1.948694E-17	2.911487E-16	1.240323E-15	99.998339	3.000000
0.17	1.732587E+16	19.833333	1.234286E-06	2.276829E-17	3.093453E-16	1.395362E-15	99.998150	3.000000
0.18	1.732584E+16	21.000000	1.234286E-06	2.638313E-17	3.275418E-16	1.559522E-15	99.997951	2.999999
0.19	1.732580E+16	22.166667	1.234286E-06	3.034708E-17	3.457383E-16	1.732801E-15	99.997742	2.999999
0.20	1.732576E+16	23.333333	1.234286E-06	3.467574E-17	3.639348E-16	1.915201E-15	99.997522	2.999999
0.21	1.732572E+16	24.500000	1.234286E-06	3.938473E-17	3.821312E-16	2.106720E-15	99.997293	2.999999
0.22	1.732568E+16	25.666667	1.234286E-06	4.448965E-17	4.003276E-16	2.307358E-15	99.997053	2.999999
0.23	1.732564E+16	26.833333	1.234286E-06	5.000611E-17	4.185240E-16	2.517117E-15	99.996803	2.999999
0.24	1.732559E+16	28.000000	1.234286E-06	5.594972E-17	4.367203E-16	2.735995E-15	99.996542	2.999999
0.25	1.732555E+16	29.166667	1.234286E-06	6.233608E-17	4.549165E-16	2.963993E-15	99.996272	2.999999
0.26	1.732550E+16	30.333333	1.234286E-06	6.918080E-17	4.731127E-16	3.201110E-15	99.995991	2.999999
0.27	1.732545E+16	31.500000	1.234286E-06	7.649949E-17	4.913089E-16	3.447347E-15	99.995700	2.999999
0.28	1.732539E+16	32.666667	1.234286E-06	8.430777E-17	5.095050E-16	3.702704E-15	99.995399	2.999999
0.29	1.732534E+16	33.833333	1.234286E-06	9.262122E-17	5.277010E-16	3.967180E-15	99.995087	2.999999
0.30	1.732528E+16	35.000000	1.234286E-06	1.014555E-16	5.458970E-16	4.240776E-15	99.994765	2.999999
0.31	1.732523E+16	36.166667	1.234286E-06	1.108261E-16	5.640929E-16	4.523491E-15	99.994433	2.999998
0.32	1.732517E+16	37.333333	1.234286E-06	1.207488E-16	5.822888E-16	4.815325E-15	99.994091	2.999998
0.33	1.732511E+16	38.500000	1.234286E-06	1.312391E-16	6.004846E-16	5.116279E-15	99.993738	2.999998
0.34	1.732504E+16	39.666667	1.234286E-06	1.423126E-16	6.186803E-16	5.426353E-15	99.993374	2.999998
0.35	1.732498E+16	40.833333	1.234286E-06	1.539849E-16	6.368760E-16	5.745545E-15	99.993000	2.999998
0.36	1.732491E+16	42.000000	1.234286E-06	1.662717E-16	6.550716E-16	6.073857E-15	99.992616	2.999998
0.37	1.732484E+16	43.166667	1.234286E-06	1.791885E-16	6.732671E-16	6.411288E-15	99.992221	2.999998
0.38	1.732477E+16	44.333333	1.234286E-06	1.927509E-16	6.914626E-16	6.757839E-15	99.991816	2.999998
0.39	1.732470E+16	45.500000	1.234286E-06	2.069746E-16	7.096579E-16	7.113508E-15	99.991401	2.999997
0.40	1.732463E+16	46.666667	1.234286E-06	2.218752E-16	7.278532E-16	7.478297E-15	99.990975	2.999997
0.41	1.732455E+16	47.833333	1.234286E-06	2.374682E-16	7.460485E-16	7.852204E-15	99.990538	2.999997
0.42	1.732447E+16	49.000000	1.234286E-06	2.537694E-16	7.642436E-16	8.235231E-15	99.990091	2.999997
0.43	1.732439E+16	50.166667	1.234286E-06	2.707942E-16	7.824387E-16	8.627376E-15	99.989633	2.999997
0.44	1.732431E+16	51.333333	1.234286E-06	2.885582E-16	8.006337E-16	9.028641E-15	99.989165	2.999997
0.45	1.732423E+16	52.500000	1.234286E-06	3.070772E-16	8.188286E-16	9.439024E-15	99.988686	2.999997

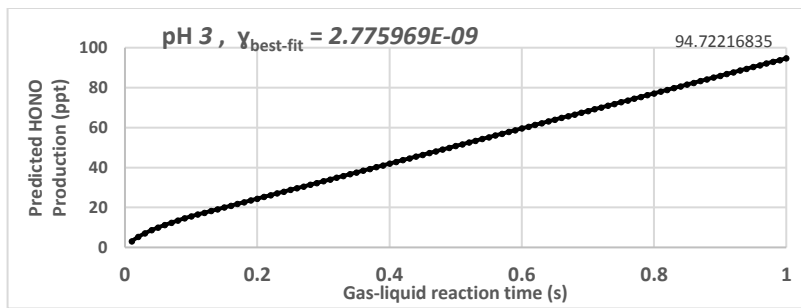
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0.47	1.732406E+16	54.833333	1.234286E-06	3.464423E-16	8.552181E-16	1.028715E-14	99.987697	2.999996
0.48	1.732397E+16	56.000000	1.234286E-06	3.673195E-16	8.734128E-16	1.072489E-14	99.987186	2.999996
0.49	1.732388E+16	57.166667	1.234286E-06	3.890141E-16	8.916073E-16	1.117174E-14	99.986665	2.999996
0.50	1.732379E+16	58.333333	1.234286E-06	4.115416E-16	9.098017E-16	1.162772E-14	99.986133	2.999996
0.51	1.732369E+16	59.500000	1.234286E-06	4.349177E-16	9.279961E-16	1.209282E-14	99.985591	2.999996
0.52	1.732360E+16	60.666667	1.234286E-06	4.591578E-16	9.461903E-16	1.256703E-14	99.985037	2.999996
0.53	1.732350E+16	61.833333	1.234286E-06	4.842777E-16	9.643845E-16	1.305036E-14	99.984473	2.999995
0.54	1.732340E+16	63.000000	1.234286E-06	5.102930E-16	9.825786E-16	1.354281E-14	99.983899	2.999995
0.55	1.732330E+16	64.166667	1.234286E-06	5.372191E-16	1.000772E-15	1.404438E-14	99.983313	2.999995
0.56	1.732320E+16	65.333333	1.234286E-06	5.650719E-16	1.018966E-15	1.455507E-14	99.982717	2.999995
0.57	1.732309E+16	66.500000	1.234286E-06	5.938667E-16	1.037160E-15	1.507487E-14	99.982110	2.999995
0.58	1.732298E+16	67.666667	1.234286E-06	6.236193E-16	1.055354E-15	1.560380E-14	99.981492	2.999995
0.59	1.732288E+16	68.833333	1.234286E-06	6.543453E-16	1.073547E-15	1.614184E-14	99.980864	2.999994
0.60	1.732276E+16	70.000000	1.234286E-06	6.860602E-16	1.091741E-15	1.668900E-14	99.980224	2.999994
0.61	1.732265E+16	71.166667	1.234286E-06	7.187797E-16	1.109934E-15	1.724527E-14	99.979574	2.999994
0.62	1.732254E+16	72.333333	1.234286E-06	7.525194E-16	1.128127E-15	1.781067E-14	99.978913	2.999994
0.63	1.732242E+16	73.500000	1.234286E-06	7.872948E-16	1.146320E-15	1.838518E-14	99.978241	2.999994
0.64	1.732230E+16	74.666667	1.234286E-06	8.231216E-16	1.164513E-15	1.896881E-14	99.977558	2.999993
0.65	1.732218E+16	75.833333	1.234286E-06	8.600153E-16	1.182706E-15	1.956156E-14	99.976864	2.999993
0.66	1.732206E+16	77.000000	1.234286E-06	8.979916E-16	1.200898E-15	2.016342E-14	99.976160	2.999993
0.67	1.732194E+16	78.166667	1.234286E-06	9.370661E-16	1.219091E-15	2.077441E-14	99.975444	2.999993
0.68	1.732181E+16	79.333333	1.234286E-06	9.772544E-16	1.237283E-15	2.139451E-14	99.974718	2.999992
0.69	1.732168E+16	80.500000	1.234286E-06	1.018572E-15	1.255476E-15	2.202372E-14	99.973980	2.999992
0.70	1.732155E+16	81.666667	1.234286E-06	1.061035E-15	1.273668E-15	2.266206E-14	99.973232	2.999992
0.71	1.732142E+16	82.833333	1.234286E-06	1.104658E-15	1.291860E-15	2.330951E-14	99.972472	2.999992
0.72	1.732129E+16	84.000000	1.234286E-06	1.149457E-15	1.310052E-15	2.396608E-14	99.971701	2.999992
0.73	1.732115E+16	85.166667	1.234286E-06	1.195448E-15	1.328244E-15	2.463176E-14	99.970920	2.999991
0.74	1.732102E+16	86.333333	1.234286E-06	1.242647E-15	1.346435E-15	2.530657E-14	99.970127	2.999991
0.75	1.732088E+16	87.500000	1.234286E-06	1.291068E-15	1.364627E-15	2.599048E-14	99.969323	2.999991
0.76	1.732073E+16	88.666667	1.234286E-06	1.340729E-15	1.382818E-15	2.668352E-14	99.968509	2.999991
0.77	1.732059E+16	89.833333	1.234286E-06	1.391643E-15	1.401009E-15	2.738567E-14	99.967683	2.999990
0.78	1.732045E+16	91.000000	1.234286E-06	1.443827E-15	1.419200E-15	2.809694E-14	99.966846	2.999990
0.79	1.732030E+16	92.166667	1.234286E-06	1.497296E-15	1.437391E-15	2.881733E-14	99.965998	2.999990
0.80	1.732015E+16	93.333333	1.234286E-06	1.552067E-15	1.455582E-15	2.954683E-14	99.965138	2.999990
0.81	1.732000E+16	94.500000	1.234286E-06	1.608154E-15	1.473772E-15	3.028545E-14	99.964268	2.999989
0.82	1.731985E+16	95.666667	1.234286E-06	1.665573E-15	1.491963E-15	3.103318E-14	99.963386	2.999989
0.83	1.731969E+16	96.833333	1.234286E-06	1.724340E-15	1.510153E-15	3.179003E-14	99.962493	2.999989
0.84	1.731954E+16	98.000000	1.234286E-06	1.784470E-15	1.528343E-15	3.255599E-14	99.961589	2.999989
0.85	1.731938E+16	99.166667	1.234286E-06	1.845979E-15	1.546533E-15	3.333108E-14	99.960674	2.999988
0.86	1.731922E+16	100.333333	1.234286E-06	1.908883E-15	1.564723E-15	3.411527E-14	99.959747	2.999988
0.87	1.731905E+16	101.500000	1.234286E-06	1.973197E-15	1.582912E-15	3.490859E-14	99.958809	2.999988
0.88	1.731889E+16	102.666667	1.234286E-06	2.038937E-15	1.601102E-15	3.571102E-14	99.957860	2.999987
0.89	1.731872E+16	103.833333	1.234286E-06	2.106118E-15	1.619291E-15	3.652256E-14	99.956899	2.999987
0.90	1.731856E+16	105.000000	1.234286E-06	2.174756E-15	1.637480E-15	3.734322E-14	99.955928	2.999987
0.91	1.731838E+16	106.166667	1.234286E-06	2.244866E-15	1.655669E-15	3.817299E-14	99.954944	2.999987
0.92	1.731821E+16	107.333333	1.234286E-06	2.316465E-15	1.673858E-15	3.901188E-14	99.953950	2.999986
0.93	1.731804E+16	108.500000	1.234286E-06	2.389567E-15	1.692046E-15	3.985989E-14	99.952944	2.999986
0.94	1.731786E+16	109.666667	1.234286E-06	2.464189E-15	1.710235E-15	4.071701E-14	99.951927	2.999986
0.95	1.731768E+16	110.833333	1.234286E-06	2.540346E-15	1.728423E-15	4.158324E-14	99.950898	2.999985
0.96	1.731750E+16	112.000000	1.234286E-06	2.618053E-15	1.746611E-15	4.245859E-14	99.949858	2.999985
0.97	1.731732E+16	113.166667	1.234286E-06	2.697326E-15	1.764799E-15	4.334305E-14	99.948807	2.999985
0.98	1.731714E+16	114.333333	1.234286E-06	2.778181E-15	1.782986E-15	4.423663E-14	99.947744	2.999984
0.99	1.731695E+16	115.500000	1.234286E-06	2.860633E-15	1.801174E-15	4.513932E-14	99.946669	2.999984
1.00	1.731676E+16	116.666667	1.234286E-06	2.944698E-15	1.819361E-15	4.605113E-14	99.945583	2.999984

## LEONARDITE HA STANDARD



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732617E+16	1.166667	3.509920E-07	9.217758E-20	6.111681E-17	3.063096E-17	99.999902	3.000000
0.02	1.732615E+16	2.333333	4.963770E-07	4.068915E-19	1.222335E-16	9.189284E-17	99.999770	3.000000
0.03	1.732612E+16	3.500000	6.079342E-07	1.038619E-18	1.833502E-16	1.837856E-16	99.999606	3.000000
0.04	1.732609E+16	4.666667	7.019806E-07	2.065277E-18	2.444667E-16	3.063091E-16	99.999408	3.000000
0.05	1.732605E+16	5.833333	7.848364E-07	3.554715E-18	3.055831E-16	4.594633E-16	99.999177	3.000000
0.06	1.732600E+16	7.000000	8.597429E-07	5.567829E-18	3.666993E-16	6.432482E-16	99.998913	3.000000
0.07	1.732595E+16	8.166667	9.286257E-07	8.160340E-18	4.278153E-16	8.576636E-16	99.998615	3.000000
0.08	1.732589E+16	9.333333	9.927393E-07	1.138393E-17	4.889312E-16	1.102709E-15	99.998283	3.000000
0.09	1.732583E+16	10.500000	1.052955E-06	1.528700E-17	5.500468E-16	1.378385E-15	99.997919	2.999999
0.10	1.732576E+16	11.666667	1.109908E-06	1.991523E-17	6.111622E-16	1.684692E-15	99.997520	2.999999
0.11	1.732569E+16	12.833333	1.164076E-06	2.531201E-17	6.722773E-16	2.021628E-15	99.997088	2.999999
0.12	1.732561E+16	14.000000	1.215832E-06	3.151872E-17	7.333921E-16	2.389194E-15	99.996622	2.999999
0.13	1.732552E+16	15.166667	1.234286E-06	3.858340E-17	7.945067E-16	2.787390E-15	99.996123	2.999999
0.14	1.732543E+16	16.333333	1.234286E-06	4.655847E-17	8.556209E-16	3.216215E-15	99.995590	2.999999
0.15	1.732533E+16	17.500000	1.234286E-06	5.549636E-17	9.167348E-16	3.675669E-15	99.995023	2.999999
0.16	1.732522E+16	18.666667	1.234286E-06	6.544949E-17	9.778483E-16	4.165753E-15	99.994422	2.999999
0.17	1.732511E+16	19.833333	1.234286E-06	7.647027E-17	1.038961E-15	4.686465E-15	99.993787	2.999998
0.18	1.732500E+16	21.000000	1.234286E-06	8.861112E-17	1.100074E-15	5.237806E-15	99.993118	2.999998
0.19	1.732488E+16	22.166667	1.234286E-06	1.019245E-16	1.161187E-15	5.819775E-15	99.992415	2.999998
0.20	1.732475E+16	23.333333	1.234286E-06	1.164627E-16	1.222298E-15	6.432372E-15	99.991678	2.999998
0.21	1.732462E+16	24.500000	1.234286E-06	1.322783E-16	1.283410E-15	7.075597E-15	99.990907	2.999998
0.22	1.732448E+16	25.666667	1.234286E-06	1.494236E-16	1.344521E-15	7.749449E-15	99.990101	2.999997
0.23	1.732433E+16	26.833333	1.234286E-06	1.679511E-16	1.405631E-15	8.453929E-15	99.989262	2.999997
0.24	1.732418E+16	28.000000	1.234286E-06	1.879131E-16	1.466741E-15	9.189035E-15	99.988388	2.999997
0.25	1.732402E+16	29.166667	1.234286E-06	2.093622E-16	1.527851E-15	9.954768E-15	99.987479	2.999996
0.26	1.732386E+16	30.333333	1.234286E-06	2.323506E-16	1.588959E-15	1.075113E-14	99.986536	2.999996
0.27	1.732369E+16	31.500000	1.234286E-06	2.569308E-16	1.650068E-15	1.157811E-14	99.985559	2.999996
0.28	1.732351E+16	32.666667	1.234286E-06	2.831552E-16	1.711175E-15	1.243572E-14	99.984547	2.999996
0.29	1.732333E+16	33.833333	1.234286E-06	3.110763E-16	1.772282E-15	1.332396E-14	99.983501	2.999995
0.30	1.732315E+16	35.000000	1.234286E-06	3.407464E-16	1.833389E-15	1.424282E-14	99.982419	2.999995
0.31	1.732295E+16	36.166667	1.234286E-06	3.722179E-16	1.894494E-15	1.519230E-14	99.981304	2.999995
0.32	1.732275E+16	37.333333	1.234286E-06	4.055433E-16	1.955599E-15	1.617241E-14	99.980153	2.999994
0.33	1.732255E+16	38.500000	1.234286E-06	4.407750E-16	2.016704E-15	1.718314E-14	99.978967	2.999994
0.34	1.732234E+16	39.666667	1.234286E-06	4.779653E-16	2.077807E-15	1.822450E-14	99.977747	2.999994
0.35	1.732212E+16	40.833333	1.234286E-06	5.171666E-16	2.138910E-15	1.929648E-14	99.976492	2.999993
0.36	1.732189E+16	42.000000	1.234286E-06	5.584314E-16	2.200012E-15	2.039908E-14	99.975201	2.999993
0.37	1.732166E+16	43.166667	1.234286E-06	6.018121E-16	2.261113E-15	2.153230E-14	99.973876	2.999992
0.38	1.732143E+16	44.333333	1.234286E-06	6.473610E-16	2.322214E-15	2.269614E-14	99.972515	2.999992
0.39	1.732119E+16	45.500000	1.234286E-06	6.951305E-16	2.383313E-15	2.389060E-14	99.971119	2.999992
0.40	1.732094E+16	46.666667	1.234286E-06	7.451732E-16	2.444412E-15	2.511569E-14	99.969689	2.999991
0.41	1.732069E+16	47.833333	1.234286E-06	7.975412E-16	2.505510E-15	2.637139E-14	99.968222	2.999991
0.42	1.732043E+16	49.000000	1.234286E-06	8.522871E-16	2.566607E-15	2.765771E-14	99.966721	2.999990
0.43	1.732016E+16	50.166667	1.234286E-06	9.094632E-16	2.627703E-15	2.897465E-14	99.965184	2.999990
0.44	1.731989E+16	51.333333	1.234286E-06	9.691219E-16	2.688798E-15	3.032221E-14	99.963611	2.999989
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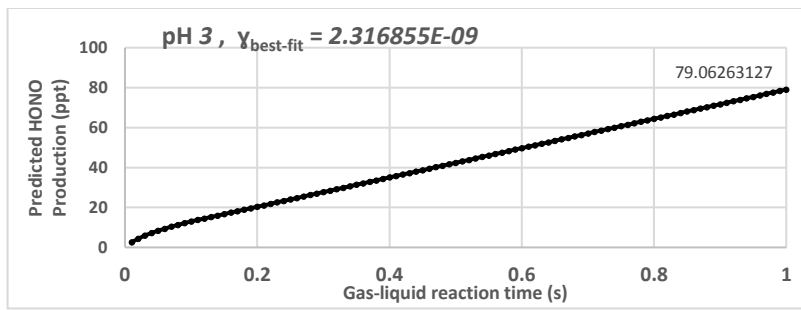
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0.49	1.731843E+16	57.166667	1.234286E-06	1.306488E-15	2.994259E-15	3.751925E-14	99.955216	2.999987
0.50	1.731812E+16	58.333333	1.234286E-06	1.382143E-15	3.055348E-15	3.905050E-14	99.953430	2.999986
0.51	1.731781E+16	59.500000	1.234286E-06	1.460647E-15	3.116436E-15	4.061237E-14	99.951608	2.999986
0.52	1.731748E+16	60.666667	1.234286E-06	1.542052E-15	3.177523E-15	4.220485E-14	99.949750	2.999985
0.53	1.731716E+16	61.833333	1.234286E-06	1.626411E-15	3.238609E-15	4.382794E-14	99.947856	2.999985
0.54	1.731682E+16	63.000000	1.234286E-06	1.713777E-15	3.299693E-15	4.548164E-14	99.945926	2.999984
0.55	1.731648E+16	64.166667	1.234286E-06	1.804202E-15	3.360777E-15	4.716596E-14	99.943960	2.999983
0.56	1.731613E+16	65.333333	1.234286E-06	1.897738E-15	3.421859E-15	4.888088E-14	99.941958	2.999983
0.57	1.731578E+16	66.500000	1.234286E-06	1.994437E-15	3.482940E-15	5.062641E-14	99.939920	2.999982
0.58	1.731542E+16	67.666667	1.234286E-06	2.094352E-15	3.544019E-15	5.240256E-14	99.937845	2.999982
0.59	1.731506E+16	68.833333	1.234286E-06	2.197536E-15	3.605098E-15	5.420931E-14	99.935735	2.999981
0.60	1.731468E+16	70.000000	1.234286E-06	2.304040E-15	3.666175E-15	5.604666E-14	99.933588	2.999980
0.61	1.731431E+16	71.166667	1.234286E-06	2.413917E-15	3.727251E-15	5.791462E-14	99.931404	2.999980
0.62	1.731392E+16	72.333333	1.234286E-06	2.527219E-15	3.788326E-15	5.981319E-14	99.929184	2.999979
0.63	1.731353E+16	73.500000	1.234286E-06	2.643999E-15	3.849399E-15	6.174237E-14	99.926928	2.999978
0.64	1.731313E+16	74.666667	1.234286E-06	2.764309E-15	3.910471E-15	6.370214E-14	99.924635	2.999978
0.65	1.731273E+16	75.833333	1.234286E-06	2.888202E-15	3.971541E-15	6.569252E-14	99.922305	2.999977
0.66	1.731232E+16	77.000000	1.234286E-06	3.015729E-15	4.032610E-15	6.771350E-14	99.919939	2.999976
0.67	1.731190E+16	78.166667	1.234286E-06	3.146943E-15	4.093678E-15	6.976509E-14	99.917536	2.999975
0.68	1.731148E+16	79.333333	1.234286E-06	3.281896E-15	4.154744E-15	7.184727E-14	99.915097	2.999975
0.69	1.731105E+16	80.500000	1.234286E-06	3.420641E-15	4.215809E-15	7.396005E-14	99.912620	2.999974
0.70	1.731062E+16	81.666667	1.234286E-06	3.563231E-15	4.276872E-15	7.610344E-14	99.910107	2.999973
0.71	1.731017E+16	82.833333	1.234286E-06	3.709716E-15	4.337934E-15	7.827741E-14	99.907556	2.999972
0.72	1.730973E+16	84.000000	1.234286E-06	3.860151E-15	4.398994E-15	8.048199E-14	99.904969	2.999972
0.73	1.730927E+16	85.166667	1.234286E-06	4.014586E-15	4.460052E-15	8.271716E-14	99.902345	2.999971
0.74	1.730881E+16	86.333333	1.234286E-06	4.173075E-15	4.521109E-15	8.498293E-14	99.899683	2.999970
0.75	1.730834E+16	87.500000	1.234286E-06	4.335670E-15	4.582165E-15	8.727929E-14	99.896985	2.999969
0.76	1.730787E+16	88.666667	1.234286E-06	4.502422E-15	4.643218E-15	8.960624E-14	99.894249	2.999968
0.77	1.730739E+16	89.833333	1.234286E-06	4.673385E-15	4.704270E-15	9.196379E-14	99.891476	2.999968
0.78	1.730690E+16	91.000000	1.234286E-06	4.848610E-15	4.765321E-15	9.435192E-14	99.888665	2.999967
0.79	1.730641E+16	92.166667	1.234286E-06	5.028151E-15	4.826369E-15	9.677065E-14	99.885818	2.999966
0.80	1.730591E+16	93.333333	1.234286E-06	5.212058E-15	4.887416E-15	9.921996E-14	99.882932	2.999965
0.81	1.730540E+16	94.500000	1.234286E-06	5.400386E-15	4.948462E-15	1.016999E-13	99.880010	2.999964
0.82	1.730489E+16	95.666667	1.234286E-06	5.593185E-15	5.009505E-15	1.042103E-13	99.877049	2.999963
0.83	1.730437E+16	96.833333	1.234286E-06	5.790508E-15	5.070547E-15	1.067514E-13	99.874052	2.999962
0.84	1.730384E+16	98.000000	1.234286E-06	5.992408E-15	5.131586E-15	1.093231E-13	99.871016	2.999962
0.85	1.730331E+16	99.166667	1.234286E-06	6.198936E-15	5.192624E-15	1.119253E-13	99.867943	2.999961
0.86	1.730277E+16	100.333333	1.234286E-06	6.410146E-15	5.253661E-15	1.145581E-13	99.864832	2.999960
0.87	1.730223E+16	101.500000	1.234286E-06	6.626089E-15	5.314695E-15	1.172215E-13	99.861683	2.999959
0.88	1.730167E+16	102.666667	1.234286E-06	6.846817E-15	5.375727E-15	1.199155E-13	99.858496	2.999958
0.89	1.730112E+16	103.833333	1.234286E-06	7.072383E-15	5.436758E-15	1.226401E-13	99.855272	2.999957
0.90	1.730055E+16	105.000000	1.234286E-06	7.302840E-15	5.497786E-15	1.253952E-13	99.852009	2.999956
0.91	1.729998E+16	106.166667	1.234286E-06	7.538239E-15	5.558813E-15	1.281810E-13	99.848709	2.999955
0.92	1.729940E+16	107.333333	1.234286E-06	7.778633E-15	5.619837E-15	1.309972E-13	99.845370	2.999954
0.93	1.729881E+16	108.500000	1.234286E-06	8.024073E-15	5.680860E-15	1.338441E-13	99.841993	2.999953
0.94	1.729822E+16	109.666667	1.234286E-06	8.274613E-15	5.741880E-15	1.367215E-13	99.838578	2.999952
0.95	1.729762E+16	110.833333	1.234286E-06	8.530304E-15	5.802899E-15	1.396296E-13	99.835125	2.999951
0.96	1.729702E+16	112.000000	1.234286E-06	8.791199E-15	5.863915E-15	1.425681E-13	99.831633	2.999950
0.97	1.729641E+16	113.166667	1.234286E-06	9.057350E-15	5.924929E-15	1.455373E-13	99.828103	2.999949
0.98	1.729579E+16	114.333333	1.234286E-06	9.328810E-15	5.985941E-15	1.485370E-13	99.824535	2.999948
0.99	1.729516E+16	115.500000	1.234286E-06	9.605629E-15	6.046951E-15	1.515673E-13	99.820928	2.999947
1.00	1.729453E+16	116.666667	1.234286E-06	9.887862E-15	6.107959E-15	1.546281E-13	99.817283	2.999946



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732618E+16	1.166667	3.509921E-07	8.024097E-20	5.320244E-17	2.666438E-17	99.999914	3.000000
0.02	1.732616E+16	2.333333	4.963772E-07	3.542008E-19	1.064048E-16	7.999311E-17	99.999800	3.000000
0.03	1.732613E+16	3.500000	6.079346E-07	9.041219E-19	1.596071E-16	1.599861E-16	99.999657	3.000000
0.04	1.732610E+16	4.666667	7.019811E-07	1.797832E-18	2.128094E-16	2.666434E-16	99.999485	3.000000
0.05	1.732607E+16	5.833333	7.848372E-07	3.094394E-18	2.660115E-16	3.999649E-16	99.999284	3.000000
0.06	1.732603E+16	7.000000	8.597441E-07	4.846818E-18	3.192135E-16	5.599505E-16	99.999053	3.000000
0.07	1.732598E+16	8.166667	9.286274E-07	7.103610E-18	3.724153E-16	7.466002E-16	99.998794	3.000000
0.08	1.732593E+16	9.333333	9.927415E-07	9.909757E-18	4.256170E-16	9.599138E-16	99.998506	3.000000
0.09	1.732588E+16	10.500000	1.052958E-06	1.330739E-17	4.788186E-16	1.199891E-15	99.998188	3.000000
0.10	1.732582E+16	11.666667	1.109911E-06	1.733629E-17	5.320199E-16	1.466533E-15	99.997841	2.999999
0.11	1.732575E+16	12.833333	1.164081E-06	2.203421E-17	5.852211E-16	1.759837E-15	99.997465	2.999999
0.12	1.732568E+16	14.000000	1.215838E-06	2.743717E-17	6.384220E-16	2.079806E-15	99.997060	2.999999
0.13	1.732561E+16	15.166667	1.234286E-06	3.358701E-17	6.916228E-16	2.426438E-15	99.996625	2.999999
0.14	1.732553E+16	16.333333	1.234286E-06	4.052935E-17	7.448233E-16	2.799733E-15	99.996161	2.999999
0.15	1.732544E+16	17.500000	1.234286E-06	4.830982E-17	7.980235E-16	3.199691E-15	99.995667	2.999999
0.16	1.732535E+16	18.666667	1.234286E-06	5.697407E-17	8.512234E-16	3.626312E-15	99.995144	2.999999
0.17	1.732525E+16	19.833333	1.234286E-06	6.656772E-17	9.044231E-16	4.079596E-15	99.994591	2.999999
0.18	1.732515E+16	21.000000	1.234286E-06	7.713640E-17	9.576225E-16	4.559542E-15	99.994009	2.999998
0.19	1.732505E+16	22.166667	1.234286E-06	8.872574E-17	1.010822E-15	5.066151E-15	99.993397	2.999998
0.20	1.732494E+16	23.333333	1.234286E-06	1.013814E-16	1.064020E-15	5.599422E-15	99.992756	2.999998
0.21	1.732482E+16	24.500000	1.234286E-06	1.151489E-16	1.117219E-15	6.159355E-15	99.992084	2.999998
0.22	1.732470E+16	25.666667	1.234286E-06	1.300741E-16	1.170417E-15	6.745949E-15	99.991383	2.999998
0.23	1.732457E+16	26.833333	1.234286E-06	1.462023E-16	1.223614E-15	7.359206E-15	99.990652	2.999997
0.24	1.732444E+16	28.000000	1.234286E-06	1.635794E-16	1.276811E-15	7.999123E-15	99.989891	2.999997
0.25	1.732430E+16	29.166667	1.234286E-06	1.822510E-16	1.330008E-15	8.665701E-15	99.989101	2.999997
0.26	1.732416E+16	30.333333	1.234286E-06	2.022626E-16	1.383205E-15	9.358941E-15	99.988280	2.999997
0.27	1.732401E+16	31.500000	1.234286E-06	2.236599E-16	1.436401E-15	1.007884E-14	99.987429	2.999996
0.28	1.732386E+16	32.666667	1.234286E-06	2.464885E-16	1.489596E-15	1.082540E-14	99.986548	2.999996
0.29	1.732370E+16	33.833333	1.234286E-06	2.707940E-16	1.542791E-15	1.159862E-14	99.985637	2.999996
0.30	1.732354E+16	35.000000	1.234286E-06	2.966221E-16	1.595986E-15	1.239850E-14	99.984696	2.999996
0.31	1.732337E+16	36.166667	1.234286E-06	3.240184E-16	1.649180E-15	1.322504E-14	99.983725	2.999995
0.32	1.732320E+16	37.333333	1.234286E-06	3.530285E-16	1.702373E-15	1.407824E-14	99.982723	2.999995
0.33	1.732302E+16	38.500000	1.234286E-06	3.836980E-16	1.755566E-15	1.495809E-14	99.981691	2.999995
0.34	1.732283E+16	39.666667	1.234286E-06	4.160725E-16	1.808758E-15	1.586461E-14	99.980628	2.999994
0.35	1.732265E+16	40.833333	1.234286E-06	4.501978E-16	1.861950E-15	1.679778E-14	99.979536	2.999994
0.36	1.732245E+16	42.000000	1.234286E-06	4.861193E-16	1.915142E-15	1.775761E-14	99.978412	2.999994
0.37	1.732225E+16	43.166667	1.234286E-06	5.238827E-16	1.968332E-15	1.874410E-14	99.977259	2.999993
0.38	1.732205E+16	44.333333	1.234286E-06	5.635336E-16	2.021522E-15	1.975725E-14	99.976074	2.999993
0.39	1.732184E+16	45.500000	1.234286E-06	6.051176E-16	2.074712E-15	2.079705E-14	99.974859	2.999993
0.40	1.732162E+16	46.666667	1.234286E-06	6.486804E-16	2.127900E-15	2.186350E-14	99.973614	2.999992
0.41	1.732140E+16	47.833333	1.234286E-06	6.942676E-16	2.181089E-15	2.295662E-14	99.972337	2.999992
0.42	1.732117E+16	49.000000	1.234286E-06	7.419247E-16	2.234276E-15	2.407639E-14	99.971030	2.999992
0.43	1.732094E+16	50.166667	1.234286E-06	7.916974E-16	2.287463E-15	2.522281E-14	99.969692	2.999991
0.44	1.732070E+16	51.333333	1.234286E-06	8.436313E-16	2.340649E-15	2.639589E-14	99.968323	2.999991
0.45	1.732046E+16	52.500000	1.234286E-06	8.977719E-16	2.393834E-15	2.759562E-14	99.966924	2.999990

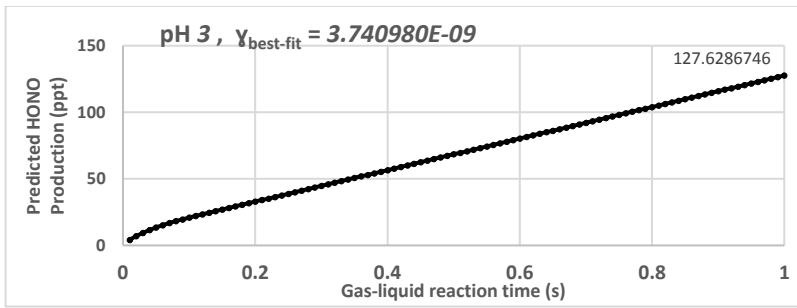


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0.47	1.731996E+16	54.833333	1.234286E-06	1.012856E-15	2.500202E-15	3.007505E-14	99.964031	2.999989
0.48	1.731970E+16	56.000000	1.234286E-06	1.073891E-15	2.553385E-15	3.135474E-14	99.962539	2.999989
0.49	1.731944E+16	57.166667	1.234286E-06	1.137315E-15	2.606568E-15	3.266108E-14	99.961015	2.999989
0.50	1.731917E+16	58.333333	1.234286E-06	1.203173E-15	2.659749E-15	3.399408E-14	99.959460	2.999988
0.51	1.731889E+16	59.500000	1.234286E-06	1.271513E-15	2.712930E-15	3.535372E-14	99.957874	2.999988
0.52	1.731861E+16	60.666667	1.234286E-06	1.342378E-15	2.766109E-15	3.674002E-14	99.956256	2.999987
0.53	1.731833E+16	61.833333	1.234286E-06	1.415814E-15	2.819288E-15	3.815297E-14	99.954608	2.999987
0.54	1.731804E+16	63.000000	1.234286E-06	1.491868E-15	2.872466E-15	3.959256E-14	99.952928	2.999986
0.55	1.731774E+16	64.166667	1.234286E-06	1.570585E-15	2.925643E-15	4.105881E-14	99.951216	2.999986
0.56	1.731744E+16	65.333333	1.234286E-06	1.652010E-15	2.978819E-15	4.255171E-14	99.949473	2.999985
0.57	1.731713E+16	66.500000	1.234286E-06	1.736189E-15	3.031995E-15	4.407125E-14	99.947699	2.999984
0.58	1.731682E+16	67.666667	1.234286E-06	1.823168E-15	3.085169E-15	4.561744E-14	99.945893	2.999984
0.59	1.731650E+16	68.833333	1.234286E-06	1.912992E-15	3.138343E-15	4.719028E-14	99.944056	2.999983
0.60	1.731617E+16	70.000000	1.234286E-06	2.005707E-15	3.191515E-15	4.878976E-14	99.942187	2.999983
0.61	1.731584E+16	71.166667	1.234286E-06	2.101358E-15	3.244686E-15	5.041589E-14	99.940286	2.999982
0.62	1.731551E+16	72.333333	1.234286E-06	2.199990E-15	3.297857E-15	5.206866E-14	99.938353	2.999982
0.63	1.731517E+16	73.500000	1.234286E-06	2.301651E-15	3.351026E-15	5.374808E-14	99.936389	2.999981
0.64	1.731482E+16	74.666667	1.234286E-06	2.406384E-15	3.404195E-15	5.545414E-14	99.934393	2.999980
0.65	1.731447E+16	75.833333	1.234286E-06	2.514236E-15	3.457362E-15	5.718685E-14	99.932365	2.999980
0.66	1.731412E+16	77.000000	1.234286E-06	2.625253E-15	3.510528E-15	5.894620E-14	99.930305	2.999979
0.67	1.731375E+16	78.166667	1.234286E-06	2.739479E-15	3.563693E-15	6.073219E-14	99.928213	2.999979
0.68	1.731339E+16	79.333333	1.234286E-06	2.856960E-15	3.616857E-15	6.254482E-14	99.926090	2.999978
0.69	1.731301E+16	80.500000	1.234286E-06	2.977743E-15	3.670020E-15	6.438409E-14	99.923934	2.999977
0.70	1.731263E+16	81.666667	1.234286E-06	3.101872E-15	3.723182E-15	6.625000E-14	99.921746	2.999977
0.71	1.731225E+16	82.833333	1.234286E-06	3.229393E-15	3.776343E-15	6.814255E-14	99.919525	2.999976
0.72	1.731186E+16	84.000000	1.234286E-06	3.360351E-15	3.829502E-15	7.006174E-14	99.917273	2.999975
0.73	1.731146E+16	85.166667	1.234286E-06	3.494793E-15	3.882661E-15	7.200757E-14	99.914988	2.999975
0.74	1.731106E+16	86.333333	1.234286E-06	3.632764E-15	3.935818E-15	7.398003E-14	99.912671	2.999974
0.75	1.731065E+16	87.500000	1.234286E-06	3.774309E-15	3.988974E-15	7.597913E-14	99.910322	2.999973
0.76	1.731024E+16	88.666667	1.234286E-06	3.919474E-15	4.042128E-15	7.800486E-14	99.907941	2.999973
0.77	1.730982E+16	89.833333	1.234286E-06	4.068304E-15	4.095282E-15	8.005723E-14	99.905526	2.999972
0.78	1.730940E+16	91.000000	1.234286E-06	4.220845E-15	4.148434E-15	8.213624E-14	99.903080	2.999971
0.79	1.730897E+16	92.166667	1.234286E-06	4.377143E-15	4.201584E-15	8.424187E-14	99.900601	2.999970
0.80	1.730853E+16	93.333333	1.234286E-06	4.537243E-15	4.254734E-15	8.637414E-14	99.898089	2.999970
0.81	1.730809E+16	94.500000	1.234286E-06	4.701190E-15	4.307882E-15	8.853304E-14	99.895544	2.999969
0.82	1.730765E+16	95.666667	1.234286E-06	4.869031E-15	4.361029E-15	9.071857E-14	99.892967	2.999968
0.83	1.730719E+16	96.833333	1.234286E-06	5.040810E-15	4.414175E-15	9.293074E-14	99.890358	2.999967
0.84	1.730674E+16	98.000000	1.234286E-06	5.216574E-15	4.467319E-15	9.516953E-14	99.887715	2.999967
0.85	1.730627E+16	99.166667	1.234286E-06	5.396367E-15	4.520461E-15	9.743495E-14	99.885039	2.999966
0.86	1.730580E+16	100.333333	1.234286E-06	5.580236E-15	4.573603E-15	9.972699E-14	99.882331	2.999965
0.87	1.730533E+16	101.500000	1.234286E-06	5.768225E-15	4.626743E-15	1.020457E-13	99.879590	2.999964
0.88	1.730485E+16	102.666667	1.234286E-06	5.960381E-15	4.679881E-15	1.043910E-13	99.876816	2.999963
0.89	1.730436E+16	103.833333	1.234286E-06	6.156749E-15	4.733018E-15	1.067629E-13	99.874009	2.999962
0.90	1.730387E+16	105.000000	1.234286E-06	6.357374E-15	4.786154E-15	1.091614E-13	99.871168	2.999962
0.91	1.730337E+16	106.166667	1.234286E-06	6.562302E-15	4.839288E-15	1.115866E-13	99.868295	2.999961
0.92	1.730287E+16	107.333333	1.234286E-06	6.771579E-15	4.892420E-15	1.140384E-13	99.865388	2.999960
0.93	1.730236E+16	108.500000	1.234286E-06	6.985249E-15	4.945551E-15	1.165168E-13	99.862448	2.999959
0.94	1.730184E+16	109.666667	1.234286E-06	7.203359E-15	4.998680E-15	1.190218E-13	99.859475	2.999958
0.95	1.730132E+16	110.833333	1.234286E-06	7.425954E-15	5.051808E-15	1.215535E-13	99.856469	2.999957
0.96	1.730080E+16	112.000000	1.234286E-06	7.653080E-15	5.104935E-15	1.241118E-13	99.853429	2.999956
0.97	1.730026E+16	113.166667	1.234286E-06	7.884781E-15	5.158059E-15	1.266967E-13	99.850356	2.999955
0.98	1.729973E+16	114.333333	1.234286E-06	8.121104E-15	5.211182E-15	1.293082E-13	99.847250	2.999955
0.99	1.729918E+16	115.500000	1.234286E-06	8.362094E-15	5.264304E-15	1.319463E-13	99.844110	2.999954
1.00	1.729863E+16	116.666667	1.234286E-06	8.607797E-15	5.317424E-15	1.346110E-13	99.840936	2.999953



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi\text{HONO}$ (mol)	$\Phi\text{HNO}_2$ (mol)	$\Phi\text{NO}_2$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732618E+16	1.166667	3.509921E-07	6.697003E-20	4.440337E-17	2.225440E-17	99.999929	3.000000
0.02	1.732616E+16	2.333333	4.963774E-07	2.956200E-19	8.880670E-17	6.676318E-17	99.999833	3.000000
0.03	1.732614E+16	3.500000	6.079349E-07	7.545905E-19	1.332100E-16	1.335263E-16	99.999714	3.000000
0.04	1.732612E+16	4.666667	7.019817E-07	1.500491E-18	1.776132E-16	2.225437E-16	99.999570	3.000000
0.05	1.732609E+16	5.833333	7.848381E-07	2.582617E-18	2.220163E-16	3.338155E-16	99.999402	3.000000
0.06	1.732605E+16	7.000000	8.597455E-07	4.045209E-18	2.664194E-16	4.673414E-16	99.999210	3.000000
0.07	1.732602E+16	8.166667	9.286292E-07	5.928754E-18	3.108224E-16	6.231215E-16	99.998994	3.000000
0.08	1.732598E+16	9.333333	9.927440E-07	8.270796E-18	3.552252E-16	8.011557E-16	99.998753	3.000000
0.09	1.732593E+16	10.500000	1.052961E-06	1.110650E-17	3.996280E-16	1.001444E-15	99.998488	3.000000
0.10	1.732588E+16	11.666667	1.109915E-06	1.446907E-17	4.440306E-16	1.223986E-15	99.998198	3.000000
0.11	1.732582E+16	12.833333	1.164085E-06	1.839000E-17	4.884331E-16	1.468782E-15	99.997884	2.999999
0.12	1.732577E+16	14.000000	1.215843E-06	2.289938E-17	5.328354E-16	1.735832E-15	99.997546	2.999999
0.13	1.732570E+16	15.166667	1.234286E-06	2.803210E-17	5.772376E-16	2.025136E-15	99.997183	2.999999
0.14	1.732564E+16	16.333333	1.234286E-06	3.382626E-17	6.216396E-16	2.336693E-15	99.996796	2.999999
0.15	1.732556E+16	17.500000	1.234286E-06	4.031994E-17	6.660414E-16	2.670504E-15	99.996384	2.999999
0.16	1.732549E+16	18.666667	1.234286E-06	4.755123E-17	7.104431E-16	3.026568E-15	99.995947	2.999999
0.17	1.732541E+16	19.833333	1.234286E-06	5.555820E-17	7.548445E-16	3.404885E-15	99.995486	2.999999
0.18	1.732532E+16	21.000000	1.234286E-06	6.437896E-17	7.992457E-16	3.805456E-15	99.995000	2.999999
0.19	1.732524E+16	22.166667	1.234286E-06	7.405158E-17	8.436467E-16	4.228279E-15	99.994489	2.999999
0.20	1.732514E+16	23.333333	1.234286E-06	8.461414E-17	8.880475E-16	4.673356E-15	99.993954	2.999998
0.21	1.732505E+16	24.500000	1.234286E-06	9.610474E-17	9.324480E-16	5.140685E-15	99.993394	2.999998
0.22	1.732495E+16	25.666667	1.234286E-06	1.085614E-16	9.768483E-16	5.630266E-15	99.992808	2.999998
0.23	1.732484E+16	26.833333	1.234286E-06	1.220224E-16	1.021248E-15	6.142101E-15	99.992198	2.999998
0.24	1.732473E+16	28.000000	1.234286E-06	1.365255E-16	1.065648E-15	6.676187E-15	99.991563	2.999998
0.25	1.732462E+16	29.166667	1.234286E-06	1.521091E-16	1.110048E-15	7.232525E-15	99.990903	2.999997
0.26	1.732450E+16	30.333333	1.234286E-06	1.688111E-16	1.154447E-15	7.811115E-15	99.990218	2.999997
0.27	1.732437E+16	31.500000	1.234286E-06	1.866696E-16	1.198845E-15	8.411957E-15	99.989508	2.999997
0.28	1.732425E+16	32.666667	1.234286E-06	2.057227E-16	1.243244E-15	9.035051E-15	99.988773	2.999997
0.29	1.732411E+16	33.833333	1.234286E-06	2.260085E-16	1.287642E-15	9.680396E-15	99.988013	2.999997
0.30	1.732398E+16	35.000000	1.234286E-06	2.475651E-16	1.332040E-15	1.034799E-14	99.987227	2.999996
0.31	1.732384E+16	36.166667	1.234286E-06	2.704305E-16	1.376438E-15	1.103784E-14	99.986416	2.999996
0.32	1.732369E+16	37.333333	1.234286E-06	2.946428E-16	1.420835E-15	1.174994E-14	99.985580	2.999996
0.33	1.732354E+16	38.500000	1.234286E-06	3.202402E-16	1.465231E-15	1.248428E-14	99.984719	2.999996
0.34	1.732339E+16	39.666667	1.234286E-06	3.472606E-16	1.509628E-15	1.324088E-14	99.983832	2.999995
0.35	1.732323E+16	40.833333	1.234286E-06	3.757421E-16	1.554024E-15	1.401973E-14	99.982920	2.999995
0.36	1.732307E+16	42.000000	1.234286E-06	4.057229E-16	1.598419E-15	1.482083E-14	99.981983	2.999995
0.37	1.732290E+16	43.166667	1.234286E-06	4.372410E-16	1.642815E-15	1.564417E-14	99.981020	2.999994
0.38	1.732273E+16	44.333333	1.234286E-06	4.703345E-16	1.687209E-15	1.648977E-14	99.980031	2.999994
0.39	1.732256E+16	45.500000	1.234286E-06	5.050414E-16	1.731604E-15	1.735762E-14	99.979017	2.999994
0.40	1.732238E+16	46.666667	1.234286E-06	5.413999E-16	1.775997E-15	1.824771E-14	99.977977	2.999994
0.41	1.732219E+16	47.833333	1.234286E-06	5.794480E-16	1.820391E-15	1.916005E-14	99.976912	2.999993
0.42	1.732200E+16	49.000000	1.234286E-06	6.192237E-16	1.864784E-15	2.009464E-14	99.975821	2.999993
0.43	1.732181E+16	50.166667	1.234286E-06	6.607651E-16	1.909176E-15	2.105148E-14	99.974704	2.999993
0.44	1.732161E+16	51.333333	1.234286E-06	7.041104E-16	1.953568E-15	2.203057E-14	99.973562	2.999992
0.45	1.732141E+16	52.500000	1.234286E-06	7.492975E-16	1.997960E-15	2.303190E-14	99.972394	2.999992

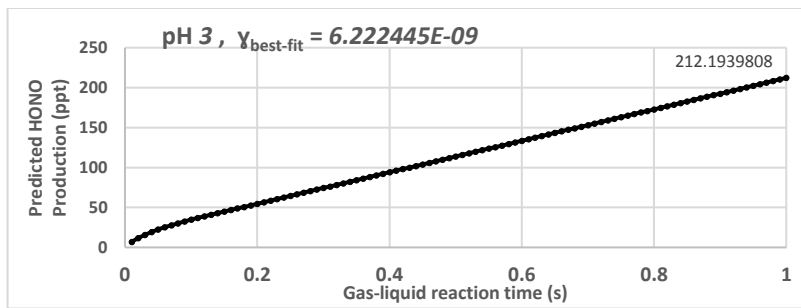
0.46	1.732120E+16	53.666667	1.234286E-06	7.963646E-16	2.042350E-15	2.405548E-14	99.971200	2.999992
0.47	1.732099E+16	54.833333	1.234286E-06	8.453497E-16	2.086741E-15	2.510131E-14	99.969980	2.999991
0.48	1.732077E+16	56.000000	1.234286E-06	8.962909E-16	2.131131E-15	2.616938E-14	99.968734	2.999991
0.49	1.732055E+16	57.166667	1.234286E-06	9.492262E-16	2.175520E-15	2.725970E-14	99.967462	2.999990
0.50	1.732033E+16	58.333333	1.234286E-06	1.004194E-15	2.219909E-15	2.837226E-14	99.966164	2.999990
0.51	1.732010E+16	59.500000	1.234286E-06	1.061232E-15	2.264297E-15	2.950707E-14	99.964840	2.999990
0.52	1.731987E+16	60.666667	1.234286E-06	1.120378E-15	2.308684E-15	3.066413E-14	99.963490	2.999989
0.53	1.731963E+16	61.833333	1.234286E-06	1.181670E-15	2.353071E-15	3.184343E-14	99.962114	2.999989
0.54	1.731938E+16	63.000000	1.234286E-06	1.245147E-15	2.397458E-15	3.304497E-14	99.960712	2.999988
0.55	1.731914E+16	64.166667	1.234286E-06	1.310847E-15	2.441843E-15	3.426876E-14	99.959284	2.999988
0.56	1.731888E+16	65.333333	1.234286E-06	1.378807E-15	2.486228E-15	3.551479E-14	99.957829	2.999988
0.57	1.731863E+16	66.500000	1.234286E-06	1.449065E-15	2.530613E-15	3.678306E-14	99.956348	2.999987
0.58	1.731837E+16	67.666667	1.234286E-06	1.521661E-15	2.574997E-15	3.807358E-14	99.954841	2.999987
0.59	1.731810E+16	68.833333	1.234286E-06	1.596631E-15	2.619380E-15	3.938633E-14	99.953307	2.999986
0.60	1.731783E+16	70.000000	1.234286E-06	1.674014E-15	2.663762E-15	4.072133E-14	99.951747	2.999986
0.61	1.731756E+16	71.166667	1.234286E-06	1.753848E-15	2.708144E-15	4.207857E-14	99.950161	2.999985
0.62	1.731728E+16	72.333333	1.234286E-06	1.836170E-15	2.752525E-15	4.345806E-14	99.948548	2.999985
0.63	1.731699E+16	73.500000	1.234286E-06	1.921020E-15	2.796906E-15	4.485978E-14	99.946908	2.999984
0.64	1.731670E+16	74.666667	1.234286E-06	2.008434E-15	2.841285E-15	4.628374E-14	99.945242	2.999984
0.65	1.731641E+16	75.833333	1.234286E-06	2.098452E-15	2.885664E-15	4.772994E-14	99.943550	2.999983
0.66	1.731611E+16	77.000000	1.234286E-06	2.191111E-15	2.930042E-15	4.919838E-14	99.941830	2.999983
0.67	1.731581E+16	78.166667	1.234286E-06	2.286449E-15	2.974420E-15	5.068906E-14	99.940085	2.999982
0.68	1.731550E+16	79.333333	1.234286E-06	2.384504E-15	3.018796E-15	5.220198E-14	99.938312	2.999982
0.69	1.731519E+16	80.500000	1.234286E-06	2.485314E-15	3.063172E-15	5.373714E-14	99.936512	2.999981
0.70	1.731487E+16	81.666667	1.234286E-06	2.588917E-15	3.107547E-15	5.529453E-14	99.934686	2.999981
0.71	1.731455E+16	82.833333	1.234286E-06	2.695352E-15	3.151922E-15	5.687416E-14	99.932833	2.999980
0.72	1.731423E+16	84.000000	1.234286E-06	2.804656E-15	3.196295E-15	5.847603E-14	99.930953	2.999979
0.73	1.731390E+16	85.166667	1.234286E-06	2.916868E-15	3.240668E-15	6.010013E-14	99.929046	2.999979
0.74	1.731356E+16	86.333333	1.234286E-06	3.032025E-15	3.285039E-15	6.174647E-14	99.927112	2.999978
0.75	1.731322E+16	87.500000	1.234286E-06	3.150165E-15	3.329410E-15	6.341504E-14	99.925151	2.999978
0.76	1.731288E+16	88.666667	1.234286E-06	3.271327E-15	3.373780E-15	6.510585E-14	99.923164	2.999977
0.77	1.731253E+16	89.833333	1.234286E-06	3.395548E-15	3.418150E-15	6.681889E-14	99.921149	2.999976
0.78	1.731218E+16	91.000000	1.234286E-06	3.522867E-15	3.462518E-15	6.855416E-14	99.919106	2.999976
0.79	1.731182E+16	92.166667	1.234286E-06	3.653322E-15	3.506885E-15	7.031167E-14	99.917037	2.999975
0.80	1.731145E+16	93.333333	1.234286E-06	3.786950E-15	3.551252E-15	7.209140E-14	99.914941	2.999975
0.81	1.731109E+16	94.500000	1.234286E-06	3.923789E-15	3.595617E-15	7.389337E-14	99.912817	2.999974
0.82	1.731071E+16	95.666667	1.234286E-06	4.063879E-15	3.639982E-15	7.571757E-14	99.910666	2.999973
0.83	1.731034E+16	96.833333	1.234286E-06	4.207256E-15	3.684346E-15	7.756400E-14	99.908488	2.999973
0.84	1.730995E+16	98.000000	1.234286E-06	4.353958E-15	3.728708E-15	7.943267E-14	99.906282	2.999972
0.85	1.730957E+16	99.166667	1.234286E-06	4.504025E-15	3.773070E-15	8.132356E-14	99.904049	2.999971
0.86	1.730917E+16	100.333333	1.234286E-06	4.657493E-15	3.817431E-15	8.323667E-14	99.901788	2.999971
0.87	1.730878E+16	101.500000	1.234286E-06	4.814401E-15	3.861791E-15	8.517202E-14	99.899500	2.999970
0.88	1.730838E+16	102.666667	1.234286E-06	4.974786E-15	3.906150E-15	8.712960E-14	99.897185	2.999969
0.89	1.730797E+16	103.833333	1.234286E-06	5.138687E-15	3.950507E-15	8.910940E-14	99.894841	2.999969
0.90	1.730756E+16	105.000000	1.234286E-06	5.306142E-15	3.994864E-15	9.111142E-14	99.892471	2.999968
0.91	1.730714E+16	106.166667	1.234286E-06	5.477189E-15	4.039220E-15	9.313568E-14	99.890072	2.999967
0.92	1.730672E+16	107.333333	1.234286E-06	5.651866E-15	4.083574E-15	9.518215E-14	99.887646	2.999967
0.93	1.730630E+16	108.500000	1.234286E-06	5.830210E-15	4.127928E-15	9.725086E-14	99.885192	2.999966
0.94	1.730587E+16	109.666667	1.234286E-06	6.012260E-15	4.172281E-15	9.934178E-14	99.882711	2.999965
0.95	1.730543E+16	110.833333	1.234286E-06	6.198054E-15	4.216632E-15	1.014549E-13	99.880201	2.999964
0.96	1.730500E+16	112.000000	1.234286E-06	6.387630E-15	4.260982E-15	1.035903E-13	99.877664	2.999964
0.97	1.730455E+16	113.166667	1.234286E-06	6.581026E-15	4.305332E-15	1.057479E-13	99.875099	2.999963
0.98	1.730410E+16	114.333333	1.234286E-06	6.778279E-15	4.349680E-15	1.079277E-13	99.872506	2.999962
0.99	1.730365E+16	115.500000	1.234286E-06	6.979428E-15	4.394027E-15	1.101297E-13	99.869885	2.999961
1.00	1.730319E+16	116.666667	1.234286E-06	7.184511E-15	4.438372E-15	1.123540E-13	99.867236	2.999960



$t_{reac}$ (s)	$Z_{collisions}$ (/mol)	$t_{diffusion}$ (s)	$V_{film,diff}$ (L)	$\Phi_{HONO}$ (mol)	$\Phi_{HNO2}$ (mol)	$\Phi_{NO2}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732617E+16	1.166667	3.509920E-07	1.081352E-19	7.169722E-17	3.593373E-17	99.999885	3.000000
0.02	1.732614E+16	2.333333	4.963769E-07	4.773318E-19	1.433943E-16	1.078011E-16	99.999730	3.000000
0.03	1.732611E+16	3.500000	6.079338E-07	1.218422E-18	2.150913E-16	2.156021E-16	99.999537	3.000000
0.04	1.732607E+16	4.666667	7.019799E-07	2.422813E-18	2.867881E-16	3.593366E-16	99.999305	3.000000
0.05	1.732602E+16	5.833333	7.848353E-07	4.170100E-18	3.584847E-16	5.390044E-16	99.999034	3.000000
0.06	1.732597E+16	7.000000	8.597413E-07	6.531720E-18	4.301811E-16	7.546055E-16	99.998724	3.000000
0.07	1.732591E+16	8.166667	9.286235E-07	9.573042E-18	5.018773E-16	1.006140E-15	99.998375	3.000000
0.08	1.732584E+16	9.333333	9.927364E-07	1.335469E-17	5.735732E-16	1.293607E-15	99.997986	2.999999
0.09	1.732577E+16	10.500000	1.052951E-06	1.793345E-17	6.452688E-16	1.617007E-15	99.997558	2.999999
0.10	1.732569E+16	11.666667	1.109903E-06	2.336292E-17	7.169640E-16	1.976339E-15	99.997091	2.999999
0.11	1.732560E+16	12.833333	1.164070E-06	2.969398E-17	7.886589E-16	2.371604E-15	99.996584	2.999999
0.12	1.732550E+16	14.000000	1.215825E-06	3.697517E-17	8.603534E-16	2.802802E-15	99.996038	2.999999
0.13	1.732540E+16	15.166667	1.234286E-06	4.526288E-17	9.320475E-16	3.269931E-15	99.995452	2.999999
0.14	1.732529E+16	16.333333	1.234286E-06	5.461857E-17	1.003741E-15	3.772991E-15	99.994826	2.999999
0.15	1.732518E+16	17.500000	1.234286E-06	6.510376E-17	1.075434E-15	4.311983E-15	99.994161	2.999998
0.16	1.732506E+16	18.666667	1.234286E-06	7.677994E-17	1.147127E-15	4.886907E-15	99.993456	2.999998
0.17	1.732493E+16	19.833333	1.234286E-06	8.970860E-17	1.218819E-15	5.497761E-15	99.992711	2.999998
0.18	1.732479E+16	21.000000	1.234286E-06	1.039512E-16	1.290511E-15	6.144545E-15	99.991927	2.999998
0.19	1.732465E+16	22.166667	1.234286E-06	1.195693E-16	1.362202E-15	6.827259E-15	99.991102	2.999998
0.20	1.732450E+16	23.333333	1.234286E-06	1.366243E-16	1.433892E-15	7.545903E-15	99.990237	2.999997
0.21	1.732434E+16	24.500000	1.234286E-06	1.551778E-16	1.505582E-15	8.300477E-15	99.989333	2.999997
0.22	1.732418E+16	25.666667	1.234286E-06	1.752912E-16	1.577271E-15	9.090979E-15	99.988388	2.999997
0.23	1.732401E+16	26.833333	1.234286E-06	1.970260E-16	1.648960E-15	9.917410E-15	99.987403	2.999997
0.24	1.732383E+16	28.000000	1.234286E-06	2.204438E-16	1.720648E-15	1.077977E-14	99.986378	2.999996
0.25	1.732365E+16	29.166667	1.234286E-06	2.456059E-16	1.792335E-15	1.167806E-14	99.985312	2.999996
0.26	1.732345E+16	30.333333	1.234286E-06	2.725738E-16	1.864021E-15	1.261227E-14	99.984206	2.999996
0.27	1.732326E+16	31.500000	1.234286E-06	3.014092E-16	1.935706E-15	1.358241E-14	99.983059	2.999995
0.28	1.732305E+16	32.666667	1.234286E-06	3.321733E-16	2.007391E-15	1.458848E-14	99.981872	2.999995
0.29	1.732284E+16	33.833333	1.234286E-06	3.649278E-16	2.079074E-15	1.563047E-14	99.980644	2.999995
0.30	1.732262E+16	35.000000	1.234286E-06	3.997340E-16	2.150757E-15	1.670839E-14	99.979376	2.999994
0.31	1.732239E+16	36.166667	1.234286E-06	4.366535E-16	2.222439E-15	1.782223E-14	99.978067	2.999994
0.32	1.732216E+16	37.333333	1.234286E-06	4.757478E-16	2.294120E-15	1.897200E-14	99.976717	2.999993
0.33	1.732192E+16	38.500000	1.234286E-06	5.170782E-16	2.365800E-15	2.015768E-14	99.975326	2.999993
0.34	1.732167E+16	39.666667	1.234286E-06	5.607064E-16	2.437479E-15	2.137930E-14	99.973895	2.999992
0.35	1.732141E+16	40.833333	1.234286E-06	6.066937E-16	2.509157E-15	2.263683E-14	99.972422	2.999992
0.36	1.732115E+16	42.000000	1.234286E-06	6.551016E-16	2.580834E-15	2.393029E-14	99.970908	2.999992
0.37	1.732088E+16	43.166667	1.234286E-06	7.059915E-16	2.652510E-15	2.525966E-14	99.969353	2.999991
0.38	1.732060E+16	44.333333	1.234286E-06	7.594251E-16	2.724185E-15	2.662496E-14	99.967757	2.999991
0.39	1.732032E+16	45.500000	1.234286E-06	8.154636E-16	2.795858E-15	2.802618E-14	99.966120	2.999990
0.40	1.732003E+16	46.666667	1.234286E-06	8.741686E-16	2.867530E-15	2.946331E-14	99.964442	2.999990
0.41	1.731973E+16	47.833333	1.234286E-06	9.356016E-16	2.939202E-15	3.093637E-14	99.962722	2.999989
0.42	1.731943E+16	49.000000	1.234286E-06	9.998239E-16	3.010872E-15	3.244534E-14	99.960960	2.999989
0.43	1.731911E+16	50.166667	1.234286E-06	1.066897E-15	3.082540E-15	3.399022E-14	99.959157	2.999988
0.44	1.731880E+16	51.333333	1.234286E-06	1.136883E-15	3.154208E-15	3.557103E-14	99.957313	2.999987
0.45	1.731847E+16	52.500000	1.234286E-06	1.209842E-15	3.225874E-15	3.718775E-14	99.955426	2.999987

0.46	1.731813E+16	53.666667	1.234286E-06	1.285836E-15	3.297538E-15	3.884038E-14	99.953499	2.999986
0.47	1.731779E+16	54.833333	1.234286E-06	1.364927E-15	3.369202E-15	4.052892E-14	99.951529	2.999986
0.48	1.731744E+16	56.000000	1.234286E-06	1.447176E-15	3.440864E-15	4.225338E-14	99.949517	2.999985
0.49	1.731709E+16	57.166667	1.234286E-06	1.532645E-15	3.512524E-15	4.401375E-14	99.947464	2.999985
0.50	1.731673E+16	58.333333	1.234286E-06	1.621394E-15	3.584183E-15	4.581003E-14	99.945369	2.999984
0.51	1.731636E+16	59.500000	1.234286E-06	1.713486E-15	3.655841E-15	4.764222E-14	99.943231	2.999983
0.52	1.731598E+16	60.666667	1.234286E-06	1.808982E-15	3.727497E-15	4.951032E-14	99.941052	2.999983
0.53	1.731559E+16	61.833333	1.234286E-06	1.907943E-15	3.799151E-15	5.141433E-14	99.938830	2.999982
0.54	1.731520E+16	63.000000	1.234286E-06	2.010431E-15	3.870804E-15	5.335424E-14	99.936566	2.999981
0.55	1.731480E+16	64.166667	1.234286E-06	2.116506E-15	3.942455E-15	5.533006E-14	99.934260	2.999981
0.56	1.731439E+16	65.333333	1.234286E-06	2.226232E-15	4.014105E-15	5.734178E-14	99.931911	2.999980
0.57	1.731398E+16	66.500000	1.234286E-06	2.339668E-15	4.085753E-15	5.938941E-14	99.929520	2.999979
0.58	1.731356E+16	67.666667	1.234286E-06	2.456876E-15	4.157399E-15	6.147294E-14	99.927087	2.999978
0.59	1.731313E+16	68.833333	1.234286E-06	2.577919E-15	4.229043E-15	6.359238E-14	99.924611	2.999978
0.60	1.731269E+16	70.000000	1.234286E-06	2.702856E-15	4.300686E-15	6.574771E-14	99.922092	2.999977
0.61	1.731225E+16	71.166667	1.234286E-06	2.831750E-15	4.372327E-15	6.793895E-14	99.919531	2.999976
0.62	1.731180E+16	72.333333	1.234286E-06	2.964662E-15	4.443966E-15	7.016608E-14	99.916927	2.999975
0.63	1.731134E+16	73.500000	1.234286E-06	3.101654E-15	4.515603E-15	7.242911E-14	99.914280	2.999975
0.64	1.731087E+16	74.666667	1.234286E-06	3.242786E-15	4.587239E-15	7.472803E-14	99.911590	2.999974
0.65	1.731040E+16	75.833333	1.234286E-06	3.388120E-15	4.658872E-15	7.706286E-14	99.908858	2.999973
0.66	1.730992E+16	77.000000	1.234286E-06	3.537718E-15	4.730504E-15	7.943357E-14	99.906082	2.999972
0.67	1.730943E+16	78.166667	1.234286E-06	3.691641E-15	4.802133E-15	8.184018E-14	99.903263	2.999971
0.68	1.730893E+16	79.333333	1.234286E-06	3.849951E-15	4.873761E-15	8.428268E-14	99.900402	2.999970
0.69	1.730843E+16	80.500000	1.234286E-06	4.012708E-15	4.945386E-15	8.676107E-14	99.897497	2.999969
0.70	1.730792E+16	81.666667	1.234286E-06	4.179974E-15	5.017010E-15	8.927535E-14	99.894548	2.999969
0.71	1.730740E+16	82.833333	1.234286E-06	4.351810E-15	5.088631E-15	9.182552E-14	99.891557	2.999968
0.72	1.730688E+16	84.000000	1.234286E-06	4.528279E-15	5.160250E-15	9.441157E-14	99.888522	2.999967
0.73	1.730634E+16	85.166667	1.234286E-06	4.709441E-15	5.231867E-15	9.703351E-14	99.885443	2.999966
0.74	1.730580E+16	86.333333	1.234286E-06	4.895357E-15	5.303482E-15	9.969133E-14	99.882321	2.999965
0.75	1.730525E+16	87.500000	1.234286E-06	5.086089E-15	5.375095E-15	1.023850E-13	99.879156	2.999964
0.76	1.730470E+16	88.666667	1.234286E-06	5.281698E-15	5.446705E-15	1.051146E-13	99.875946	2.999963
0.77	1.730413E+16	89.833333	1.234286E-06	5.482246E-15	5.518313E-15	1.078801E-13	99.872693	2.999962
0.78	1.730356E+16	91.000000	1.234286E-06	5.687794E-15	5.589919E-15	1.106814E-13	99.869397	2.999961
0.79	1.730298E+16	92.166667	1.234286E-06	5.898404E-15	5.661522E-15	1.135187E-13	99.866056	2.999960
0.80	1.730240E+16	93.333333	1.234286E-06	6.114136E-15	5.733123E-15	1.163918E-13	99.862672	2.999959
0.81	1.730180E+16	94.500000	1.234286E-06	6.335052E-15	5.804722E-15	1.193007E-13	99.859243	2.999958
0.82	1.730120E+16	95.666667	1.234286E-06	6.561213E-15	5.876318E-15	1.222456E-13	99.855771	2.999957
0.83	1.730059E+16	96.833333	1.234286E-06	6.792681E-15	5.947912E-15	1.252263E-13	99.852254	2.999956
0.84	1.729998E+16	98.000000	1.234286E-06	7.029517E-15	6.019503E-15	1.282429E-13	99.848694	2.999955
0.85	1.729935E+16	99.166667	1.234286E-06	7.271782E-15	6.091092E-15	1.312953E-13	99.845089	2.999954
0.86	1.729872E+16	100.333333	1.234286E-06	7.519538E-15	6.162678E-15	1.343836E-13	99.841440	2.999953
0.87	1.729808E+16	101.500000	1.234286E-06	7.772846E-15	6.234262E-15	1.375078E-13	99.837746	2.999952
0.88	1.729743E+16	102.666667	1.234286E-06	8.031767E-15	6.305843E-15	1.406679E-13	99.834008	2.999951
0.89	1.729678E+16	103.833333	1.234286E-06	8.296363E-15	6.377421E-15	1.438638E-13	99.830226	2.999949
0.90	1.729611E+16	105.000000	1.234286E-06	8.566694E-15	6.448997E-15	1.470956E-13	99.826399	2.999948
0.91	1.729544E+16	106.166667	1.234286E-06	8.842822E-15	6.520570E-15	1.503632E-13	99.822527	2.999947
0.92	1.729476E+16	107.333333	1.234286E-06	9.124809E-15	6.592140E-15	1.536667E-13	99.818611	2.999946
0.93	1.729408E+16	108.500000	1.234286E-06	9.412716E-15	6.663708E-15	1.570060E-13	99.814650	2.999945
0.94	1.729338E+16	109.666667	1.234286E-06	9.706603E-15	6.735272E-15	1.603812E-13	99.810644	2.999944
0.95	1.729268E+16	110.833333	1.234286E-06	1.000653E-14	6.806834E-15	1.637922E-13	99.806594	2.999942
0.96	1.729197E+16	112.000000	1.234286E-06	1.031257E-14	6.878393E-15	1.672391E-13	99.802498	2.999941
0.97	1.729125E+16	113.166667	1.234286E-06	1.062476E-14	6.949949E-15	1.707219E-13	99.798358	2.999940
0.98	1.729053E+16	114.333333	1.234286E-06	1.094319E-14	7.021502E-15	1.742405E-13	99.794172	2.999939
0.99	1.728980E+16	115.500000	1.234286E-06	1.126790E-14	7.093052E-15	1.777949E-13	99.789941	2.999937
1.00	1.728906E+16	116.666667	1.234286E-06	1.159896E-14	7.164600E-15	1.813852E-13	99.785665	2.999936

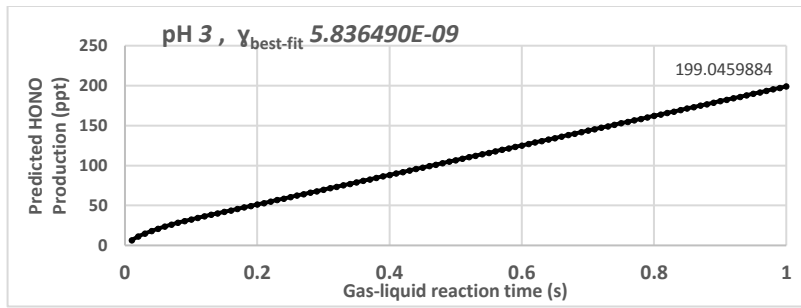
## PAHOKEE PEAT HA STANDARD



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO2}}$ (mol)	$\Phi_{\text{NO2}}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732616E+16	1.166667	3.509917E-07	1.798634E-19	1.192553E-16	5.976922E-17	99.999808	3.000000
0.02	1.732611E+16	2.333333	4.963760E-07	7.939553E-19	2.385103E-16	1.793075E-16	99.999552	3.000000
0.03	1.732606E+16	3.500000	6.079320E-07	2.026626E-18	3.577649E-16	3.586146E-16	99.999231	3.000000
0.04	1.732599E+16	4.666667	7.019767E-07	4.029913E-18	4.770191E-16	5.976902E-16	99.998845	3.000000
0.05	1.732591E+16	5.833333	7.848302E-07	6.936209E-18	5.962727E-16	8.965342E-16	99.998394	3.000000
0.06	1.732582E+16	7.000000	8.597340E-07	1.086434E-17	7.155257E-16	1.255146E-15	99.997878	2.999999
0.07	1.732572E+16	8.166667	9.286135E-07	1.592303E-17	8.347781E-16	1.673525E-15	99.997297	2.999999
0.08	1.732561E+16	9.333333	9.927231E-07	2.221312E-17	9.540297E-16	2.151672E-15	99.996650	2.999999
0.09	1.732549E+16	10.500000	1.052934E-06	2.982906E-17	1.073280E-15	2.689585E-15	99.995938	2.999999
0.10	1.732535E+16	11.666667	1.109882E-06	3.886000E-17	1.192530E-15	3.287264E-15	99.995161	2.999999
0.11	1.732521E+16	12.833333	1.164044E-06	4.939057E-17	1.311779E-15	3.944709E-15	99.994318	2.999999
0.12	1.732505E+16	14.000000	1.215793E-06	6.150154E-17	1.431027E-15	4.661919E-15	99.993409	2.999998
0.13	1.732488E+16	15.166667	1.234286E-06	7.528661E-17	1.550274E-15	5.438893E-15	99.992435	2.999998
0.14	1.732470E+16	16.333333	1.234286E-06	9.084809E-17	1.669519E-15	6.275630E-15	99.991394	2.999998
0.15	1.732451E+16	17.500000	1.234286E-06	1.082882E-16	1.788763E-15	7.172130E-15	99.990288	2.999997
0.16	1.732431E+16	18.666667	1.234286E-06	1.277093E-16	1.908006E-15	8.128392E-15	99.989115	2.999997
0.17	1.732409E+16	19.833333	1.234286E-06	1.492137E-16	2.027247E-15	9.144415E-15	99.987877	2.999997
0.18	1.732386E+16	21.000000	1.234286E-06	1.729035E-16	2.146487E-15	1.022020E-14	99.986572	2.999996
0.19	1.732363E+16	22.166667	1.234286E-06	1.988810E-16	2.265725E-15	1.135574E-14	99.985200	2.999996
0.20	1.732338E+16	23.333333	1.234286E-06	2.272487E-16	2.384962E-15	1.255104E-14	99.983762	2.999996
0.21	1.732312E+16	24.500000	1.234286E-06	2.581085E-16	2.504197E-15	1.380610E-14	99.982257	2.999995
0.22	1.732284E+16	25.666667	1.234286E-06	2.915630E-16	2.623430E-15	1.512091E-14	99.980686	2.999995
0.23	1.732256E+16	26.833333	1.234286E-06	3.277143E-16	2.742661E-15	1.649548E-14	99.979047	2.999994
0.24	1.732227E+16	28.000000	1.234286E-06	3.666646E-16	2.861890E-15	1.792980E-14	99.977342	2.999994
0.25	1.732196E+16	29.166667	1.234286E-06	4.085162E-16	2.981117E-15	1.942388E-14	99.975570	2.999993
0.26	1.732164E+16	30.333333	1.234286E-06	4.533714E-16	3.100342E-15	2.097770E-14	99.973730	2.999993
0.27	1.732131E+16	31.500000	1.234286E-06	5.013324E-16	3.219564E-15	2.259128E-14	99.971823	2.999992
0.28	1.732097E+16	32.666667	1.234286E-06	5.525014E-16	3.338785E-15	2.426460E-14	99.969849	2.999991
0.29	1.732061E+16	33.833333	1.234286E-06	6.069808E-16	3.458003E-15	2.599767E-14	99.967807	2.999991
0.30	1.732025E+16	35.000000	1.234286E-06	6.648726E-16	3.577218E-15	2.779049E-14	99.965697	2.999990
0.31	1.731987E+16	36.166667	1.234286E-06	7.262791E-16	3.696431E-15	2.964305E-14	99.963520	2.999990
0.32	1.731948E+16	37.333333	1.234286E-06	7.913026E-16	3.815642E-15	3.155535E-14	99.961275	2.999989
0.33	1.731908E+16	38.500000	1.234286E-06	8.600453E-16	3.934849E-15	3.352739E-14	99.958962	2.999988
0.34	1.731867E+16	39.666667	1.234286E-06	9.326094E-16	4.054054E-15	3.555917E-14	99.956580	2.999987
0.35	1.731824E+16	40.833333	1.234286E-06	1.009097E-15	4.173256E-15	3.765069E-14	99.954131	2.999987
0.36	1.731781E+16	42.000000	1.234286E-06	1.089611E-15	4.292455E-15	3.980194E-14	99.951613	2.999986
0.37	1.731736E+16	43.166667	1.234286E-06	1.174252E-15	4.411651E-15	4.201293E-14	99.949028	2.999985
0.38	1.731690E+16	44.333333	1.234286E-06	1.263124E-15	4.530844E-15	4.428365E-14	99.946373	2.999984
0.39	1.731643E+16	45.500000	1.234286E-06	1.356328E-15	4.650034E-15	4.661410E-14	99.943650	2.999984
0.40	1.731594E+16	46.666667	1.234286E-06	1.453966E-15	4.769221E-15	4.900428E-14	99.940858	2.999983
0.41	1.731545E+16	47.833333	1.234286E-06	1.556142E-15	4.888404E-15	5.145418E-14	99.937998	2.999982
0.42	1.731494E+16	49.000000	1.234286E-06	1.662956E-15	5.007584E-15	5.396381E-14	99.935068	2.999981
0.43	1.731442E+16	50.166667	1.234286E-06	1.774511E-15	5.126760E-15	5.653316E-14	99.932070	2.999980
0.44	1.731389E+16	51.333333	1.234286E-06	1.890910E-15	5.245933E-15	5.916223E-14	99.929002	2.999979
0.45	1.731335E+16	52.500000	1.234286E-06	2.012254E-15	5.365102E-15	6.185101E-14	99.925865	2.999978

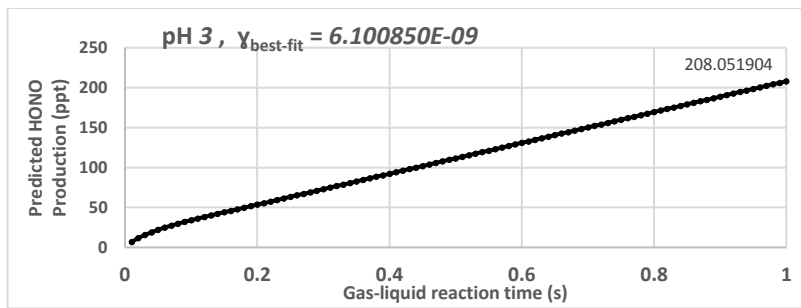
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0.47	1.731222E+16	54.833333	1.234286E-06	2.270187E-15	5.603429E-15	6.740773E-14	99.919383	2.999976
0.48	1.731164E+16	56.000000	1.234286E-06	2.406980E-15	5.722586E-15	7.027565E-14	99.916038	2.999975
0.49	1.731105E+16	57.166667	1.234286E-06	2.549127E-15	5.841740E-15	7.320328E-14	99.912623	2.999974
0.50	1.731045E+16	58.333333	1.234286E-06	2.696730E-15	5.960890E-15	7.619062E-14	99.909138	2.999973
0.51	1.730983E+16	59.500000	1.234286E-06	2.849891E-15	6.080035E-15	7.923766E-14	99.905583	2.999972
0.52	1.730920E+16	60.666667	1.234286E-06	3.008713E-15	6.199176E-15	8.234440E-14	99.901959	2.999971
0.53	1.730856E+16	61.833333	1.234286E-06	3.173296E-15	6.318313E-15	8.551084E-14	99.898264	2.999970
0.54	1.730791E+16	63.000000	1.234286E-06	3.343745E-15	6.437446E-15	8.873697E-14	99.894499	2.999969
0.55	1.730725E+16	64.166667	1.234286E-06	3.520160E-15	6.556574E-15	9.202280E-14	99.890664	2.999968
0.56	1.730657E+16	65.333333	1.234286E-06	3.702643E-15	6.675697E-15	9.536832E-14	99.886758	2.999966
0.57	1.730588E+16	66.500000	1.234286E-06	3.891298E-15	6.794816E-15	9.877352E-14	99.882782	2.999965
0.58	1.730518E+16	67.666667	1.234286E-06	4.086225E-15	6.913931E-15	1.022384E-13	99.878735	2.999964
0.59	1.730447E+16	68.833333	1.234286E-06	4.287526E-15	7.033040E-15	1.057630E-13	99.874618	2.999963
0.60	1.730374E+16	70.000000	1.234286E-06	4.495305E-15	7.152144E-15	1.093472E-13	99.870430	2.999962
0.61	1.730300E+16	71.166667	1.234286E-06	4.709663E-15	7.271244E-15	1.129911E-13	99.866170	2.999960
0.62	1.730225E+16	72.333333	1.234286E-06	4.930701E-15	7.390339E-15	1.166947E-13	99.861840	2.999959
0.63	1.730149E+16	73.500000	1.234286E-06	5.158523E-15	7.509428E-15	1.204580E-13	99.857439	2.999958
0.64	1.730072E+16	74.666667	1.234286E-06	5.393229E-15	7.628512E-15	1.242809E-13	99.852966	2.999956
0.65	1.729993E+16	75.833333	1.234286E-06	5.634923E-15	7.747591E-15	1.281635E-13	99.848422	2.999955
0.66	1.729913E+16	77.000000	1.234286E-06	5.883705E-15	7.866664E-15	1.321058E-13	99.843806	2.999954
0.67	1.729832E+16	78.166667	1.234286E-06	6.139678E-15	7.985732E-15	1.361077E-13	99.839119	2.999952
0.68	1.729749E+16	79.333333	1.234286E-06	6.402944E-15	8.104795E-15	1.401692E-13	99.834360	2.999951
0.69	1.729666E+16	80.500000	1.234286E-06	6.673605E-15	8.223852E-15	1.442904E-13	99.829529	2.999949
0.70	1.729581E+16	81.666667	1.234286E-06	6.951763E-15	8.342903E-15	1.484713E-13	99.824627	2.999948
0.71	1.729494E+16	82.833333	1.234286E-06	7.237520E-15	8.461948E-15	1.527118E-13	99.819652	2.999946
0.72	1.729407E+16	84.000000	1.234286E-06	7.530977E-15	8.580988E-15	1.570119E-13	99.814606	2.999945
0.73	1.729318E+16	85.166667	1.234286E-06	7.832237E-15	8.700021E-15	1.613717E-13	99.809487	2.999943
0.74	1.729228E+16	86.333333	1.234286E-06	8.141401E-15	8.819049E-15	1.657911E-13	99.804296	2.999942
0.75	1.729137E+16	87.500000	1.234286E-06	8.458572E-15	8.938070E-15	1.702701E-13	99.799032	2.999940
0.76	1.729045E+16	88.666667	1.234286E-06	8.783851E-15	9.057085E-15	1.748088E-13	99.793696	2.999938
0.77	1.728951E+16	89.833333	1.234286E-06	9.117341E-15	9.176094E-15	1.794070E-13	99.788287	2.999937
0.78	1.728856E+16	91.000000	1.234286E-06	9.459142E-15	9.295096E-15	1.840649E-13	99.782806	2.999935
0.79	1.728760E+16	92.166667	1.234286E-06	9.809358E-15	9.414092E-15	1.887824E-13	99.777251	2.999934
0.80	1.728662E+16	93.333333	1.234286E-06	1.016809E-14	9.533082E-15	1.935595E-13	99.771624	2.999932
0.81	1.728563E+16	94.500000	1.234286E-06	1.053544E-14	9.652065E-15	1.983963E-13	99.765924	2.999930
0.82	1.728463E+16	95.666667	1.234286E-06	1.091151E-14	9.771041E-15	2.032926E-13	99.760150	2.999928
0.83	1.728362E+16	96.833333	1.234286E-06	1.129640E-14	9.890010E-15	2.082485E-13	99.754303	2.999927
0.84	1.728260E+16	98.000000	1.234286E-06	1.169021E-14	1.000897E-14	2.132640E-13	99.748383	2.999925
0.85	1.728156E+16	99.166667	1.234286E-06	1.209305E-14	1.012793E-14	2.183391E-13	99.742390	2.999923
0.86	1.728051E+16	100.333333	1.234286E-06	1.250501E-14	1.024688E-14	2.234738E-13	99.736323	2.999921
0.87	1.727944E+16	101.500000	1.234286E-06	1.292620E-14	1.036582E-14	2.286680E-13	99.730182	2.999920
0.88	1.727837E+16	102.666667	1.234286E-06	1.335672E-14	1.048475E-14	2.339218E-13	99.723967	2.999918
0.89	1.727728E+16	103.833333	1.234286E-06	1.379668E-14	1.060368E-14	2.392352E-13	99.717679	2.999916
0.90	1.727617E+16	105.000000	1.234286E-06	1.424617E-14	1.072260E-14	2.446082E-13	99.711316	2.999914
0.91	1.727506E+16	106.166667	1.234286E-06	1.470529E-14	1.084151E-14	2.500407E-13	99.704880	2.999912
0.92	1.727393E+16	107.333333	1.234286E-06	1.517415E-14	1.096041E-14	2.555328E-13	99.698369	2.999910
0.93	1.727279E+16	108.500000	1.234286E-06	1.565285E-14	1.107931E-14	2.610844E-13	99.691784	2.999908
0.94	1.727164E+16	109.666667	1.234286E-06	1.614149E-14	1.119820E-14	2.666956E-13	99.685124	2.999906
0.95	1.727047E+16	110.833333	1.234286E-06	1.664017E-14	1.131708E-14	2.723663E-13	99.678390	2.999904
0.96	1.726929E+16	112.000000	1.234286E-06	1.714899E-14	1.143595E-14	2.780966E-13	99.671582	2.999902
0.97	1.726810E+16	113.166667	1.234286E-06	1.766806E-14	1.155482E-14	2.838864E-13	99.664699	2.999900
0.98	1.726689E+16	114.333333	1.234286E-06	1.819748E-14	1.167367E-14	2.897357E-13	99.657740	2.999898
0.99	1.726567E+16	115.500000	1.234286E-06	1.873735E-14	1.179252E-14	2.956446E-13	99.650707	2.999896
1.00	1.726444E+16	116.666667	1.234286E-06	1.928776E-14	1.191136E-14	3.016129E-13	99.643599	2.999894





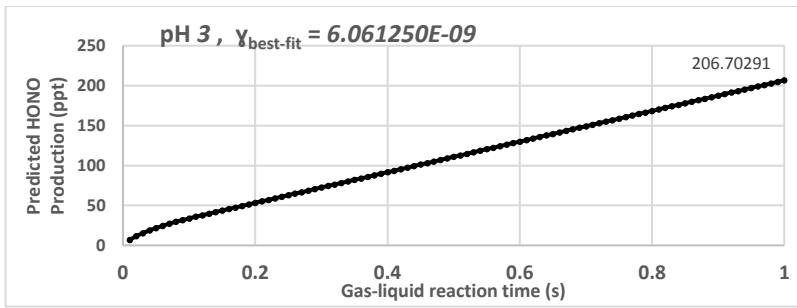
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732616E+16	1.166667	3.509918E-07	1.687071E-19	1.118583E-16	5.606196E-17	99.999820	3.000000
0.02	1.732612E+16	2.333333	4.963761E-07	7.447092E-19	2.237164E-16	1.681857E-16	99.999580	3.000000
0.03	1.732607E+16	3.500000	6.079323E-07	1.900922E-18	3.355742E-16	3.363711E-16	99.999278	3.000000
0.04	1.732600E+16	4.666667	7.019772E-07	3.779953E-18	4.474315E-16	5.606179E-16	99.998916	3.000000
0.05	1.732593E+16	5.833333	7.848310E-07	6.505982E-18	5.592884E-16	8.409258E-16	99.998494	3.000000
0.06	1.732585E+16	7.000000	8.597351E-07	1.019046E-17	6.711448E-16	1.177295E-15	99.998010	2.999999
0.07	1.732575E+16	8.166667	9.286150E-07	1.493538E-17	7.830005E-16	1.569724E-15	99.997465	2.999999
0.08	1.732565E+16	9.333333	9.927252E-07	2.083532E-17	8.948556E-16	2.018213E-15	99.996858	2.999999
0.09	1.732553E+16	10.500000	1.052937E-06	2.797888E-17	1.006710E-15	2.522762E-15	99.996190	2.999999
0.10	1.732540E+16	11.666667	1.109885E-06	3.644966E-17	1.118564E-15	3.083370E-15	99.995461	2.999999
0.11	1.732527E+16	12.833333	1.164048E-06	4.632706E-17	1.230416E-15	3.700037E-15	99.994670	2.999999
0.12	1.732512E+16	14.000000	1.215798E-06	5.768683E-17	1.342268E-15	4.372762E-15	99.993818	2.999998
0.13	1.732496E+16	15.166667	1.234286E-06	7.061687E-17	1.454119E-15	5.101545E-15	99.992904	2.999998
0.14	1.732479E+16	16.333333	1.234286E-06	8.521313E-17	1.565968E-15	5.886385E-15	99.991928	2.999998
0.15	1.732461E+16	17.500000	1.234286E-06	1.015715E-16	1.677817E-15	6.727281E-15	99.990890	2.999998
0.16	1.732442E+16	18.666667	1.234286E-06	1.197880E-16	1.789664E-15	7.624232E-15	99.989791	2.999997
0.17	1.732422E+16	19.833333	1.234286E-06	1.399585E-16	1.901510E-15	8.577238E-15	99.988629	2.999997
0.18	1.732401E+16	21.000000	1.234286E-06	1.621790E-16	2.013355E-15	9.586298E-15	99.987405	2.999997
0.19	1.732379E+16	22.166667	1.234286E-06	1.865453E-16	2.125199E-15	1.065141E-14	99.986118	2.999996
0.20	1.732355E+16	23.333333	1.234286E-06	2.131535E-16	2.237040E-15	1.177258E-14	99.984769	2.999996
0.21	1.732331E+16	24.500000	1.234286E-06	2.420993E-16	2.348881E-15	1.294979E-14	99.983358	2.999995
0.22	1.732305E+16	25.666667	1.234286E-06	2.734788E-16	2.460719E-15	1.418306E-14	99.981884	2.999995
0.23	1.732279E+16	26.833333	1.234286E-06	3.073878E-16	2.572556E-15	1.547238E-14	99.980347	2.999995
0.24	1.732251E+16	28.000000	1.234286E-06	3.439223E-16	2.684392E-15	1.681774E-14	99.978747	2.999994
0.25	1.732222E+16	29.166667	1.234286E-06	3.831782E-16	2.796225E-15	1.821915E-14	99.977085	2.999994
0.26	1.732192E+16	30.333333	1.234286E-06	4.252513E-16	2.908057E-15	1.967661E-14	99.975359	2.999993
0.27	1.732161E+16	31.500000	1.234286E-06	4.702377E-16	3.019886E-15	2.119011E-14	99.973571	2.999993
0.28	1.732129E+16	32.666667	1.234286E-06	5.182331E-16	3.131714E-15	2.275966E-14	99.971719	2.999992
0.29	1.732096E+16	33.833333	1.234286E-06	5.693336E-16	3.243539E-15	2.438525E-14	99.969803	2.999991
0.30	1.732062E+16	35.000000	1.234286E-06	6.236349E-16	3.355363E-15	2.606688E-14	99.967825	2.999991
0.31	1.732026E+16	36.166667	1.234286E-06	6.812330E-16	3.467184E-15	2.780455E-14	99.965782	2.999990
0.32	1.731990E+16	37.333333	1.234286E-06	7.422237E-16	3.579003E-15	2.959825E-14	99.963676	2.999990
0.33	1.731952E+16	38.500000	1.234286E-06	8.067030E-16	3.690819E-15	3.144800E-14	99.961507	2.999989
0.34	1.731913E+16	39.666667	1.234286E-06	8.747667E-16	3.802633E-15	3.335378E-14	99.959273	2.999988
0.35	1.731874E+16	40.833333	1.234286E-06	9.465107E-16	3.914445E-15	3.531559E-14	99.956976	2.999988
0.36	1.731833E+16	42.000000	1.234286E-06	1.022031E-15	4.026253E-15	3.733344E-14	99.954614	2.999987
0.37	1.731791E+16	43.166667	1.234286E-06	1.101423E-15	4.138060E-15	3.940731E-14	99.952189	2.999986
0.38	1.731748E+16	44.333333	1.234286E-06	1.184783E-15	4.249863E-15	4.153722E-14	99.949699	2.999985
0.39	1.731703E+16	45.500000	1.234286E-06	1.272207E-15	4.361664E-15	4.372315E-14	99.947145	2.999985
0.40	1.731658E+16	46.666667	1.234286E-06	1.363790E-15	4.473462E-15	4.596511E-14	99.944526	2.999984
0.41	1.731611E+16	47.833333	1.234286E-06	1.459629E-15	4.585257E-15	4.826309E-14	99.941843	2.999983
0.42	1.731564E+16	49.000000	1.234286E-06	1.559819E-15	4.697049E-15	5.061710E-14	99.939095	2.999982
0.43	1.731515E+16	50.166667	1.234286E-06	1.664457E-15	4.808838E-15	5.302712E-14	99.936282	2.999981
0.44	1.731465E+16	51.333333	1.234286E-06	1.773637E-15	4.920623E-15	5.549316E-14	99.933405	2.999980
0.45	1.731414E+16	52.500000	1.234286E-06	1.887456E-15	5.032406E-15	5.801522E-14	99.930463	2.999980

0.46	1.731362E+16	53.666667	1.234286E-06	2.006010E-15	5.144185E-15	6.059330E-14	99.927455	2.999979
0.47	1.731309E+16	54.833333	1.234286E-06	2.129394E-15	5.255961E-15	6.322738E-14	99.924382	2.999978
0.48	1.731255E+16	56.000000	1.234286E-06	2.257704E-15	5.367733E-15	6.591748E-14	99.921245	2.999977
0.49	1.731199E+16	57.166667	1.234286E-06	2.391036E-15	5.479502E-15	6.866358E-14	99.918041	2.999976
0.50	1.731142E+16	58.333333	1.234286E-06	2.529486E-15	5.591268E-15	7.146569E-14	99.914773	2.999975
0.51	1.731085E+16	59.500000	1.234286E-06	2.673150E-15	5.703029E-15	7.432380E-14	99.911439	2.999974
0.52	1.731026E+16	60.666667	1.234286E-06	2.822123E-15	5.814787E-15	7.723792E-14	99.908039	2.999973
0.53	1.730966E+16	61.833333	1.234286E-06	2.976501E-15	5.926542E-15	8.020803E-14	99.904573	2.999972
0.54	1.730905E+16	63.000000	1.234286E-06	3.136380E-15	6.038292E-15	8.323414E-14	99.901042	2.999971
0.55	1.730842E+16	64.166667	1.234286E-06	3.301856E-15	6.150038E-15	8.631625E-14	99.897444	2.999970
0.56	1.730779E+16	65.333333	1.234286E-06	3.473025E-15	6.261781E-15	8.945435E-14	99.893781	2.999969
0.57	1.730714E+16	66.500000	1.234286E-06	3.649981E-15	6.373519E-15	9.264843E-14	99.890051	2.999967
0.58	1.730648E+16	67.666667	1.234286E-06	3.832822E-15	6.485253E-15	9.589851E-14	99.886255	2.999966
0.59	1.730581E+16	68.833333	1.234286E-06	4.021642E-15	6.596983E-15	9.920457E-14	99.882393	2.999965
0.60	1.730513E+16	70.000000	1.234286E-06	4.216538E-15	6.708709E-15	1.025666E-13	99.878464	2.999964
0.61	1.730444E+16	71.166667	1.234286E-06	4.417605E-15	6.820430E-15	1.059846E-13	99.874469	2.999963
0.62	1.730374E+16	72.333333	1.234286E-06	4.624938E-15	6.932147E-15	1.094586E-13	99.870407	2.999961
0.63	1.730302E+16	73.500000	1.234286E-06	4.838635E-15	7.043860E-15	1.129886E-13	99.866278	2.999960
0.64	1.730230E+16	74.666667	1.234286E-06	5.058789E-15	7.155567E-15	1.165745E-13	99.862083	2.999959
0.65	1.730156E+16	75.833333	1.234286E-06	5.285498E-15	7.267271E-15	1.202164E-13	99.857821	2.999958
0.66	1.730081E+16	77.000000	1.234286E-06	5.518856E-15	7.378969E-15	1.239143E-13	99.853491	2.999956
0.67	1.730004E+16	78.166667	1.234286E-06	5.758959E-15	7.490663E-15	1.276681E-13	99.849094	2.999955
0.68	1.729927E+16	79.333333	1.234286E-06	6.005904E-15	7.602351E-15	1.314779E-13	99.844631	2.999954
0.69	1.729849E+16	80.500000	1.234286E-06	6.259785E-15	7.714035E-15	1.353437E-13	99.840099	2.999952
0.70	1.729769E+16	81.666667	1.234286E-06	6.520698E-15	7.825714E-15	1.392654E-13	99.835501	2.999951
0.71	1.729688E+16	82.833333	1.234286E-06	6.788739E-15	7.937387E-15	1.432431E-13	99.830834	2.999950
0.72	1.729606E+16	84.000000	1.234286E-06	7.064004E-15	8.049056E-15	1.472767E-13	99.826101	2.999948
0.73	1.729523E+16	85.166667	1.234286E-06	7.346588E-15	8.160719E-15	1.513662E-13	99.821299	2.999947
0.74	1.729439E+16	86.333333	1.234286E-06	7.636587E-15	8.272377E-15	1.555117E-13	99.816430	2.999945
0.75	1.729353E+16	87.500000	1.234286E-06	7.934096E-15	8.384029E-15	1.597131E-13	99.811492	2.999944
0.76	1.729266E+16	88.666667	1.234286E-06	8.239212E-15	8.495676E-15	1.639705E-13	99.806487	2.999942
0.77	1.729178E+16	89.833333	1.234286E-06	8.552028E-15	8.607318E-15	1.682838E-13	99.801413	2.999941
0.78	1.729089E+16	91.000000	1.234286E-06	8.872642E-15	8.718954E-15	1.726530E-13	99.796271	2.999939
0.79	1.728999E+16	92.166667	1.234286E-06	9.201149E-15	8.830584E-15	1.770781E-13	99.791061	2.999938
0.80	1.728908E+16	93.333333	1.234286E-06	9.537644E-15	8.942208E-15	1.815592E-13	99.785783	2.999936
0.81	1.728815E+16	94.500000	1.234286E-06	9.882223E-15	9.053827E-15	1.860962E-13	99.780436	2.999935
0.82	1.728721E+16	95.666667	1.234286E-06	1.023498E-14	9.165440E-15	1.906891E-13	99.775020	2.999933
0.83	1.728626E+16	96.833333	1.234286E-06	1.059601E-14	9.277046E-15	1.953379E-13	99.769536	2.999931
0.84	1.728530E+16	98.000000	1.234286E-06	1.096542E-14	9.388647E-15	2.000426E-13	99.763982	2.999930
0.85	1.728432E+16	99.166667	1.234286E-06	1.134329E-14	9.500241E-15	2.048032E-13	99.758360	2.999928
0.86	1.728334E+16	100.333333	1.234286E-06	1.172972E-14	9.611829E-15	2.096197E-13	99.752669	2.999926
0.87	1.728234E+16	101.500000	1.234286E-06	1.212481E-14	9.723411E-15	2.144921E-13	99.746909	2.999925
0.88	1.728133E+16	102.666667	1.234286E-06	1.252865E-14	9.834987E-15	2.194204E-13	99.741079	2.999923
0.89	1.728031E+16	103.833333	1.234286E-06	1.294133E-14	9.946556E-15	2.244046E-13	99.735180	2.999921
0.90	1.727927E+16	105.000000	1.234286E-06	1.336296E-14	1.005812E-14	2.294446E-13	99.729212	2.999919
0.91	1.727823E+16	106.166667	1.234286E-06	1.379363E-14	1.016967E-14	2.345406E-13	99.723174	2.999917
0.92	1.727717E+16	107.333333	1.234286E-06	1.423344E-14	1.028122E-14	2.396924E-13	99.717067	2.999916
0.93	1.727610E+16	108.500000	1.234286E-06	1.468247E-14	1.039277E-14	2.449001E-13	99.710890	2.999914
0.94	1.727502E+16	109.666667	1.234286E-06	1.514083E-14	1.050430E-14	2.501636E-13	99.704643	2.999912
0.95	1.727392E+16	110.833333	1.234286E-06	1.560861E-14	1.061583E-14	2.554830E-13	99.698326	2.999910
0.96	1.727282E+16	112.000000	1.234286E-06	1.608590E-14	1.072735E-14	2.608583E-13	99.691939	2.999908
0.97	1.727170E+16	113.166667	1.234286E-06	1.657281E-14	1.083887E-14	2.662895E-13	99.685482	2.999906
0.98	1.727057E+16	114.333333	1.234286E-06	1.706942E-14	1.095037E-14	2.717764E-13	99.678955	2.999904
0.99	1.726942E+16	115.500000	1.234286E-06	1.757584E-14	1.106188E-14	2.773193E-13	99.672358	2.999902
1.00	1.726827E+16	116.666667	1.234286E-06	1.809215E-14	1.117337E-14	2.829179E-13	99.665690	2.999900



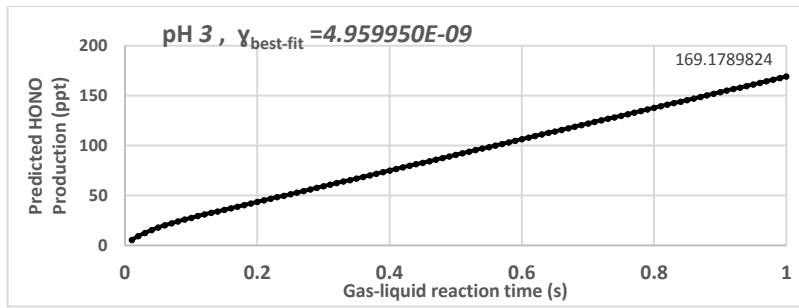
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732616E+16	1.166667	3.509917E-07	1.763486E-19	1.169249E-16	5.860125E-17	99.999812	3.000000
0.02	1.732612E+16	2.333333	4.963760E-07	7.784403E-19	2.338495E-16	1.758036E-16	99.999560	3.000000
0.03	1.732606E+16	3.500000	6.079321E-07	1.987023E-18	3.507737E-16	3.516068E-16	99.999246	3.000000
0.04	1.732599E+16	4.666667	7.019768E-07	3.951163E-18	4.676975E-16	5.860106E-16	99.998867	3.000000
0.05	1.732592E+16	5.833333	7.848305E-07	6.800666E-18	5.846208E-16	8.790148E-16	99.998425	3.000000
0.06	1.732583E+16	7.000000	8.597344E-07	1.065203E-17	7.015435E-16	1.230619E-15	99.997919	2.999999
0.07	1.732573E+16	8.166667	9.286139E-07	1.561187E-17	8.184656E-16	1.640823E-15	99.997350	2.999999
0.08	1.732562E+16	9.333333	9.927238E-07	2.177905E-17	9.353870E-16	2.109626E-15	99.996716	2.999999
0.09	1.732550E+16	10.500000	1.052935E-06	2.924616E-17	1.052307E-15	2.637028E-15	99.996018	2.999999
0.10	1.732537E+16	11.666667	1.109883E-06	3.810063E-17	1.169227E-15	3.223028E-15	99.995256	2.999999
0.11	1.732523E+16	12.833333	1.164045E-06	4.842542E-17	1.286146E-15	3.867625E-15	99.994429	2.999999
0.12	1.732507E+16	14.000000	1.215795E-06	6.029971E-17	1.403064E-15	4.570820E-15	99.993538	2.999998
0.13	1.732491E+16	15.166667	1.234286E-06	7.381541E-17	1.519980E-15	5.332612E-15	99.992583	2.999998
0.14	1.732473E+16	16.333333	1.234286E-06	8.907280E-17	1.636896E-15	6.152999E-15	99.991563	2.999998
0.15	1.732454E+16	17.500000	1.234286E-06	1.061721E-16	1.753810E-15	7.031981E-15	99.990478	2.999998
0.16	1.732434E+16	18.666667	1.234286E-06	1.252137E-16	1.870723E-15	7.969557E-15	99.989328	2.999997
0.17	1.732413E+16	19.833333	1.234286E-06	1.462978E-16	1.987634E-15	8.965726E-15	99.988114	2.999997
0.18	1.732391E+16	21.000000	1.234286E-06	1.695247E-16	2.104544E-15	1.002049E-14	99.986834	2.999996
0.19	1.732368E+16	22.166667	1.234286E-06	1.949947E-16	2.221453E-15	1.113384E-14	99.985489	2.999996
0.20	1.732343E+16	23.333333	1.234286E-06	2.228080E-16	2.338359E-15	1.230579E-14	99.984079	2.999996
0.21	1.732318E+16	24.500000	1.234286E-06	2.530648E-16	2.455265E-15	1.353632E-14	99.982604	2.999995
0.22	1.732291E+16	25.666667	1.234286E-06	2.858656E-16	2.572168E-15	1.482544E-14	99.981063	2.999995
0.23	1.732263E+16	26.833333	1.234286E-06	3.213104E-16	2.689070E-15	1.617315E-14	99.979457	2.999994
0.24	1.732234E+16	28.000000	1.234286E-06	3.594996E-16	2.805969E-15	1.757945E-14	99.977785	2.999994
0.25	1.732204E+16	29.166667	1.234286E-06	4.005335E-16	2.922867E-15	1.904433E-14	99.976047	2.999993
0.26	1.732173E+16	30.333333	1.234286E-06	4.445122E-16	3.039763E-15	2.056779E-14	99.974243	2.999993
0.27	1.732140E+16	31.500000	1.234286E-06	4.915360E-16	3.156656E-15	2.214984E-14	99.972373	2.999992
0.28	1.732107E+16	32.666667	1.234286E-06	5.417052E-16	3.273547E-15	2.379047E-14	99.970438	2.999992
0.29	1.732072E+16	33.833333	1.234286E-06	5.951200E-16	3.390436E-15	2.548968E-14	99.968436	2.999991
0.30	1.732036E+16	35.000000	1.234286E-06	6.518807E-16	3.507323E-15	2.724747E-14	99.966367	2.999990
0.31	1.731999E+16	36.166667	1.234286E-06	7.120874E-16	3.624207E-15	2.906383E-14	99.964233	2.999990
0.32	1.731961E+16	37.333333	1.234286E-06	7.758404E-16	3.741089E-15	3.093877E-14	99.962031	2.999989
0.33	1.731922E+16	38.500000	1.234286E-06	8.432399E-16	3.857968E-15	3.287228E-14	99.959763	2.999988
0.34	1.731882E+16	39.666667	1.234286E-06	9.143861E-16	3.974844E-15	3.486437E-14	99.957429	2.999988
0.35	1.731840E+16	40.833333	1.234286E-06	9.893793E-16	4.091718E-15	3.691502E-14	99.955027	2.999987
0.36	1.731797E+16	42.000000	1.234286E-06	1.068320E-15	4.208589E-15	3.902425E-14	99.952559	2.999986
0.37	1.731753E+16	43.166667	1.234286E-06	1.151307E-15	4.325457E-15	4.119204E-14	99.950023	2.999986
0.38	1.731708E+16	44.333333	1.234286E-06	1.238443E-15	4.442322E-15	4.341839E-14	99.947421	2.999985
0.39	1.731662E+16	45.500000	1.234286E-06	1.329826E-15	4.559184E-15	4.570331E-14	99.944751	2.999984
0.40	1.731614E+16	46.666667	1.234286E-06	1.425557E-15	4.676043E-15	4.804680E-14	99.942014	2.999983
0.41	1.731566E+16	47.833333	1.234286E-06	1.525736E-15	4.792898E-15	5.044884E-14	99.939209	2.999982
0.42	1.731516E+16	49.000000	1.234286E-06	1.630463E-15	4.909751E-15	5.290944E-14	99.936337	2.999981
0.43	1.731465E+16	50.166667	1.234286E-06	1.739839E-15	5.026600E-15	5.542859E-14	99.933397	2.999980
0.44	1.731413E+16	51.333333	1.234286E-06	1.853963E-15	5.143445E-15	5.800630E-14	99.930389	2.999980
0.45	1.731360E+16	52.500000	1.234286E-06	1.972937E-15	5.260287E-15	6.064256E-14	99.927313	2.999979

0.46	1.731305E+16	53.666667	1.234286E-06	2.096859E-15	5.377126E-15	6.333737E-14	99.924170	2.999978
0.47	1.731250E+16	54.833333	1.234286E-06	2.225830E-15	5.493960E-15	6.609072E-14	99.920958	2.999977
0.48	1.731193E+16	56.000000	1.234286E-06	2.359951E-15	5.610791E-15	6.890262E-14	99.917678	2.999976
0.49	1.731135E+16	57.166667	1.234286E-06	2.499321E-15	5.727619E-15	7.177306E-14	99.914330	2.999975
0.50	1.731076E+16	58.333333	1.234286E-06	2.644040E-15	5.844442E-15	7.470205E-14	99.910913	2.999974
0.51	1.731015E+16	59.500000	1.234286E-06	2.794209E-15	5.961261E-15	7.768957E-14	99.907428	2.999973
0.52	1.730954E+16	60.666667	1.234286E-06	2.949928E-15	6.078076E-15	8.073562E-14	99.903874	2.999972
0.53	1.730891E+16	61.833333	1.234286E-06	3.111297E-15	6.194888E-15	8.384021E-14	99.900252	2.999971
0.54	1.730827E+16	63.000000	1.234286E-06	3.278415E-15	6.311694E-15	8.700333E-14	99.896560	2.999969
0.55	1.730762E+16	64.166667	1.234286E-06	3.451384E-15	6.428497E-15	9.022497E-14	99.892800	2.999968
0.56	1.730695E+16	65.333333	1.234286E-06	3.630303E-15	6.545295E-15	9.350514E-14	99.888971	2.999967
0.57	1.730628E+16	66.500000	1.234286E-06	3.815272E-15	6.662089E-15	9.684383E-14	99.885072	2.999966
0.58	1.730559E+16	67.666667	1.234286E-06	4.006391E-15	6.778878E-15	1.002410E-13	99.881104	2.999965
0.59	1.730489E+16	68.833333	1.234286E-06	4.203760E-15	6.895663E-15	1.036968E-13	99.877067	2.999964
0.60	1.730418E+16	70.000000	1.234286E-06	4.407480E-15	7.012443E-15	1.072110E-13	99.872961	2.999962
0.61	1.730346E+16	71.166667	1.234286E-06	4.617651E-15	7.129218E-15	1.107838E-13	99.868785	2.999961
0.62	1.730272E+16	72.333333	1.234286E-06	4.834372E-15	7.245988E-15	1.144150E-13	99.864539	2.999960
0.63	1.730197E+16	73.500000	1.234286E-06	5.057743E-15	7.362754E-15	1.181048E-13	99.860223	2.999958
0.64	1.730121E+16	74.666667	1.234286E-06	5.287865E-15	7.479514E-15	1.218531E-13	99.855838	2.999957
0.65	1.730044E+16	75.833333	1.234286E-06	5.524838E-15	7.596269E-15	1.256598E-13	99.851383	2.999956
0.66	1.729966E+16	77.000000	1.234286E-06	5.768761E-15	7.713020E-15	1.295251E-13	99.846857	2.999954
0.67	1.729886E+16	78.166667	1.234286E-06	6.019734E-15	7.829764E-15	1.334488E-13	99.842262	2.999953
0.68	1.729805E+16	79.333333	1.234286E-06	6.277858E-15	7.946504E-15	1.374311E-13	99.837596	2.999952
0.69	1.729723E+16	80.500000	1.234286E-06	6.543233E-15	8.063238E-15	1.414718E-13	99.832859	2.999950
0.70	1.729640E+16	81.666667	1.234286E-06	6.815958E-15	8.179967E-15	1.455710E-13	99.828053	2.999949
0.71	1.729555E+16	82.833333	1.234286E-06	7.096134E-15	8.296690E-15	1.497287E-13	99.823175	2.999947
0.72	1.729470E+16	84.000000	1.234286E-06	7.383860E-15	8.413407E-15	1.539449E-13	99.818227	2.999946
0.73	1.729383E+16	85.166667	1.234286E-06	7.679236E-15	8.530119E-15	1.582195E-13	99.813208	2.999944
0.74	1.729295E+16	86.333333	1.234286E-06	7.982362E-15	8.646825E-15	1.625526E-13	99.808118	2.999943
0.75	1.729205E+16	87.500000	1.234286E-06	8.293339E-15	8.763525E-15	1.669442E-13	99.802958	2.999941
0.76	1.729114E+16	88.666667	1.234286E-06	8.612266E-15	8.880219E-15	1.713942E-13	99.797726	2.999940
0.77	1.729023E+16	89.833333	1.234286E-06	8.939242E-15	8.996907E-15	1.759027E-13	99.792422	2.999938
0.78	1.728929E+16	91.000000	1.234286E-06	9.274369E-15	9.113589E-15	1.804697E-13	99.787048	2.999937
0.79	1.728835E+16	92.166667	1.234286E-06	9.617745E-15	9.230264E-15	1.850951E-13	99.781602	2.999935
0.80	1.728740E+16	93.333333	1.234286E-06	9.969471E-15	9.346933E-15	1.897789E-13	99.776085	2.999933
0.81	1.728643E+16	94.500000	1.234286E-06	1.032965E-14	9.463596E-15	1.945212E-13	99.770496	2.999932
0.82	1.728545E+16	95.666667	1.234286E-06	1.069837E-14	9.580253E-15	1.993219E-13	99.764835	2.999930
0.83	1.728445E+16	96.833333	1.234286E-06	1.107574E-14	9.696903E-15	2.041811E-13	99.759102	2.999928
0.84	1.728345E+16	98.000000	1.234286E-06	1.146187E-14	9.813546E-15	2.090987E-13	99.753298	2.999926
0.85	1.728243E+16	99.166667	1.234286E-06	1.185684E-14	9.930182E-15	2.140747E-13	99.747421	2.999925
0.86	1.728140E+16	100.333333	1.234286E-06	1.226076E-14	1.004681E-14	2.191091E-13	99.741472	2.999923
0.87	1.728035E+16	101.500000	1.234286E-06	1.267373E-14	1.016343E-14	2.242020E-13	99.735451	2.999921
0.88	1.727930E+16	102.666667	1.234286E-06	1.309584E-14	1.028005E-14	2.293533E-13	99.729358	2.999919
0.89	1.727823E+16	103.833333	1.234286E-06	1.352721E-14	1.039666E-14	2.345629E-13	99.723192	2.999917
0.90	1.727715E+16	105.000000	1.234286E-06	1.396792E-14	1.051326E-14	2.398310E-13	99.716954	2.999916
0.91	1.727606E+16	106.166667	1.234286E-06	1.441808E-14	1.062986E-14	2.451575E-13	99.710643	2.999914
0.92	1.727495E+16	107.333333	1.234286E-06	1.487779E-14	1.074644E-14	2.505424E-13	99.704260	2.999912
0.93	1.727383E+16	108.500000	1.234286E-06	1.534714E-14	1.086302E-14	2.559857E-13	99.697803	2.999910
0.94	1.727270E+16	109.666667	1.234286E-06	1.582624E-14	1.097960E-14	2.614874E-13	99.691274	2.999908
0.95	1.727156E+16	110.833333	1.234286E-06	1.631518E-14	1.109616E-14	2.670474E-13	99.684671	2.999906
0.96	1.727040E+16	112.000000	1.234286E-06	1.681408E-14	1.121272E-14	2.726658E-13	99.677995	2.999904
0.97	1.726923E+16	113.166667	1.234286E-06	1.732301E-14	1.132927E-14	2.783426E-13	99.671246	2.999902
0.98	1.726805E+16	114.333333	1.234286E-06	1.784210E-14	1.144581E-14	2.840778E-13	99.664424	2.999900
0.99	1.726685E+16	115.500000	1.234286E-06	1.837142E-14	1.156234E-14	2.898714E-13	99.657528	2.999898
1.00	1.726565E+16	116.666667	1.234286E-06	1.891110E-14	1.167887E-14	2.957233E-13	99.650559	2.999896



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732616E+16	1.166667	3.509917E-07	1.752039E-19	1.161659E-16	5.822088E-17	99.999813	3.000000
0.02	1.732612E+16	2.333333	4.963760E-07	7.733875E-19	2.323316E-16	1.746625E-16	99.999563	3.000000
0.03	1.732606E+16	3.500000	6.079321E-07	1.974125E-18	3.484969E-16	3.493246E-16	99.999251	3.000000
0.04	1.732600E+16	4.666667	7.019769E-07	3.925516E-18	4.646618E-16	5.822069E-16	99.998875	3.000000
0.05	1.732592E+16	5.833333	7.848306E-07	6.756524E-18	5.808261E-16	8.733092E-16	99.998436	3.000000
0.06	1.732583E+16	7.000000	8.597345E-07	1.058289E-17	6.969899E-16	1.222631E-15	99.997933	2.999999
0.07	1.732573E+16	8.166667	9.286141E-07	1.551054E-17	8.131531E-16	1.630172E-15	99.997367	2.999999
0.08	1.732563E+16	9.333333	9.927240E-07	2.163768E-17	9.293155E-16	2.095933E-15	99.996737	2.999999
0.09	1.732551E+16	10.500000	1.052935E-06	2.905633E-17	1.045477E-15	2.619911E-15	99.996044	2.999999
0.10	1.732537E+16	11.666667	1.109883E-06	3.785332E-17	1.161638E-15	3.202107E-15	99.995286	2.999999
0.11	1.732523E+16	12.833333	1.164046E-06	4.811109E-17	1.277798E-15	3.842521E-15	99.994465	2.999999
0.12	1.732508E+16	14.000000	1.215795E-06	5.990831E-17	1.393957E-15	4.541152E-15	99.993580	2.999998
0.13	1.732491E+16	15.166667	1.234286E-06	7.333628E-17	1.510114E-15	5.297999E-15	99.992631	2.999998
0.14	1.732474E+16	16.333333	1.234286E-06	8.849463E-17	1.626271E-15	6.113061E-15	99.991617	2.999998
0.15	1.732455E+16	17.500000	1.234286E-06	1.054830E-16	1.742426E-15	6.986338E-15	99.990540	2.999998
0.16	1.732435E+16	18.666667	1.234286E-06	1.244010E-16	1.858580E-15	7.917829E-15	99.989397	2.999997
0.17	1.732415E+16	19.833333	1.234286E-06	1.453482E-16	1.974733E-15	8.907533E-15	99.988191	2.999997
0.18	1.732392E+16	21.000000	1.234286E-06	1.684244E-16	2.090884E-15	9.955449E-15	99.986919	2.999996
0.19	1.732369E+16	22.166667	1.234286E-06	1.937290E-16	2.207034E-15	1.106158E-14	99.985583	2.999996
0.20	1.732345E+16	23.333333	1.234286E-06	2.213618E-16	2.323182E-15	1.222591E-14	99.984183	2.999996
0.21	1.732320E+16	24.500000	1.234286E-06	2.514223E-16	2.439329E-15	1.344846E-14	99.982717	2.999995
0.22	1.732293E+16	25.666667	1.234286E-06	2.840101E-16	2.555474E-15	1.472922E-14	99.981186	2.999995
0.23	1.732265E+16	26.833333	1.234286E-06	3.192249E-16	2.671617E-15	1.606818E-14	99.979590	2.999994
0.24	1.732237E+16	28.000000	1.234286E-06	3.571662E-16	2.787758E-15	1.746535E-14	99.977929	2.999994
0.25	1.732207E+16	29.166667	1.234286E-06	3.979337E-16	2.903897E-15	1.892072E-14	99.976202	2.999993
0.26	1.732176E+16	30.333333	1.234286E-06	4.416270E-16	3.020034E-15	2.043430E-14	99.974410	2.999993
0.27	1.732144E+16	31.500000	1.234286E-06	4.883456E-16	3.136169E-15	2.200608E-14	99.972553	2.999992
0.28	1.732110E+16	32.666667	1.234286E-06	5.381892E-16	3.252301E-15	2.363606E-14	99.970630	2.999992
0.29	1.732076E+16	33.833333	1.234286E-06	5.912573E-16	3.368432E-15	2.532424E-14	99.968641	2.999991
0.30	1.732040E+16	35.000000	1.234286E-06	6.476496E-16	3.484560E-15	2.707062E-14	99.966586	2.999990
0.31	1.732003E+16	36.166667	1.234286E-06	7.074655E-16	3.600686E-15	2.887519E-14	99.964465	2.999990
0.32	1.731966E+16	37.333333	1.234286E-06	7.708048E-16	3.716809E-15	3.073797E-14	99.962278	2.999989
0.33	1.731926E+16	38.500000	1.234286E-06	8.377668E-16	3.832930E-15	3.265893E-14	99.960025	2.999989
0.34	1.731886E+16	39.666667	1.234286E-06	9.084513E-16	3.949048E-15	3.463809E-14	99.957705	2.999988
0.35	1.731845E+16	40.833333	1.234286E-06	9.829578E-16	4.065163E-15	3.667543E-14	99.955319	2.999987
0.36	1.731802E+16	42.000000	1.234286E-06	1.061386E-15	4.181276E-15	3.877097E-14	99.952867	2.999986
0.37	1.731759E+16	43.166667	1.234286E-06	1.143835E-15	4.297386E-15	4.092469E-14	99.950348	2.999986
0.38	1.731714E+16	44.333333	1.234286E-06	1.230405E-15	4.413493E-15	4.313660E-14	99.947762	2.999985
0.39	1.731668E+16	45.500000	1.234286E-06	1.321195E-15	4.529596E-15	4.540670E-14	99.945110	2.999984
0.40	1.731621E+16	46.666667	1.234286E-06	1.416304E-15	4.645697E-15	4.773497E-14	99.942390	2.999983
0.41	1.731573E+16	47.833333	1.234286E-06	1.515833E-15	4.761795E-15	5.012142E-14	99.939604	2.999982
0.42	1.731523E+16	49.000000	1.234286E-06	1.619881E-15	4.877889E-15	5.256606E-14	99.936750	2.999982
0.43	1.731473E+16	50.166667	1.234286E-06	1.728547E-15	4.993980E-15	5.506886E-14	99.933829	2.999981
0.44	1.731421E+16	51.333333	1.234286E-06	1.841931E-15	5.110068E-15	5.762984E-14	99.930841	2.999980
0.45	1.731368E+16	52.500000	1.234286E-06	1.960132E-15	5.226152E-15	6.024900E-14	99.927785	2.999979

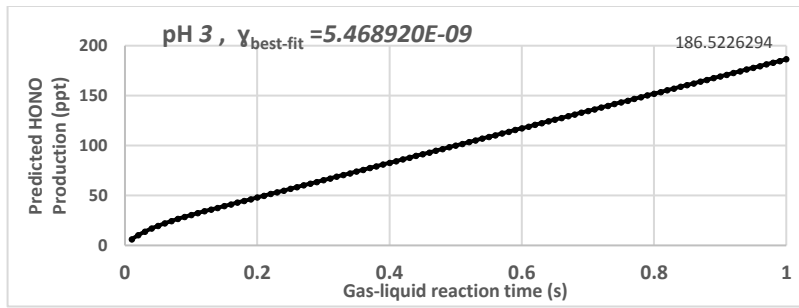
0.46	1.731314E+16	53.666667	1.234286E-06	2.083250E-15	5.342232E-15	6.292632E-14	99.924662	2.999978
0.47	1.731259E+16	54.833333	1.234286E-06	2.211384E-15	5.458309E-15	6.566181E-14	99.921471	2.999977
0.48	1.731202E+16	56.000000	1.234286E-06	2.344635E-15	5.574383E-15	6.845546E-14	99.918212	2.999976
0.49	1.731144E+16	57.166667	1.234286E-06	2.483100E-15	5.690452E-15	7.130728E-14	99.914886	2.999975
0.50	1.731086E+16	58.333333	1.234286E-06	2.626881E-15	5.806518E-15	7.421726E-14	99.911491	2.999974
0.51	1.731026E+16	59.500000	1.234286E-06	2.776075E-15	5.922580E-15	7.718539E-14	99.908029	2.999973
0.52	1.730964E+16	60.666667	1.234286E-06	2.930783E-15	6.038637E-15	8.021168E-14	99.904498	2.999972
0.53	1.730902E+16	61.833333	1.234286E-06	3.091105E-15	6.154691E-15	8.329613E-14	99.900899	2.999971
0.54	1.730839E+16	63.000000	1.234286E-06	3.257139E-15	6.270740E-15	8.643872E-14	99.897232	2.999970
0.55	1.730774E+16	64.166667	1.234286E-06	3.428985E-15	6.386786E-15	8.963947E-14	99.893496	2.999968
0.56	1.730708E+16	65.333333	1.234286E-06	3.606743E-15	6.502827E-15	9.289836E-14	99.889691	2.999967
0.57	1.730641E+16	66.500000	1.234286E-06	3.790512E-15	6.618863E-15	9.621539E-14	99.885818	2.999966
0.58	1.730572E+16	67.666667	1.234286E-06	3.980391E-15	6.734895E-15	9.959056E-14	99.881876	2.999965
0.59	1.730503E+16	68.833333	1.234286E-06	4.176480E-15	6.850923E-15	1.030239E-13	99.877865	2.999964
0.60	1.730432E+16	70.000000	1.234286E-06	4.378878E-15	6.966946E-15	1.065153E-13	99.873785	2.999963
0.61	1.730360E+16	71.166667	1.234286E-06	4.587685E-15	7.082964E-15	1.100649E-13	99.869636	2.999961
0.62	1.730287E+16	72.333333	1.234286E-06	4.803000E-15	7.198977E-15	1.136726E-13	99.865418	2.999960
0.63	1.730213E+16	73.500000	1.234286E-06	5.024922E-15	7.314986E-15	1.173384E-13	99.861130	2.999959
0.64	1.730138E+16	74.666667	1.234286E-06	5.253551E-15	7.430989E-15	1.210624E-13	99.856774	2.999957
0.65	1.730061E+16	75.833333	1.234286E-06	5.488986E-15	7.546988E-15	1.248444E-13	99.852347	2.999956
0.66	1.729983E+16	77.000000	1.234286E-06	5.731326E-15	7.662981E-15	1.286846E-13	99.847851	2.999955
0.67	1.729904E+16	78.166667	1.234286E-06	5.980672E-15	7.778969E-15	1.325829E-13	99.843285	2.999953
0.68	1.729824E+16	79.333333	1.234286E-06	6.237121E-15	7.894952E-15	1.365393E-13	99.838649	2.999952
0.69	1.729742E+16	80.500000	1.234286E-06	6.500774E-15	8.010930E-15	1.405539E-13	99.833944	2.999951
0.70	1.729659E+16	81.666667	1.234286E-06	6.771730E-15	8.126902E-15	1.446265E-13	99.829168	2.999949
0.71	1.729575E+16	82.833333	1.234286E-06	7.050088E-15	8.242869E-15	1.487572E-13	99.824322	2.999948
0.72	1.729490E+16	84.000000	1.234286E-06	7.335947E-15	8.358830E-15	1.529460E-13	99.819406	2.999946
0.73	1.729404E+16	85.166667	1.234286E-06	7.629407E-15	8.474786E-15	1.571929E-13	99.814420	2.999945
0.74	1.729316E+16	86.333333	1.234286E-06	7.930567E-15	8.590736E-15	1.614979E-13	99.809363	2.999943
0.75	1.729227E+16	87.500000	1.234286E-06	8.239527E-15	8.706679E-15	1.658610E-13	99.804236	2.999942
0.76	1.729137E+16	88.666667	1.234286E-06	8.556384E-15	8.822617E-15	1.702822E-13	99.799038	2.999940
0.77	1.729046E+16	89.833333	1.234286E-06	8.881240E-15	8.938550E-15	1.747615E-13	99.793769	2.999939
0.78	1.728953E+16	91.000000	1.234286E-06	9.214193E-15	9.054476E-15	1.792988E-13	99.788430	2.999937
0.79	1.728860E+16	92.166667	1.234286E-06	9.555342E-15	9.170395E-15	1.838942E-13	99.783019	2.999935
0.80	1.728765E+16	93.333333	1.234286E-06	9.904786E-15	9.286309E-15	1.885477E-13	99.777537	2.999934
0.81	1.728668E+16	94.500000	1.234286E-06	1.026263E-14	9.402216E-15	1.932592E-13	99.771985	2.999932
0.82	1.728571E+16	95.666667	1.234286E-06	1.062896E-14	9.518117E-15	1.980288E-13	99.766361	2.999930
0.83	1.728472E+16	96.833333	1.234286E-06	1.100388E-14	9.634012E-15	2.028564E-13	99.760665	2.999929
0.84	1.728372E+16	98.000000	1.234286E-06	1.138750E-14	9.749900E-15	2.077421E-13	99.754898	2.999927
0.85	1.728271E+16	99.166667	1.234286E-06	1.177991E-14	9.865781E-15	2.126859E-13	99.749060	2.999925
0.86	1.728169E+16	100.333333	1.234286E-06	1.218121E-14	9.981656E-15	2.176877E-13	99.743150	2.999923
0.87	1.728065E+16	101.500000	1.234286E-06	1.259150E-14	1.009752E-14	2.227475E-13	99.737168	2.999922
0.88	1.727960E+16	102.666667	1.234286E-06	1.301088E-14	1.021338E-14	2.278654E-13	99.731114	2.999920
0.89	1.727854E+16	103.833333	1.234286E-06	1.343945E-14	1.032924E-14	2.330413E-13	99.724988	2.999918
0.90	1.727747E+16	105.000000	1.234286E-06	1.387730E-14	1.044509E-14	2.382752E-13	99.718790	2.999916
0.91	1.727638E+16	106.166667	1.234286E-06	1.432454E-14	1.056093E-14	2.435672E-13	99.712520	2.999914
0.92	1.727528E+16	107.333333	1.234286E-06	1.478127E-14	1.067676E-14	2.489172E-13	99.706178	2.999912
0.93	1.727417E+16	108.500000	1.234286E-06	1.524758E-14	1.079258E-14	2.543252E-13	99.699763	2.999911
0.94	1.727305E+16	109.666667	1.234286E-06	1.572357E-14	1.090840E-14	2.597912E-13	99.693276	2.999909
0.95	1.727191E+16	110.833333	1.234286E-06	1.620935E-14	1.102421E-14	2.653152E-13	99.686716	2.999907
0.96	1.727076E+16	112.000000	1.234286E-06	1.670500E-14	1.114001E-14	2.708972E-13	99.680084	2.999905
0.97	1.726960E+16	113.166667	1.234286E-06	1.721064E-14	1.125581E-14	2.765372E-13	99.673379	2.999903
0.98	1.726843E+16	114.333333	1.234286E-06	1.772636E-14	1.137160E-14	2.822352E-13	99.666601	2.999901
0.99	1.726724E+16	115.500000	1.234286E-06	1.825225E-14	1.148738E-14	2.879912E-13	99.659749	2.999899
1.00	1.726604E+16	116.666667	1.234286E-06	1.878842E-14	1.160315E-14	2.938051E-13	99.652825	2.999897



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO2}}$ (mol)	$\Phi_{\text{NO2}}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732616E+16	1.166667	3.509918E-07	1.433702E-19	9.505918E-17	4.764244E-17	99.999847	3.000000
0.02	1.732613E+16	2.333333	4.963764E-07	6.328667E-19	1.901182E-16	1.429272E-16	99.999643	3.000000
0.03	1.732608E+16	3.500000	6.079329E-07	1.615436E-18	2.851769E-16	2.858542E-16	99.999387	3.000000
0.04	1.732603E+16	4.666667	7.019783E-07	3.212269E-18	3.802354E-16	4.764232E-16	99.999079	3.000000
0.05	1.732597E+16	5.833333	7.848328E-07	5.528896E-18	4.752935E-16	7.146340E-16	99.998720	3.000000
0.06	1.732590E+16	7.000000	8.597377E-07	8.660032E-18	5.703513E-16	1.000486E-15	99.998309	2.999999
0.07	1.732582E+16	8.166667	9.286186E-07	1.269235E-17	6.654086E-16	1.333980E-15	99.997845	2.999999
0.08	1.732573E+16	9.333333	9.927299E-07	1.770622E-17	7.604654E-16	1.715115E-15	99.997330	2.999999
0.09	1.732563E+16	10.500000	1.052943E-06	2.377693E-17	8.555217E-16	2.143891E-15	99.996763	2.999999
0.10	1.732552E+16	11.666667	1.109893E-06	3.097555E-17	9.505774E-16	2.620307E-15	99.996143	2.999999
0.11	1.732541E+16	12.833333	1.164057E-06	3.936953E-17	1.045633E-15	3.144363E-15	99.995471	2.999999
0.12	1.732528E+16	14.000000	1.215809E-06	4.902326E-17	1.140687E-15	3.716059E-15	99.994747	2.999999
0.13	1.732515E+16	15.166667	1.234286E-06	6.001144E-17	1.235741E-15	4.335394E-15	99.993970	2.999998
0.14	1.732500E+16	16.333333	1.234286E-06	7.241560E-17	1.330794E-15	5.002368E-15	99.993140	2.999998
0.15	1.732485E+16	17.500000	1.234286E-06	8.631728E-17	1.425846E-15	5.716981E-15	99.992258	2.999998
0.16	1.732469E+16	18.666667	1.234286E-06	1.017980E-16	1.520897E-15	6.479231E-15	99.991324	2.999998
0.17	1.732452E+16	19.833333	1.234286E-06	1.189393E-16	1.615947E-15	7.289118E-15	99.990336	2.999997
0.18	1.732434E+16	21.000000	1.234286E-06	1.378227E-16	1.710997E-15	8.146642E-15	99.989296	2.999997
0.19	1.732415E+16	22.166667	1.234286E-06	1.585297E-16	1.806045E-15	9.051802E-15	99.988203	2.999997
0.20	1.732395E+16	23.333333	1.234286E-06	1.811418E-16	1.901092E-15	1.000460E-14	99.987056	2.999996
0.21	1.732374E+16	24.500000	1.234286E-06	2.057407E-16	1.996138E-15	1.100503E-14	99.985857	2.999996
0.22	1.732352E+16	25.666667	1.234286E-06	2.324076E-16	2.091183E-15	1.205309E-14	99.984604	2.999996
0.23	1.732330E+16	26.833333	1.234286E-06	2.612243E-16	2.186227E-15	1.314879E-14	99.983298	2.999995
0.24	1.732306E+16	28.000000	1.234286E-06	2.922722E-16	2.281270E-15	1.429212E-14	99.981939	2.999995
0.25	1.732282E+16	29.166667	1.234286E-06	3.256328E-16	2.376311E-15	1.548308E-14	99.980526	2.999995
0.26	1.732256E+16	30.333333	1.234286E-06	3.613876E-16	2.471351E-15	1.672167E-14	99.979060	2.999994
0.27	1.732230E+16	31.500000	1.234286E-06	3.996182E-16	2.566389E-15	1.800790E-14	99.977540	2.999994
0.28	1.732203E+16	32.666667	1.234286E-06	4.404060E-16	2.661426E-15	1.934175E-14	99.975966	2.999993
0.29	1.732174E+16	33.833333	1.234286E-06	4.838325E-16	2.756462E-15	2.072323E-14	99.974338	2.999993
0.30	1.732145E+16	35.000000	1.234286E-06	5.299793E-16	2.851495E-15	2.215234E-14	99.972656	2.999992
0.31	1.732115E+16	36.166667	1.234286E-06	5.789278E-16	2.946528E-15	2.362907E-14	99.970921	2.999992
0.32	1.732084E+16	37.333333	1.234286E-06	6.307596E-16	3.041558E-15	2.515343E-14	99.969131	2.999991
0.33	1.732052E+16	38.500000	1.234286E-06	6.855561E-16	3.136587E-15	2.672541E-14	99.967287	2.999991
0.34	1.732019E+16	39.666667	1.234286E-06	7.433987E-16	3.231614E-15	2.834502E-14	99.965389	2.999990
0.35	1.731986E+16	40.833333	1.234286E-06	8.043691E-16	3.326640E-15	3.001225E-14	99.963437	2.999989
0.36	1.731951E+16	42.000000	1.234286E-06	8.685487E-16	3.421663E-15	3.172710E-14	99.961430	2.999989
0.37	1.731915E+16	43.166667	1.234286E-06	9.360189E-16	3.516685E-15	3.348957E-14	99.959369	2.999988
0.38	1.731878E+16	44.333333	1.234286E-06	1.006861E-15	3.611704E-15	3.529966E-14	99.957253	2.999988
0.39	1.731841E+16	45.500000	1.234286E-06	1.081157E-15	3.706722E-15	3.715736E-14	99.955082	2.999987
0.40	1.731802E+16	46.666667	1.234286E-06	1.158988E-15	3.801737E-15	3.906268E-14	99.952856	2.999986
0.41	1.731763E+16	47.833333	1.234286E-06	1.240436E-15	3.896751E-15	4.101562E-14	99.950576	2.999986
0.42	1.731722E+16	49.000000	1.234286E-06	1.325581E-15	3.991762E-15	4.301617E-14	99.948241	2.999985
0.43	1.731681E+16	50.166667	1.234286E-06	1.414506E-15	4.086771E-15	4.506433E-14	99.945850	2.999984
0.44	1.731639E+16	51.333333	1.234286E-06	1.507292E-15	4.181778E-15	4.716011E-14	99.943405	2.999983
0.45	1.731595E+16	52.500000	1.234286E-06	1.604021E-15	4.276782E-15	4.930349E-14	99.940904	2.999983

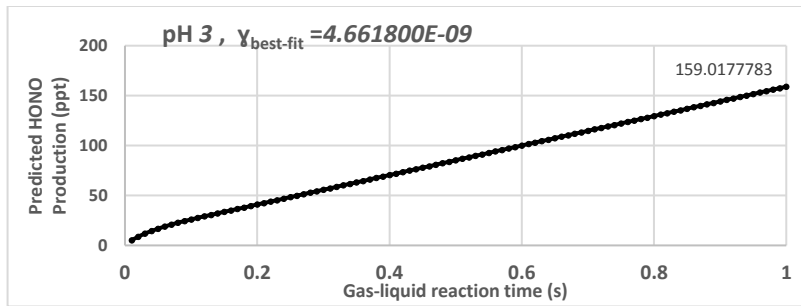
0.46	1.731551E+16	53.666667	1.234286E-06	1.704773E-15	4.371784E-15	5.149448E-14	99.938349	2.999982
0.47	1.731506E+16	54.833333	1.234286E-06	1.809630E-15	4.466784E-15	5.373308E-14	99.935737	2.999981
0.48	1.731459E+16	56.000000	1.234286E-06	1.918674E-15	4.561781E-15	5.601928E-14	99.933070	2.999980
0.49	1.731412E+16	57.166667	1.234286E-06	2.031986E-15	4.656776E-15	5.835309E-14	99.930348	2.999979
0.50	1.731364E+16	58.333333	1.234286E-06	2.149648E-15	4.751768E-15	6.073450E-14	99.927570	2.999979
0.51	1.731315E+16	59.500000	1.234286E-06	2.271741E-15	4.846757E-15	6.316350E-14	99.924737	2.999978
0.52	1.731265E+16	60.666667	1.234286E-06	2.398346E-15	4.941744E-15	6.564011E-14	99.921847	2.999977
0.53	1.731214E+16	61.833333	1.234286E-06	2.529545E-15	5.036728E-15	6.816431E-14	99.918902	2.999976
0.54	1.731162E+16	63.000000	1.234286E-06	2.665419E-15	5.131709E-15	7.073611E-14	99.915901	2.999975
0.55	1.731109E+16	64.166667	1.234286E-06	2.806050E-15	5.226687E-15	7.335551E-14	99.912843	2.999974
0.56	1.731055E+16	65.333333	1.234286E-06	2.951518E-15	5.321663E-15	7.602249E-14	99.909730	2.999973
0.57	1.731000E+16	66.500000	1.234286E-06	3.101906E-15	5.416635E-15	7.873707E-14	99.906560	2.999972
0.58	1.730944E+16	67.666667	1.234286E-06	3.257296E-15	5.511605E-15	8.149923E-14	99.903334	2.999971
0.59	1.730887E+16	68.833333	1.234286E-06	3.417767E-15	5.606571E-15	8.430898E-14	99.900052	2.999970
0.60	1.730830E+16	70.000000	1.234286E-06	3.583402E-15	5.701535E-15	8.716632E-14	99.896713	2.999969
0.61	1.730771E+16	71.166667	1.234286E-06	3.754281E-15	5.796495E-15	9.007123E-14	99.893317	2.999968
0.62	1.730711E+16	72.333333	1.234286E-06	3.930487E-15	5.891452E-15	9.302373E-14	99.889865	2.999967
0.63	1.730650E+16	73.500000	1.234286E-06	4.112101E-15	5.986406E-15	9.602381E-14	99.886356	2.999966
0.64	1.730588E+16	74.666667	1.234286E-06	4.299204E-15	6.081356E-15	9.907146E-14	99.882790	2.999965
0.65	1.730526E+16	75.833333	1.234286E-06	4.491877E-15	6.176303E-15	1.021667E-13	99.879168	2.999964
0.66	1.730462E+16	77.000000	1.234286E-06	4.690202E-15	6.271247E-15	1.053095E-13	99.875488	2.999963
0.67	1.730397E+16	78.166667	1.234286E-06	4.894260E-15	6.366187E-15	1.084999E-13	99.871751	2.999962
0.68	1.730331E+16	79.333333	1.234286E-06	5.104133E-15	6.461124E-15	1.117378E-13	99.867958	2.999961
0.69	1.730265E+16	80.500000	1.234286E-06	5.319901E-15	6.556057E-15	1.150233E-13	99.864107	2.999960
0.70	1.730197E+16	81.666667	1.234286E-06	5.541646E-15	6.650986E-15	1.183564E-13	99.860198	2.999958
0.71	1.730128E+16	82.833333	1.234286E-06	5.769450E-15	6.745912E-15	1.217370E-13	99.856232	2.999957
0.72	1.730058E+16	84.000000	1.234286E-06	6.003394E-15	6.840834E-15	1.251652E-13	99.852209	2.999956
0.73	1.729988E+16	85.166667	1.234286E-06	6.243558E-15	6.935752E-15	1.286409E-13	99.848128	2.999955
0.74	1.729916E+16	86.333333	1.234286E-06	6.490025E-15	7.030667E-15	1.321642E-13	99.843989	2.999953
0.75	1.729843E+16	87.500000	1.234286E-06	6.742875E-15	7.125577E-15	1.357351E-13	99.839793	2.999952
0.76	1.729770E+16	88.666667	1.234286E-06	7.002190E-15	7.220484E-15	1.393535E-13	99.835539	2.999951
0.77	1.729695E+16	89.833333	1.234286E-06	7.268052E-15	7.315386E-15	1.430195E-13	99.831227	2.999950
0.78	1.729619E+16	91.000000	1.234286E-06	7.540541E-15	7.410285E-15	1.467330E-13	99.826857	2.999948
0.79	1.729542E+16	92.166667	1.234286E-06	7.819738E-15	7.505179E-15	1.504940E-13	99.822428	2.999947
0.80	1.729465E+16	93.333333	1.234286E-06	8.105726E-15	7.600069E-15	1.543026E-13	99.817942	2.999946
0.81	1.729386E+16	94.500000	1.234286E-06	8.398584E-15	7.694955E-15	1.581587E-13	99.813397	2.999944
0.82	1.729306E+16	95.666667	1.234286E-06	8.698395E-15	7.789837E-15	1.620624E-13	99.808794	2.999943
0.83	1.729225E+16	96.833333	1.234286E-06	9.005240E-15	7.884714E-15	1.660135E-13	99.804133	2.999942
0.84	1.729144E+16	98.000000	1.234286E-06	9.319200E-15	7.979587E-15	1.700123E-13	99.799413	2.999940
0.85	1.729061E+16	99.166667	1.234286E-06	9.640356E-15	8.074456E-15	1.740585E-13	99.794634	2.999939
0.86	1.728977E+16	100.333333	1.234286E-06	9.968789E-15	8.169320E-15	1.781523E-13	99.789797	2.999937
0.87	1.728892E+16	101.500000	1.234286E-06	1.030458E-14	8.264180E-15	1.822936E-13	99.784901	2.999936
0.88	1.728806E+16	102.666667	1.234286E-06	1.064781E-14	8.359034E-15	1.864824E-13	99.779946	2.999934
0.89	1.728720E+16	103.833333	1.234286E-06	1.099856E-14	8.453885E-15	1.907187E-13	99.774933	2.999933
0.90	1.728632E+16	105.000000	1.234286E-06	1.135692E-14	8.548730E-15	1.950025E-13	99.769860	2.999931
0.91	1.728543E+16	106.166667	1.234286E-06	1.172296E-14	8.643571E-15	1.993339E-13	99.764728	2.999930
0.92	1.728453E+16	107.333333	1.234286E-06	1.209676E-14	8.738407E-15	2.037127E-13	99.759537	2.999928
0.93	1.728362E+16	108.500000	1.234286E-06	1.247841E-14	8.833238E-15	2.081391E-13	99.754287	2.999927
0.94	1.728270E+16	109.666667	1.234286E-06	1.286798E-14	8.928064E-15	2.126130E-13	99.748977	2.999925
0.95	1.728177E+16	110.833333	1.234286E-06	1.326556E-14	9.022885E-15	2.171343E-13	99.743608	2.999924
0.96	1.728083E+16	112.000000	1.234286E-06	1.367123E-14	9.117702E-15	2.217032E-13	99.738179	2.999922
0.97	1.727988E+16	113.166667	1.234286E-06	1.408507E-14	9.212513E-15	2.263195E-13	99.732691	2.999920
0.98	1.727892E+16	114.333333	1.234286E-06	1.450717E-14	9.307318E-15	2.309834E-13	99.727143	2.999919
0.99	1.727794E+16	115.500000	1.234286E-06	1.493759E-14	9.402119E-15	2.356947E-13	99.721535	2.999917
1.00	1.727696E+16	116.666667	1.234286E-06	1.537643E-14	9.496914E-15	2.404535E-13	99.715868	2.999915





$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732616E+16	1.166667	3.509918E-07	1.580823E-19	1.048137E-16	5.253130E-17	99.999831	3.000000
0.02	1.732612E+16	2.333333	4.963762E-07	6.978090E-19	2.096273E-16	1.575938E-16	99.999606	3.000000
0.03	1.732607E+16	3.500000	6.079325E-07	1.781206E-18	3.144405E-16	3.151873E-16	99.999324	3.000000
0.04	1.732602E+16	4.666667	7.019776E-07	3.541899E-18	4.192534E-16	5.253115E-16	99.998985	3.000000
0.05	1.732595E+16	5.833333	7.848318E-07	6.096249E-18	5.240659E-16	7.879664E-16	99.998588	3.000000
0.06	1.732587E+16	7.000000	8.597362E-07	9.548689E-18	6.288779E-16	1.103152E-15	99.998135	2.999999
0.07	1.732578E+16	8.166667	9.286165E-07	1.399478E-17	7.336893E-16	1.470867E-15	99.997624	2.999999
0.08	1.732568E+16	9.333333	9.927272E-07	1.952316E-17	8.385002E-16	1.891112E-15	99.997056	2.999999
0.09	1.732557E+16	10.500000	1.052940E-06	2.621683E-17	9.433105E-16	2.363886E-15	99.996430	2.999999
0.10	1.732545E+16	11.666667	1.109888E-06	3.415414E-17	1.048120E-15	2.889189E-15	99.995747	2.999999
0.11	1.732533E+16	12.833333	1.164052E-06	4.340948E-17	1.152929E-15	3.467020E-15	99.995006	2.999999
0.12	1.732519E+16	14.000000	1.215803E-06	5.405383E-17	1.257737E-15	4.097380E-15	99.994207	2.999999
0.13	1.732504E+16	15.166667	1.234286E-06	6.616957E-17	1.362544E-15	4.780267E-15	99.993351	2.999998
0.14	1.732488E+16	16.333333	1.234286E-06	7.984659E-17	1.467350E-15	5.515680E-15	99.992437	2.999998
0.15	1.732471E+16	17.500000	1.234286E-06	9.517479E-17	1.572155E-15	6.303621E-15	99.991464	2.999998
0.16	1.732453E+16	18.666667	1.234286E-06	1.122441E-16	1.676959E-15	7.144086E-15	99.990434	2.999997
0.17	1.732435E+16	19.833333	1.234286E-06	1.311443E-16	1.781762E-15	8.037077E-15	99.989345	2.999997
0.18	1.732415E+16	21.000000	1.234286E-06	1.519654E-16	1.886564E-15	8.982592E-15	99.988198	2.999997
0.19	1.732394E+16	22.166667	1.234286E-06	1.747972E-16	1.991365E-15	9.980630E-15	99.986992	2.999996
0.20	1.732372E+16	23.333333	1.234286E-06	1.997297E-16	2.096164E-15	1.103119E-14	99.985728	2.999996
0.21	1.732349E+16	24.500000	1.234286E-06	2.268526E-16	2.200962E-15	1.213427E-14	99.984406	2.999996
0.22	1.732325E+16	25.666667	1.234286E-06	2.562560E-16	2.305758E-15	1.328988E-14	99.983025	2.999995
0.23	1.732300E+16	26.833333	1.234286E-06	2.880296E-16	2.410553E-15	1.449800E-14	99.981585	2.999995
0.24	1.732274E+16	28.000000	1.234286E-06	3.222633E-16	2.515347E-15	1.575865E-14	99.980086	2.999994
0.25	1.732247E+16	29.166667	1.234286E-06	3.590470E-16	2.620139E-15	1.707181E-14	99.978528	2.999994
0.26	1.732219E+16	30.333333	1.234286E-06	3.984707E-16	2.724929E-15	1.843749E-14	99.976911	2.999994
0.27	1.732190E+16	31.500000	1.234286E-06	4.406241E-16	2.829718E-15	1.985568E-14	99.975235	2.999993
0.28	1.732160E+16	32.666667	1.234286E-06	4.855971E-16	2.934504E-15	2.132639E-14	99.973500	2.999992
0.29	1.732129E+16	33.833333	1.234286E-06	5.334795E-16	3.039289E-15	2.284962E-14	99.971705	2.999992
0.30	1.732097E+16	35.000000	1.234286E-06	5.843613E-16	3.144072E-15	2.442536E-14	99.969851	2.999991
0.31	1.732064E+16	36.166667	1.234286E-06	6.383323E-16	3.248853E-15	2.605361E-14	99.967937	2.999991
0.32	1.732029E+16	37.333333	1.234286E-06	6.954823E-16	3.353632E-15	2.773437E-14	99.965964	2.999990
0.33	1.731994E+16	38.500000	1.234286E-06	7.559013E-16	3.458409E-15	2.946764E-14	99.963931	2.999990
0.34	1.731958E+16	39.666667	1.234286E-06	8.196789E-16	3.563184E-15	3.125341E-14	99.961838	2.999989
0.35	1.731921E+16	40.833333	1.234286E-06	8.869051E-16	3.667957E-15	3.309170E-14	99.959685	2.999988
0.36	1.731882E+16	42.000000	1.234286E-06	9.576697E-16	3.772727E-15	3.498249E-14	99.957472	2.999988
0.37	1.731843E+16	43.166667	1.234286E-06	1.032063E-15	3.877495E-15	3.692578E-14	99.955200	2.999987
0.38	1.731802E+16	44.333333	1.234286E-06	1.110174E-15	3.982261E-15	3.892157E-14	99.952866	2.999986
0.39	1.731761E+16	45.500000	1.234286E-06	1.192092E-15	4.087024E-15	4.096987E-14	99.950473	2.999986
0.40	1.731718E+16	46.666667	1.234286E-06	1.277909E-15	4.191784E-15	4.307066E-14	99.948019	2.999985
0.41	1.731675E+16	47.833333	1.234286E-06	1.367713E-15	4.296543E-15	4.522396E-14	99.945505	2.999984
0.42	1.731630E+16	49.000000	1.234286E-06	1.461594E-15	4.401298E-15	4.742975E-14	99.942930	2.999983
0.43	1.731585E+16	50.166667	1.234286E-06	1.559643E-15	4.506051E-15	4.968803E-14	99.940295	2.999983
0.44	1.731538E+16	51.333333	1.234286E-06	1.661949E-15	4.610801E-15	5.199881E-14	99.937598	2.999982
0.45	1.731490E+16	52.500000	1.234286E-06	1.768601E-15	4.715548E-15	5.436208E-14	99.934841	2.999981

0.46	1.731441E+16	53.666667	1.234286E-06	1.879690E-15	4.820292E-15	5.677784E-14	99.932023	2.999980
0.47	1.731391E+16	54.833333	1.234286E-06	1.995305E-15	4.925033E-15	5.924608E-14	99.929144	2.999979
0.48	1.731341E+16	56.000000	1.234286E-06	2.115536E-15	5.029772E-15	6.176681E-14	99.926204	2.999978
0.49	1.731289E+16	57.166667	1.234286E-06	2.240473E-15	5.134507E-15	6.434003E-14	99.923202	2.999977
0.50	1.731235E+16	58.333333	1.234286E-06	2.370206E-15	5.239239E-15	6.696572E-14	99.920139	2.999976
0.51	1.731181E+16	59.500000	1.234286E-06	2.504824E-15	5.343968E-15	6.964390E-14	99.917015	2.999975
0.52	1.731126E+16	60.666667	1.234286E-06	2.644418E-15	5.448694E-15	7.237456E-14	99.913829	2.999975
0.53	1.731070E+16	61.833333	1.234286E-06	2.789076E-15	5.553416E-15	7.515769E-14	99.910582	2.999974
0.54	1.731013E+16	63.000000	1.234286E-06	2.938889E-15	5.658135E-15	7.799329E-14	99.907272	2.999973
0.55	1.730954E+16	64.166667	1.234286E-06	3.093947E-15	5.762850E-15	8.088137E-14	99.903901	2.999972
0.56	1.730895E+16	65.333333	1.234286E-06	3.254339E-15	5.867562E-15	8.382192E-14	99.900469	2.999971
0.57	1.730834E+16	66.500000	1.234286E-06	3.420154E-15	5.972271E-15	8.681494E-14	99.896974	2.999969
0.58	1.730772E+16	67.666667	1.234286E-06	3.591484E-15	6.076976E-15	8.986042E-14	99.893417	2.999968
0.59	1.730710E+16	68.833333	1.234286E-06	3.768416E-15	6.181677E-15	9.295836E-14	99.889798	2.999967
0.60	1.730646E+16	70.000000	1.234286E-06	3.951042E-15	6.286374E-15	9.610877E-14	99.886116	2.999966
0.61	1.730581E+16	71.166667	1.234286E-06	4.139451E-15	6.391067E-15	9.931163E-14	99.882373	2.999965
0.62	1.730515E+16	72.333333	1.234286E-06	4.333732E-15	6.495757E-15	1.025669E-13	99.878566	2.999964
0.63	1.730448E+16	73.500000	1.234286E-06	4.533975E-15	6.600442E-15	1.058747E-13	99.874698	2.999963
0.64	1.730380E+16	74.666667	1.234286E-06	4.740270E-15	6.705124E-15	1.092349E-13	99.870766	2.999962
0.65	1.730311E+16	75.833333	1.234286E-06	4.952707E-15	6.809801E-15	1.126476E-13	99.866772	2.999960
0.66	1.730240E+16	77.000000	1.234286E-06	5.171374E-15	6.914475E-15	1.161127E-13	99.862715	2.999959
0.67	1.730169E+16	78.166667	1.234286E-06	5.396363E-15	7.019144E-15	1.196303E-13	99.858595	2.999958
0.68	1.730097E+16	79.333333	1.234286E-06	5.627762E-15	7.123809E-15	1.232003E-13	99.854412	2.999957
0.69	1.730023E+16	80.500000	1.234286E-06	5.865662E-15	7.228469E-15	1.268228E-13	99.850166	2.999955
0.70	1.729948E+16	81.666667	1.234286E-06	6.110151E-15	7.333125E-15	1.304976E-13	99.845857	2.999954
0.71	1.729873E+16	82.833333	1.234286E-06	6.361320E-15	7.437777E-15	1.342250E-13	99.841484	2.999953
0.72	1.729796E+16	84.000000	1.234286E-06	6.619258E-15	7.542424E-15	1.380047E-13	99.837049	2.999951
0.73	1.729718E+16	85.166667	1.234286E-06	6.884054E-15	7.647066E-15	1.418369E-13	99.832549	2.999950
0.74	1.729639E+16	86.333333	1.234286E-06	7.155799E-15	7.751704E-15	1.457215E-13	99.827986	2.999949
0.75	1.729559E+16	87.500000	1.234286E-06	7.434582E-15	7.856337E-15	1.496585E-13	99.823360	2.999947
0.76	1.729477E+16	88.666667	1.234286E-06	7.720493E-15	7.960965E-15	1.536479E-13	99.818669	2.999946
0.77	1.729395E+16	89.833333	1.234286E-06	8.013620E-15	8.065589E-15	1.576898E-13	99.813915	2.999945
0.78	1.729311E+16	91.000000	1.234286E-06	8.314054E-15	8.170207E-15	1.617840E-13	99.809097	2.999943
0.79	1.729227E+16	92.166667	1.234286E-06	8.621885E-15	8.274820E-15	1.659307E-13	99.804214	2.999942
0.80	1.729141E+16	93.333333	1.234286E-06	8.937201E-15	8.379429E-15	1.701298E-13	99.799268	2.999940
0.81	1.729054E+16	94.500000	1.234286E-06	9.260093E-15	8.484032E-15	1.743813E-13	99.794257	2.999939
0.82	1.728966E+16	95.666667	1.234286E-06	9.590649E-15	8.588630E-15	1.786852E-13	99.789182	2.999937
0.83	1.728877E+16	96.833333	1.234286E-06	9.928960E-15	8.693223E-15	1.830415E-13	99.784043	2.999936
0.84	1.728787E+16	98.000000	1.234286E-06	1.027512E-14	8.797810E-15	1.874501E-13	99.778839	2.999934
0.85	1.728696E+16	99.166667	1.234286E-06	1.062920E-14	8.902392E-15	1.919112E-13	99.773571	2.999932
0.86	1.728604E+16	100.333333	1.234286E-06	1.099132E-14	9.006969E-15	1.964247E-13	99.768238	2.999931
0.87	1.728510E+16	101.500000	1.234286E-06	1.136154E-14	9.111540E-15	2.009905E-13	99.762840	2.999929
0.88	1.728415E+16	102.666667	1.234286E-06	1.173997E-14	9.216105E-15	2.056087E-13	99.757377	2.999928
0.89	1.728320E+16	103.833333	1.234286E-06	1.212668E-14	9.320665E-15	2.102793E-13	99.751849	2.999926
0.90	1.728223E+16	105.000000	1.234286E-06	1.252178E-14	9.425219E-15	2.150023E-13	99.746256	2.999924
0.91	1.728125E+16	106.166667	1.234286E-06	1.292535E-14	9.529767E-15	2.197777E-13	99.740599	2.999923
0.92	1.728026E+16	107.333333	1.234286E-06	1.333748E-14	9.634310E-15	2.246054E-13	99.734875	2.999921
0.93	1.727925E+16	108.500000	1.234286E-06	1.375826E-14	9.738846E-15	2.294855E-13	99.729087	2.999919
0.94	1.727824E+16	109.666667	1.234286E-06	1.418777E-14	9.843376E-15	2.344179E-13	99.723233	2.999918
0.95	1.727721E+16	110.833333	1.234286E-06	1.462612E-14	9.947901E-15	2.394027E-13	99.717313	2.999916
0.96	1.727618E+16	112.000000	1.234286E-06	1.507338E-14	1.005242E-14	2.444398E-13	99.711328	2.999914
0.97	1.727513E+16	113.166667	1.234286E-06	1.552965E-14	1.015693E-14	2.495293E-13	99.705278	2.999912
0.98	1.727407E+16	114.333333	1.234286E-06	1.599502E-14	1.026144E-14	2.546712E-13	99.699161	2.999910
0.99	1.727300E+16	115.500000	1.234286E-06	1.646957E-14	1.036594E-14	2.598654E-13	99.692979	2.999909
1.00	1.727191E+16	116.666667	1.234286E-06	1.695339E-14	1.047043E-14	2.651119E-13	99.686730	2.999907



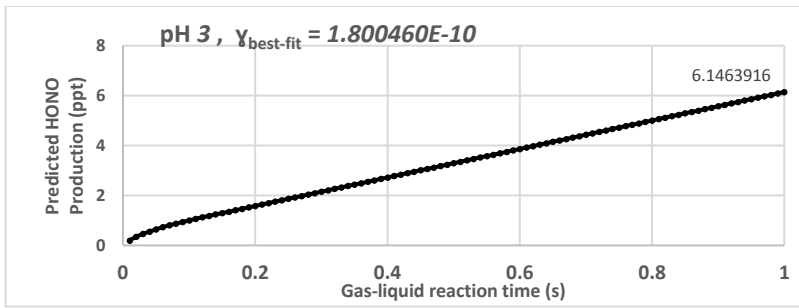
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO2}}$ (mol)	$\Phi_{\text{NO2}}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732617E+16	1.166667	3.509919E-07	1.347520E-19	8.934503E-17	4.477859E-17	99.999856	3.000000
0.02	1.732613E+16	2.333333	4.963765E-07	5.948242E-19	1.786899E-16	1.343357E-16	99.999664	3.000000
0.03	1.732609E+16	3.500000	6.079331E-07	1.518330E-18	2.680346E-16	2.686711E-16	99.999424	3.000000
0.04	1.732604E+16	4.666667	7.019787E-07	3.019175E-18	3.573790E-16	4.477848E-16	99.999135	3.000000
0.05	1.732598E+16	5.833333	7.848334E-07	5.196545E-18	4.467231E-16	6.716765E-16	99.998797	3.000000
0.06	1.732592E+16	7.000000	8.597386E-07	8.139464E-18	5.360668E-16	9.403460E-16	99.998410	3.000000
0.07	1.732584E+16	8.166667	9.286198E-07	1.192939E-17	6.254102E-16	1.253793E-15	99.997975	2.999999
0.08	1.732576E+16	9.333333	9.927315E-07	1.664187E-17	7.147532E-16	1.612018E-15	99.997490	2.999999
0.09	1.732566E+16	10.500000	1.052945E-06	2.234767E-17	8.040957E-16	2.015020E-15	99.996957	2.999999
0.10	1.732556E+16	11.666667	1.109895E-06	2.911356E-17	8.934377E-16	2.462798E-15	99.996375	2.999999
0.11	1.732545E+16	12.833333	1.164060E-06	3.700297E-17	9.827791E-16	2.955353E-15	99.995743	2.999999
0.12	1.732534E+16	14.000000	1.215813E-06	4.607640E-17	1.072120E-15	3.492685E-15	99.995062	2.999999
0.13	1.732521E+16	15.166667	1.234286E-06	5.640406E-17	1.161460E-15	4.074792E-15	99.994332	2.999999
0.14	1.732507E+16	16.333333	1.234286E-06	6.806260E-17	1.250800E-15	4.701674E-15	99.993553	2.999998
0.15	1.732493E+16	17.500000	1.234286E-06	8.112863E-17	1.340138E-15	5.373331E-15	99.992724	2.999998
0.16	1.732478E+16	18.666667	1.234286E-06	9.567880E-17	1.429476E-15	6.089763E-15	99.991845	2.999998
0.17	1.732462E+16	19.833333	1.234286E-06	1.117897E-16	1.518814E-15	6.850969E-15	99.990917	2.999998
0.18	1.732445E+16	21.000000	1.234286E-06	1.295380E-16	1.608150E-15	7.656948E-15	99.989940	2.999997
0.19	1.732427E+16	22.166667	1.234286E-06	1.490003E-16	1.697485E-15	8.507700E-15	99.988912	2.999997
0.20	1.732408E+16	23.333333	1.234286E-06	1.702533E-16	1.786820E-15	9.403225E-15	99.987835	2.999997
0.21	1.732389E+16	24.500000	1.234286E-06	1.933734E-16	1.876154E-15	1.034352E-14	99.986707	2.999996
0.22	1.732368E+16	25.666667	1.234286E-06	2.184375E-16	1.965486E-15	1.132859E-14	99.985530	2.999996
0.23	1.732347E+16	26.833333	1.234286E-06	2.455220E-16	2.054817E-15	1.235843E-14	99.984302	2.999996
0.24	1.732325E+16	28.000000	1.234286E-06	2.747036E-16	2.144148E-15	1.343303E-14	99.983025	2.999995
0.25	1.732302E+16	29.166667	1.234286E-06	3.060590E-16	2.233477E-15	1.455241E-14	99.981697	2.999995
0.26	1.732278E+16	30.333333	1.234286E-06	3.396646E-16	2.322805E-15	1.571656E-14	99.980318	2.999994
0.27	1.732253E+16	31.500000	1.234286E-06	3.755972E-16	2.412132E-15	1.692547E-14	99.978890	2.999994
0.28	1.732228E+16	32.666667	1.234286E-06	4.139333E-16	2.501457E-15	1.817915E-14	99.977410	2.999994
0.29	1.732201E+16	33.833333	1.234286E-06	4.547496E-16	2.590781E-15	1.947760E-14	99.975881	2.999993
0.30	1.732174E+16	35.000000	1.234286E-06	4.981226E-16	2.680104E-15	2.082081E-14	99.974300	2.999993
0.31	1.732146E+16	36.166667	1.234286E-06	5.441290E-16	2.769425E-15	2.220878E-14	99.972669	2.999992
0.32	1.732116E+16	37.333333	1.234286E-06	5.928453E-16	2.858745E-15	2.364152E-14	99.970987	2.999992
0.33	1.732086E+16	38.500000	1.234286E-06	6.443481E-16	2.948063E-15	2.511902E-14	99.969254	2.999991
0.34	1.732055E+16	39.666667	1.234286E-06	6.987141E-16	3.037380E-15	2.664129E-14	99.967470	2.999991
0.35	1.732024E+16	40.833333	1.234286E-06	7.560198E-16	3.126695E-15	2.820831E-14	99.965634	2.999990
0.36	1.731991E+16	42.000000	1.234286E-06	8.163418E-16	3.216009E-15	2.982009E-14	99.963748	2.999990
0.37	1.731957E+16	43.166667	1.234286E-06	8.797568E-16	3.305320E-15	3.147664E-14	99.961811	2.999989
0.38	1.731923E+16	44.333333	1.234286E-06	9.463412E-16	3.394630E-15	3.317794E-14	99.959822	2.999988
0.39	1.731888E+16	45.500000	1.234286E-06	1.016172E-15	3.483939E-15	3.492399E-14	99.957782	2.999988
0.40	1.731851E+16	46.666667	1.234286E-06	1.089325E-15	3.573245E-15	3.671480E-14	99.955690	2.999987
0.41	1.731814E+16	47.833333	1.234286E-06	1.165877E-15	3.662550E-15	3.855037E-14	99.953547	2.999986
0.42	1.731776E+16	49.000000	1.234286E-06	1.245905E-15	3.751852E-15	4.043069E-14	99.951352	2.999986
0.43	1.731737E+16	50.166667	1.234286E-06	1.329485E-15	3.841153E-15	4.235576E-14	99.949105	2.999985
0.44	1.731697E+16	51.333333	1.234286E-06	1.416695E-15	3.930452E-15	4.432558E-14	99.946807	2.999984
0.45	1.731657E+16	52.500000	1.234286E-06	1.507609E-15	4.019749E-15	4.634015E-14	99.944456	2.999984

0.46	1.731615E+16	53.666667	1.234286E-06	1.602306E-15	4.109043E-15	4.839947E-14	99.942054	2.999983
0.47	1.731573E+16	54.833333	1.234286E-06	1.700862E-15	4.198335E-15	5.050354E-14	99.939600	2.999982
0.48	1.731529E+16	56.000000	1.234286E-06	1.803352E-15	4.287626E-15	5.265235E-14	99.937093	2.999981
0.49	1.731485E+16	57.166667	1.234286E-06	1.909854E-15	4.376914E-15	5.484590E-14	99.934534	2.999981
0.50	1.731440E+16	58.333333	1.234286E-06	2.020444E-15	4.466199E-15	5.708420E-14	99.931923	2.999980
0.51	1.731393E+16	59.500000	1.234286E-06	2.135199E-15	4.555483E-15	5.936724E-14	99.929260	2.999979
0.52	1.731346E+16	60.666667	1.234286E-06	2.254196E-15	4.644764E-15	6.169502E-14	99.926544	2.999978
0.53	1.731298E+16	61.833333	1.234286E-06	2.377510E-15	4.734042E-15	6.406754E-14	99.923776	2.999977
0.54	1.731250E+16	63.000000	1.234286E-06	2.505218E-15	4.823319E-15	6.648480E-14	99.920955	2.999977
0.55	1.731200E+16	64.166667	1.234286E-06	2.637398E-15	4.912592E-15	6.894679E-14	99.918081	2.999976
0.56	1.731149E+16	65.333333	1.234286E-06	2.774124E-15	5.001863E-15	7.145351E-14	99.915155	2.999975
0.57	1.731097E+16	66.500000	1.234286E-06	2.915475E-15	5.091132E-15	7.400497E-14	99.912176	2.999974
0.58	1.731045E+16	67.666667	1.234286E-06	3.061526E-15	5.180398E-15	7.660116E-14	99.909144	2.999973
0.59	1.730991E+16	68.833333	1.234286E-06	3.212354E-15	5.269661E-15	7.924207E-14	99.906058	2.999972
0.60	1.730937E+16	70.000000	1.234286E-06	3.368035E-15	5.358921E-15	8.192772E-14	99.902920	2.999971
0.61	1.730882E+16	71.166667	1.234286E-06	3.528646E-15	5.448179E-15	8.465809E-14	99.899729	2.999970
0.62	1.730826E+16	72.333333	1.234286E-06	3.694263E-15	5.537434E-15	8.743318E-14	99.896484	2.999969
0.63	1.730768E+16	73.500000	1.234286E-06	3.864963E-15	5.626685E-15	9.025300E-14	99.893186	2.999968
0.64	1.730710E+16	74.666667	1.234286E-06	4.040823E-15	5.715934E-15	9.311754E-14	99.889834	2.999967
0.65	1.730651E+16	75.833333	1.234286E-06	4.221918E-15	5.805180E-15	9.602679E-14	99.886429	2.999966
0.66	1.730591E+16	77.000000	1.234286E-06	4.408326E-15	5.894423E-15	9.898077E-14	99.882971	2.999965
0.67	1.730531E+16	78.166667	1.234286E-06	4.600122E-15	5.983663E-15	1.019795E-13	99.879459	2.999964
0.68	1.730469E+16	79.333333	1.234286E-06	4.797384E-15	6.072900E-15	1.050229E-13	99.875893	2.999963
0.69	1.730406E+16	80.500000	1.234286E-06	5.000187E-15	6.162134E-15	1.081110E-13	99.872273	2.999962
0.70	1.730342E+16	81.666667	1.234286E-06	5.208608E-15	6.251364E-15	1.112438E-13	99.868599	2.999961
0.71	1.730278E+16	82.833333	1.234286E-06	5.422724E-15	6.340591E-15	1.144213E-13	99.864872	2.999960
0.72	1.730212E+16	84.000000	1.234286E-06	5.642611E-15	6.429815E-15	1.176436E-13	99.861090	2.999959
0.73	1.730146E+16	85.166667	1.234286E-06	5.868345E-15	6.519036E-15	1.209105E-13	99.857254	2.999957
0.74	1.730078E+16	86.333333	1.234286E-06	6.100003E-15	6.608253E-15	1.242221E-13	99.853364	2.999956
0.75	1.730010E+16	87.500000	1.234286E-06	6.337661E-15	6.697467E-15	1.275785E-13	99.849420	2.999955
0.76	1.729941E+16	88.666667	1.234286E-06	6.581395E-15	6.786677E-15	1.309795E-13	99.845422	2.999954
0.77	1.729871E+16	89.833333	1.234286E-06	6.831283E-15	6.875884E-15	1.344252E-13	99.841368	2.999953
0.78	1.729799E+16	91.000000	1.234286E-06	7.087401E-15	6.965087E-15	1.379157E-13	99.837261	2.999951
0.79	1.729727E+16	92.166667	1.234286E-06	7.349824E-15	7.054286E-15	1.414508E-13	99.833099	2.999950
0.80	1.729654E+16	93.333333	1.234286E-06	7.618629E-15	7.143482E-15	1.450306E-13	99.828882	2.999949
0.81	1.729580E+16	94.500000	1.234286E-06	7.893893E-15	7.232674E-15	1.486551E-13	99.824610	2.999948
0.82	1.729505E+16	95.666667	1.234286E-06	8.175692E-15	7.321862E-15	1.523242E-13	99.820284	2.999946
0.83	1.729429E+16	96.833333	1.234286E-06	8.464102E-15	7.411047E-15	1.560381E-13	99.815902	2.999945
0.84	1.729353E+16	98.000000	1.234286E-06	8.759200E-15	7.500227E-15	1.597966E-13	99.811466	2.999944
0.85	1.729275E+16	99.166667	1.234286E-06	9.061062E-15	7.589404E-15	1.635998E-13	99.806974	2.999942
0.86	1.729196E+16	100.333333	1.234286E-06	9.369765E-15	7.678577E-15	1.674477E-13	99.802427	2.999941
0.87	1.729116E+16	101.500000	1.234286E-06	9.685384E-15	7.767745E-15	1.713403E-13	99.797826	2.999940
0.88	1.729036E+16	102.666667	1.234286E-06	1.000800E-14	7.856910E-15	1.752775E-13	99.793168	2.999938
0.89	1.728954E+16	103.833333	1.234286E-06	1.033768E-14	7.946070E-15	1.792594E-13	99.788456	2.999937
0.90	1.728871E+16	105.000000	1.234286E-06	1.067451E-14	8.035227E-15	1.832859E-13	99.783688	2.999936
0.91	1.728788E+16	106.166667	1.234286E-06	1.101855E-14	8.124379E-15	1.873571E-13	99.778864	2.999934
0.92	1.728703E+16	107.333333	1.234286E-06	1.136990E-14	8.213527E-15	1.914730E-13	99.773985	2.999933
0.93	1.728618E+16	108.500000	1.234286E-06	1.172863E-14	8.302670E-15	1.956336E-13	99.769050	2.999931
0.94	1.728531E+16	109.666667	1.234286E-06	1.209480E-14	8.391809E-15	1.998387E-13	99.764059	2.999930
0.95	1.728444E+16	110.833333	1.234286E-06	1.246850E-14	8.480944E-15	2.040886E-13	99.759012	2.999928
0.96	1.728355E+16	112.000000	1.234286E-06	1.284980E-14	8.570074E-15	2.083831E-13	99.753909	2.999927
0.97	1.728266E+16	113.166667	1.234286E-06	1.323879E-14	8.659200E-15	2.127222E-13	99.748751	2.999925
0.98	1.728176E+16	114.333333	1.234286E-06	1.363553E-14	8.748321E-15	2.171060E-13	99.743536	2.999924
0.99	1.728084E+16	115.500000	1.234286E-06	1.404010E-14	8.837438E-15	2.215344E-13	99.738265	2.999922
1.00	1.727992E+16	116.666667	1.234286E-06	1.445258E-14	8.926550E-15	2.260074E-13	99.732938	2.999920

### APPENDIX C1-3: DEPENDENCE OF $\gamma_{\text{best-fit}}$ ON IRRADIANCE

( $[\text{HA}]_{\text{solution}} (\text{pH } 3) = 0.84 \text{ g L}^{-1}$ ;  $[\text{NO}_2]_0 = 36 \text{ ppbv}$ ; 0 to 4 lamps;  $t_{\text{reac}}$  of 1 s)

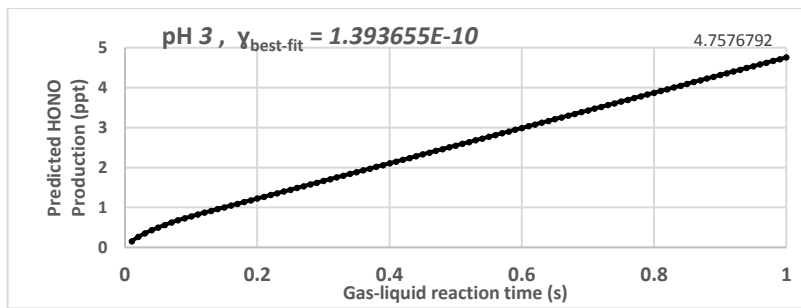
ZERO LAMPS



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732619E+16	1.166667	3.509924E-07	5.204333E-21	3.450649E-18	1.729421E-18	99.999994	3.000000
0.02	1.732619E+16	2.333333	4.963781E-07	2.297304E-20	6.901299E-18	5.188264E-18	99.999987	3.000000
0.03	1.732619E+16	3.500000	6.079365E-07	5.864026E-20	1.035195E-17	1.037653E-17	99.999978	3.000000
0.04	1.732619E+16	4.666667	7.019845E-07	1.166052E-19	1.380260E-17	1.729421E-17	99.999967	3.000000
0.05	1.732618E+16	5.833333	7.848425E-07	2.006987E-19	1.725324E-17	2.594132E-17	99.999954	3.000000
0.06	1.732618E+16	7.000000	8.597517E-07	3.143588E-19	2.070389E-17	3.631784E-17	99.999939	3.000000
0.07	1.732618E+16	8.166667	9.286378E-07	4.607316E-19	2.415454E-17	4.842379E-17	99.999922	3.000000
0.08	1.732617E+16	9.333333	9.927554E-07	6.427349E-19	2.760519E-17	6.225916E-17	99.999903	3.000000
0.09	1.732617E+16	10.500000	1.052976E-06	8.631016E-19	3.105583E-17	7.782394E-17	99.999882	3.000000
0.10	1.732617E+16	11.666667	1.109934E-06	1.124411E-18	3.450648E-17	9.511814E-17	99.999860	3.000000
0.11	1.732616E+16	12.833333	1.164108E-06	1.429112E-18	3.795712E-17	1.141418E-16	99.999836	3.000000
0.12	1.732616E+16	14.000000	1.215871E-06	1.779542E-18	4.140776E-17	1.348948E-16	99.999809	3.000000
0.13	1.732615E+16	15.166667	1.234286E-06	2.178413E-18	4.485841E-17	1.573773E-16	99.999781	3.000000
0.14	1.732615E+16	16.333333	1.234286E-06	2.628687E-18	4.830905E-17	1.815891E-16	99.999751	3.000000
0.15	1.732614E+16	17.500000	1.234286E-06	3.133321E-18	5.175969E-17	2.075304E-16	99.999719	3.000000
0.16	1.732614E+16	18.666667	1.234286E-06	3.695277E-18	5.521033E-17	2.352011E-16	99.999685	3.000000
0.17	1.732613E+16	19.833333	1.234286E-06	4.317515E-18	5.866096E-17	2.646013E-16	99.999649	3.000000
0.18	1.732612E+16	21.000000	1.234286E-06	5.002993E-18	6.211160E-17	2.957308E-16	99.999611	3.000000
0.19	1.732612E+16	22.166667	1.234286E-06	5.754673E-18	6.556224E-17	3.285897E-16	99.999572	3.000000
0.20	1.732611E+16	23.333333	1.234286E-06	6.575514E-18	6.901287E-17	3.631781E-16	99.999530	3.000000
0.21	1.732610E+16	24.500000	1.234286E-06	7.468475E-18	7.246350E-17	3.994959E-16	99.999487	3.000000
0.22	1.732609E+16	25.666667	1.234286E-06	8.436518E-18	7.591413E-17	4.375430E-16	99.999441	3.000000
0.23	1.732609E+16	26.833333	1.234286E-06	9.482600E-18	7.936476E-17	4.773196E-16	99.999394	3.000000
0.24	1.732608E+16	28.000000	1.234286E-06	1.060968E-17	8.281539E-17	5.188256E-16	99.999344	3.000000
0.25	1.732607E+16	29.166667	1.234286E-06	1.182073E-17	8.626601E-17	5.620610E-16	99.999293	3.000000
0.26	1.732606E+16	30.333333	1.234286E-06	1.311869E-17	8.971664E-17	6.070258E-16	99.999240	3.000000
0.27	1.732605E+16	31.500000	1.234286E-06	1.450653E-17	9.316726E-17	6.537201E-16	99.999185	3.000000
0.28	1.732604E+16	32.666667	1.234286E-06	1.598722E-17	9.661788E-17	7.021437E-16	99.999128	3.000000
0.29	1.732603E+16	33.833333	1.234286E-06	1.756370E-17	1.000685E-16	7.522967E-16	99.999068	3.000000
0.30	1.732602E+16	35.000000	1.234286E-06	1.923894E-17	1.035191E-16	8.041791E-16	99.999007	3.000000
0.31	1.732601E+16	36.166667	1.234286E-06	2.101591E-17	1.069697E-16	8.577910E-16	99.998944	3.000000
0.32	1.732600E+16	37.333333	1.234286E-06	2.289755E-17	1.104203E-16	9.131322E-16	99.998879	3.000000
0.33	1.732599E+16	38.500000	1.234286E-06	2.488683E-17	1.138710E-16	9.702028E-16	99.998812	3.000000
0.34	1.732597E+16	39.666667	1.234286E-06	2.698671E-17	1.173216E-16	1.029003E-15	99.998744	3.000000
0.35	1.732596E+16	40.833333	1.234286E-06	2.920015E-17	1.207722E-16	1.089532E-15	99.998673	3.000000
0.36	1.732595E+16	42.000000	1.234286E-06	3.153010E-17	1.242228E-16	1.151791E-15	99.998600	3.000000
0.37	1.732594E+16	43.166667	1.234286E-06	3.397954E-17	1.276734E-16	1.215779E-15	99.998525	3.000000
0.38	1.732592E+16	44.333333	1.234286E-06	3.655141E-17	1.311240E-16	1.281497E-15	99.998448	3.000000
0.39	1.732591E+16	45.500000	1.234286E-06	3.924868E-17	1.345746E-16	1.348944E-15	99.998369	3.000000
0.40	1.732589E+16	46.666667	1.234286E-06	4.207431E-17	1.380251E-16	1.418120E-15	99.998289	3.000000
0.41	1.732588E+16	47.833333	1.234286E-06	4.503126E-17	1.414757E-16	1.489026E-15	99.998206	2.999999
0.42	1.732587E+16	49.000000	1.234286E-06	4.812248E-17	1.449263E-16	1.561661E-15	99.998121	2.999999
0.43	1.732585E+16	50.166667	1.234286E-06	5.135094E-17	1.483769E-16	1.636026E-15	99.998034	2.999999
0.44	1.732584E+16	51.333333	1.234286E-06	5.471960E-17	1.518275E-16	1.712119E-15	99.997945	2.999999
0.45	1.732582E+16	52.500000	1.234286E-06	5.823142E-17	1.552781E-16	1.789943E-15	99.997855	2.999999

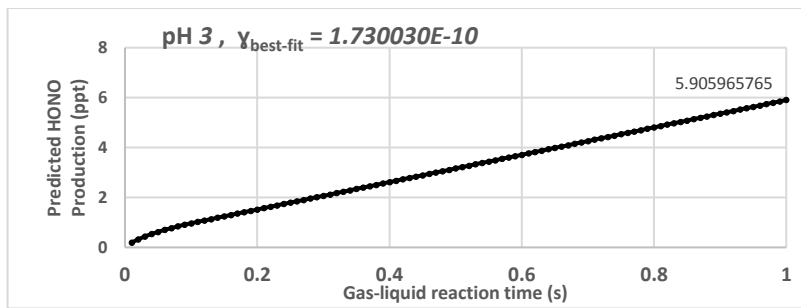
0.46	1.732580E+16	53.666667	1.234286E-06	6.188935E-17	1.587286E-16	1.869495E-15	99.997762	2.999999
0.47	1.732579E+16	54.833333	1.234286E-06	6.569636E-17	1.621792E-16	1.950777E-15	99.997667	2.999999
0.48	1.732577E+16	56.000000	1.234286E-06	6.965540E-17	1.656298E-16	2.033789E-15	99.997570	2.999999
0.49	1.732575E+16	57.166667	1.234286E-06	7.376944E-17	1.690803E-16	2.118530E-15	99.997471	2.999999
0.50	1.732574E+16	58.333333	1.234286E-06	7.804144E-17	1.725309E-16	2.205000E-15	99.997370	2.999999
0.51	1.732572E+16	59.500000	1.234286E-06	8.247435E-17	1.759815E-16	2.293199E-15	99.997267	2.999999
0.52	1.732570E+16	60.666667	1.234286E-06	8.707114E-17	1.794320E-16	2.383128E-15	99.997163	2.999999
0.53	1.732568E+16	61.833333	1.234286E-06	9.183476E-17	1.828826E-16	2.474786E-15	99.997056	2.999999
0.54	1.732566E+16	63.000000	1.234286E-06	9.676817E-17	1.863331E-16	2.568174E-15	99.996947	2.999999
0.55	1.732564E+16	64.166667	1.234286E-06	1.018743E-16	1.897837E-16	2.663291E-15	99.996836	2.999999
0.56	1.732562E+16	65.333333	1.234286E-06	1.071562E-16	1.932342E-16	2.760137E-15	99.996723	2.999999
0.57	1.732560E+16	66.500000	1.234286E-06	1.126168E-16	1.966847E-16	2.858713E-15	99.996607	2.999999
0.58	1.732558E+16	67.666667	1.234286E-06	1.182590E-16	2.001353E-16	2.959018E-15	99.996490	2.999999
0.59	1.732556E+16	68.833333	1.234286E-06	1.240858E-16	2.035858E-16	3.061052E-15	99.996371	2.999999
0.60	1.732554E+16	70.000000	1.234286E-06	1.301001E-16	2.070363E-16	3.164816E-15	99.996250	2.999999
0.61	1.732552E+16	71.166667	1.234286E-06	1.363049E-16	2.104868E-16	3.270309E-15	99.996127	2.999999
0.62	1.732550E+16	72.333333	1.234286E-06	1.427033E-16	2.139373E-16	3.377531E-15	99.996001	2.999999
0.63	1.732548E+16	73.500000	1.234286E-06	1.492980E-16	2.173879E-16	3.486483E-15	99.995874	2.999999
0.64	1.732545E+16	74.666667	1.234286E-06	1.560922E-16	2.208384E-16	3.597164E-15	99.995744	2.999999
0.65	1.732543E+16	75.833333	1.234286E-06	1.630887E-16	2.242889E-16	3.709574E-15	99.995613	2.999999
0.66	1.732541E+16	77.000000	1.234286E-06	1.702905E-16	2.277394E-16	3.823714E-15	99.995479	2.999999
0.67	1.732538E+16	78.166667	1.234286E-06	1.777005E-16	2.311899E-16	3.939583E-15	99.995343	2.999999
0.68	1.732536E+16	79.333333	1.234286E-06	1.853219E-16	2.346403E-16	4.057181E-15	99.995206	2.999999
0.69	1.732534E+16	80.500000	1.234286E-06	1.931573E-16	2.380908E-16	4.176509E-15	99.995066	2.999999
0.70	1.732531E+16	81.666667	1.234286E-06	2.012100E-16	2.415413E-16	4.297566E-15	99.994924	2.999998
0.71	1.732529E+16	82.833333	1.234286E-06	2.094827E-16	2.449918E-16	4.420352E-15	99.994780	2.999998
0.72	1.732526E+16	84.000000	1.234286E-06	2.179786E-16	2.484422E-16	4.544868E-15	99.994634	2.999998
0.73	1.732524E+16	85.166667	1.234286E-06	2.267004E-16	2.518927E-16	4.671113E-15	99.994485	2.999998
0.74	1.732521E+16	86.333333	1.234286E-06	2.356513E-16	2.553432E-16	4.799087E-15	99.994335	2.999998
0.75	1.732518E+16	87.500000	1.234286E-06	2.448340E-16	2.587936E-16	4.928791E-15	99.994183	2.999998
0.76	1.732516E+16	88.666667	1.234286E-06	2.542517E-16	2.622441E-16	5.060224E-15	99.994028	2.999998
0.77	1.732513E+16	89.833333	1.234286E-06	2.639073E-16	2.656945E-16	5.193386E-15	99.993871	2.999998
0.78	1.732510E+16	91.000000	1.234286E-06	2.738037E-16	2.691450E-16	5.328277E-15	99.993713	2.999998
0.79	1.732507E+16	92.166667	1.234286E-06	2.839439E-16	2.725954E-16	5.464898E-15	99.993552	2.999998
0.80	1.732505E+16	93.333333	1.234286E-06	2.943308E-16	2.760458E-16	5.603248E-15	99.993389	2.999998
0.81	1.732502E+16	94.500000	1.234286E-06	3.049674E-16	2.794962E-16	5.743327E-15	99.993224	2.999998
0.82	1.732499E+16	95.666667	1.234286E-06	3.158567E-16	2.829466E-16	5.885136E-15	99.993057	2.999998
0.83	1.732496E+16	96.833333	1.234286E-06	3.270016E-16	2.863971E-16	6.028674E-15	99.992887	2.999998
0.84	1.732493E+16	98.000000	1.234286E-06	3.384051E-16	2.898475E-16	6.173941E-15	99.992716	2.999998
0.85	1.732490E+16	99.166667	1.234286E-06	3.500701E-16	2.932979E-16	6.320937E-15	99.992542	2.999998
0.86	1.732487E+16	100.333333	1.234286E-06	3.619996E-16	2.967483E-16	6.469663E-15	99.992366	2.999998
0.87	1.732484E+16	101.500000	1.234286E-06	3.741966E-16	3.001986E-16	6.620118E-15	99.992188	2.999998
0.88	1.732481E+16	102.666667	1.234286E-06	3.866641E-16	3.036490E-16	6.772302E-15	99.992008	2.999998
0.89	1.732477E+16	103.833333	1.234286E-06	3.994049E-16	3.070994E-16	6.926215E-15	99.991826	2.999998
0.90	1.732474E+16	105.000000	1.234286E-06	4.124220E-16	3.105498E-16	7.081858E-15	99.991642	2.999998
0.91	1.732471E+16	106.166667	1.234286E-06	4.257184E-16	3.140001E-16	7.239230E-15	99.991456	2.999997
0.92	1.732468E+16	107.333333	1.234286E-06	4.392971E-16	3.174505E-16	7.398331E-15	99.991267	2.999997
0.93	1.732464E+16	108.500000	1.234286E-06	4.531610E-16	3.209008E-16	7.559161E-15	99.991076	2.999997
0.94	1.732461E+16	109.666667	1.234286E-06	4.673131E-16	3.243512E-16	7.721721E-15	99.990883	2.999997
0.95	1.732458E+16	110.833333	1.234286E-06	4.817564E-16	3.278015E-16	7.886010E-15	99.990688	2.999997
0.96	1.732454E+16	112.000000	1.234286E-06	4.964937E-16	3.312518E-16	8.052028E-15	99.990491	2.999997
0.97	1.732451E+16	113.166667	1.234286E-06	5.115281E-16	3.347022E-16	8.219775E-15	99.990291	2.999997
0.98	1.732447E+16	114.333333	1.234286E-06	5.268624E-16	3.381525E-16	8.389252E-15	99.990090	2.999997
0.99	1.732444E+16	115.500000	1.234286E-06	5.424998E-16	3.416028E-16	8.560458E-15	99.989886	2.999997
1.00	1.732440E+16	116.666667	1.234286E-06	5.584431E-16	3.450531E-16	8.733393E-15	99.989680	2.999997





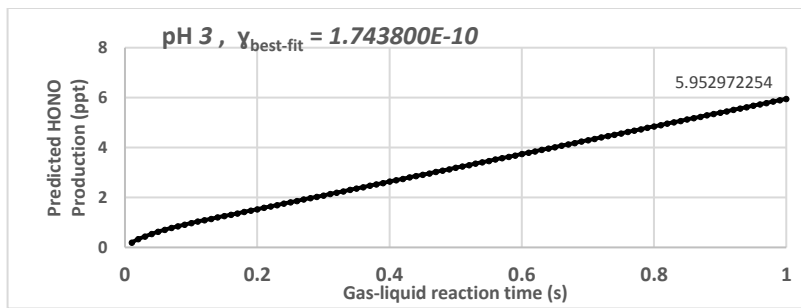
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732619E+16	1.166667	3.509924E-07	4.028440E-21	2.670992E-18	1.338667E-18	99.999996	3.000000
0.02	1.732619E+16	2.333333	4.963781E-07	1.778239E-20	5.341985E-18	4.016002E-18	99.999990	3.000000
0.03	1.732619E+16	3.500000	6.079365E-07	4.539079E-20	8.012977E-18	8.032003E-18	99.999983	3.000000
0.04	1.732619E+16	4.666667	7.019846E-07	9.025886E-20	1.068397E-17	1.338667E-17	99.999974	3.000000
0.05	1.732618E+16	5.833333	7.848425E-07	1.553518E-19	1.335496E-17	2.008001E-17	99.999964	3.000000
0.06	1.732618E+16	7.000000	8.597518E-07	2.433310E-19	1.602595E-17	2.811201E-17	99.999952	3.000000
0.07	1.732618E+16	8.166667	9.286380E-07	3.566316E-19	1.869694E-17	3.748268E-17	99.999939	3.000000
0.08	1.732618E+16	9.333333	9.927556E-07	4.975122E-19	2.136793E-17	4.819201E-17	99.999925	3.000000
0.09	1.732618E+16	10.500000	1.052976E-06	6.680881E-19	2.403892E-17	6.024001E-17	99.999909	3.000000
0.10	1.732617E+16	11.666667	1.109934E-06	8.703560E-19	2.670991E-17	7.362668E-17	99.999892	3.000000
0.11	1.732617E+16	12.833333	1.164109E-06	1.106211E-18	2.938090E-17	8.835201E-17	99.999873	3.000000
0.12	1.732617E+16	14.000000	1.215871E-06	1.377463E-18	3.205189E-17	1.044160E-16	99.999852	3.000000
0.13	1.732616E+16	15.166667	1.234286E-06	1.686212E-18	3.472288E-17	1.218187E-16	99.999831	3.000000
0.14	1.732616E+16	16.333333	1.234286E-06	2.034748E-18	3.739387E-17	1.405600E-16	99.999807	3.000000
0.15	1.732615E+16	17.500000	1.234286E-06	2.425363E-18	4.006485E-17	1.606400E-16	99.999782	3.000000
0.16	1.732615E+16	18.666667	1.234286E-06	2.860348E-18	4.273584E-17	1.820586E-16	99.999756	3.000000
0.17	1.732614E+16	19.833333	1.234286E-06	3.341994E-18	4.540682E-17	2.048160E-16	99.999728	3.000000
0.18	1.732614E+16	21.000000	1.234286E-06	3.872592E-18	4.807781E-17	2.289119E-16	99.999699	3.000000
0.19	1.732613E+16	22.166667	1.234286E-06	4.454434E-18	5.074879E-17	2.543466E-16	99.999669	3.000000
0.20	1.732613E+16	23.333333	1.234286E-06	5.089810E-18	5.341978E-17	2.811199E-16	99.999636	3.000000
0.21	1.732612E+16	24.500000	1.234286E-06	5.781011E-18	5.609076E-17	3.092318E-16	99.999603	3.000000
0.22	1.732612E+16	25.666667	1.234286E-06	6.530329E-18	5.876174E-17	3.386825E-16	99.999567	3.000000
0.23	1.732611E+16	26.833333	1.234286E-06	7.340055E-18	6.143272E-17	3.694718E-16	99.999531	3.000000
0.24	1.732610E+16	28.000000	1.234286E-06	8.212480E-18	6.410370E-17	4.015997E-16	99.999492	3.000000
0.25	1.732610E+16	29.166667	1.234286E-06	9.149894E-18	6.677468E-17	4.350663E-16	99.999453	3.000000
0.26	1.732609E+16	30.333333	1.234286E-06	1.015459E-17	6.944565E-17	4.698716E-16	99.999412	3.000000
0.27	1.732608E+16	31.500000	1.234286E-06	1.122886E-17	7.211663E-17	5.060155E-16	99.999369	3.000000
0.28	1.732607E+16	32.666667	1.234286E-06	1.237499E-17	7.478760E-17	5.434981E-16	99.999325	3.000000
0.29	1.732607E+16	33.833333	1.234286E-06	1.359527E-17	7.745858E-17	5.823193E-16	99.999279	3.000000
0.30	1.732606E+16	35.000000	1.234286E-06	1.489200E-17	8.012955E-17	6.224792E-16	99.999232	3.000000
0.31	1.732605E+16	36.166667	1.234286E-06	1.626747E-17	8.280052E-17	6.639777E-16	99.999183	3.000000
0.32	1.732604E+16	37.333333	1.234286E-06	1.772397E-17	8.547149E-17	7.068149E-16	99.999133	3.000000
0.33	1.732603E+16	38.500000	1.234286E-06	1.926378E-17	8.814246E-17	7.509908E-16	99.999081	3.000000
0.34	1.732602E+16	39.666667	1.234286E-06	2.088920E-17	9.081343E-17	7.965053E-16	99.999027	3.000000
0.35	1.732601E+16	40.833333	1.234286E-06	2.260253E-17	9.348439E-17	8.433584E-16	99.998973	3.000000
0.36	1.732600E+16	42.000000	1.234286E-06	2.440604E-17	9.615536E-17	8.915502E-16	99.998916	3.000000
0.37	1.732599E+16	43.166667	1.234286E-06	2.630204E-17	9.882632E-17	9.410807E-16	99.998858	3.000000
0.38	1.732598E+16	44.333333	1.234286E-06	2.829282E-17	1.014973E-16	9.919498E-16	99.998799	3.000000
0.39	1.732597E+16	45.500000	1.234286E-06	3.038066E-17	1.041682E-16	1.044158E-15	99.998738	3.000000
0.40	1.732596E+16	46.666667	1.234286E-06	3.256785E-17	1.068392E-16	1.097704E-15	99.998675	3.000000
0.41	1.732595E+16	47.833333	1.234286E-06	3.485669E-17	1.095102E-16	1.152589E-15	99.998611	3.000000
0.42	1.732594E+16	49.000000	1.234286E-06	3.724947E-17	1.121811E-16	1.208813E-15	99.998545	3.000000
0.43	1.732593E+16	50.166667	1.234286E-06	3.974848E-17	1.148521E-16	1.266375E-15	99.998478	3.000000
0.44	1.732592E+16	51.333333	1.234286E-06	4.235601E-17	1.175230E-16	1.325276E-15	99.998410	3.000000
0.45	1.732590E+16	52.500000	1.234286E-06	4.507435E-17	1.201940E-16	1.385516E-15	99.998339	3.000000

0.46	1.732589E+16	53.666667	1.234286E-06	4.790580E-17	1.228649E-16	1.447094E-15	99.998267	2.999999
0.47	1.732588E+16	54.833333	1.234286E-06	5.085264E-17	1.255359E-16	1.510011E-15	99.998194	2.999999
0.48	1.732587E+16	56.000000	1.234286E-06	5.391716E-17	1.282068E-16	1.574266E-15	99.998119	2.999999
0.49	1.732585E+16	57.166667	1.234286E-06	5.710166E-17	1.308777E-16	1.639860E-15	99.998043	2.999999
0.50	1.732584E+16	58.333333	1.234286E-06	6.040842E-17	1.335487E-16	1.706793E-15	99.997965	2.999999
0.51	1.732582E+16	59.500000	1.234286E-06	6.383975E-17	1.362196E-16	1.775065E-15	99.997885	2.999999
0.52	1.732581E+16	60.666667	1.234286E-06	6.739792E-17	1.388906E-16	1.844675E-15	99.997804	2.999999
0.53	1.732580E+16	61.833333	1.234286E-06	7.108523E-17	1.415615E-16	1.915623E-15	99.997721	2.999999
0.54	1.732578E+16	63.000000	1.234286E-06	7.490397E-17	1.442324E-16	1.987911E-15	99.997637	2.999999
0.55	1.732577E+16	64.166667	1.234286E-06	7.885644E-17	1.469033E-16	2.061537E-15	99.997551	2.999999
0.56	1.732575E+16	65.333333	1.234286E-06	8.294491E-17	1.495743E-16	2.136501E-15	99.997463	2.999999
0.57	1.732574E+16	66.500000	1.234286E-06	8.717170E-17	1.522452E-16	2.212804E-15	99.997374	2.999999
0.58	1.732572E+16	67.666667	1.234286E-06	9.153907E-17	1.549161E-16	2.290446E-15	99.997283	2.999999
0.59	1.732570E+16	68.833333	1.234286E-06	9.604933E-17	1.575870E-16	2.369427E-15	99.997191	2.999999
0.60	1.732569E+16	70.000000	1.234286E-06	1.007048E-16	1.602580E-16	2.449746E-15	99.997097	2.999999
0.61	1.732567E+16	71.166667	1.234286E-06	1.055077E-16	1.629289E-16	2.531404E-15	99.997002	2.999999
0.62	1.732565E+16	72.333333	1.234286E-06	1.104603E-16	1.655998E-16	2.614400E-15	99.996905	2.999999
0.63	1.732564E+16	73.500000	1.234286E-06	1.155651E-16	1.682707E-16	2.698735E-15	99.996806	2.999999
0.64	1.732562E+16	74.666667	1.234286E-06	1.208241E-16	1.709416E-16	2.784408E-15	99.996706	2.999999
0.65	1.732560E+16	75.833333	1.234286E-06	1.262398E-16	1.736125E-16	2.871421E-15	99.996604	2.999999
0.66	1.732558E+16	77.000000	1.234286E-06	1.318144E-16	1.762834E-16	2.959771E-15	99.996501	2.999999
0.67	1.732557E+16	78.166667	1.234286E-06	1.375502E-16	1.789543E-16	3.049461E-15	99.996395	2.999999
0.68	1.732555E+16	79.333333	1.234286E-06	1.434496E-16	1.816252E-16	3.140489E-15	99.996289	2.999999
0.69	1.732553E+16	80.500000	1.234286E-06	1.495147E-16	1.842961E-16	3.232855E-15	99.996181	2.999999
0.70	1.732551E+16	81.666667	1.234286E-06	1.557479E-16	1.869670E-16	3.326560E-15	99.996071	2.999999
0.71	1.732549E+16	82.833333	1.234286E-06	1.621515E-16	1.896379E-16	3.421604E-15	99.995959	2.999999
0.72	1.732547E+16	84.000000	1.234286E-06	1.687278E-16	1.923087E-16	3.517987E-15	99.995846	2.999999
0.73	1.732545E+16	85.166667	1.234286E-06	1.754790E-16	1.949796E-16	3.615708E-15	99.995731	2.999999
0.74	1.732543E+16	86.333333	1.234286E-06	1.824074E-16	1.976505E-16	3.714767E-15	99.995615	2.999999
0.75	1.732541E+16	87.500000	1.234286E-06	1.895155E-16	2.003214E-16	3.815166E-15	99.995497	2.999999
0.76	1.732539E+16	88.666667	1.234286E-06	1.968053E-16	2.029923E-16	3.916902E-15	99.995377	2.999999
0.77	1.732537E+16	89.833333	1.234286E-06	2.042793E-16	2.056631E-16	4.019978E-15	99.995256	2.999999
0.78	1.732535E+16	91.000000	1.234286E-06	2.119396E-16	2.083340E-16	4.124392E-15	99.995133	2.999999
0.79	1.732533E+16	92.166667	1.234286E-06	2.197887E-16	2.110048E-16	4.230144E-15	99.995009	2.999999
0.80	1.732530E+16	93.333333	1.234286E-06	2.278288E-16	2.136757E-16	4.337235E-15	99.994883	2.999998
0.81	1.732528E+16	94.500000	1.234286E-06	2.360622E-16	2.163466E-16	4.445665E-15	99.994755	2.999998
0.82	1.732526E+16	95.666667	1.234286E-06	2.444911E-16	2.190174E-16	4.555434E-15	99.994625	2.999998
0.83	1.732524E+16	96.833333	1.234286E-06	2.531179E-16	2.216883E-16	4.666540E-15	99.994494	2.999998
0.84	1.732521E+16	98.000000	1.234286E-06	2.619449E-16	2.243591E-16	4.778986E-15	99.994362	2.999998
0.85	1.732519E+16	99.166667	1.234286E-06	2.709743E-16	2.270300E-16	4.892770E-15	99.994227	2.999998
0.86	1.732517E+16	100.333333	1.234286E-06	2.802085E-16	2.297008E-16	5.007893E-15	99.994091	2.999998
0.87	1.732514E+16	101.500000	1.234286E-06	2.896497E-16	2.323716E-16	5.124354E-15	99.993953	2.999998
0.88	1.732512E+16	102.666667	1.234286E-06	2.993002E-16	2.350425E-16	5.242154E-15	99.993814	2.999998
0.89	1.732509E+16	103.833333	1.234286E-06	3.091624E-16	2.377133E-16	5.361292E-15	99.993673	2.999998
0.90	1.732507E+16	105.000000	1.234286E-06	3.192384E-16	2.403841E-16	5.481769E-15	99.993530	2.999998
0.91	1.732505E+16	106.166667	1.234286E-06	3.295306E-16	2.430549E-16	5.603584E-15	99.993386	2.999998
0.92	1.732502E+16	107.333333	1.234286E-06	3.400413E-16	2.457257E-16	5.726738E-15	99.993240	2.999998
0.93	1.732499E+16	108.500000	1.234286E-06	3.507728E-16	2.483966E-16	5.851231E-15	99.993092	2.999998
0.94	1.732497E+16	109.666667	1.234286E-06	3.617274E-16	2.510674E-16	5.977062E-15	99.992943	2.999998
0.95	1.732494E+16	110.833333	1.234286E-06	3.729073E-16	2.537382E-16	6.104232E-15	99.992792	2.999998
0.96	1.732492E+16	112.000000	1.234286E-06	3.843149E-16	2.564090E-16	6.232740E-15	99.992639	2.999998
0.97	1.732489E+16	113.166667	1.234286E-06	3.959524E-16	2.590798E-16	6.362587E-15	99.992485	2.999998
0.98	1.732486E+16	114.333333	1.234286E-06	4.078222E-16	2.617506E-16	6.493772E-15	99.992329	2.999998
0.99	1.732483E+16	115.500000	1.234286E-06	4.199264E-16	2.644213E-16	6.626296E-15	99.992171	2.999998
1.00	1.732481E+16	116.666667	1.234286E-06	4.322675E-16	2.670921E-16	6.760159E-15	99.992012	2.999998



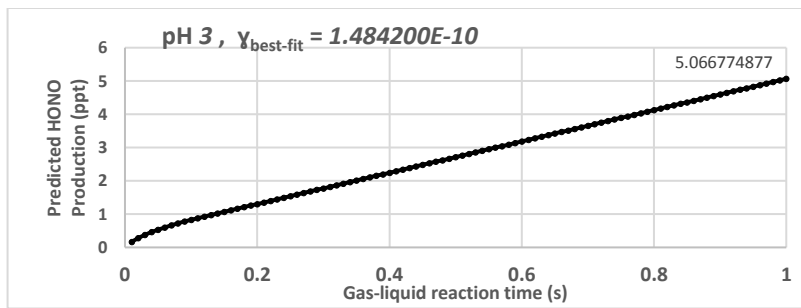
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732619E+16	1.166667	3.509924E-07	5.000751E-21	3.315668E-18	1.661770E-18	99.999995	3.000000
0.02	1.732619E+16	2.333333	4.963781E-07	2.207438E-20	6.631335E-18	4.985311E-18	99.999988	3.000000
0.03	1.732619E+16	3.500000	6.079365E-07	5.634639E-20	9.947002E-18	9.970621E-18	99.999979	3.000000
0.04	1.732619E+16	4.666667	7.019845E-07	1.120439E-19	1.326267E-17	1.661770E-17	99.999968	3.000000
0.05	1.732618E+16	5.833333	7.848425E-07	1.928478E-19	1.657834E-17	2.492655E-17	99.999955	3.000000
0.06	1.732618E+16	7.000000	8.597517E-07	3.020618E-19	1.989400E-17	3.489717E-17	99.999941	3.000000
0.07	1.732618E+16	8.166667	9.286379E-07	4.427088E-19	2.320967E-17	4.652956E-17	99.999925	3.000000
0.08	1.732618E+16	9.333333	9.927555E-07	6.175926E-19	2.652533E-17	5.982372E-17	99.999907	3.000000
0.09	1.732617E+16	10.500000	1.052976E-06	8.293390E-19	2.984100E-17	7.477964E-17	99.999887	3.000000
0.10	1.732617E+16	11.666667	1.109934E-06	1.080427E-18	3.315666E-17	9.139734E-17	99.999865	3.000000
0.11	1.732616E+16	12.833333	1.164108E-06	1.373209E-18	3.647232E-17	1.096768E-16	99.999842	3.000000
0.12	1.732616E+16	14.000000	1.215871E-06	1.709930E-18	3.978798E-17	1.296180E-16	99.999817	3.000000
0.13	1.732615E+16	15.166667	1.234286E-06	2.093199E-18	4.310365E-17	1.512210E-16	99.999790	3.000000
0.14	1.732615E+16	16.333333	1.234286E-06	2.525858E-18	4.641931E-17	1.744858E-16	99.999761	3.000000
0.15	1.732614E+16	17.500000	1.234286E-06	3.010753E-18	4.973496E-17	1.994123E-16	99.999730	3.000000
0.16	1.732614E+16	18.666667	1.234286E-06	3.550726E-18	5.305062E-17	2.260006E-16	99.999697	3.000000
0.17	1.732613E+16	19.833333	1.234286E-06	4.148623E-18	5.636628E-17	2.542506E-16	99.999663	3.000000
0.18	1.732613E+16	21.000000	1.234286E-06	4.807288E-18	5.968194E-17	2.841625E-16	99.999627	3.000000
0.19	1.732612E+16	22.166667	1.234286E-06	5.529563E-18	6.299759E-17	3.157360E-16	99.999589	3.000000
0.20	1.732611E+16	23.333333	1.234286E-06	6.318294E-18	6.631324E-17	3.489714E-16	99.999549	3.000000
0.21	1.732611E+16	24.500000	1.234286E-06	7.176325E-18	6.962890E-17	3.838685E-16	99.999507	3.000000
0.22	1.732610E+16	25.666667	1.234286E-06	8.106500E-18	7.294455E-17	4.204274E-16	99.999463	3.000000
0.23	1.732609E+16	26.833333	1.234286E-06	9.111662E-18	7.626019E-17	4.586480E-16	99.999417	3.000000
0.24	1.732608E+16	28.000000	1.234286E-06	1.019466E-17	7.957584E-17	4.985304E-16	99.999370	3.000000
0.25	1.732607E+16	29.166667	1.234286E-06	1.135833E-17	8.289149E-17	5.400745E-16	99.999321	3.000000
0.26	1.732606E+16	30.333333	1.234286E-06	1.260552E-17	8.620713E-17	5.832804E-16	99.999270	3.000000
0.27	1.732606E+16	31.500000	1.234286E-06	1.393907E-17	8.952278E-17	6.281480E-16	99.999217	3.000000
0.28	1.732605E+16	32.666667	1.234286E-06	1.536183E-17	9.283842E-17	6.746774E-16	99.999162	3.000000
0.29	1.732604E+16	33.833333	1.234286E-06	1.687665E-17	9.615405E-17	7.228686E-16	99.999105	3.000000
0.30	1.732603E+16	35.000000	1.234286E-06	1.848636E-17	9.946969E-17	7.727215E-16	99.999046	3.000000
0.31	1.732602E+16	36.166667	1.234286E-06	2.019381E-17	1.027853E-16	8.242362E-16	99.998986	3.000000
0.32	1.732600E+16	37.333333	1.234286E-06	2.200185E-17	1.061010E-16	8.774126E-16	99.998923	3.000000
0.33	1.732599E+16	38.500000	1.234286E-06	2.391331E-17	1.094166E-16	9.322507E-16	99.998859	3.000000
0.34	1.732598E+16	39.666667	1.234286E-06	2.593105E-17	1.127322E-16	9.887506E-16	99.998793	3.000000
0.35	1.732597E+16	40.833333	1.234286E-06	2.805790E-17	1.160478E-16	1.046912E-15	99.998725	3.000000
0.36	1.732596E+16	42.000000	1.234286E-06	3.029672E-17	1.193635E-16	1.106736E-15	99.998655	3.000000
0.37	1.732595E+16	43.166667	1.234286E-06	3.265034E-17	1.226791E-16	1.168221E-15	99.998583	3.000000
0.38	1.732593E+16	44.333333	1.234286E-06	3.512160E-17	1.259947E-16	1.231368E-15	99.998509	3.000000
0.39	1.732592E+16	45.500000	1.234286E-06	3.771337E-17	1.293103E-16	1.296176E-15	99.998433	3.000000
0.40	1.732591E+16	46.666667	1.234286E-06	4.042846E-17	1.326259E-16	1.362647E-15	99.998355	3.000000
0.41	1.732589E+16	47.833333	1.234286E-06	4.326974E-17	1.359416E-16	1.430779E-15	99.998276	2.999999
0.42	1.732588E+16	49.000000	1.234286E-06	4.624004E-17	1.392572E-16	1.500573E-15	99.998194	2.999999
0.43	1.732586E+16	50.166667	1.234286E-06	4.934222E-17	1.425728E-16	1.572028E-15	99.998111	2.999999
0.44	1.732585E+16	51.333333	1.234286E-06	5.257910E-17	1.458884E-16	1.645145E-15	99.998026	2.999999
0.45	1.732583E+16	52.500000	1.234286E-06	5.595354E-17	1.492040E-16	1.719924E-15	99.997938	2.999999

0.46	1.732582E+16	53.666667	1.234286E-06	5.946838E-17	1.525196E-16	1.796365E-15	99.997849	2.999999
0.47	1.732580E+16	54.833333	1.234286E-06	6.312647E-17	1.558352E-16	1.874468E-15	99.997758	2.999999
0.48	1.732579E+16	56.000000	1.234286E-06	6.693065E-17	1.591508E-16	1.954232E-15	99.997665	2.999999
0.49	1.732577E+16	57.166667	1.234286E-06	7.088376E-17	1.624664E-16	2.035658E-15	99.997570	2.999999
0.50	1.732575E+16	58.333333	1.234286E-06	7.498864E-17	1.657819E-16	2.118745E-15	99.997473	2.999999
0.51	1.732574E+16	59.500000	1.234286E-06	7.924815E-17	1.690975E-16	2.203495E-15	99.997374	2.999999
0.52	1.732572E+16	60.666667	1.234286E-06	8.366512E-17	1.724131E-16	2.289906E-15	99.997274	2.999999
0.53	1.732570E+16	61.833333	1.234286E-06	8.824240E-17	1.757287E-16	2.377979E-15	99.997171	2.999999
0.54	1.732568E+16	63.000000	1.234286E-06	9.298283E-17	1.790442E-16	2.467713E-15	99.997066	2.999999
0.55	1.732566E+16	64.166667	1.234286E-06	9.788926E-17	1.823598E-16	2.559109E-15	99.996959	2.999999
0.56	1.732565E+16	65.333333	1.234286E-06	1.029645E-16	1.856754E-16	2.652167E-15	99.996851	2.999999
0.57	1.732563E+16	66.500000	1.234286E-06	1.082115E-16	1.889909E-16	2.746887E-15	99.996740	2.999999
0.58	1.732561E+16	67.666667	1.234286E-06	1.136330E-16	1.923065E-16	2.843268E-15	99.996628	2.999999
0.59	1.732559E+16	68.833333	1.234286E-06	1.192318E-16	1.956221E-16	2.941311E-15	99.996513	2.999999
0.60	1.732557E+16	70.000000	1.234286E-06	1.250109E-16	1.989376E-16	3.041016E-15	99.996397	2.999999
0.61	1.732555E+16	71.166667	1.234286E-06	1.309730E-16	2.022532E-16	3.142383E-15	99.996278	2.999999
0.62	1.732553E+16	72.333333	1.234286E-06	1.371211E-16	2.055687E-16	3.245411E-15	99.996158	2.999999
0.63	1.732550E+16	73.500000	1.234286E-06	1.434579E-16	2.088842E-16	3.350101E-15	99.996035	2.999999
0.64	1.732548E+16	74.666667	1.234286E-06	1.499862E-16	2.121998E-16	3.456452E-15	99.995911	2.999999
0.65	1.732546E+16	75.833333	1.234286E-06	1.567090E-16	2.155153E-16	3.564465E-15	99.995784	2.999999
0.66	1.732544E+16	77.000000	1.234286E-06	1.636291E-16	2.188308E-16	3.674140E-15	99.995656	2.999999
0.67	1.732542E+16	78.166667	1.234286E-06	1.707493E-16	2.221464E-16	3.785477E-15	99.995525	2.999999
0.68	1.732539E+16	79.333333	1.234286E-06	1.780725E-16	2.254619E-16	3.898475E-15	99.995393	2.999999
0.69	1.732537E+16	80.500000	1.234286E-06	1.856015E-16	2.287774E-16	4.013135E-15	99.995259	2.999999
0.70	1.732535E+16	81.666667	1.234286E-06	1.933392E-16	2.320929E-16	4.129457E-15	99.995122	2.999999
0.71	1.732532E+16	82.833333	1.234286E-06	2.012883E-16	2.354084E-16	4.247440E-15	99.994984	2.999999
0.72	1.732530E+16	84.000000	1.234286E-06	2.094518E-16	2.387239E-16	4.367085E-15	99.994843	2.999998
0.73	1.732527E+16	85.166667	1.234286E-06	2.178325E-16	2.420394E-16	4.488391E-15	99.994701	2.999998
0.74	1.732525E+16	86.333333	1.234286E-06	2.264332E-16	2.453549E-16	4.611360E-15	99.994557	2.999998
0.75	1.732522E+16	87.500000	1.234286E-06	2.352568E-16	2.486704E-16	4.735990E-15	99.994410	2.999998
0.76	1.732520E+16	88.666667	1.234286E-06	2.443061E-16	2.519859E-16	4.862281E-15	99.994262	2.999998
0.77	1.732517E+16	89.833333	1.234286E-06	2.535839E-16	2.553013E-16	4.990235E-15	99.994111	2.999998
0.78	1.732514E+16	91.000000	1.234286E-06	2.630932E-16	2.586168E-16	5.119849E-15	99.993959	2.999998
0.79	1.732512E+16	92.166667	1.234286E-06	2.728367E-16	2.619323E-16	5.251126E-15	99.993804	2.999998
0.80	1.732509E+16	93.333333	1.234286E-06	2.828173E-16	2.652477E-16	5.384064E-15	99.993647	2.999998
0.81	1.732506E+16	94.500000	1.234286E-06	2.930379E-16	2.685632E-16	5.518664E-15	99.993489	2.999998
0.82	1.732504E+16	95.666667	1.234286E-06	3.035012E-16	2.718787E-16	5.654926E-15	99.993328	2.999998
0.83	1.732501E+16	96.833333	1.234286E-06	3.142102E-16	2.751941E-16	5.792849E-15	99.993165	2.999998
0.84	1.732498E+16	98.000000	1.234286E-06	3.251676E-16	2.785095E-16	5.932433E-15	99.993001	2.999998
0.85	1.732495E+16	99.166667	1.234286E-06	3.363763E-16	2.818250E-16	6.073680E-15	99.992834	2.999998
0.86	1.732492E+16	100.333333	1.234286E-06	3.478392E-16	2.851404E-16	6.216588E-15	99.992665	2.999998
0.87	1.732489E+16	101.500000	1.234286E-06	3.595591E-16	2.884558E-16	6.361157E-15	99.992494	2.999998
0.88	1.732486E+16	102.666667	1.234286E-06	3.715388E-16	2.917712E-16	6.507389E-15	99.992321	2.999998
0.89	1.732483E+16	103.833333	1.234286E-06	3.837813E-16	2.950867E-16	6.655282E-15	99.992146	2.999998
0.90	1.732480E+16	105.000000	1.234286E-06	3.962892E-16	2.984021E-16	6.804836E-15	99.991969	2.999998
0.91	1.732477E+16	106.166667	1.234286E-06	4.090655E-16	3.017175E-16	6.956052E-15	99.991790	2.999998
0.92	1.732474E+16	107.333333	1.234286E-06	4.221131E-16	3.050329E-16	7.108930E-15	99.991609	2.999997
0.93	1.732471E+16	108.500000	1.234286E-06	4.354347E-16	3.083483E-16	7.263469E-15	99.991425	2.999997
0.94	1.732467E+16	109.666667	1.234286E-06	4.490332E-16	3.116636E-16	7.419670E-15	99.991240	2.999997
0.95	1.732464E+16	110.833333	1.234286E-06	4.629114E-16	3.149790E-16	7.577533E-15	99.991052	2.999997
0.96	1.732461E+16	112.000000	1.234286E-06	4.770723E-16	3.182944E-16	7.737057E-15	99.990863	2.999997
0.97	1.732457E+16	113.166667	1.234286E-06	4.915186E-16	3.216098E-16	7.898242E-15	99.990671	2.999997
0.98	1.732454E+16	114.333333	1.234286E-06	5.062531E-16	3.249251E-16	8.061090E-15	99.990477	2.999997
0.99	1.732451E+16	115.500000	1.234286E-06	5.212788E-16	3.282405E-16	8.225598E-15	99.990282	2.999997
1.00	1.732447E+16	116.666667	1.234286E-06	5.365985E-16	3.315558E-16	8.391769E-15	99.990084	2.999997



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO2}}$ (mol)	$\Phi_{\text{NO2}}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732619E+16	1.166667	3.509924E-07	5.040554E-21	3.342058E-18	1.674997E-18	99.999995	3.000000
0.02	1.732619E+16	2.333333	4.963781E-07	2.225008E-20	6.684117E-18	5.024991E-18	99.999987	3.000000
0.03	1.732619E+16	3.500000	6.079365E-07	5.679487E-20	1.002617E-17	1.004998E-17	99.999978	3.000000
0.04	1.732619E+16	4.666667	7.019845E-07	1.129357E-19	1.336823E-17	1.674997E-17	99.999968	3.000000
0.05	1.732618E+16	5.833333	7.848425E-07	1.943827E-19	1.671029E-17	2.512495E-17	99.999955	3.000000
0.06	1.732618E+16	7.000000	8.597517E-07	3.044660E-19	2.005235E-17	3.517493E-17	99.999941	3.000000
0.07	1.732618E+16	8.166667	9.286379E-07	4.462325E-19	2.339440E-17	4.689991E-17	99.999924	3.000000
0.08	1.732617E+16	9.333333	9.927554E-07	6.225082E-19	2.673646E-17	6.029988E-17	99.999906	3.000000
0.09	1.732617E+16	10.500000	1.052976E-06	8.359401E-19	3.007851E-17	7.537484E-17	99.999886	3.000000
0.10	1.732617E+16	11.666667	1.109934E-06	1.089026E-18	3.342057E-17	9.212480E-17	99.999864	3.000000
0.11	1.732616E+16	12.833333	1.164108E-06	1.384139E-18	3.676262E-17	1.105498E-16	99.999841	3.000000
0.12	1.732616E+16	14.000000	1.215871E-06	1.723540E-18	4.010467E-17	1.306497E-16	99.999815	3.000000
0.13	1.732615E+16	15.166667	1.234286E-06	2.109859E-18	4.344672E-17	1.524246E-16	99.999788	3.000000
0.14	1.732615E+16	16.333333	1.234286E-06	2.545962E-18	4.678878E-17	1.758746E-16	99.999759	3.000000
0.15	1.732614E+16	17.500000	1.234286E-06	3.034716E-18	5.013083E-17	2.009995E-16	99.999728	3.000000
0.16	1.732614E+16	18.666667	1.234286E-06	3.578988E-18	5.347287E-17	2.277994E-16	99.999695	3.000000
0.17	1.732613E+16	19.833333	1.234286E-06	4.181644E-18	5.681492E-17	2.562743E-16	99.999660	3.000000
0.18	1.732613E+16	21.000000	1.234286E-06	4.845551E-18	6.015697E-17	2.864242E-16	99.999624	3.000000
0.19	1.732612E+16	22.166667	1.234286E-06	5.573575E-18	6.349901E-17	3.182491E-16	99.999585	3.000000
0.20	1.732611E+16	23.333333	1.234286E-06	6.368584E-18	6.684106E-17	3.517490E-16	99.999545	3.000000
0.21	1.732611E+16	24.500000	1.234286E-06	7.233445E-18	7.018310E-17	3.869238E-16	99.999503	3.000000
0.22	1.732610E+16	25.666667	1.234286E-06	8.171023E-18	7.352514E-17	4.237737E-16	99.999459	3.000000
0.23	1.732609E+16	26.833333	1.234286E-06	9.184186E-18	7.686718E-17	4.622985E-16	99.999413	3.000000
0.24	1.732608E+16	28.000000	1.234286E-06	1.027580E-17	8.020922E-17	5.024984E-16	99.999365	3.000000
0.25	1.732607E+16	29.166667	1.234286E-06	1.144873E-17	8.355125E-17	5.443732E-16	99.999315	3.000000
0.26	1.732606E+16	30.333333	1.234286E-06	1.270585E-17	8.689329E-17	5.879229E-16	99.999264	3.000000
0.27	1.732605E+16	31.500000	1.234286E-06	1.405002E-17	9.023532E-17	6.331477E-16	99.999210	3.000000
0.28	1.732604E+16	32.666667	1.234286E-06	1.548411E-17	9.357735E-17	6.800475E-16	99.999155	3.000000
0.29	1.732603E+16	33.833333	1.234286E-06	1.701098E-17	9.691938E-17	7.286222E-16	99.999098	3.000000
0.30	1.732602E+16	35.000000	1.234286E-06	1.863350E-17	1.002614E-16	7.788719E-16	99.999039	3.000000
0.31	1.732601E+16	36.166667	1.234286E-06	2.035454E-17	1.036034E-16	8.307966E-16	99.998978	3.000000
0.32	1.732600E+16	37.333333	1.234286E-06	2.217697E-17	1.069455E-16	8.843962E-16	99.998915	3.000000
0.33	1.732599E+16	38.500000	1.234286E-06	2.410365E-17	1.102875E-16	9.396709E-16	99.998850	3.000000
0.34	1.732598E+16	39.666667	1.234286E-06	2.613744E-17	1.136295E-16	9.966205E-16	99.998783	3.000000
0.35	1.732597E+16	40.833333	1.234286E-06	2.828123E-17	1.169715E-16	1.055245E-15	99.998714	3.000000
0.36	1.732596E+16	42.000000	1.234286E-06	3.053786E-17	1.203135E-16	1.115545E-15	99.998644	3.000000
0.37	1.732594E+16	43.166667	1.234286E-06	3.291021E-17	1.236555E-16	1.177519E-15	99.998571	3.000000
0.38	1.732593E+16	44.333333	1.234286E-06	3.540115E-17	1.269975E-16	1.241169E-15	99.998497	3.000000
0.39	1.732592E+16	45.500000	1.234286E-06	3.801354E-17	1.303396E-16	1.306493E-15	99.998421	3.000000
0.40	1.732590E+16	46.666667	1.234286E-06	4.075025E-17	1.336816E-16	1.373492E-15	99.998342	3.000000
0.41	1.732589E+16	47.833333	1.234286E-06	4.361414E-17	1.370236E-16	1.442167E-15	99.998262	2.999999
0.42	1.732588E+16	49.000000	1.234286E-06	4.660809E-17	1.403656E-16	1.512516E-15	99.998180	2.999999
0.43	1.732586E+16	50.166667	1.234286E-06	4.973495E-17	1.437076E-16	1.584540E-15	99.998096	2.999999
0.44	1.732585E+16	51.333333	1.234286E-06	5.299760E-17	1.470496E-16	1.658240E-15	99.998010	2.999999
0.45	1.732583E+16	52.500000	1.234286E-06	5.639890E-17	1.503915E-16	1.733614E-15	99.997922	2.999999

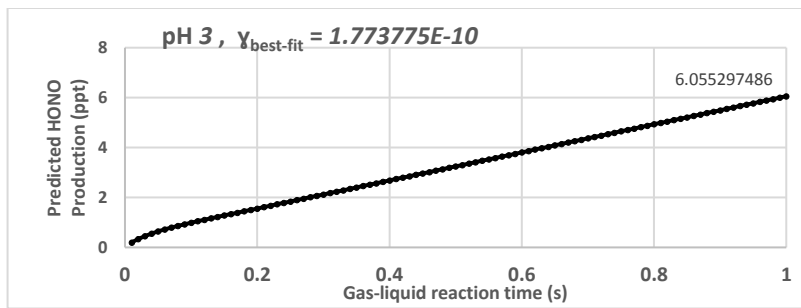
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0.47	1.732580E+16	54.833333	1.234286E-06	6.362892E-17	1.570755E-16	1.889387E-15	99.997740	2.999999
0.48	1.732578E+16	56.000000	1.234286E-06	6.746337E-17	1.604175E-16	1.969786E-15	99.997647	2.999999
0.49	1.732577E+16	57.166667	1.234286E-06	7.144795E-17	1.637595E-16	2.051860E-15	99.997551	2.999999
0.50	1.732575E+16	58.333333	1.234286E-06	7.558551E-17	1.671015E-16	2.135609E-15	99.997453	2.999999
0.51	1.732573E+16	59.500000	1.234286E-06	7.987892E-17	1.704434E-16	2.221033E-15	99.997353	2.999999
0.52	1.732572E+16	60.666667	1.234286E-06	8.433104E-17	1.737854E-16	2.308132E-15	99.997252	2.999999
0.53	1.732570E+16	61.833333	1.234286E-06	8.894475E-17	1.771274E-16	2.396906E-15	99.997148	2.999999
0.54	1.732568E+16	63.000000	1.234286E-06	9.372292E-17	1.804693E-16	2.487355E-15	99.997043	2.999999
0.55	1.732566E+16	64.166667	1.234286E-06	9.866840E-17	1.838113E-16	2.579478E-15	99.996935	2.999999
0.56	1.732564E+16	65.333333	1.234286E-06	1.037841E-16	1.871532E-16	2.673277E-15	99.996826	2.999999
0.57	1.732562E+16	66.500000	1.234286E-06	1.090728E-16	1.904952E-16	2.768750E-15	99.996714	2.999999
0.58	1.732560E+16	67.666667	1.234286E-06	1.145374E-16	1.938371E-16	2.865899E-15	99.996601	2.999999
0.59	1.732558E+16	68.833333	1.234286E-06	1.201808E-16	1.971791E-16	2.964722E-15	99.996485	2.999999
0.60	1.732556E+16	70.000000	1.234286E-06	1.260059E-16	2.005210E-16	3.065221E-15	99.996368	2.999999
0.61	1.732554E+16	71.166667	1.234286E-06	1.320155E-16	2.038630E-16	3.167394E-15	99.996248	2.999999
0.62	1.732552E+16	72.333333	1.234286E-06	1.382125E-16	2.072049E-16	3.271242E-15	99.996127	2.999999
0.63	1.732550E+16	73.500000	1.234286E-06	1.445997E-16	2.105468E-16	3.376765E-15	99.996004	2.999999
0.64	1.732548E+16	74.666667	1.234286E-06	1.511800E-16	2.138887E-16	3.483963E-15	99.995878	2.999999
0.65	1.732545E+16	75.833333	1.234286E-06	1.579563E-16	2.172307E-16	3.592836E-15	99.995751	2.999999
0.66	1.732543E+16	77.000000	1.234286E-06	1.649315E-16	2.205726E-16	3.703384E-15	99.995621	2.999999
0.67	1.732541E+16	78.166667	1.234286E-06	1.721084E-16	2.239145E-16	3.815607E-15	99.995490	2.999999
0.68	1.732539E+16	79.333333	1.234286E-06	1.794899E-16	2.272564E-16	3.929504E-15	99.995356	2.999999
0.69	1.732536E+16	80.500000	1.234286E-06	1.870788E-16	2.305983E-16	4.045077E-15	99.995221	2.999999
0.70	1.732534E+16	81.666667	1.234286E-06	1.948780E-16	2.339402E-16	4.162324E-15	99.995083	2.999999
0.71	1.732532E+16	82.833333	1.234286E-06	2.028904E-16	2.372821E-16	4.281247E-15	99.994944	2.999998
0.72	1.732529E+16	84.000000	1.234286E-06	2.111189E-16	2.406240E-16	4.401844E-15	99.994802	2.999998
0.73	1.732527E+16	85.166667	1.234286E-06	2.195663E-16	2.439659E-16	4.524116E-15	99.994659	2.999998
0.74	1.732524E+16	86.333333	1.234286E-06	2.282355E-16	2.473077E-16	4.648063E-15	99.994513	2.999998
0.75	1.732521E+16	87.500000	1.234286E-06	2.371293E-16	2.506496E-16	4.773685E-15	99.994366	2.999998
0.76	1.732519E+16	88.666667	1.234286E-06	2.462506E-16	2.539915E-16	4.900982E-15	99.994216	2.999998
0.77	1.732516E+16	89.833333	1.234286E-06	2.556023E-16	2.573333E-16	5.029953E-15	99.994064	2.999998
0.78	1.732514E+16	91.000000	1.234286E-06	2.651873E-16	2.606752E-16	5.160600E-15	99.993910	2.999998
0.79	1.732511E+16	92.166667	1.234286E-06	2.750083E-16	2.640171E-16	5.292921E-15	99.993755	2.999998
0.80	1.732508E+16	93.333333	1.234286E-06	2.850684E-16	2.673589E-16	5.426918E-15	99.993597	2.999998
0.81	1.732505E+16	94.500000	1.234286E-06	2.953703E-16	2.707008E-16	5.562589E-15	99.993437	2.999998
0.82	1.732503E+16	95.666667	1.234286E-06	3.059169E-16	2.740426E-16	5.699935E-15	99.993275	2.999998
0.83	1.732500E+16	96.833333	1.234286E-06	3.167111E-16	2.773844E-16	5.838956E-15	99.993111	2.999998
0.84	1.732497E+16	98.000000	1.234286E-06	3.277557E-16	2.807263E-16	5.979651E-15	99.992945	2.999998
0.85	1.732494E+16	99.166667	1.234286E-06	3.390536E-16	2.840681E-16	6.122022E-15	99.992777	2.999998
0.86	1.732491E+16	100.333333	1.234286E-06	3.506078E-16	2.874099E-16	6.266067E-15	99.992607	2.999998
0.87	1.732488E+16	101.500000	1.234286E-06	3.624209E-16	2.907517E-16	6.411788E-15	99.992434	2.999998
0.88	1.732485E+16	102.666667	1.234286E-06	3.744960E-16	2.940935E-16	6.559183E-15	99.992260	2.999998
0.89	1.732482E+16	103.833333	1.234286E-06	3.868359E-16	2.974353E-16	6.708253E-15	99.992084	2.999998
0.90	1.732479E+16	105.000000	1.234286E-06	3.994434E-16	3.007771E-16	6.858998E-15	99.991905	2.999998
0.91	1.732476E+16	106.166667	1.234286E-06	4.123214E-16	3.041189E-16	7.011417E-15	99.991724	2.999998
0.92	1.732473E+16	107.333333	1.234286E-06	4.254728E-16	3.074607E-16	7.165512E-15	99.991542	2.999997
0.93	1.732469E+16	108.500000	1.234286E-06	4.389004E-16	3.108025E-16	7.321281E-15	99.991357	2.999997
0.94	1.732466E+16	109.666667	1.234286E-06	4.526071E-16	3.141442E-16	7.478725E-15	99.991170	2.999997
0.95	1.732463E+16	110.833333	1.234286E-06	4.665959E-16	3.174860E-16	7.637844E-15	99.990981	2.999997
0.96	1.732460E+16	112.000000	1.234286E-06	4.808694E-16	3.208277E-16	7.798638E-15	99.990790	2.999997
0.97	1.732456E+16	113.166667	1.234286E-06	4.954307E-16	3.241695E-16	7.961106E-15	99.990597	2.999997
0.98	1.732453E+16	114.333333	1.234286E-06	5.102825E-16	3.275112E-16	8.125250E-15	99.990402	2.999997
0.99	1.732449E+16	115.500000	1.234286E-06	5.254278E-16	3.308530E-16	8.291068E-15	99.990204	2.999997
1.00	1.732446E+16	116.666667	1.234286E-06	5.408694E-16	3.341947E-16	8.458561E-15	99.990005	2.999997



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732619E+16	1.166667	3.509924E-07	4.290165E-21	2.844525E-18	1.425640E-18	99.999995	3.000000
0.02	1.732619E+16	2.333333	4.963781E-07	1.893771E-20	5.689050E-18	4.276919E-18	99.999989	3.000000
0.03	1.732619E+16	3.500000	6.079365E-07	4.833980E-20	8.533575E-18	8.553838E-18	99.999982	3.000000
0.04	1.732619E+16	4.666667	7.019846E-07	9.612293E-20	1.137810E-17	1.425640E-17	99.999972	3.000000
0.05	1.732618E+16	5.833333	7.848425E-07	1.654449E-19	1.422262E-17	2.138459E-17	99.999962	3.000000
0.06	1.732618E+16	7.000000	8.597518E-07	2.591401E-19	1.706715E-17	2.993843E-17	99.999949	3.000000
0.07	1.732618E+16	8.166667	9.286380E-07	3.798017E-19	1.991167E-17	3.991791E-17	99.999936	3.000000
0.08	1.732618E+16	9.333333	9.927556E-07	5.298352E-19	2.275620E-17	5.132302E-17	99.999920	3.000000
0.09	1.732617E+16	10.500000	1.052976E-06	7.114934E-19	2.560072E-17	6.415377E-17	99.999903	3.000000
0.10	1.732617E+16	11.666667	1.109934E-06	9.269025E-19	2.844524E-17	7.841016E-17	99.999885	3.000000
0.11	1.732617E+16	12.833333	1.164108E-06	1.178081E-18	3.128976E-17	9.409219E-17	99.999864	3.000000
0.12	1.732616E+16	14.000000	1.215871E-06	1.466956E-18	3.413428E-17	1.111999E-16	99.999843	3.000000
0.13	1.732616E+16	15.166667	1.234286E-06	1.795764E-18	3.697880E-17	1.297332E-16	99.999820	3.000000
0.14	1.732616E+16	16.333333	1.234286E-06	2.166944E-18	3.982332E-17	1.496921E-16	99.999795	3.000000
0.15	1.732615E+16	17.500000	1.234286E-06	2.582937E-18	4.266784E-17	1.710767E-16	99.999768	3.000000
0.16	1.732615E+16	18.666667	1.234286E-06	3.046183E-18	4.551236E-17	1.938869E-16	99.999740	3.000000
0.17	1.732614E+16	19.833333	1.234286E-06	3.559121E-18	4.835688E-17	2.181227E-16	99.999711	3.000000
0.18	1.732614E+16	21.000000	1.234286E-06	4.124192E-18	5.120139E-17	2.437842E-16	99.999680	3.000000
0.19	1.732613E+16	22.166667	1.234286E-06	4.743836E-18	5.404591E-17	2.708713E-16	99.999647	3.000000
0.20	1.732612E+16	23.333333	1.234286E-06	5.420492E-18	5.689042E-17	2.993841E-16	99.999613	3.000000
0.21	1.732612E+16	24.500000	1.234286E-06	6.156600E-18	5.973494E-17	3.293224E-16	99.999577	3.000000
0.22	1.732611E+16	25.666667	1.234286E-06	6.954601E-18	6.257945E-17	3.606865E-16	99.999539	3.000000
0.23	1.732610E+16	26.833333	1.234286E-06	7.816934E-18	6.542396E-17	3.934761E-16	99.999500	3.000000
0.24	1.732610E+16	28.000000	1.234286E-06	8.746040E-18	6.826847E-17	4.276914E-16	99.999460	3.000000
0.25	1.732609E+16	29.166667	1.234286E-06	9.744357E-18	7.111298E-17	4.633323E-16	99.999417	3.000000
0.26	1.732608E+16	30.333333	1.234286E-06	1.081433E-17	7.395749E-17	5.003988E-16	99.999373	3.000000
0.27	1.732607E+16	31.500000	1.234286E-06	1.195839E-17	7.680200E-17	5.388910E-16	99.999328	3.000000
0.28	1.732607E+16	32.666667	1.234286E-06	1.317898E-17	7.964650E-17	5.788088E-16	99.999281	3.000000
0.29	1.732606E+16	33.833333	1.234286E-06	1.447855E-17	8.249101E-17	6.201522E-16	99.999232	3.000000
0.30	1.732605E+16	35.000000	1.234286E-06	1.585953E-17	8.533551E-17	6.629212E-16	99.999182	3.000000
0.31	1.732604E+16	36.166667	1.234286E-06	1.732436E-17	8.818001E-17	7.071159E-16	99.999130	3.000000
0.32	1.732603E+16	37.333333	1.234286E-06	1.887548E-17	9.102451E-17	7.527362E-16	99.999076	3.000000
0.33	1.732602E+16	38.500000	1.234286E-06	2.051534E-17	9.386901E-17	7.997821E-16	99.999021	3.000000
0.34	1.732601E+16	39.666667	1.234286E-06	2.224636E-17	9.671350E-17	8.482537E-16	99.998964	3.000000
0.35	1.732600E+16	40.833333	1.234286E-06	2.407100E-17	9.955800E-17	8.981508E-16	99.998906	3.000000
0.36	1.732599E+16	42.000000	1.234286E-06	2.599169E-17	1.024025E-16	9.494736E-16	99.998846	3.000000
0.37	1.732598E+16	43.166667	1.234286E-06	2.801087E-17	1.052470E-16	1.002222E-15	99.998784	3.000000
0.38	1.732597E+16	44.333333	1.234286E-06	3.013098E-17	1.080915E-16	1.056396E-15	99.998721	3.000000
0.39	1.732596E+16	45.500000	1.234286E-06	3.235447E-17	1.109360E-16	1.111996E-15	99.998656	3.000000
0.40	1.732595E+16	46.666667	1.234286E-06	3.468376E-17	1.137804E-16	1.169021E-15	99.998589	3.000000
0.41	1.732593E+16	47.833333	1.234286E-06	3.712131E-17	1.166249E-16	1.227472E-15	99.998521	3.000000
0.42	1.732592E+16	49.000000	1.234286E-06	3.966954E-17	1.194694E-16	1.287348E-15	99.998451	3.000000
0.43	1.732591E+16	50.166667	1.234286E-06	4.233091E-17	1.223139E-16	1.348650E-15	99.998379	3.000000
0.44	1.732590E+16	51.333333	1.234286E-06	4.510785E-17	1.251584E-16	1.411378E-15	99.998306	3.000000
0.45	1.732588E+16	52.500000	1.234286E-06	4.800280E-17	1.280028E-16	1.475531E-15	99.998231	2.999999

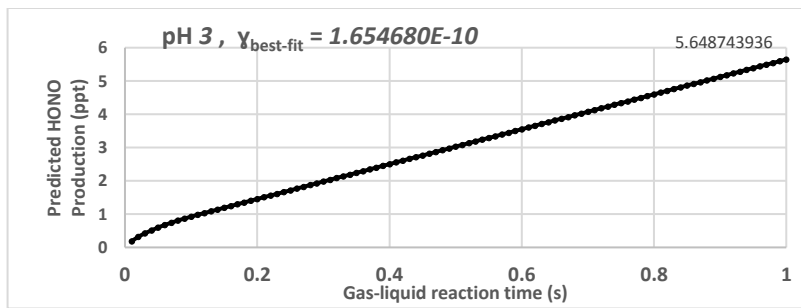
0.46	1.732587E+16	53.666667	1.234286E-06	5.101820E-17	1.308473E-16	1.541110E-15	99.998155	2.999999
0.47	1.732586E+16	54.833333	1.234286E-06	5.415649E-17	1.336918E-16	1.608115E-15	99.998077	2.999999
0.48	1.732584E+16	56.000000	1.234286E-06	5.742012E-17	1.365363E-16	1.676545E-15	99.997997	2.999999
0.49	1.732583E+16	57.166667	1.234286E-06	6.081151E-17	1.393807E-16	1.746401E-15	99.997915	2.999999
0.50	1.732582E+16	58.333333	1.234286E-06	6.433311E-17	1.422252E-16	1.817682E-15	99.997832	2.999999
0.51	1.732580E+16	59.500000	1.234286E-06	6.798736E-17	1.450697E-16	1.890389E-15	99.997747	2.999999
0.52	1.732579E+16	60.666667	1.234286E-06	7.177671E-17	1.479141E-16	1.964522E-15	99.997661	2.999999
0.53	1.732577E+16	61.833333	1.234286E-06	7.570358E-17	1.507586E-16	2.040080E-15	99.997573	2.999999
0.54	1.732576E+16	63.000000	1.234286E-06	7.977042E-17	1.536030E-16	2.117063E-15	99.997483	2.999999
0.55	1.732574E+16	64.166667	1.234286E-06	8.397967E-17	1.564475E-16	2.195473E-15	99.997391	2.999999
0.56	1.732572E+16	65.333333	1.234286E-06	8.833378E-17	1.592919E-16	2.275308E-15	99.997298	2.999999
0.57	1.732571E+16	66.500000	1.234286E-06	9.283517E-17	1.621364E-16	2.356568E-15	99.997203	2.999999
0.58	1.732569E+16	67.666667	1.234286E-06	9.748629E-17	1.649808E-16	2.439254E-15	99.997107	2.999999
0.59	1.732567E+16	68.833333	1.234286E-06	1.022896E-16	1.678253E-16	2.523366E-15	99.997009	2.999999
0.60	1.732566E+16	70.000000	1.234286E-06	1.072475E-16	1.706697E-16	2.608903E-15	99.996909	2.999999
0.61	1.732564E+16	71.166667	1.234286E-06	1.123624E-16	1.735141E-16	2.695866E-15	99.996807	2.999999
0.62	1.732562E+16	72.333333	1.234286E-06	1.176369E-16	1.763586E-16	2.784255E-15	99.996704	2.999999
0.63	1.732560E+16	73.500000	1.234286E-06	1.230732E-16	1.792030E-16	2.874069E-15	99.996599	2.999999
0.64	1.732558E+16	74.666667	1.234286E-06	1.286739E-16	1.820474E-16	2.965308E-15	99.996492	2.999999
0.65	1.732556E+16	75.833333	1.234286E-06	1.344415E-16	1.848919E-16	3.057974E-15	99.996383	2.999999
0.66	1.732555E+16	77.000000	1.234286E-06	1.403783E-16	1.877363E-16	3.152064E-15	99.996273	2.999999
0.67	1.732553E+16	78.166667	1.234286E-06	1.464867E-16	1.905807E-16	3.247581E-15	99.996161	2.999999
0.68	1.732551E+16	79.333333	1.234286E-06	1.527693E-16	1.934251E-16	3.344523E-15	99.996048	2.999999
0.69	1.732549E+16	80.500000	1.234286E-06	1.592285E-16	1.962695E-16	3.442890E-15	99.995932	2.999999
0.70	1.732547E+16	81.666667	1.234286E-06	1.658667E-16	1.991139E-16	3.542683E-15	99.995815	2.999999
0.71	1.732545E+16	82.833333	1.234286E-06	1.726863E-16	2.019583E-16	3.643902E-15	99.995697	2.999999
0.72	1.732542E+16	84.000000	1.234286E-06	1.796898E-16	2.048028E-16	3.746546E-15	99.995576	2.999999
0.73	1.732540E+16	85.166667	1.234286E-06	1.868797E-16	2.076472E-16	3.850616E-15	99.995454	2.999999
0.74	1.732538E+16	86.333333	1.234286E-06	1.942583E-16	2.104915E-16	3.956111E-15	99.995330	2.999999
0.75	1.732536E+16	87.500000	1.234286E-06	2.018281E-16	2.133359E-16	4.063032E-15	99.995204	2.999999
0.76	1.732534E+16	88.666667	1.234286E-06	2.095915E-16	2.161803E-16	4.171379E-15	99.995077	2.999999
0.77	1.732532E+16	89.833333	1.234286E-06	2.175511E-16	2.190247E-16	4.281151E-15	99.994948	2.999998
0.78	1.732529E+16	91.000000	1.234286E-06	2.257091E-16	2.218691E-16	4.392348E-15	99.994817	2.999998
0.79	1.732527E+16	92.166667	1.234286E-06	2.340681E-16	2.247135E-16	4.504971E-15	99.994684	2.999998
0.80	1.732525E+16	93.333333	1.234286E-06	2.426306E-16	2.275578E-16	4.619020E-15	99.994550	2.999998
0.81	1.732522E+16	94.500000	1.234286E-06	2.513989E-16	2.304022E-16	4.734494E-15	99.994414	2.999998
0.82	1.732520E+16	95.666667	1.234286E-06	2.603754E-16	2.332466E-16	4.851394E-15	99.994276	2.999998
0.83	1.732518E+16	96.833333	1.234286E-06	2.695627E-16	2.360909E-16	4.969719E-15	99.994137	2.999998
0.84	1.732515E+16	98.000000	1.234286E-06	2.789631E-16	2.389353E-16	5.089470E-15	99.993995	2.999998
0.85	1.732513E+16	99.166667	1.234286E-06	2.885792E-16	2.417797E-16	5.210646E-15	99.993852	2.999998
0.86	1.732510E+16	100.333333	1.234286E-06	2.984133E-16	2.446240E-16	5.333248E-15	99.993707	2.999998
0.87	1.732508E+16	101.500000	1.234286E-06	3.084679E-16	2.474684E-16	5.457276E-15	99.993561	2.999998
0.88	1.732505E+16	102.666667	1.234286E-06	3.187454E-16	2.503127E-16	5.582729E-15	99.993412	2.999998
0.89	1.732502E+16	103.833333	1.234286E-06	3.292482E-16	2.531570E-16	5.709607E-15	99.993262	2.999998
0.90	1.732500E+16	105.000000	1.234286E-06	3.399789E-16	2.560014E-16	5.837911E-15	99.993110	2.999998
0.91	1.732497E+16	106.166667	1.234286E-06	3.509398E-16	2.588457E-16	5.967641E-15	99.992956	2.999998
0.92	1.732494E+16	107.333333	1.234286E-06	3.621334E-16	2.616900E-16	6.098796E-15	99.992801	2.999998
0.93	1.732492E+16	108.500000	1.234286E-06	3.735621E-16	2.645343E-16	6.231376E-15	99.992644	2.999998
0.94	1.732489E+16	109.666667	1.234286E-06	3.852283E-16	2.673787E-16	6.365383E-15	99.992485	2.999998
0.95	1.732486E+16	110.833333	1.234286E-06	3.971346E-16	2.702230E-16	6.500814E-15	99.992324	2.999998
0.96	1.732483E+16	112.000000	1.234286E-06	4.092833E-16	2.730673E-16	6.637671E-15	99.992161	2.999998
0.97	1.732480E+16	113.166667	1.234286E-06	4.216769E-16	2.759116E-16	6.775954E-15	99.991997	2.999998
0.98	1.732478E+16	114.333333	1.234286E-06	4.343177E-16	2.787559E-16	6.915662E-15	99.991831	2.999998
0.99	1.732475E+16	115.500000	1.234286E-06	4.472084E-16	2.816002E-16	7.056796E-15	99.991663	2.999998
1.00	1.732472E+16	116.666667	1.234286E-06	4.603513E-16	2.844445E-16	7.199355E-15	99.991493	2.999997





$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732619E+16	1.166667	3.509924E-07	5.127199E-21	3.399507E-18	1.703789E-18	99.999995	3.000000
0.02	1.732619E+16	2.333333	4.963781E-07	2.263255E-20	6.799013E-18	5.111368E-18	99.999987	3.000000
0.03	1.732619E+16	3.500000	6.079365E-07	5.777114E-20	1.019852E-17	1.022274E-17	99.999978	3.000000
0.04	1.732619E+16	4.666667	7.019845E-07	1.148770E-19	1.359802E-17	1.703789E-17	99.999967	3.000000
0.05	1.732618E+16	5.833333	7.848425E-07	1.977241E-19	1.699753E-17	2.555684E-17	99.999954	3.000000
0.06	1.732618E+16	7.000000	8.597517E-07	3.096996E-19	2.039704E-17	3.577957E-17	99.999940	3.000000
0.07	1.732618E+16	8.166667	9.286378E-07	4.539030E-19	2.379654E-17	4.770609E-17	99.999923	3.000000
0.08	1.732617E+16	9.333333	9.927554E-07	6.332088E-19	2.719604E-17	6.133640E-17	99.999905	3.000000
0.09	1.732617E+16	10.500000	1.052976E-06	8.503094E-19	3.059555E-17	7.667050E-17	99.999884	3.000000
0.10	1.732617E+16	11.666667	1.109934E-06	1.107746E-18	3.399505E-17	9.370838E-17	99.999862	3.000000
0.11	1.732616E+16	12.833333	1.164108E-06	1.407931E-18	3.739455E-17	1.124500E-16	99.999838	3.000000
0.12	1.732616E+16	14.000000	1.215871E-06	1.753167E-18	4.079405E-17	1.328955E-16	99.999812	3.000000
0.13	1.732615E+16	15.166667	1.234286E-06	2.146127E-18	4.419355E-17	1.550447E-16	99.999784	3.000000
0.14	1.732615E+16	16.333333	1.234286E-06	2.589726E-18	4.759305E-17	1.788978E-16	99.999755	3.000000
0.15	1.732614E+16	17.500000	1.234286E-06	3.086882E-18	5.099255E-17	2.044546E-16	99.999723	3.000000
0.16	1.732614E+16	18.666667	1.234286E-06	3.640509E-18	5.439204E-17	2.317152E-16	99.999690	3.000000
0.17	1.732613E+16	19.833333	1.234286E-06	4.253524E-18	5.779154E-17	2.606795E-16	99.999654	3.000000
0.18	1.732612E+16	21.000000	1.234286E-06	4.928843E-18	6.119103E-17	2.913477E-16	99.999617	3.000000
0.19	1.732612E+16	22.166667	1.234286E-06	5.669382E-18	6.459053E-17	3.237196E-16	99.999578	3.000000
0.20	1.732611E+16	23.333333	1.234286E-06	6.478057E-18	6.799002E-17	3.577954E-16	99.999537	3.000000
0.21	1.732610E+16	24.500000	1.234286E-06	7.357784E-18	7.138951E-17	3.935749E-16	99.999494	3.000000
0.22	1.732610E+16	25.666667	1.234286E-06	8.311478E-18	7.478900E-17	4.310581E-16	99.999449	3.000000
0.23	1.732609E+16	26.833333	1.234286E-06	9.342057E-18	7.818848E-17	4.702452E-16	99.999403	3.000000
0.24	1.732608E+16	28.000000	1.234286E-06	1.045244E-17	8.158797E-17	5.111360E-16	99.999354	3.000000
0.25	1.732607E+16	29.166667	1.234286E-06	1.164553E-17	8.498745E-17	5.537306E-16	99.999304	3.000000
0.26	1.732606E+16	30.333333	1.234286E-06	1.292426E-17	8.838693E-17	5.980290E-16	99.999251	3.000000
0.27	1.732605E+16	31.500000	1.234286E-06	1.429153E-17	9.178641E-17	6.440312E-16	99.999197	3.000000
0.28	1.732604E+16	32.666667	1.234286E-06	1.575027E-17	9.518589E-17	6.917371E-16	99.999140	3.000000
0.29	1.732603E+16	33.833333	1.234286E-06	1.730339E-17	9.858537E-17	7.411468E-16	99.999082	3.000000
0.30	1.732602E+16	35.000000	1.234286E-06	1.895380E-17	1.019848E-16	7.922603E-16	99.999022	3.000000
0.31	1.732601E+16	36.166667	1.234286E-06	2.070443E-17	1.053843E-16	8.450775E-16	99.998960	3.000000
0.32	1.732600E+16	37.333333	1.234286E-06	2.255818E-17	1.087838E-16	8.995985E-16	99.998896	3.000000
0.33	1.732599E+16	38.500000	1.234286E-06	2.451798E-17	1.121833E-16	9.558233E-16	99.998830	3.000000
0.34	1.732598E+16	39.666667	1.234286E-06	2.658673E-17	1.155827E-16	1.013752E-15	99.998762	3.000000
0.35	1.732596E+16	40.833333	1.234286E-06	2.876737E-17	1.189822E-16	1.073384E-15	99.998692	3.000000
0.36	1.732595E+16	42.000000	1.234286E-06	3.106279E-17	1.223816E-16	1.134720E-15	99.998621	3.000000
0.37	1.732594E+16	43.166667	1.234286E-06	3.347592E-17	1.257811E-16	1.197760E-15	99.998547	3.000000
0.38	1.732593E+16	44.333333	1.234286E-06	3.600968E-17	1.291806E-16	1.262504E-15	99.998471	3.000000
0.39	1.732591E+16	45.500000	1.234286E-06	3.866697E-17	1.325800E-16	1.328951E-15	99.998393	3.000000
0.40	1.732590E+16	46.666667	1.234286E-06	4.145072E-17	1.359795E-16	1.397102E-15	99.998314	3.000000
0.41	1.732588E+16	47.833333	1.234286E-06	4.436384E-17	1.393789E-16	1.466957E-15	99.998232	2.999999
0.42	1.732587E+16	49.000000	1.234286E-06	4.740925E-17	1.427784E-16	1.538515E-15	99.998149	2.999999
0.43	1.732586E+16	50.166667	1.234286E-06	5.058986E-17	1.461778E-16	1.611778E-15	99.998063	2.999999
0.44	1.732584E+16	51.333333	1.234286E-06	5.390860E-17	1.495772E-16	1.686744E-15	99.997976	2.999999
0.45	1.732582E+16	52.500000	1.234286E-06	5.736836E-17	1.529767E-16	1.763414E-15	99.997886	2.999999

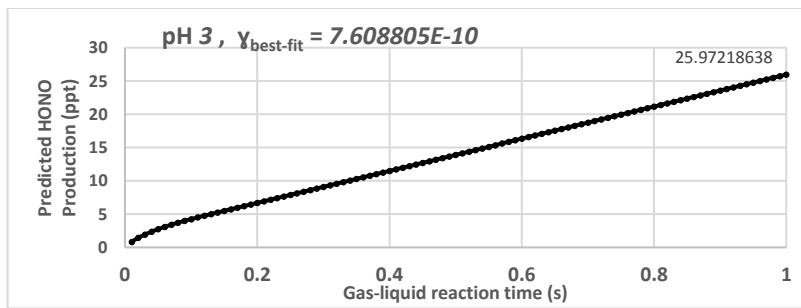
0.46	1.732581E+16	53.666667	1.234286E-06	6.097208E-17	1.563761E-16	1.841787E-15	99.997795	2.999999
0.47	1.732579E+16	54.833333	1.234286E-06	6.472266E-17	1.597755E-16	1.921865E-15	99.997702	2.999999
0.48	1.732578E+16	56.000000	1.234286E-06	6.862303E-17	1.631750E-16	2.003646E-15	99.997606	2.999999
0.49	1.732576E+16	57.166667	1.234286E-06	7.267609E-17	1.665744E-16	2.087131E-15	99.997509	2.999999
0.50	1.732574E+16	58.333333	1.234286E-06	7.688477E-17	1.699738E-16	2.172319E-15	99.997409	2.999999
0.51	1.732572E+16	59.500000	1.234286E-06	8.125198E-17	1.733732E-16	2.259211E-15	99.997308	2.999999
0.52	1.732571E+16	60.666667	1.234286E-06	8.578064E-17	1.767726E-16	2.347807E-15	99.997205	2.999999
0.53	1.732569E+16	61.833333	1.234286E-06	9.047366E-17	1.801721E-16	2.438107E-15	99.997099	2.999999
0.54	1.732567E+16	63.000000	1.234286E-06	9.533396E-17	1.835715E-16	2.530111E-15	99.996992	2.999999
0.55	1.732565E+16	64.166667	1.234286E-06	1.003644E-16	1.869709E-16	2.623818E-15	99.996883	2.999999
0.56	1.732563E+16	65.333333	1.234286E-06	1.055680E-16	1.903703E-16	2.719229E-15	99.996771	2.999999
0.57	1.732561E+16	66.500000	1.234286E-06	1.109477E-16	1.937697E-16	2.816343E-15	99.996658	2.999999
0.58	1.732559E+16	67.666667	1.234286E-06	1.165062E-16	1.971690E-16	2.915162E-15	99.996542	2.999999
0.59	1.732557E+16	68.833333	1.234286E-06	1.222467E-16	2.005684E-16	3.015684E-15	99.996425	2.999999
0.60	1.732555E+16	70.000000	1.234286E-06	1.281719E-16	2.039678E-16	3.117910E-15	99.996305	2.999999
0.61	1.732553E+16	71.166667	1.234286E-06	1.342848E-16	2.073672E-16	3.221839E-15	99.996184	2.999999
0.62	1.732551E+16	72.333333	1.234286E-06	1.405882E-16	2.107666E-16	3.327472E-15	99.996060	2.999999
0.63	1.732549E+16	73.500000	1.234286E-06	1.470853E-16	2.141659E-16	3.434809E-15	99.995935	2.999999
0.64	1.732546E+16	74.666667	1.234286E-06	1.537787E-16	2.175653E-16	3.543850E-15	99.995807	2.999999
0.65	1.732544E+16	75.833333	1.234286E-06	1.606715E-16	2.209647E-16	3.654594E-15	99.995678	2.999999
0.66	1.732542E+16	77.000000	1.234286E-06	1.677666E-16	2.243640E-16	3.767042E-15	99.995546	2.999999
0.67	1.732540E+16	78.166667	1.234286E-06	1.750668E-16	2.277634E-16	3.881194E-15	99.995412	2.999999
0.68	1.732537E+16	79.333333	1.234286E-06	1.825752E-16	2.311627E-16	3.997050E-15	99.995277	2.999999
0.69	1.732535E+16	80.500000	1.234286E-06	1.902945E-16	2.345621E-16	4.114609E-15	99.995139	2.999999
0.70	1.732532E+16	81.666667	1.234286E-06	1.982278E-16	2.379614E-16	4.233872E-15	99.994999	2.999999
0.71	1.732530E+16	82.833333	1.234286E-06	2.063780E-16	2.413608E-16	4.354838E-15	99.994857	2.999998
0.72	1.732528E+16	84.000000	1.234286E-06	2.147479E-16	2.447601E-16	4.477508E-15	99.994713	2.999998
0.73	1.732525E+16	85.166667	1.234286E-06	2.233405E-16	2.481594E-16	4.601882E-15	99.994567	2.999998
0.74	1.732522E+16	86.333333	1.234286E-06	2.321587E-16	2.515587E-16	4.727960E-15	99.994419	2.999998
0.75	1.732520E+16	87.500000	1.234286E-06	2.412053E-16	2.549581E-16	4.855741E-15	99.994269	2.999998
0.76	1.732517E+16	88.666667	1.234286E-06	2.504835E-16	2.583574E-16	4.985226E-15	99.994117	2.999998
0.77	1.732515E+16	89.833333	1.234286E-06	2.599959E-16	2.617567E-16	5.116414E-15	99.993962	2.999998
0.78	1.732512E+16	91.000000	1.234286E-06	2.697456E-16	2.651560E-16	5.249307E-15	99.993806	2.999998
0.79	1.732509E+16	92.166667	1.234286E-06	2.797355E-16	2.685553E-16	5.383903E-15	99.993647	2.999998
0.80	1.732506E+16	93.333333	1.234286E-06	2.899685E-16	2.719546E-16	5.520202E-15	99.993487	2.999998
0.81	1.732503E+16	94.500000	1.234286E-06	3.004475E-16	2.753539E-16	5.658205E-15	99.993324	2.999998
0.82	1.732501E+16	95.666667	1.234286E-06	3.111754E-16	2.787531E-16	5.797912E-15	99.993159	2.999998
0.83	1.732498E+16	96.833333	1.234286E-06	3.221551E-16	2.821524E-16	5.939323E-15	99.992993	2.999998
0.84	1.732495E+16	98.000000	1.234286E-06	3.333896E-16	2.855517E-16	6.082437E-15	99.992824	2.999998
0.85	1.732492E+16	99.166667	1.234286E-06	3.448817E-16	2.889509E-16	6.227255E-15	99.992653	2.999998
0.86	1.732489E+16	100.333333	1.234286E-06	3.566344E-16	2.923502E-16	6.373776E-15	99.992479	2.999998
0.87	1.732486E+16	101.500000	1.234286E-06	3.686507E-16	2.957494E-16	6.522001E-15	99.992304	2.999998
0.88	1.732483E+16	102.666667	1.234286E-06	3.809333E-16	2.991487E-16	6.671930E-15	99.992127	2.999998
0.89	1.732480E+16	103.833333	1.234286E-06	3.934853E-16	3.025479E-16	6.823562E-15	99.991947	2.999998
0.90	1.732476E+16	105.000000	1.234286E-06	4.063095E-16	3.059472E-16	6.976898E-15	99.991766	2.999998
0.91	1.732473E+16	106.166667	1.234286E-06	4.194089E-16	3.093464E-16	7.131938E-15	99.991582	2.999997
0.92	1.732470E+16	107.333333	1.234286E-06	4.327863E-16	3.127456E-16	7.288681E-15	99.991396	2.999997
0.93	1.732467E+16	108.500000	1.234286E-06	4.464448E-16	3.161448E-16	7.447128E-15	99.991208	2.999997
0.94	1.732463E+16	109.666667	1.234286E-06	4.603871E-16	3.195440E-16	7.607278E-15	99.991018	2.999997
0.95	1.732460E+16	110.833333	1.234286E-06	4.746163E-16	3.229432E-16	7.769132E-15	99.990826	2.999997
0.96	1.732457E+16	112.000000	1.234286E-06	4.891352E-16	3.263424E-16	7.932690E-15	99.990632	2.999997
0.97	1.732453E+16	113.166667	1.234286E-06	5.039467E-16	3.297416E-16	8.097951E-15	99.990435	2.999997
0.98	1.732450E+16	114.333333	1.234286E-06	5.190538E-16	3.331408E-16	8.264916E-15	99.990237	2.999997
0.99	1.732446E+16	115.500000	1.234286E-06	5.344595E-16	3.365400E-16	8.433584E-15	99.990036	2.999997
1.00	1.732443E+16	116.666667	1.234286E-06	5.501665E-16	3.399391E-16	8.603956E-15	99.989833	2.999997



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732619E+16	1.166667	3.509924E-07	4.782948E-21	3.171257E-18	1.589393E-18	99.999995	3.000000
0.02	1.732619E+16	2.333333	4.963781E-07	2.111295E-20	6.342513E-18	4.768180E-18	99.999988	3.000000
0.03	1.732619E+16	3.500000	6.079365E-07	5.389227E-20	9.513769E-18	9.536359E-18	99.999980	3.000000
0.04	1.732619E+16	4.666667	7.019846E-07	1.071639E-19	1.268503E-17	1.589393E-17	99.999969	3.000000
0.05	1.732618E+16	5.833333	7.848425E-07	1.844485E-19	1.585628E-17	2.384090E-17	99.999957	3.000000
0.06	1.732618E+16	7.000000	8.597518E-07	2.889057E-19	1.902754E-17	3.337725E-17	99.999944	3.000000
0.07	1.732618E+16	8.166667	9.286379E-07	4.234270E-19	2.219879E-17	4.450300E-17	99.999928	3.000000
0.08	1.732618E+16	9.333333	9.927555E-07	5.906938E-19	2.537004E-17	5.721815E-17	99.999911	3.000000
0.09	1.732617E+16	10.500000	1.052976E-06	7.932179E-19	2.854130E-17	7.152268E-17	99.999892	3.000000
0.10	1.732617E+16	11.666667	1.109934E-06	1.033370E-18	3.171255E-17	8.741660E-17	99.999871	3.000000
0.11	1.732616E+16	12.833333	1.164108E-06	1.313400E-18	3.488380E-17	1.048999E-16	99.999849	3.000000
0.12	1.732616E+16	14.000000	1.215871E-06	1.635456E-18	3.805505E-17	1.239726E-16	99.999825	3.000000
0.13	1.732616E+16	15.166667	1.234286E-06	2.002031E-18	4.122630E-17	1.446347E-16	99.999799	3.000000
0.14	1.732615E+16	16.333333	1.234286E-06	2.415847E-18	4.439755E-17	1.668862E-16	99.999771	3.000000
0.15	1.732615E+16	17.500000	1.234286E-06	2.879622E-18	4.756880E-17	1.907271E-16	99.999742	3.000000
0.16	1.732614E+16	18.666667	1.234286E-06	3.396077E-18	5.074005E-17	2.161573E-16	99.999711	3.000000
0.17	1.732614E+16	19.833333	1.234286E-06	3.967933E-18	5.391130E-17	2.431770E-16	99.999678	3.000000
0.18	1.732613E+16	21.000000	1.234286E-06	4.597910E-18	5.708254E-17	2.717860E-16	99.999643	3.000000
0.19	1.732612E+16	22.166667	1.234286E-06	5.288728E-18	6.025379E-17	3.019844E-16	99.999606	3.000000
0.20	1.732612E+16	23.333333	1.234286E-06	6.043107E-18	6.342503E-17	3.337722E-16	99.999568	3.000000
0.21	1.732611E+16	24.500000	1.234286E-06	6.863767E-18	6.659627E-17	3.671494E-16	99.999528	3.000000
0.22	1.732610E+16	25.666667	1.234286E-06	7.753428E-18	6.976751E-17	4.021160E-16	99.999486	3.000000
0.23	1.732609E+16	26.833333	1.234286E-06	8.714812E-18	7.293875E-17	4.386720E-16	99.999443	3.000000
0.24	1.732609E+16	28.000000	1.234286E-06	9.750637E-18	7.610999E-17	4.768173E-16	99.999397	3.000000
0.25	1.732608E+16	29.166667	1.234286E-06	1.086362E-17	7.928123E-17	5.165520E-16	99.999350	3.000000
0.26	1.732607E+16	30.333333	1.234286E-06	1.205649E-17	8.245246E-17	5.578761E-16	99.999301	3.000000
0.27	1.732606E+16	31.500000	1.234286E-06	1.333197E-17	8.562370E-17	6.007896E-16	99.999251	3.000000
0.28	1.732605E+16	32.666667	1.234286E-06	1.469276E-17	8.879493E-17	6.452925E-16	99.999198	3.000000
0.29	1.732604E+16	33.833333	1.234286E-06	1.614160E-17	9.196616E-17	6.913847E-16	99.999144	3.000000
0.30	1.732603E+16	35.000000	1.234286E-06	1.768120E-17	9.513739E-17	7.390663E-16	99.999088	3.000000
0.31	1.732602E+16	36.166667	1.234286E-06	1.931429E-17	9.830861E-17	7.883373E-16	99.999030	3.000000
0.32	1.732601E+16	37.333333	1.234286E-06	2.104358E-17	1.014798E-16	8.391977E-16	99.998970	3.000000
0.33	1.732600E+16	38.500000	1.234286E-06	2.287179E-17	1.046511E-16	8.916474E-16	99.998909	3.000000
0.34	1.732599E+16	39.666667	1.234286E-06	2.480165E-17	1.078223E-16	9.456865E-16	99.998845	3.000000
0.35	1.732598E+16	40.833333	1.234286E-06	2.683587E-17	1.109935E-16	1.001315E-15	99.998780	3.000000
0.36	1.732597E+16	42.000000	1.234286E-06	2.897717E-17	1.141647E-16	1.058533E-15	99.998713	3.000000
0.37	1.732596E+16	43.166667	1.234286E-06	3.122828E-17	1.173359E-16	1.117340E-15	99.998644	3.000000
0.38	1.732594E+16	44.333333	1.234286E-06	3.359192E-17	1.205071E-16	1.177737E-15	99.998574	3.000000
0.39	1.732593E+16	45.500000	1.234286E-06	3.607080E-17	1.236784E-16	1.239723E-15	99.998501	3.000000
0.40	1.732592E+16	46.666667	1.234286E-06	3.866764E-17	1.268496E-16	1.303298E-15	99.998427	3.000000
0.41	1.732591E+16	47.833333	1.234286E-06	4.138517E-17	1.300208E-16	1.368463E-15	99.998351	3.000000
0.42	1.732589E+16	49.000000	1.234286E-06	4.422610E-17	1.331920E-16	1.435217E-15	99.998273	2.999999
0.43	1.732588E+16	50.166667	1.234286E-06	4.719316E-17	1.363632E-16	1.503560E-15	99.998193	2.999999
0.44	1.732586E+16	51.333333	1.234286E-06	5.028907E-17	1.395344E-16	1.573493E-15	99.998112	2.999999
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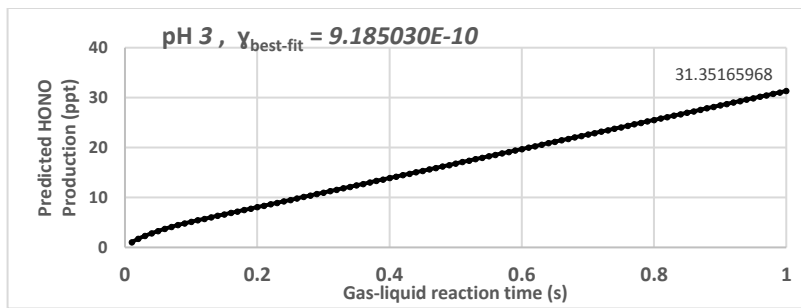
0.46	1.732583E+16	53.666667	1.234286E-06	5.687830E-17	1.458768E-16	1.718126E-15	99.997943	2.999999
0.47	1.732582E+16	54.833333	1.234286E-06	6.037706E-17	1.490480E-16	1.792827E-15	99.997856	2.999999
0.48	1.732580E+16	56.000000	1.234286E-06	6.401555E-17	1.522191E-16	1.869117E-15	99.997767	2.999999
0.49	1.732579E+16	57.166667	1.234286E-06	6.779649E-17	1.553903E-16	1.946997E-15	99.997676	2.999999
0.50	1.732577E+16	58.333333	1.234286E-06	7.172259E-17	1.585615E-16	2.026466E-15	99.997583	2.999999
0.51	1.732576E+16	59.500000	1.234286E-06	7.579658E-17	1.617327E-16	2.107524E-15	99.997489	2.999999
0.52	1.732574E+16	60.666667	1.234286E-06	8.002117E-17	1.649039E-16	2.190172E-15	99.997392	2.999999
0.53	1.732572E+16	61.833333	1.234286E-06	8.439910E-17	1.680750E-16	2.274408E-15	99.997294	2.999999
0.54	1.732570E+16	63.000000	1.234286E-06	8.893307E-17	1.712462E-16	2.360235E-15	99.997194	2.999999
0.55	1.732569E+16	64.166667	1.234286E-06	9.362580E-17	1.744174E-16	2.447650E-15	99.997092	2.999999
0.56	1.732567E+16	65.333333	1.234286E-06	9.848002E-17	1.775885E-16	2.536655E-15	99.996988	2.999999
0.57	1.732565E+16	66.500000	1.234286E-06	1.034985E-16	1.807597E-16	2.627249E-15	99.996882	2.999999
0.58	1.732563E+16	67.666667	1.234286E-06	1.086838E-16	1.839309E-16	2.719433E-15	99.996774	2.999999
0.59	1.732561E+16	68.833333	1.234286E-06	1.140388E-16	1.871020E-16	2.813206E-15	99.996665	2.999999
0.60	1.732559E+16	70.000000	1.234286E-06	1.195662E-16	1.902732E-16	2.908568E-15	99.996553	2.999999
0.61	1.732557E+16	71.166667	1.234286E-06	1.252686E-16	1.934443E-16	3.005520E-15	99.996440	2.999999
0.62	1.732555E+16	72.333333	1.234286E-06	1.311489E-16	1.966154E-16	3.104061E-15	99.996325	2.999999
0.63	1.732553E+16	73.500000	1.234286E-06	1.372097E-16	1.997866E-16	3.204191E-15	99.996208	2.999999
0.64	1.732551E+16	74.666667	1.234286E-06	1.434537E-16	2.029577E-16	3.305911E-15	99.996089	2.999999
0.65	1.732549E+16	75.833333	1.234286E-06	1.498838E-16	2.061288E-16	3.409219E-15	99.995968	2.999999
0.66	1.732547E+16	77.000000	1.234286E-06	1.565025E-16	2.093000E-16	3.514118E-15	99.995845	2.999999
0.67	1.732545E+16	78.166667	1.234286E-06	1.633126E-16	2.124711E-16	3.620605E-15	99.995720	2.999999
0.68	1.732543E+16	79.333333	1.234286E-06	1.703168E-16	2.156422E-16	3.728682E-15	99.995594	2.999999
0.69	1.732541E+16	80.500000	1.234286E-06	1.775179E-16	2.188133E-16	3.838348E-15	99.995465	2.999999
0.70	1.732538E+16	81.666667	1.234286E-06	1.849185E-16	2.219845E-16	3.949603E-15	99.995335	2.999999
0.71	1.732536E+16	82.833333	1.234286E-06	1.925215E-16	2.251556E-16	4.062448E-15	99.995202	2.999999
0.72	1.732534E+16	84.000000	1.234286E-06	2.003294E-16	2.283267E-16	4.176882E-15	99.995068	2.999999
0.73	1.732531E+16	85.166667	1.234286E-06	2.083451E-16	2.314978E-16	4.292905E-15	99.994932	2.999998
0.74	1.732529E+16	86.333333	1.234286E-06	2.165712E-16	2.346689E-16	4.410518E-15	99.994794	2.999998
0.75	1.732526E+16	87.500000	1.234286E-06	2.250105E-16	2.378399E-16	4.529720E-15	99.994654	2.999998
0.76	1.732524E+16	88.666667	1.234286E-06	2.336656E-16	2.410110E-16	4.650511E-15	99.994512	2.999998
0.77	1.732522E+16	89.833333	1.234286E-06	2.425394E-16	2.441821E-16	4.772892E-15	99.994368	2.999998
0.78	1.732519E+16	91.000000	1.234286E-06	2.516345E-16	2.473532E-16	4.896861E-15	99.994222	2.999998
0.79	1.732516E+16	92.166667	1.234286E-06	2.609537E-16	2.505243E-16	5.022420E-15	99.994074	2.999998
0.80	1.732514E+16	93.333333	1.234286E-06	2.704996E-16	2.536953E-16	5.149569E-15	99.993924	2.999998
0.81	1.732511E+16	94.500000	1.234286E-06	2.802750E-16	2.568664E-16	5.278306E-15	99.993772	2.999998
0.82	1.732509E+16	95.666667	1.234286E-06	2.902826E-16	2.600375E-16	5.408633E-15	99.993619	2.999998
0.83	1.732506E+16	96.833333	1.234286E-06	3.005252E-16	2.632085E-16	5.540549E-15	99.993463	2.999998
0.84	1.732503E+16	98.000000	1.234286E-06	3.110054E-16	2.663796E-16	5.674055E-15	99.993305	2.999998
0.85	1.732500E+16	99.166667	1.234286E-06	3.217259E-16	2.695506E-16	5.809150E-15	99.993146	2.999998
0.86	1.732498E+16	100.333333	1.234286E-06	3.326896E-16	2.727216E-16	5.945834E-15	99.992984	2.999998
0.87	1.732495E+16	101.500000	1.234286E-06	3.438990E-16	2.758927E-16	6.084107E-15	99.992821	2.999998
0.88	1.732492E+16	102.666667	1.234286E-06	3.553570E-16	2.790637E-16	6.223969E-15	99.992656	2.999998
0.89	1.732489E+16	103.833333	1.234286E-06	3.670662E-16	2.822347E-16	6.365421E-15	99.992488	2.999998
0.90	1.732486E+16	105.000000	1.234286E-06	3.790294E-16	2.854058E-16	6.508462E-15	99.992319	2.999998
0.91	1.732483E+16	106.166667	1.234286E-06	3.912493E-16	2.885768E-16	6.653092E-15	99.992147	2.999998
0.92	1.732480E+16	107.333333	1.234286E-06	4.037286E-16	2.917478E-16	6.799312E-15	99.991974	2.999998
0.93	1.732477E+16	108.500000	1.234286E-06	4.164700E-16	2.949188E-16	6.947120E-15	99.991799	2.999998
0.94	1.732474E+16	109.666667	1.234286E-06	4.294762E-16	2.980898E-16	7.096518E-15	99.991621	2.999998
0.95	1.732471E+16	110.833333	1.234286E-06	4.427500E-16	3.012608E-16	7.247505E-15	99.991442	2.999997
0.96	1.732468E+16	112.000000	1.234286E-06	4.562941E-16	3.044318E-16	7.400082E-15	99.991261	2.999997
0.97	1.732465E+16	113.166667	1.234286E-06	4.701112E-16	3.076027E-16	7.554247E-15	99.991077	2.999997
0.98	1.732461E+16	114.333333	1.234286E-06	4.842041E-16	3.107737E-16	7.710002E-15	99.990892	2.999997
0.99	1.732458E+16	115.500000	1.234286E-06	4.985753E-16	3.139447E-16	7.867346E-15	99.990705	2.999997
1.00	1.732455E+16	116.666667	1.234286E-06	5.132278E-16	3.171156E-16	8.026280E-15	99.990516	2.999997

TWO LAMPS



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732619E+16	1.166667	3.509923E-07	2.199369E-20	1.458256E-17	7.308592E-18	99.999977	3.000000
0.02	1.732618E+16	2.333333	4.963779E-07	9.708483E-20	2.916511E-17	2.192577E-17	99.999945	3.000000
0.03	1.732617E+16	3.500000	6.079361E-07	2.478157E-19	4.374766E-17	4.385154E-17	99.999906	3.000000
0.04	1.732617E+16	4.666667	7.019838E-07	4.927776E-19	5.833020E-17	7.308589E-17	99.999859	3.000000
0.05	1.732616E+16	5.833333	7.848413E-07	8.481594E-19	7.291274E-17	1.096288E-16	99.999804	3.000000
0.06	1.732615E+16	7.000000	8.597500E-07	1.328491E-18	8.749526E-17	1.534803E-16	99.999741	3.000000
0.07	1.732613E+16	8.166667	9.286355E-07	1.947067E-18	1.020778E-16	2.046404E-16	99.999669	3.000000
0.08	1.732612E+16	9.333333	9.927523E-07	2.716219E-18	1.166603E-16	2.631090E-16	99.999590	3.000000
0.09	1.732611E+16	10.500000	1.052972E-06	3.647497E-18	1.312428E-16	3.288862E-16	99.999503	3.000000
0.10	1.732609E+16	11.666667	1.109929E-06	4.751799E-18	1.458252E-16	4.019719E-16	99.999408	3.000000
0.11	1.732607E+16	12.833333	1.164102E-06	6.039477E-18	1.604077E-16	4.823662E-16	99.999305	3.000000
0.12	1.732605E+16	14.000000	1.215863E-06	7.520405E-18	1.749902E-16	5.700690E-16	99.999194	3.000000
0.13	1.732603E+16	15.166667	1.234286E-06	9.206048E-18	1.895726E-16	6.650803E-16	99.999075	3.000000
0.14	1.732601E+16	16.333333	1.234286E-06	1.110892E-17	2.041550E-16	7.674001E-16	99.998948	3.000000
0.15	1.732599E+16	17.500000	1.234286E-06	1.324152E-17	2.187374E-16	8.770284E-16	99.998812	3.000000
0.16	1.732596E+16	18.666667	1.234286E-06	1.561636E-17	2.333198E-16	9.939652E-16	99.998669	3.000000
0.17	1.732593E+16	19.833333	1.234286E-06	1.824595E-17	2.479021E-16	1.118210E-15	99.998518	3.000000
0.18	1.732591E+16	21.000000	1.234286E-06	2.114280E-17	2.624844E-16	1.249764E-15	99.998358	3.000000
0.19	1.732588E+16	22.166667	1.234286E-06	2.431942E-17	2.770667E-16	1.388626E-15	99.998190	3.000000
0.20	1.732585E+16	23.333333	1.234286E-06	2.778831E-17	2.916490E-16	1.534797E-15	99.998014	2.999999
0.21	1.732582E+16	24.500000	1.234286E-06	3.156198E-17	3.062313E-16	1.688276E-15	99.997830	2.999999
0.22	1.732578E+16	25.666667	1.234286E-06	3.565294E-17	3.208135E-16	1.849063E-15	99.997638	2.999999
0.23	1.732575E+16	26.833333	1.234286E-06	4.007370E-17	3.353957E-16	2.017159E-15	99.997438	2.999999
0.24	1.732571E+16	28.000000	1.234286E-06	4.483677E-17	3.499779E-16	2.192563E-15	99.997229	2.999999
0.25	1.732567E+16	29.166667	1.234286E-06	4.995465E-17	3.645600E-16	2.375276E-15	99.997012	2.999999
0.26	1.732563E+16	30.333333	1.234286E-06	5.543986E-17	3.791421E-16	2.565296E-15	99.996787	2.999999
0.27	1.732559E+16	31.500000	1.234286E-06	6.130489E-17	3.937242E-16	2.762626E-15	99.996554	2.999999
0.28	1.732555E+16	32.666667	1.234286E-06	6.756227E-17	4.083062E-16	2.967263E-15	99.996313	2.999999
0.29	1.732551E+16	33.833333	1.234286E-06	7.422449E-17	4.228882E-16	3.179208E-15	99.996063	2.999999
0.30	1.732546E+16	35.000000	1.234286E-06	8.130406E-17	4.374702E-16	3.398462E-15	99.995805	2.999999
0.31	1.732542E+16	36.166667	1.234286E-06	8.881349E-17	4.520521E-16	3.625024E-15	99.995539	2.999999
0.32	1.732537E+16	37.333333	1.234286E-06	9.676530E-17	4.666340E-16	3.858895E-15	99.995264	2.999999
0.33	1.732532E+16	38.500000	1.234286E-06	1.051720E-16	4.812158E-16	4.100073E-15	99.994981	2.999999
0.34	1.732527E+16	39.666667	1.234286E-06	1.140460E-16	4.957976E-16	4.348560E-15	99.994690	2.999998
0.35	1.732522E+16	40.833333	1.234286E-06	1.234000E-16	5.103794E-16	4.604354E-15	99.994391	2.999998
0.36	1.732517E+16	42.000000	1.234286E-06	1.332463E-16	5.249611E-16	4.867457E-15	99.994083	2.999998
0.37	1.732511E+16	43.166667	1.234286E-06	1.435976E-16	5.395428E-16	5.137868E-15	99.993766	2.999998
0.38	1.732505E+16	44.333333	1.234286E-06	1.544663E-16	5.541244E-16	5.415587E-15	99.993442	2.999998
0.39	1.732500E+16	45.500000	1.234286E-06	1.658649E-16	5.687060E-16	5.700614E-15	99.993109	2.999998
0.40	1.732494E+16	46.666667	1.234286E-06	1.778059E-16	5.832875E-16	5.992949E-15	99.992767	2.999998
0.41	1.732488E+16	47.833333	1.234286E-06	1.903018E-16	5.978690E-16	6.292591E-15	99.992417	2.999998
0.42	1.732482E+16	49.000000	1.234286E-06	2.033652E-16	6.124504E-16	6.599542E-15	99.992059	2.999998
0.43	1.732475E+16	50.166667	1.234286E-06	2.170086E-16	6.270318E-16	6.913801E-15	99.991692	2.999998
0.44	1.732469E+16	51.333333	1.234286E-06	2.312443E-16	6.416131E-16	7.235367E-15	99.991317	2.999997
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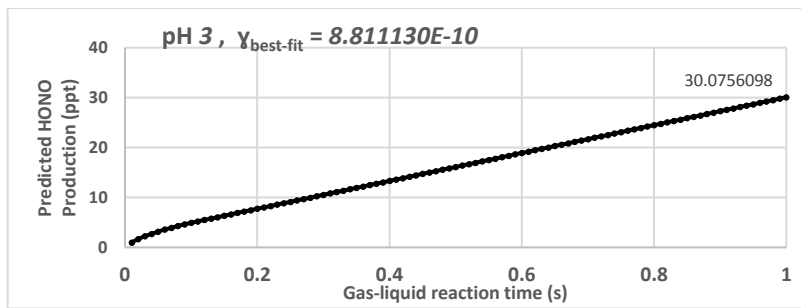
0.46	1.732455E+16	53.666667	1.234286E-06	2.615433E-16	6.707756E-16	7.900423E-15	99.990541	2.999997
0.47	1.732448E+16	54.833333	1.234286E-06	2.776315E-16	6.853568E-16	8.243913E-15	99.990141	2.999997
0.48	1.732441E+16	56.000000	1.234286E-06	2.943622E-16	6.999379E-16	8.594710E-15	99.989731	2.999997
0.49	1.732434E+16	57.166667	1.234286E-06	3.117478E-16	7.145189E-16	8.952816E-15	99.989314	2.999997
0.50	1.732427E+16	58.333333	1.234286E-06	3.298010E-16	7.290999E-16	9.318228E-15	99.988887	2.999997
0.51	1.732419E+16	59.500000	1.234286E-06	3.485341E-16	7.436808E-16	9.690949E-15	99.988453	2.999997
0.52	1.732411E+16	60.666667	1.234286E-06	3.679598E-16	7.582617E-16	1.007098E-14	99.988009	2.999996
0.53	1.732404E+16	61.833333	1.234286E-06	3.880904E-16	7.728424E-16	1.045831E-14	99.987557	2.999996
0.54	1.732396E+16	63.000000	1.234286E-06	4.089386E-16	7.874232E-16	1.085296E-14	99.987097	2.999996
0.55	1.732387E+16	64.166667	1.234286E-06	4.305168E-16	8.020038E-16	1.125491E-14	99.986628	2.999996
0.56	1.732379E+16	65.333333	1.234286E-06	4.528375E-16	8.165844E-16	1.166416E-14	99.986150	2.999996
0.57	1.732371E+16	66.500000	1.234286E-06	4.759132E-16	8.311649E-16	1.208073E-14	99.985663	2.999996
0.58	1.732362E+16	67.666667	1.234286E-06	4.997565E-16	8.457454E-16	1.250460E-14	99.985168	2.999996
0.59	1.732353E+16	68.833333	1.234286E-06	5.243798E-16	8.603258E-16	1.293578E-14	99.984665	2.999995
0.60	1.732345E+16	70.000000	1.234286E-06	5.497957E-16	8.749061E-16	1.337427E-14	99.984152	2.999995
0.61	1.732336E+16	71.166667	1.234286E-06	5.760166E-16	8.894863E-16	1.382006E-14	99.983631	2.999995
0.62	1.732326E+16	72.333333	1.234286E-06	6.030551E-16	9.040664E-16	1.427316E-14	99.983101	2.999995
0.63	1.732317E+16	73.500000	1.234286E-06	6.309236E-16	9.186465E-16	1.473357E-14	99.982563	2.999995
0.64	1.732308E+16	74.666667	1.234286E-06	6.596347E-16	9.332265E-16	1.520129E-14	99.982016	2.999995
0.65	1.732298E+16	75.833333	1.234286E-06	6.892009E-16	9.478064E-16	1.567631E-14	99.981460	2.999994
0.66	1.732288E+16	77.000000	1.234286E-06	7.196346E-16	9.623863E-16	1.615864E-14	99.980895	2.999994
0.67	1.732278E+16	78.166667	1.234286E-06	7.509484E-16	9.769660E-16	1.664828E-14	99.980321	2.999994
0.68	1.732268E+16	79.333333	1.234286E-06	7.831548E-16	9.915457E-16	1.714522E-14	99.979739	2.999994
0.69	1.732258E+16	80.500000	1.234286E-06	8.162663E-16	1.006125E-15	1.764947E-14	99.979148	2.999994
0.70	1.732247E+16	81.666667	1.234286E-06	8.502953E-16	1.020705E-15	1.816103E-14	99.978548	2.999994
0.71	1.732237E+16	82.833333	1.234286E-06	8.852545E-16	1.035284E-15	1.867989E-14	99.977939	2.999993
0.72	1.732226E+16	84.000000	1.234286E-06	9.211562E-16	1.049864E-15	1.920606E-14	99.977322	2.999993
0.73	1.732215E+16	85.166667	1.234286E-06	9.580131E-16	1.064443E-15	1.973954E-14	99.976696	2.999993
0.74	1.732204E+16	86.333333	1.234286E-06	9.958375E-16	1.079022E-15	2.028032E-14	99.976060	2.999993
0.75	1.732193E+16	87.500000	1.234286E-06	1.034642E-15	1.093601E-15	2.082841E-14	99.975416	2.999993
0.76	1.732182E+16	88.666667	1.234286E-06	1.074439E-15	1.108180E-15	2.138380E-14	99.974763	2.999992
0.77	1.732170E+16	89.833333	1.234286E-06	1.115241E-15	1.122759E-15	2.194651E-14	99.974101	2.999992
0.78	1.732159E+16	91.000000	1.234286E-06	1.157061E-15	1.137338E-15	2.251652E-14	99.973431	2.999992
0.79	1.732147E+16	92.166667	1.234286E-06	1.199911E-15	1.151916E-15	2.309383E-14	99.972751	2.999992
0.80	1.732135E+16	93.333333	1.234286E-06	1.243804E-15	1.166495E-15	2.367845E-14	99.972062	2.999992
0.81	1.732123E+16	94.500000	1.234286E-06	1.288752E-15	1.181073E-15	2.427038E-14	99.971365	2.999991
0.82	1.732111E+16	95.666667	1.234286E-06	1.334767E-15	1.195652E-15	2.486961E-14	99.970658	2.999991
0.83	1.732098E+16	96.833333	1.234286E-06	1.381862E-15	1.210230E-15	2.547615E-14	99.969942	2.999991
0.84	1.732086E+16	98.000000	1.234286E-06	1.430050E-15	1.224808E-15	2.609000E-14	99.969218	2.999991
0.85	1.732073E+16	99.166667	1.234286E-06	1.479344E-15	1.239386E-15	2.671115E-14	99.968484	2.999991
0.86	1.732060E+16	100.333333	1.234286E-06	1.529754E-15	1.253964E-15	2.733960E-14	99.967742	2.999990
0.87	1.732047E+16	101.500000	1.234286E-06	1.581295E-15	1.268542E-15	2.797537E-14	99.966990	2.999990
0.88	1.732034E+16	102.666667	1.234286E-06	1.633979E-15	1.283120E-15	2.861844E-14	99.966229	2.999990
0.89	1.732021E+16	103.833333	1.234286E-06	1.687818E-15	1.297697E-15	2.926881E-14	99.965460	2.999990
0.90	1.732007E+16	105.000000	1.234286E-06	1.742824E-15	1.312275E-15	2.992649E-14	99.964681	2.999989
0.91	1.731994E+16	106.166667	1.234286E-06	1.799010E-15	1.326852E-15	3.059147E-14	99.963893	2.999989
0.92	1.731980E+16	107.333333	1.234286E-06	1.856389E-15	1.341430E-15	3.126376E-14	99.963096	2.999989
0.93	1.731966E+16	108.500000	1.234286E-06	1.914973E-15	1.356007E-15	3.194336E-14	99.962290	2.999989
0.94	1.731952E+16	109.666667	1.234286E-06	1.974775E-15	1.370584E-15	3.263026E-14	99.961475	2.999989
0.95	1.731937E+16	110.833333	1.234286E-06	2.035807E-15	1.385161E-15	3.332447E-14	99.960650	2.999988
0.96	1.731923E+16	112.000000	1.234286E-06	2.098082E-15	1.399738E-15	3.402598E-14	99.959817	2.999988
0.97	1.731908E+16	113.166667	1.234286E-06	2.161611E-15	1.414314E-15	3.473480E-14	99.958974	2.999988
0.98	1.731894E+16	114.333333	1.234286E-06	2.226409E-15	1.428891E-15	3.545092E-14	99.958122	2.999988
0.99	1.731879E+16	115.500000	1.234286E-06	2.292486E-15	1.443468E-15	3.617434E-14	99.957261	2.999987
1.00	1.731864E+16	116.666667	1.234286E-06	2.359856E-15	1.458044E-15	3.690507E-14	99.956391	2.999987



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732619E+16	1.166667	3.509923E-07	2.654986E-20	1.760345E-17	8.822625E-18	99.999972	3.000000
0.02	1.732618E+16	2.333333	4.963779E-07	1.171967E-19	3.520690E-17	2.646787E-17	99.999934	3.000000
0.03	1.732617E+16	3.500000	6.079360E-07	2.991528E-19	5.281034E-17	5.293574E-17	99.999886	3.000000
0.04	1.732616E+16	4.666667	7.019836E-07	5.948605E-19	7.041376E-17	8.822621E-17	99.999829	3.000000
0.05	1.732615E+16	5.833333	7.848410E-07	1.023862E-18	8.801718E-17	1.323393E-16	99.999763	3.000000
0.06	1.732614E+16	7.000000	8.597496E-07	1.603698E-18	1.056206E-16	1.852750E-16	99.999687	3.000000
0.07	1.732612E+16	8.166667	9.286349E-07	2.350418E-18	1.232240E-16	2.470332E-16	99.999601	3.000000
0.08	1.732611E+16	9.333333	9.927515E-07	3.278906E-18	1.408273E-16	3.176141E-16	99.999506	3.000000
0.09	1.732609E+16	10.500000	1.052971E-06	4.403105E-18	1.584307E-16	3.970175E-16	99.999400	3.000000
0.10	1.732607E+16	11.666667	1.109927E-06	5.736173E-18	1.760340E-16	4.852435E-16	99.999286	3.000000
0.11	1.732605E+16	12.833333	1.164100E-06	7.290603E-18	1.936373E-16	5.822920E-16	99.999161	3.000000
0.12	1.732602E+16	14.000000	1.215861E-06	9.078317E-18	2.112406E-16	6.881630E-16	99.999027	3.000000
0.13	1.732600E+16	15.166667	1.234286E-06	1.111316E-17	2.288439E-16	8.028566E-16	99.998883	3.000000
0.14	1.732597E+16	16.333333	1.234286E-06	1.341022E-17	2.464471E-16	9.263727E-16	99.998730	3.000000
0.15	1.732594E+16	17.500000	1.234286E-06	1.598460E-17	2.640503E-16	1.058711E-15	99.998566	3.000000
0.16	1.732591E+16	18.666667	1.234286E-06	1.885141E-17	2.816535E-16	1.199872E-15	99.998393	3.000000
0.17	1.732588E+16	19.833333	1.234286E-06	2.202574E-17	2.992567E-16	1.349856E-15	99.998210	3.000000
0.18	1.732585E+16	21.000000	1.234286E-06	2.552270E-17	3.168598E-16	1.508662E-15	99.998018	2.999999
0.19	1.732581E+16	22.166667	1.234286E-06	2.935737E-17	3.344629E-16	1.676290E-15	99.997815	2.999999
0.20	1.732578E+16	23.333333	1.234286E-06	3.354487E-17	3.520659E-16	1.852741E-15	99.997603	2.999999
0.21	1.732574E+16	24.500000	1.234286E-06	3.810028E-17	3.696689E-16	2.038014E-15	99.997381	2.999999
0.22	1.732570E+16	25.666667	1.234286E-06	4.303871E-17	3.872719E-16	2.232109E-15	99.997149	2.999999
0.23	1.732566E+16	26.833333	1.234286E-06	4.837527E-17	4.048748E-16	2.435027E-15	99.996907	2.999999
0.24	1.732561E+16	28.000000	1.234286E-06	5.412503E-17	4.224777E-16	2.646767E-15	99.996655	2.999999
0.25	1.732557E+16	29.166667	1.234286E-06	6.030312E-17	4.400805E-16	2.867329E-15	99.996394	2.999999
0.26	1.732552E+16	30.333333	1.234286E-06	6.692462E-17	4.576833E-16	3.096713E-15	99.996122	2.999999
0.27	1.732547E+16	31.500000	1.234286E-06	7.400463E-17	4.752861E-16	3.334920E-15	99.995840	2.999999
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0.29	1.732537E+16	33.833333	1.234286E-06	8.960059E-17	5.104914E-16	3.837800E-15	99.995248	2.999999
0.30	1.732531E+16	35.000000	1.234286E-06	9.814673E-17	5.280940E-16	4.102473E-15	99.994936	2.999999
0.31	1.732526E+16	36.166667	1.234286E-06	1.072118E-16	5.456965E-16	4.375968E-15	99.994615	2.999998
0.32	1.732520E+16	37.333333	1.234286E-06	1.168108E-16	5.632990E-16	4.658285E-15	99.994283	2.999998
0.33	1.732514E+16	38.500000	1.234286E-06	1.269590E-16	5.809014E-16	4.949424E-15	99.993942	2.999998
0.34	1.732508E+16	39.666667	1.234286E-06	1.376714E-16	5.985037E-16	5.249386E-15	99.993590	2.999998
0.35	1.732502E+16	40.833333	1.234286E-06	1.489630E-16	6.161060E-16	5.558169E-15	99.993229	2.999998
0.36	1.732495E+16	42.000000	1.234286E-06	1.608491E-16	6.337083E-16	5.875774E-15	99.992857	2.999998
0.37	1.732489E+16	43.166667	1.234286E-06	1.733447E-16	6.513104E-16	6.202200E-15	99.992475	2.999998
0.38	1.732482E+16	44.333333	1.234286E-06	1.864648E-16	6.689125E-16	6.537449E-15	99.992083	2.999998
0.39	1.732475E+16	45.500000	1.234286E-06	2.002247E-16	6.865145E-16	6.881520E-15	99.991681	2.999998
0.40	1.732468E+16	46.666667	1.234286E-06	2.146393E-16	7.041165E-16	7.234412E-15	99.991269	2.999997
0.41	1.732461E+16	47.833333	1.234286E-06	2.297238E-16	7.217184E-16	7.596125E-15	99.990847	2.999997
0.42	1.732453E+16	49.000000	1.234286E-06	2.454933E-16	7.393202E-16	7.966661E-15	99.990414	2.999997
0.43	1.732445E+16	50.166667	1.234286E-06	2.619629E-16	7.569219E-16	8.346018E-15	99.989971	2.999997
0.44	1.732438E+16	51.333333	1.234286E-06	2.791476E-16	7.745236E-16	8.734197E-15	99.989518	2.999997
0.45	1.732429E+16	52.500000	1.234286E-06	2.970627E-16	7.921252E-16	9.131197E-15	99.989055	2.999997

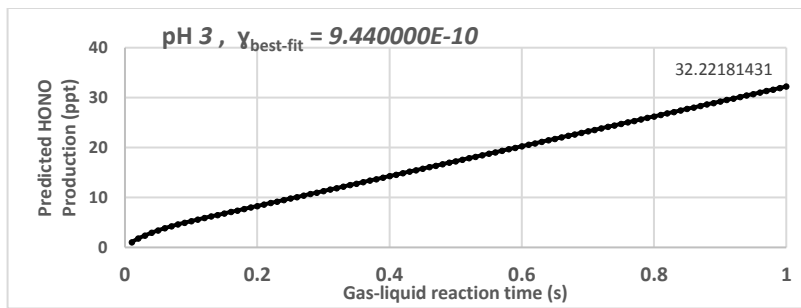


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0.47	1.732413E+16	54.833333	1.234286E-06	3.351440E-16	8.273281E-16	9.951661E-15	99.988098	2.999996
0.48	1.732404E+16	56.000000	1.234286E-06	3.553404E-16	8.449294E-16	1.037513E-14	99.987604	2.999996
0.49	1.732396E+16	57.166667	1.234286E-06	3.763275E-16	8.625306E-16	1.080741E-14	99.987100	2.999996
0.50	1.732387E+16	58.333333	1.234286E-06	3.981203E-16	8.801318E-16	1.124852E-14	99.986585	2.999996
0.51	1.732378E+16	59.500000	1.234286E-06	4.207341E-16	8.977328E-16	1.169845E-14	99.986060	2.999996
0.52	1.732368E+16	60.666667	1.234286E-06	4.441837E-16	9.153338E-16	1.215719E-14	99.985525	2.999996
0.53	1.732359E+16	61.833333	1.234286E-06	4.684844E-16	9.329347E-16	1.262476E-14	99.984980	2.999996
0.54	1.732349E+16	63.000000	1.234286E-06	4.936512E-16	9.505354E-16	1.310116E-14	99.984424	2.999995
0.55	1.732339E+16	64.166667	1.234286E-06	5.196993E-16	9.681361E-16	1.358637E-14	99.983857	2.999995
0.56	1.732329E+16	65.333333	1.234286E-06	5.466437E-16	9.857367E-16	1.408040E-14	99.983281	2.999995
0.57	1.732319E+16	66.500000	1.234286E-06	5.744995E-16	1.003337E-15	1.458326E-14	99.982693	2.999995
0.58	1.732309E+16	67.666667	1.234286E-06	6.032819E-16	1.020938E-15	1.509493E-14	99.982096	2.999995
0.59	1.732298E+16	68.833333	1.234286E-06	6.330058E-16	1.038538E-15	1.561542E-14	99.981488	2.999995
0.60	1.732288E+16	70.000000	1.234286E-06	6.636865E-16	1.056138E-15	1.614474E-14	99.980869	2.999994
0.61	1.732277E+16	71.166667	1.234286E-06	6.953390E-16	1.073738E-15	1.668288E-14	99.980240	2.999994
0.62	1.732266E+16	72.333333	1.234286E-06	7.279783E-16	1.091338E-15	1.722983E-14	99.979601	2.999994
0.63	1.732254E+16	73.500000	1.234286E-06	7.616197E-16	1.108938E-15	1.778561E-14	99.978951	2.999994
0.64	1.732243E+16	74.666667	1.234286E-06	7.962781E-16	1.126538E-15	1.835021E-14	99.978290	2.999994
0.65	1.732231E+16	75.833333	1.234286E-06	8.319687E-16	1.144137E-15	1.892363E-14	99.977619	2.999993
0.66	1.732220E+16	77.000000	1.234286E-06	8.687066E-16	1.161737E-15	1.950587E-14	99.976937	2.999993
0.67	1.732208E+16	78.166667	1.234286E-06	9.065069E-16	1.179336E-15	2.009692E-14	99.976245	2.999993
0.68	1.732195E+16	79.333333	1.234286E-06	9.453846E-16	1.196935E-15	2.069680E-14	99.975542	2.999993
0.69	1.732183E+16	80.500000	1.234286E-06	9.853548E-16	1.214534E-15	2.130550E-14	99.974829	2.999993
0.70	1.732170E+16	81.666667	1.234286E-06	1.026433E-15	1.232133E-15	2.192302E-14	99.974104	2.999992
0.71	1.732158E+16	82.833333	1.234286E-06	1.068633E-15	1.249732E-15	2.254936E-14	99.973370	2.999992
0.72	1.732145E+16	84.000000	1.234286E-06	1.111972E-15	1.267331E-15	2.318452E-14	99.972624	2.999992
0.73	1.732132E+16	85.166667	1.234286E-06	1.156463E-15	1.284930E-15	2.382850E-14	99.971868	2.999992
0.74	1.732118E+16	86.333333	1.234286E-06	1.202123E-15	1.302528E-15	2.448129E-14	99.971101	2.999991
0.75	1.732105E+16	87.500000	1.234286E-06	1.248965E-15	1.320127E-15	2.514291E-14	99.970324	2.999991
0.76	1.732091E+16	88.666667	1.234286E-06	1.297006E-15	1.337725E-15	2.581335E-14	99.969536	2.999991
0.77	1.732077E+16	89.833333	1.234286E-06	1.346260E-15	1.355323E-15	2.649260E-14	99.968737	2.999991
0.78	1.732063E+16	91.000000	1.234286E-06	1.396742E-15	1.372921E-15	2.718068E-14	99.967927	2.999990
0.79	1.732049E+16	92.166667	1.234286E-06	1.448468E-15	1.390519E-15	2.787757E-14	99.967106	2.999990
0.80	1.732035E+16	93.333333	1.234286E-06	1.501452E-15	1.408116E-15	2.858329E-14	99.966275	2.999990
0.81	1.732020E+16	94.500000	1.234286E-06	1.555710E-15	1.425714E-15	2.929782E-14	99.965433	2.999990
0.82	1.732005E+16	95.666667	1.234286E-06	1.611257E-15	1.443311E-15	3.002117E-14	99.964580	2.999989
0.83	1.731990E+16	96.833333	1.234286E-06	1.668108E-15	1.460908E-15	3.075334E-14	99.963716	2.999989
0.84	1.731975E+16	98.000000	1.234286E-06	1.726277E-15	1.478505E-15	3.149433E-14	99.962842	2.999989
0.85	1.731960E+16	99.166667	1.234286E-06	1.785780E-15	1.496102E-15	3.224414E-14	99.961956	2.999989
0.86	1.731944E+16	100.333333	1.234286E-06	1.846633E-15	1.513699E-15	3.300276E-14	99.961060	2.999988
0.87	1.731929E+16	101.500000	1.234286E-06	1.908850E-15	1.531296E-15	3.377021E-14	99.960152	2.999988
0.88	1.731913E+16	102.666667	1.234286E-06	1.972446E-15	1.548892E-15	3.454647E-14	99.959234	2.999988
0.89	1.731897E+16	103.833333	1.234286E-06	2.037436E-15	1.566488E-15	3.533155E-14	99.958305	2.999988
0.90	1.731880E+16	105.000000	1.234286E-06	2.103836E-15	1.584084E-15	3.612545E-14	99.957365	2.999987
0.91	1.731864E+16	106.166667	1.234286E-06	2.171660E-15	1.601680E-15	3.692817E-14	99.956414	2.999987
0.92	1.731847E+16	107.333333	1.234286E-06	2.240924E-15	1.619276E-15	3.773971E-14	99.955452	2.999987
0.93	1.731830E+16	108.500000	1.234286E-06	2.311643E-15	1.636872E-15	3.856006E-14	99.954479	2.999986
0.94	1.731813E+16	109.666667	1.234286E-06	2.383831E-15	1.654467E-15	3.938923E-14	99.953494	2.999986
0.95	1.731796E+16	110.833333	1.234286E-06	2.457505E-15	1.672063E-15	4.022722E-14	99.952499	2.999986
0.96	1.731779E+16	112.000000	1.234286E-06	2.532678E-15	1.689658E-15	4.107403E-14	99.951493	2.999986
0.97	1.731761E+16	113.166667	1.234286E-06	2.609366E-15	1.707253E-15	4.192965E-14	99.950476	2.999985
0.98	1.731743E+16	114.333333	1.234286E-06	2.687585E-15	1.724847E-15	4.279409E-14	99.949448	2.999985
0.99	1.731725E+16	115.500000	1.234286E-06	2.767348E-15	1.742442E-15	4.366735E-14	99.948408	2.999985
1.00	1.731707E+16	116.666667	1.234286E-06	2.848672E-15	1.760036E-15	4.454943E-14	99.947358	2.999984



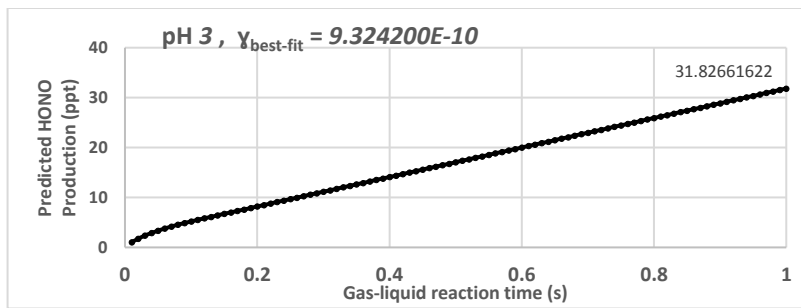
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732619E+16	1.166667	3.509923E-07	2.546908E-20	1.688686E-17	8.463478E-18	99.999973	3.000000
0.02	1.732618E+16	2.333333	4.963779E-07	1.124259E-19	3.377371E-17	2.539043E-17	99.999937	3.000000
0.03	1.732617E+16	3.500000	6.079360E-07	2.869750E-19	5.066056E-17	5.078085E-17	99.999891	3.000000
0.04	1.732616E+16	4.666667	7.019836E-07	5.706452E-19	6.754740E-17	8.463474E-17	99.999836	3.000000
0.05	1.732615E+16	5.833333	7.848410E-07	9.821836E-19	8.443422E-17	1.269521E-16	99.999773	3.000000
0.06	1.732614E+16	7.000000	8.597497E-07	1.538416E-18	1.013210E-16	1.777329E-16	99.999700	3.000000
0.07	1.732612E+16	8.166667	9.286350E-07	2.254738E-18	1.182078E-16	2.369771E-16	99.999617	3.000000
0.08	1.732611E+16	9.333333	9.927517E-07	3.145430E-18	1.350946E-16	3.046848E-16	99.999526	3.000000
0.09	1.732609E+16	10.500000	1.052971E-06	4.223866E-18	1.519814E-16	3.808559E-16	99.999425	3.000000
0.10	1.732607E+16	11.666667	1.109928E-06	5.502667E-18	1.688681E-16	4.654904E-16	99.999315	3.000000
0.11	1.732605E+16	12.833333	1.164101E-06	6.993821E-18	1.857549E-16	5.585884E-16	99.999195	3.000000
0.12	1.732603E+16	14.000000	1.215862E-06	8.708761E-18	2.026416E-16	6.601497E-16	99.999067	3.000000
0.13	1.732601E+16	15.166667	1.234286E-06	1.066077E-17	2.195283E-16	7.701744E-16	99.998929	3.000000
0.14	1.732598E+16	16.333333	1.234286E-06	1.286432E-17	2.364149E-16	8.886624E-16	99.998781	3.000000
0.15	1.732595E+16	17.500000	1.234286E-06	1.533391E-17	2.533016E-16	1.015614E-15	99.998625	3.000000
0.16	1.732592E+16	18.666667	1.234286E-06	1.808402E-17	2.701882E-16	1.151029E-15	99.998459	3.000000
0.17	1.732589E+16	19.833333	1.234286E-06	2.112913E-17	2.870748E-16	1.294907E-15	99.998283	3.000000
0.18	1.732586E+16	21.000000	1.234286E-06	2.448373E-17	3.039613E-16	1.447248E-15	99.998098	2.999999
0.19	1.732583E+16	22.166667	1.234286E-06	2.816231E-17	3.208478E-16	1.608053E-15	99.997904	2.999999
0.20	1.732579E+16	23.333333	1.234286E-06	3.217934E-17	3.377343E-16	1.777320E-15	99.997701	2.999999
0.21	1.732576E+16	24.500000	1.234286E-06	3.654932E-17	3.546208E-16	1.955052E-15	99.997487	2.999999
0.22	1.732572E+16	25.666667	1.234286E-06	4.128672E-17	3.715072E-16	2.141246E-15	99.997265	2.999999
0.23	1.732568E+16	26.833333	1.234286E-06	4.640603E-17	3.883935E-16	2.335903E-15	99.997033	2.999999
0.24	1.732564E+16	28.000000	1.234286E-06	5.192175E-17	4.052799E-16	2.539024E-15	99.996791	2.999999
0.25	1.732559E+16	29.166667	1.234286E-06	5.784834E-17	4.221662E-16	2.750608E-15	99.996540	2.999999
0.26	1.732555E+16	30.333333	1.234286E-06	6.420029E-17	4.390524E-16	2.970655E-15	99.996280	2.999999
0.27	1.732550E+16	31.500000	1.234286E-06	7.099210E-17	4.559386E-16	3.199165E-15	99.996010	2.999999
0.28	1.732545E+16	32.666667	1.234286E-06	7.823824E-17	4.728248E-16	3.436138E-15	99.995730	2.999999
0.29	1.732540E+16	33.833333	1.234286E-06	8.595319E-17	4.897109E-16	3.681574E-15	99.995441	2.999999
0.30	1.732535E+16	35.000000	1.234286E-06	9.415145E-17	5.065969E-16	3.935473E-15	99.995142	2.999999
0.31	1.732530E+16	36.166667	1.234286E-06	1.028475E-16	5.234830E-16	4.197835E-15	99.994834	2.999999
0.32	1.732524E+16	37.333333	1.234286E-06	1.120558E-16	5.403689E-16	4.468660E-15	99.994516	2.999998
0.33	1.732518E+16	38.500000	1.234286E-06	1.217909E-16	5.572548E-16	4.747948E-15	99.994188	2.999998
0.34	1.732513E+16	39.666667	1.234286E-06	1.320672E-16	5.741407E-16	5.035699E-15	99.993851	2.999998
0.35	1.732507E+16	40.833333	1.234286E-06	1.428992E-16	5.910265E-16	5.331913E-15	99.993504	2.999998
0.36	1.732500E+16	42.000000	1.234286E-06	1.543014E-16	6.079122E-16	5.636589E-15	99.993148	2.999998
0.37	1.732494E+16	43.166667	1.234286E-06	1.662883E-16	6.247979E-16	5.949728E-15	99.992781	2.999998
0.38	1.732488E+16	44.333333	1.234286E-06	1.788744E-16	6.416835E-16	6.271330E-15	99.992405	2.999998
0.39	1.732481E+16	45.500000	1.234286E-06	1.920741E-16	6.585690E-16	6.601395E-15	99.992020	2.999998
0.40	1.732474E+16	46.666667	1.234286E-06	2.059020E-16	6.754545E-16	6.939922E-15	99.991624	2.999998
0.41	1.732467E+16	47.833333	1.234286E-06	2.203724E-16	6.923399E-16	7.286912E-15	99.991219	2.999997
0.42	1.732460E+16	49.000000	1.234286E-06	2.355000E-16	7.092253E-16	7.642364E-15	99.990804	2.999997
0.43	1.732452E+16	50.166667	1.234286E-06	2.512992E-16	7.261105E-16	8.006279E-15	99.990380	2.999997
0.44	1.732445E+16	51.333333	1.234286E-06	2.677844E-16	7.429957E-16	8.378657E-15	99.989945	2.999997
0.45	1.732437E+16	52.500000	1.234286E-06	2.849702E-16	7.598809E-16	8.759497E-15	99.989501	2.999997

0.46	1.732429E+16	53.666667	1.234286E-06	3.028710E-16	7.767659E-16	9.148799E-15	99.989047	2.999997
0.47	1.732421E+16	54.833333	1.234286E-06	3.215013E-16	7.936509E-16	9.546564E-15	99.988583	2.999997
0.48	1.732413E+16	56.000000	1.234286E-06	3.408757E-16	8.105358E-16	9.952791E-15	99.988109	2.999996
0.49	1.732405E+16	57.166667	1.234286E-06	3.610084E-16	8.274206E-16	1.036748E-14	99.987625	2.999996
0.50	1.732396E+16	58.333333	1.234286E-06	3.819142E-16	8.443054E-16	1.079063E-14	99.987131	2.999996
0.51	1.732387E+16	59.500000	1.234286E-06	4.036074E-16	8.611900E-16	1.122224E-14	99.986628	2.999996
0.52	1.732379E+16	60.666667	1.234286E-06	4.261025E-16	8.780746E-16	1.166232E-14	99.986114	2.999996
0.53	1.732369E+16	61.833333	1.234286E-06	4.494140E-16	8.949591E-16	1.211086E-14	99.985591	2.999996
0.54	1.732360E+16	63.000000	1.234286E-06	4.735564E-16	9.118435E-16	1.256786E-14	99.985058	2.999996
0.55	1.732351E+16	64.166667	1.234286E-06	4.985442E-16	9.287278E-16	1.303332E-14	99.984514	2.999995
0.56	1.732341E+16	65.333333	1.234286E-06	5.243918E-16	9.456120E-16	1.350724E-14	99.983961	2.999995
0.57	1.732331E+16	66.500000	1.234286E-06	5.511137E-16	9.624961E-16	1.398963E-14	99.983398	2.999995
0.58	1.732322E+16	67.666667	1.234286E-06	5.787245E-16	9.793802E-16	1.448048E-14	99.982825	2.999995
0.59	1.732311E+16	68.833333	1.234286E-06	6.072385E-16	9.962641E-16	1.497978E-14	99.982241	2.999995
0.60	1.732301E+16	70.000000	1.234286E-06	6.366703E-16	1.013148E-15	1.548755E-14	99.981648	2.999995
0.61	1.732291E+16	71.166667	1.234286E-06	6.670344E-16	1.030032E-15	1.600379E-14	99.981045	2.999994
0.62	1.732280E+16	72.333333	1.234286E-06	6.983451E-16	1.046915E-15	1.652848E-14	99.980431	2.999994
0.63	1.732269E+16	73.500000	1.234286E-06	7.306171E-16	1.063799E-15	1.706163E-14	99.979807	2.999994
0.64	1.732258E+16	74.666667	1.234286E-06	7.638648E-16	1.080682E-15	1.760325E-14	99.979174	2.999994
0.65	1.732247E+16	75.833333	1.234286E-06	7.981026E-16	1.097566E-15	1.815333E-14	99.978530	2.999994
0.66	1.732236E+16	77.000000	1.234286E-06	8.333451E-16	1.114449E-15	1.871187E-14	99.977876	2.999993
0.67	1.732224E+16	78.166667	1.234286E-06	8.696067E-16	1.131332E-15	1.927887E-14	99.977212	2.999993
0.68	1.732213E+16	79.333333	1.234286E-06	9.069019E-16	1.148215E-15	1.985433E-14	99.976538	2.999993
0.69	1.732201E+16	80.500000	1.234286E-06	9.452452E-16	1.165098E-15	2.043825E-14	99.975853	2.999993
0.70	1.732189E+16	81.666667	1.234286E-06	9.846510E-16	1.181981E-15	2.103064E-14	99.975159	2.999993
0.71	1.732176E+16	82.833333	1.234286E-06	1.025134E-15	1.198863E-15	2.163148E-14	99.974454	2.999992
0.72	1.732164E+16	84.000000	1.234286E-06	1.066708E-15	1.215746E-15	2.224079E-14	99.973739	2.999992
0.73	1.732152E+16	85.166667	1.234286E-06	1.109389E-15	1.232628E-15	2.285855E-14	99.973013	2.999992
0.74	1.732139E+16	86.333333	1.234286E-06	1.153190E-15	1.249510E-15	2.348478E-14	99.972278	2.999992
0.75	1.732126E+16	87.500000	1.234286E-06	1.198125E-15	1.266393E-15	2.411947E-14	99.971532	2.999992
0.76	1.732113E+16	88.666667	1.234286E-06	1.244211E-15	1.283275E-15	2.476261E-14	99.970776	2.999991
0.77	1.732099E+16	89.833333	1.234286E-06	1.291460E-15	1.300157E-15	2.541422E-14	99.970009	2.999991
0.78	1.732086E+16	91.000000	1.234286E-06	1.339887E-15	1.317038E-15	2.607429E-14	99.969232	2.999991
0.79	1.732072E+16	92.166667	1.234286E-06	1.389508E-15	1.333920E-15	2.674282E-14	99.968445	2.999991
0.80	1.732059E+16	93.333333	1.234286E-06	1.440335E-15	1.350802E-15	2.741981E-14	99.967648	2.999990
0.81	1.732045E+16	94.500000	1.234286E-06	1.492385E-15	1.367683E-15	2.810526E-14	99.966840	2.999990
0.82	1.732030E+16	95.666667	1.234286E-06	1.545671E-15	1.384564E-15	2.879917E-14	99.966022	2.999990
0.83	1.732016E+16	96.833333	1.234286E-06	1.600207E-15	1.401445E-15	2.950154E-14	99.965193	2.999990
0.84	1.732002E+16	98.000000	1.234286E-06	1.656009E-15	1.418326E-15	3.021237E-14	99.964354	2.999989
0.85	1.731987E+16	99.166667	1.234286E-06	1.713091E-15	1.435207E-15	3.093166E-14	99.963505	2.999989
0.86	1.731972E+16	100.333333	1.234286E-06	1.771466E-15	1.452088E-15	3.165941E-14	99.962645	2.999989
0.87	1.731957E+16	101.500000	1.234286E-06	1.831151E-15	1.468968E-15	3.239562E-14	99.961774	2.999989
0.88	1.731942E+16	102.666667	1.234286E-06	1.892158E-15	1.485849E-15	3.314028E-14	99.960893	2.999988
0.89	1.731926E+16	103.833333	1.234286E-06	1.954503E-15	1.502729E-15	3.389341E-14	99.960002	2.999988
0.90	1.731910E+16	105.000000	1.234286E-06	2.018200E-15	1.519609E-15	3.465500E-14	99.959100	2.999988
0.91	1.731895E+16	106.166667	1.234286E-06	2.083264E-15	1.536489E-15	3.542505E-14	99.958188	2.999988
0.92	1.731879E+16	107.333333	1.234286E-06	2.149709E-15	1.553369E-15	3.620355E-14	99.957265	2.999987
0.93	1.731863E+16	108.500000	1.234286E-06	2.217549E-15	1.570249E-15	3.699052E-14	99.956331	2.999987
0.94	1.731846E+16	109.666667	1.234286E-06	2.286799E-15	1.587128E-15	3.778594E-14	99.955387	2.999987
0.95	1.731830E+16	110.833333	1.234286E-06	2.357474E-15	1.604007E-15	3.858982E-14	99.954433	2.999986
0.96	1.731813E+16	112.000000	1.234286E-06	2.429587E-15	1.620887E-15	3.940217E-14	99.953468	2.999986
0.97	1.731796E+16	113.166667	1.234286E-06	2.503154E-15	1.637766E-15	4.022297E-14	99.952492	2.999986
0.98	1.731779E+16	114.333333	1.234286E-06	2.578189E-15	1.654645E-15	4.105222E-14	99.951505	2.999986
0.99	1.731762E+16	115.500000	1.234286E-06	2.654706E-15	1.671523E-15	4.188994E-14	99.950508	2.999985
1.00	1.731744E+16	116.666667	1.234286E-06	2.732720E-15	1.688402E-15	4.273612E-14	99.949500	2.999985



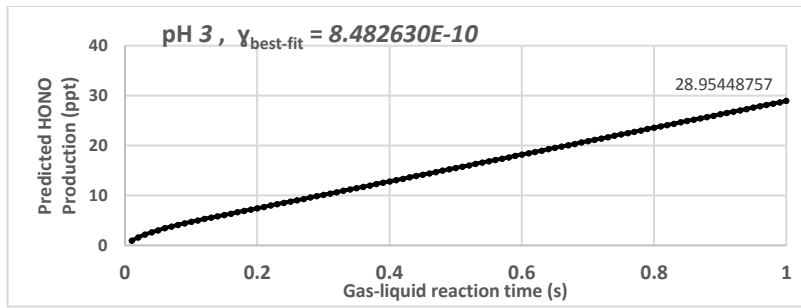
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732619E+16	1.166667	3.509923E-07	2.728686E-20	1.809211E-17	9.067535E-18	99.999971	3.000000
0.02	1.732618E+16	2.333333	4.963779E-07	1.204500E-19	3.618422E-17	2.720260E-17	99.999932	3.000000
0.03	1.732617E+16	3.500000	6.079359E-07	3.074570E-19	5.427631E-17	5.440519E-17	99.999883	3.000000
0.04	1.732616E+16	4.666667	7.019835E-07	6.113734E-19	7.236840E-17	9.067531E-17	99.999825	3.000000
0.05	1.732615E+16	5.833333	7.848409E-07	1.052284E-18	9.046047E-17	1.360129E-16	99.999756	3.000000
0.06	1.732614E+16	7.000000	8.597495E-07	1.648216E-18	1.085525E-16	1.904181E-16	99.999678	3.000000
0.07	1.732612E+16	8.166667	9.286348E-07	2.415664E-18	1.266446E-16	2.538907E-16	99.999590	3.000000
0.08	1.732610E+16	9.333333	9.927513E-07	3.369926E-18	1.447366E-16	3.264308E-16	99.999492	3.000000
0.09	1.732608E+16	10.500000	1.052971E-06	4.525332E-18	1.628286E-16	4.080384E-16	99.999384	3.000000
0.10	1.732606E+16	11.666667	1.109927E-06	5.895405E-18	1.809206E-16	4.987135E-16	99.999266	3.000000
0.11	1.732604E+16	12.833333	1.164100E-06	7.492986E-18	1.990126E-16	5.984560E-16	99.999138	3.000000
0.12	1.732602E+16	14.000000	1.215861E-06	9.330325E-18	2.171045E-16	7.072659E-16	99.999000	3.000000
0.13	1.732599E+16	15.166667	1.234286E-06	1.142165E-17	2.351964E-16	8.251433E-16	99.998852	3.000000
0.14	1.732596E+16	16.333333	1.234286E-06	1.378248E-17	2.532883E-16	9.520880E-16	99.998694	3.000000
0.15	1.732594E+16	17.500000	1.234286E-06	1.642832E-17	2.713802E-16	1.088100E-15	99.998527	3.000000
0.16	1.732591E+16	18.666667	1.234286E-06	1.937471E-17	2.894720E-16	1.233180E-15	99.998349	3.000000
0.17	1.732587E+16	19.833333	1.234286E-06	2.263716E-17	3.075638E-16	1.387327E-15	99.998161	3.000000
0.18	1.732584E+16	21.000000	1.234286E-06	2.623119E-17	3.256555E-16	1.550541E-15	99.997963	2.999999
0.19	1.732580E+16	22.166667	1.234286E-06	3.017231E-17	3.437472E-16	1.722822E-15	99.997755	2.999999
0.20	1.732576E+16	23.333333	1.234286E-06	3.447605E-17	3.618389E-16	1.904171E-15	99.997536	2.999999
0.21	1.732572E+16	24.500000	1.234286E-06	3.915792E-17	3.799306E-16	2.094587E-15	99.997308	2.999999
0.22	1.732568E+16	25.666667	1.234286E-06	4.423344E-17	3.980222E-16	2.294070E-15	99.997070	2.999999
0.23	1.732564E+16	26.833333	1.234286E-06	4.971812E-17	4.161137E-16	2.502621E-15	99.996821	2.999999
0.24	1.732560E+16	28.000000	1.234286E-06	5.562750E-17	4.342052E-16	2.720238E-15	99.996562	2.999999
0.25	1.732555E+16	29.166667	1.234286E-06	6.197708E-17	4.522967E-16	2.946923E-15	99.996293	2.999999
0.26	1.732550E+16	30.333333	1.234286E-06	6.878239E-17	4.703881E-16	3.182675E-15	99.996014	2.999999
0.27	1.732545E+16	31.500000	1.234286E-06	7.605893E-17	4.884795E-16	3.427494E-15	99.995725	2.999999
0.28	1.732540E+16	32.666667	1.234286E-06	8.382224E-17	5.065708E-16	3.681380E-15	99.995425	2.999999
0.29	1.732534E+16	33.833333	1.234286E-06	9.208782E-17	5.246620E-16	3.944333E-15	99.995116	2.999999
0.30	1.732529E+16	35.000000	1.234286E-06	1.008712E-16	5.427532E-16	4.216353E-15	99.994796	2.999999
0.31	1.732523E+16	36.166667	1.234286E-06	1.101879E-16	5.608444E-16	4.497440E-15	99.994465	2.999998
0.32	1.732517E+16	37.333333	1.234286E-06	1.200534E-16	5.789354E-16	4.787594E-15	99.994125	2.999998
0.33	1.732511E+16	38.500000	1.234286E-06	1.304833E-16	5.970264E-16	5.086815E-15	99.993774	2.999998
0.34	1.732505E+16	39.666667	1.234286E-06	1.414930E-16	6.151174E-16	5.395103E-15	99.993412	2.999998
0.35	1.732499E+16	40.833333	1.234286E-06	1.530981E-16	6.332083E-16	5.712457E-15	99.993041	2.999998
0.36	1.732492E+16	42.000000	1.234286E-06	1.653141E-16	6.512991E-16	6.038878E-15	99.992659	2.999998
0.37	1.732485E+16	43.166667	1.234286E-06	1.781565E-16	6.693899E-16	6.374366E-15	99.992266	2.999998
0.38	1.732478E+16	44.333333	1.234286E-06	1.916409E-16	6.874805E-16	6.718921E-15	99.991863	2.999998
0.39	1.732471E+16	45.500000	1.234286E-06	2.057827E-16	7.055711E-16	7.072542E-15	99.991450	2.999998
0.40	1.732464E+16	46.666667	1.234286E-06	2.205974E-16	7.236617E-16	7.435230E-15	99.991027	2.999997
0.41	1.732456E+16	47.833333	1.234286E-06	2.361007E-16	7.417521E-16	7.806984E-15	99.990593	2.999997
0.42	1.732448E+16	49.000000	1.234286E-06	2.523079E-16	7.598425E-16	8.187805E-15	99.990148	2.999997
0.43	1.732441E+16	50.166667	1.234286E-06	2.692347E-16	7.779328E-16	8.577692E-15	99.989693	2.999997
0.44	1.732432E+16	51.333333	1.234286E-06	2.868965E-16	7.960230E-16	8.976646E-15	99.989227	2.999997
0.45	1.732424E+16	52.500000	1.234286E-06	3.053088E-16	8.141131E-16	9.384666E-15	99.988751	2.999997

0.46	1.732416E+16	53.666667	1.234286E-06	3.244872E-16	8.322032E-16	9.801752E-15	99.988265	2.999997
0.47	1.732407E+16	54.833333	1.234286E-06	3.444471E-16	8.502931E-16	1.022790E-14	99.987768	2.999996
0.48	1.732398E+16	56.000000	1.234286E-06	3.652042E-16	8.683830E-16	1.066312E-14	99.987260	2.999996
0.49	1.732389E+16	57.166667	1.234286E-06	3.867738E-16	8.864728E-16	1.110741E-14	99.986742	2.999996
0.50	1.732380E+16	58.333333	1.234286E-06	4.091716E-16	9.045624E-16	1.156076E-14	99.986213	2.999996
0.51	1.732371E+16	59.500000	1.234286E-06	4.324130E-16	9.226520E-16	1.202318E-14	99.985674	2.999996
0.52	1.732361E+16	60.666667	1.234286E-06	4.565136E-16	9.407415E-16	1.249466E-14	99.985123	2.999996
0.53	1.732352E+16	61.833333	1.234286E-06	4.814889E-16	9.588309E-16	1.297521E-14	99.984563	2.999995
0.54	1.732342E+16	63.000000	1.234286E-06	5.073543E-16	9.769202E-16	1.346482E-14	99.983991	2.999995
0.55	1.732332E+16	64.166667	1.234286E-06	5.341254E-16	9.950094E-16	1.396350E-14	99.983409	2.999995
0.56	1.732321E+16	65.333333	1.234286E-06	5.618177E-16	1.013098E-15	1.447125E-14	99.982817	2.999995
0.57	1.732311E+16	66.500000	1.234286E-06	5.904467E-16	1.031187E-15	1.498806E-14	99.982213	2.999995
0.58	1.732300E+16	67.666667	1.234286E-06	6.200280E-16	1.049276E-15	1.551394E-14	99.981599	2.999995
0.59	1.732289E+16	68.833333	1.234286E-06	6.505770E-16	1.067365E-15	1.604888E-14	99.980974	2.999994
0.60	1.732278E+16	70.000000	1.234286E-06	6.821093E-16	1.085454E-15	1.659289E-14	99.980338	2.999994
0.61	1.732267E+16	71.166667	1.234286E-06	7.146404E-16	1.103542E-15	1.714596E-14	99.979692	2.999994
0.62	1.732256E+16	72.333333	1.234286E-06	7.481857E-16	1.121631E-15	1.770810E-14	99.979034	2.999994
0.63	1.732244E+16	73.500000	1.234286E-06	7.827609E-16	1.139719E-15	1.827931E-14	99.978366	2.999994
0.64	1.732233E+16	74.666667	1.234286E-06	8.183814E-16	1.157807E-15	1.885957E-14	99.977687	2.999993
0.65	1.732221E+16	75.833333	1.234286E-06	8.550627E-16	1.175895E-15	1.944891E-14	99.976998	2.999993
0.66	1.732208E+16	77.000000	1.234286E-06	8.928203E-16	1.193983E-15	2.004731E-14	99.976297	2.999993
0.67	1.732196E+16	78.166667	1.234286E-06	9.316698E-16	1.212071E-15	2.065477E-14	99.975586	2.999993
0.68	1.732184E+16	79.333333	1.234286E-06	9.716266E-16	1.230159E-15	2.127130E-14	99.974863	2.999993
0.69	1.732171E+16	80.500000	1.234286E-06	1.012706E-15	1.248246E-15	2.189690E-14	99.974130	2.999992
0.70	1.732158E+16	81.666667	1.234286E-06	1.054924E-15	1.266333E-15	2.253155E-14	99.973386	2.999992
0.71	1.732145E+16	82.833333	1.234286E-06	1.098296E-15	1.284421E-15	2.317528E-14	99.972631	2.999992
0.72	1.732132E+16	84.000000	1.234286E-06	1.142838E-15	1.302508E-15	2.382806E-14	99.971864	2.999992
0.73	1.732118E+16	85.166667	1.234286E-06	1.188564E-15	1.320595E-15	2.448992E-14	99.971087	2.999991
0.74	1.732105E+16	86.333333	1.234286E-06	1.235491E-15	1.338682E-15	2.516083E-14	99.970299	2.999991
0.75	1.732091E+16	87.500000	1.234286E-06	1.283634E-15	1.356769E-15	2.584081E-14	99.969500	2.999991
0.76	1.732077E+16	88.666667	1.234286E-06	1.333008E-15	1.374855E-15	2.652986E-14	99.968690	2.999991
0.77	1.732062E+16	89.833333	1.234286E-06	1.383629E-15	1.392942E-15	2.722797E-14	99.967869	2.999990
0.78	1.732048E+16	91.000000	1.234286E-06	1.435512E-15	1.411028E-15	2.793514E-14	99.967037	2.999990
0.79	1.732033E+16	92.166667	1.234286E-06	1.488674E-15	1.429114E-15	2.865138E-14	99.966193	2.999990
0.80	1.732019E+16	93.333333	1.234286E-06	1.543129E-15	1.447200E-15	2.937668E-14	99.965339	2.999990
0.81	1.732004E+16	94.500000	1.234286E-06	1.598893E-15	1.465286E-15	3.011104E-14	99.964473	2.999989
0.82	1.731988E+16	95.666667	1.234286E-06	1.655981E-15	1.483371E-15	3.085447E-14	99.963597	2.999989
0.83	1.731973E+16	96.833333	1.234286E-06	1.714410E-15	1.501457E-15	3.160696E-14	99.962709	2.999989
0.84	1.731957E+16	98.000000	1.234286E-06	1.774194E-15	1.519542E-15	3.236852E-14	99.961810	2.999989
0.85	1.731942E+16	99.166667	1.234286E-06	1.835349E-15	1.537628E-15	3.313914E-14	99.960900	2.999988
0.86	1.731926E+16	100.333333	1.234286E-06	1.897891E-15	1.555713E-15	3.391882E-14	99.959979	2.999988
0.87	1.731910E+16	101.500000	1.234286E-06	1.961834E-15	1.573797E-15	3.470756E-14	99.959046	2.999988
0.88	1.731893E+16	102.666667	1.234286E-06	2.027195E-15	1.591882E-15	3.550537E-14	99.958103	2.999988
0.89	1.731877E+16	103.833333	1.234286E-06	2.093990E-15	1.609967E-15	3.631224E-14	99.957148	2.999987
0.90	1.731860E+16	105.000000	1.234286E-06	2.162232E-15	1.628051E-15	3.712818E-14	99.956181	2.999987
0.91	1.731843E+16	106.166667	1.234286E-06	2.231939E-15	1.646135E-15	3.795317E-14	99.955204	2.999987
0.92	1.731826E+16	107.333333	1.234286E-06	2.303125E-15	1.664219E-15	3.878723E-14	99.954215	2.999986
0.93	1.731809E+16	108.500000	1.234286E-06	2.375807E-15	1.682303E-15	3.963036E-14	99.953215	2.999986
0.94	1.731791E+16	109.666667	1.234286E-06	2.449999E-15	1.700387E-15	4.048254E-14	99.952204	2.999986
0.95	1.731773E+16	110.833333	1.234286E-06	2.525717E-15	1.718470E-15	4.134379E-14	99.951181	2.999985
0.96	1.731755E+16	112.000000	1.234286E-06	2.602977E-15	1.736554E-15	4.221410E-14	99.950147	2.999985
0.97	1.731737E+16	113.166667	1.234286E-06	2.681794E-15	1.754637E-15	4.309347E-14	99.949101	2.999985
0.98	1.731719E+16	114.333333	1.234286E-06	2.762183E-15	1.772720E-15	4.398190E-14	99.948044	2.999985
0.99	1.731700E+16	115.500000	1.234286E-06	2.844160E-15	1.790802E-15	4.487939E-14	99.946976	2.999984
1.00	1.731682E+16	116.666667	1.234286E-06	2.927742E-15	1.808885E-15	4.578595E-14	99.945897	2.999984



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732619E+16	1.166667	3.509923E-07	2.695214E-20	1.787018E-17	8.956304E-18	99.999971	3.000000
0.02	1.732618E+16	2.333333	4.963779E-07	1.189725E-19	3.574035E-17	2.686891E-17	99.999933	3.000000
0.03	1.732617E+16	3.500000	6.079359E-07	3.036855E-19	5.361051E-17	5.373781E-17	99.999885	3.000000
0.04	1.732616E+16	4.666667	7.019836E-07	6.038737E-19	7.148066E-17	8.956300E-17	99.999827	3.000000
0.05	1.732615E+16	5.833333	7.848409E-07	1.039376E-18	8.935080E-17	1.343445E-16	99.999759	3.000000
0.06	1.732614E+16	7.000000	8.597495E-07	1.627997E-18	1.072209E-16	1.880822E-16	99.999682	3.000000
0.07	1.732612E+16	8.166667	9.286348E-07	2.386031E-18	1.250910E-16	2.507762E-16	99.999595	3.000000
0.08	1.732610E+16	9.333333	9.927514E-07	3.328588E-18	1.429611E-16	3.224265E-16	99.999498	3.000000
0.09	1.732609E+16	10.500000	1.052971E-06	4.469820E-18	1.608312E-16	4.030330E-16	99.999391	3.000000
0.10	1.732607E+16	11.666667	1.109927E-06	5.823086E-18	1.787013E-16	4.925958E-16	99.999275	3.000000
0.11	1.732604E+16	12.833333	1.164100E-06	7.401069E-18	1.965713E-16	5.911147E-16	99.999149	3.000000
0.12	1.732602E+16	14.000000	1.215861E-06	9.215870E-18	2.144413E-16	6.985899E-16	99.999012	3.000000
0.13	1.732599E+16	15.166667	1.234286E-06	1.128154E-17	2.323113E-16	8.150213E-16	99.998866	3.000000
0.14	1.732597E+16	16.333333	1.234286E-06	1.361341E-17	2.501812E-16	9.404089E-16	99.998710	3.000000
0.15	1.732594E+16	17.500000	1.234286E-06	1.622680E-17	2.680512E-16	1.074753E-15	99.998545	3.000000
0.16	1.732591E+16	18.666667	1.234286E-06	1.913705E-17	2.859211E-16	1.218052E-15	99.998369	3.000000
0.17	1.732588E+16	19.833333	1.234286E-06	2.235947E-17	3.037909E-16	1.370308E-15	99.998183	3.000000
0.18	1.732584E+16	21.000000	1.234286E-06	2.590941E-17	3.216608E-16	1.531520E-15	99.997988	2.999999
0.19	1.732581E+16	22.166667	1.234286E-06	2.980219E-17	3.395306E-16	1.701689E-15	99.997782	2.999999
0.20	1.732577E+16	23.333333	1.234286E-06	3.405313E-17	3.574003E-16	1.880813E-15	99.997567	2.999999
0.21	1.732573E+16	24.500000	1.234286E-06	3.867757E-17	3.752700E-16	2.068893E-15	99.997341	2.999999
0.22	1.732569E+16	25.666667	1.234286E-06	4.369083E-17	3.931397E-16	2.265929E-15	99.997106	2.999999
0.23	1.732565E+16	26.833333	1.234286E-06	4.910824E-17	4.110093E-16	2.471921E-15	99.996860	2.999999
0.24	1.732560E+16	28.000000	1.234286E-06	5.494512E-17	4.288789E-16	2.686870E-15	99.996605	2.999999
0.25	1.732556E+16	29.166667	1.234286E-06	6.121682E-17	4.467485E-16	2.910774E-15	99.996339	2.999999
0.26	1.732551E+16	30.333333	1.234286E-06	6.793864E-17	4.646180E-16	3.143634E-15	99.996063	2.999999
0.27	1.732546E+16	31.500000	1.234286E-06	7.512593E-17	4.824874E-16	3.385450E-15	99.995777	2.999999
0.28	1.732541E+16	32.666667	1.234286E-06	8.279400E-17	5.003568E-16	3.636221E-15	99.995482	2.999999
0.29	1.732536E+16	33.833333	1.234286E-06	9.095819E-17	5.182261E-16	3.895949E-15	99.995176	2.999999
0.30	1.732530E+16	35.000000	1.234286E-06	9.963382E-17	5.360954E-16	4.164632E-15	99.994859	2.999999
0.31	1.732524E+16	36.166667	1.234286E-06	1.088362E-16	5.539646E-16	4.442271E-15	99.994533	2.999998
0.32	1.732519E+16	37.333333	1.234286E-06	1.185807E-16	5.718338E-16	4.728866E-15	99.994197	2.999998
0.33	1.732513E+16	38.500000	1.234286E-06	1.288826E-16	5.897029E-16	5.024416E-15	99.993850	2.999998
0.34	1.732506E+16	39.666667	1.234286E-06	1.397573E-16	6.075720E-16	5.328922E-15	99.993493	2.999998
0.35	1.732500E+16	40.833333	1.234286E-06	1.512201E-16	6.254409E-16	5.642384E-15	99.993126	2.999998
0.36	1.732493E+16	42.000000	1.234286E-06	1.632862E-16	6.433099E-16	5.964801E-15	99.992749	2.999998
0.37	1.732487E+16	43.166667	1.234286E-06	1.759711E-16	6.611787E-16	6.296173E-15	99.992361	2.999998
0.38	1.732480E+16	44.333333	1.234286E-06	1.892901E-16	6.790475E-16	6.636502E-15	99.991963	2.999998
0.39	1.732473E+16	45.500000	1.234286E-06	2.032584E-16	6.969162E-16	6.985785E-15	99.991555	2.999998
0.40	1.732466E+16	46.666667	1.234286E-06	2.178914E-16	7.147848E-16	7.344024E-15	99.991137	2.999997
0.41	1.732458E+16	47.833333	1.234286E-06	2.332045E-16	7.326534E-16	7.711218E-15	99.990708	2.999997
0.42	1.732451E+16	49.000000	1.234286E-06	2.492129E-16	7.505219E-16	8.087368E-15	99.990269	2.999997
0.43	1.732443E+16	50.166667	1.234286E-06	2.659320E-16	7.683903E-16	8.472473E-15	99.989819	2.999997
0.44	1.732435E+16	51.333333	1.234286E-06	2.833772E-16	7.862586E-16	8.866532E-15	99.989360	2.999997
0.45	1.732427E+16	52.500000	1.234286E-06	3.015636E-16	8.041268E-16	9.269548E-15	99.988889	2.999997

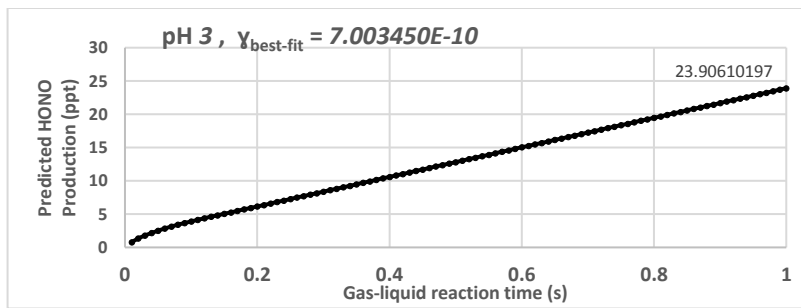
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0.47	1.732410E+16	54.833333	1.234286E-06	3.402219E-16	8.398631E-16	1.010244E-14	99.987918	2.999996
0.48	1.732401E+16	56.000000	1.234286E-06	3.607243E-16	8.577310E-16	1.053232E-14	99.987416	2.999996
0.49	1.732392E+16	57.166667	1.234286E-06	3.820294E-16	8.755989E-16	1.097116E-14	99.986904	2.999996
0.50	1.732383E+16	58.333333	1.234286E-06	4.041525E-16	8.934667E-16	1.141895E-14	99.986382	2.999996
0.51	1.732374E+16	59.500000	1.234286E-06	4.271088E-16	9.113345E-16	1.187569E-14	99.985849	2.999996
0.52	1.732365E+16	60.666667	1.234286E-06	4.509137E-16	9.292021E-16	1.234139E-14	99.985306	2.999996
0.53	1.732355E+16	61.833333	1.234286E-06	4.755826E-16	9.470696E-16	1.281605E-14	99.984752	2.999995
0.54	1.732345E+16	63.000000	1.234286E-06	5.011307E-16	9.649370E-16	1.329966E-14	99.984188	2.999995
0.55	1.732335E+16	64.166667	1.234286E-06	5.275735E-16	9.828043E-16	1.379222E-14	99.983613	2.999995
0.56	1.732325E+16	65.333333	1.234286E-06	5.549261E-16	1.000672E-15	1.429374E-14	99.983027	2.999995
0.57	1.732315E+16	66.500000	1.234286E-06	5.832040E-16	1.018539E-15	1.480421E-14	99.982431	2.999995
0.58	1.732304E+16	67.666667	1.234286E-06	6.124224E-16	1.036406E-15	1.532364E-14	99.981825	2.999995
0.59	1.732294E+16	68.833333	1.234286E-06	6.425967E-16	1.054273E-15	1.585202E-14	99.981207	2.999994
0.60	1.732283E+16	70.000000	1.234286E-06	6.737422E-16	1.072139E-15	1.638935E-14	99.980579	2.999994
0.61	1.732272E+16	71.166667	1.234286E-06	7.058742E-16	1.090006E-15	1.693564E-14	99.979941	2.999994
0.62	1.732260E+16	72.333333	1.234286E-06	7.390081E-16	1.107873E-15	1.749089E-14	99.979292	2.999994
0.63	1.732249E+16	73.500000	1.234286E-06	7.731592E-16	1.125739E-15	1.805508E-14	99.978632	2.999994
0.64	1.732237E+16	74.666667	1.234286E-06	8.083427E-16	1.143605E-15	1.862824E-14	99.977961	2.999993
0.65	1.732225E+16	75.833333	1.234286E-06	8.445741E-16	1.161472E-15	1.921034E-14	99.977280	2.999993
0.66	1.732213E+16	77.000000	1.234286E-06	8.818686E-16	1.179338E-15	1.980140E-14	99.976588	2.999993
0.67	1.732201E+16	78.166667	1.234286E-06	9.202415E-16	1.197204E-15	2.040141E-14	99.975885	2.999993
0.68	1.732189E+16	79.333333	1.234286E-06	9.597083E-16	1.215070E-15	2.101038E-14	99.975172	2.999993
0.69	1.732176E+16	80.500000	1.234286E-06	1.000284E-15	1.232935E-15	2.162830E-14	99.974447	2.999992
0.70	1.732164E+16	81.666667	1.234286E-06	1.041984E-15	1.250801E-15	2.225518E-14	99.973712	2.999992
0.71	1.732151E+16	82.833333	1.234286E-06	1.084824E-15	1.268666E-15	2.289100E-14	99.972966	2.999992
0.72	1.732138E+16	84.000000	1.234286E-06	1.128819E-15	1.286532E-15	2.353578E-14	99.972210	2.999992
0.73	1.732124E+16	85.166667	1.234286E-06	1.173985E-15	1.304397E-15	2.418952E-14	99.971442	2.999991
0.74	1.732111E+16	86.333333	1.234286E-06	1.220336E-15	1.322262E-15	2.485221E-14	99.970664	2.999991
0.75	1.732097E+16	87.500000	1.234286E-06	1.267888E-15	1.340127E-15	2.552385E-14	99.969874	2.999991
0.76	1.732083E+16	88.666667	1.234286E-06	1.316657E-15	1.357992E-15	2.620444E-14	99.969074	2.999991
0.77	1.732069E+16	89.833333	1.234286E-06	1.366657E-15	1.375856E-15	2.689399E-14	99.968263	2.999991
0.78	1.732055E+16	91.000000	1.234286E-06	1.417904E-15	1.393721E-15	2.759249E-14	99.967441	2.999990
0.79	1.732041E+16	92.166667	1.234286E-06	1.470413E-15	1.411585E-15	2.829994E-14	99.966608	2.999990
0.80	1.732026E+16	93.333333	1.234286E-06	1.524201E-15	1.429449E-15	2.901634E-14	99.965764	2.999990
0.81	1.732011E+16	94.500000	1.234286E-06	1.579281E-15	1.447313E-15	2.974170E-14	99.964909	2.999990
0.82	1.731996E+16	95.666667	1.234286E-06	1.635669E-15	1.465177E-15	3.047601E-14	99.964043	2.999989
0.83	1.731981E+16	96.833333	1.234286E-06	1.693381E-15	1.483041E-15	3.121927E-14	99.963166	2.999989
0.84	1.731966E+16	98.000000	1.234286E-06	1.752431E-15	1.500905E-15	3.197149E-14	99.962279	2.999989
0.85	1.731950E+16	99.166667	1.234286E-06	1.812836E-15	1.518768E-15	3.273265E-14	99.961380	2.999988
0.86	1.731934E+16	100.333333	1.234286E-06	1.874611E-15	1.536631E-15	3.350277E-14	99.960470	2.999988
0.87	1.731918E+16	101.500000	1.234286E-06	1.937770E-15	1.554494E-15	3.428185E-14	99.959549	2.999988
0.88	1.731902E+16	102.666667	1.234286E-06	2.002330E-15	1.572357E-15	3.506987E-14	99.958616	2.999988
0.89	1.731886E+16	103.833333	1.234286E-06	2.068305E-15	1.590220E-15	3.586684E-14	99.957673	2.999987
0.90	1.731869E+16	105.000000	1.234286E-06	2.135710E-15	1.608083E-15	3.667277E-14	99.956719	2.999987
0.91	1.731852E+16	106.166667	1.234286E-06	2.204562E-15	1.625945E-15	3.748765E-14	99.955753	2.999987
0.92	1.731836E+16	107.333333	1.234286E-06	2.274875E-15	1.643808E-15	3.831148E-14	99.954777	2.999987
0.93	1.731818E+16	108.500000	1.234286E-06	2.346665E-15	1.661670E-15	3.914426E-14	99.953789	2.999986
0.94	1.731801E+16	109.666667	1.234286E-06	2.419948E-15	1.679532E-15	3.998599E-14	99.952790	2.999986
0.95	1.731784E+16	110.833333	1.234286E-06	2.494737E-15	1.697393E-15	4.083668E-14	99.951780	2.999986
0.96	1.731766E+16	112.000000	1.234286E-06	2.571049E-15	1.715255E-15	4.169631E-14	99.950758	2.999985
0.97	1.731748E+16	113.166667	1.234286E-06	2.648899E-15	1.733116E-15	4.256490E-14	99.949726	2.999985
0.98	1.731730E+16	114.333333	1.234286E-06	2.728303E-15	1.750978E-15	4.344243E-14	99.948682	2.999985
0.99	1.731712E+16	115.500000	1.234286E-06	2.809275E-15	1.768839E-15	4.432892E-14	99.947627	2.999984
1.00	1.731693E+16	116.666667	1.234286E-06	2.891831E-15	1.786699E-15	4.522436E-14	99.946560	2.999984



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO2}}$ (mol)	$\Phi_{\text{NO2}}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732619E+16	1.166667	3.509923E-07	2.451953E-20	1.625728E-17	8.147939E-18	99.999974	3.000000
0.02	1.732618E+16	2.333333	4.963779E-07	1.082344E-19	3.251455E-17	2.444382E-17	99.999939	3.000000
0.03	1.732617E+16	3.500000	6.079360E-07	2.762759E-19	4.877181E-17	4.888762E-17	99.999895	3.000000
0.04	1.732616E+16	4.666667	7.019837E-07	5.493702E-19	6.502907E-17	8.147936E-17	99.999843	3.000000
0.05	1.732615E+16	5.833333	7.848411E-07	9.455654E-19	8.128632E-17	1.222190E-16	99.999781	3.000000
0.06	1.732614E+16	7.000000	8.597498E-07	1.481060E-18	9.754355E-17	1.711066E-16	99.999711	3.000000
0.07	1.732613E+16	8.166667	9.286351E-07	2.170676E-18	1.138008E-16	2.281421E-16	99.999631	3.000000
0.08	1.732611E+16	9.333333	9.927518E-07	3.028161E-18	1.300580E-16	2.933255E-16	99.999543	3.000000
0.09	1.732610E+16	10.500000	1.052971E-06	4.066390E-18	1.463152E-16	3.666567E-16	99.999446	3.000000
0.10	1.732608E+16	11.666667	1.109928E-06	5.297515E-18	1.625724E-16	4.481359E-16	99.999340	3.000000
0.11	1.732606E+16	12.833333	1.164101E-06	6.733075E-18	1.788295E-16	5.377629E-16	99.999225	3.000000
0.12	1.732604E+16	14.000000	1.215862E-06	8.384078E-18	1.950866E-16	6.355378E-16	99.999102	3.000000
0.13	1.732601E+16	15.166667	1.234286E-06	1.026331E-17	2.113438E-16	7.414605E-16	99.998969	3.000000
0.14	1.732599E+16	16.333333	1.234286E-06	1.238471E-17	2.276009E-16	8.555311E-16	99.998827	3.000000
0.15	1.732596E+16	17.500000	1.234286E-06	1.476223E-17	2.438579E-16	9.777495E-16	99.998676	3.000000
0.16	1.732593E+16	18.666667	1.234286E-06	1.740980E-17	2.601150E-16	1.108116E-15	99.998516	3.000000
0.17	1.732590E+16	19.833333	1.234286E-06	2.034139E-17	2.763720E-16	1.246630E-15	99.998347	3.000000
0.18	1.732587E+16	21.000000	1.234286E-06	2.357092E-17	2.926290E-16	1.393291E-15	99.998169	3.000000
0.19	1.732584E+16	22.166667	1.234286E-06	2.711235E-17	3.088859E-16	1.548101E-15	99.997982	2.999999
0.20	1.732581E+16	23.333333	1.234286E-06	3.097962E-17	3.251429E-16	1.711058E-15	99.997786	2.999999
0.21	1.732577E+16	24.500000	1.234286E-06	3.518667E-17	3.413998E-16	1.882163E-15	99.997581	2.999999
0.22	1.732573E+16	25.666667	1.234286E-06	3.974746E-17	3.576566E-16	2.061416E-15	99.997367	2.999999
0.23	1.732570E+16	26.833333	1.234286E-06	4.467591E-17	3.739135E-16	2.248816E-15	99.997144	2.999999
0.24	1.732566E+16	28.000000	1.234286E-06	4.998599E-17	3.901702E-16	2.444364E-15	99.996911	2.999999
0.25	1.732561E+16	29.166667	1.234286E-06	5.569162E-17	4.064270E-16	2.648060E-15	99.996669	2.999999
0.26	1.732557E+16	30.333333	1.234286E-06	6.180676E-17	4.226837E-16	2.859903E-15	99.996419	2.999999
0.27	1.732553E+16	31.500000	1.234286E-06	6.834536E-17	4.389404E-16	3.079893E-15	99.996159	2.999999
0.28	1.732548E+16	32.666667	1.234286E-06	7.532134E-17	4.551970E-16	3.308032E-15	99.995889	2.999999
0.29	1.732543E+16	33.833333	1.234286E-06	8.274867E-17	4.714536E-16	3.544318E-15	99.995611	2.999999
0.30	1.732538E+16	35.000000	1.234286E-06	9.064128E-17	4.877101E-16	3.788751E-15	99.995323	2.999999
0.31	1.732533E+16	36.166667	1.234286E-06	9.901311E-17	5.039666E-16	4.041332E-15	99.995027	2.999999
0.32	1.732528E+16	37.333333	1.234286E-06	1.078781E-16	5.202231E-16	4.302060E-15	99.994720	2.999998
0.33	1.732522E+16	38.500000	1.234286E-06	1.172502E-16	5.364794E-16	4.570936E-15	99.994405	2.999998
0.34	1.732517E+16	39.666667	1.234286E-06	1.271434E-16	5.527358E-16	4.847959E-15	99.994080	2.999998
0.35	1.732511E+16	40.833333	1.234286E-06	1.375716E-16	5.689921E-16	5.133129E-15	99.993746	2.999998
0.36	1.732505E+16	42.000000	1.234286E-06	1.485487E-16	5.852483E-16	5.426447E-15	99.993403	2.999998
0.37	1.732499E+16	43.166667	1.234286E-06	1.600887E-16	6.015045E-16	5.727912E-15	99.993051	2.999998
0.38	1.732492E+16	44.333333	1.234286E-06	1.722056E-16	6.177606E-16	6.037524E-15	99.992689	2.999998
0.39	1.732486E+16	45.500000	1.234286E-06	1.849132E-16	6.340167E-16	6.355283E-15	99.992317	2.999998
0.40	1.732479E+16	46.666667	1.234286E-06	1.982255E-16	6.502727E-16	6.681190E-15	99.991937	2.999998
0.41	1.732473E+16	47.833333	1.234286E-06	2.121565E-16	6.665286E-16	7.015244E-15	99.991547	2.999998
0.42	1.732466E+16	49.000000	1.234286E-06	2.267201E-16	6.827845E-16	7.357445E-15	99.991147	2.999997
0.43	1.732459E+16	50.166667	1.234286E-06	2.419303E-16	6.990403E-16	7.707792E-15	99.990738	2.999997
0.44	1.732451E+16	51.333333	1.234286E-06	2.578009E-16	7.152960E-16	8.066287E-15	99.990320	2.999997
0.45	1.732444E+16	52.500000	1.234286E-06	2.743460E-16	7.315517E-16	8.432929E-15	99.989892	2.999997



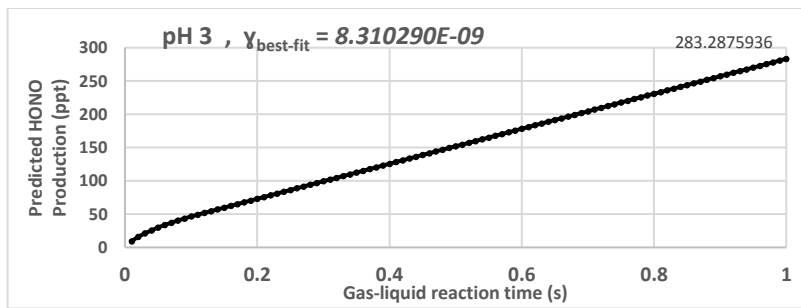
0.46	1.732436E+16	53.666667	1.234286E-06	2.915795E-16	7.478073E-16	8.807718E-15	99.989455	2.999997
0.47	1.732429E+16	54.833333	1.234286E-06	3.095152E-16	7.640628E-16	9.190654E-15	99.989008	2.999997
0.48	1.732421E+16	56.000000	1.234286E-06	3.281672E-16	7.803183E-16	9.581736E-15	99.988552	2.999997
0.49	1.732413E+16	57.166667	1.234286E-06	3.475495E-16	7.965737E-16	9.980966E-15	99.988086	2.999996
0.50	1.732404E+16	58.333333	1.234286E-06	3.676758E-16	8.128290E-16	1.038834E-14	99.987611	2.999996
0.51	1.732396E+16	59.500000	1.234286E-06	3.885603E-16	8.290842E-16	1.080386E-14	99.987126	2.999996
0.52	1.732388E+16	60.666667	1.234286E-06	4.102168E-16	8.453394E-16	1.122753E-14	99.986632	2.999996
0.53	1.732379E+16	61.833333	1.234286E-06	4.326592E-16	8.615945E-16	1.165935E-14	99.986128	2.999996
0.54	1.732370E+16	63.000000	1.234286E-06	4.559015E-16	8.778495E-16	1.209931E-14	99.985615	2.999996
0.55	1.732361E+16	64.166667	1.234286E-06	4.799578E-16	8.941044E-16	1.254742E-14	99.985092	2.999996
0.56	1.732352E+16	65.333333	1.234286E-06	5.048417E-16	9.103592E-16	1.300368E-14	99.984559	2.999995
0.57	1.732342E+16	66.500000	1.234286E-06	5.305675E-16	9.266140E-16	1.346808E-14	99.984017	2.999995
0.58	1.732333E+16	67.666667	1.234286E-06	5.571489E-16	9.428686E-16	1.394063E-14	99.983465	2.999995
0.59	1.732323E+16	68.833333	1.234286E-06	5.845999E-16	9.591232E-16	1.442132E-14	99.982903	2.999995
0.60	1.732313E+16	70.000000	1.234286E-06	6.129345E-16	9.753776E-16	1.491016E-14	99.982332	2.999995
0.61	1.732303E+16	71.166667	1.234286E-06	6.421665E-16	9.916320E-16	1.540715E-14	99.981751	2.999995
0.62	1.732293E+16	72.333333	1.234286E-06	6.723100E-16	1.007886E-15	1.591228E-14	99.981161	2.999994
0.63	1.732282E+16	73.500000	1.234286E-06	7.033789E-16	1.024141E-15	1.642556E-14	99.980560	2.999994
0.64	1.732272E+16	74.666667	1.234286E-06	7.353871E-16	1.040395E-15	1.694699E-14	99.979950	2.999994
0.65	1.732261E+16	75.833333	1.234286E-06	7.683485E-16	1.056649E-15	1.747656E-14	99.979330	2.999994
0.66	1.732250E+16	77.000000	1.234286E-06	8.022772E-16	1.072903E-15	1.801428E-14	99.978701	2.999994
0.67	1.732239E+16	78.166667	1.234286E-06	8.371870E-16	1.089156E-15	1.856014E-14	99.978062	2.999993
0.68	1.732228E+16	79.333333	1.234286E-06	8.730918E-16	1.105410E-15	1.911415E-14	99.977412	2.999993
0.69	1.732216E+16	80.500000	1.234286E-06	9.100057E-16	1.121664E-15	1.967630E-14	99.976753	2.999993
0.70	1.732205E+16	81.666667	1.234286E-06	9.479425E-16	1.137917E-15	2.024660E-14	99.976085	2.999993
0.71	1.732193E+16	82.833333	1.234286E-06	9.869162E-16	1.154170E-15	2.082505E-14	99.975406	2.999993
0.72	1.732181E+16	84.000000	1.234286E-06	1.026941E-15	1.170424E-15	2.141164E-14	99.974718	2.999992
0.73	1.732169E+16	85.166667	1.234286E-06	1.068030E-15	1.186677E-15	2.200638E-14	99.974019	2.999992
0.74	1.732157E+16	86.333333	1.234286E-06	1.110198E-15	1.202930E-15	2.260926E-14	99.973311	2.999992
0.75	1.732144E+16	87.500000	1.234286E-06	1.153459E-15	1.219183E-15	2.322029E-14	99.972593	2.999992
0.76	1.732132E+16	88.666667	1.234286E-06	1.197826E-15	1.235436E-15	2.383946E-14	99.971865	2.999992
0.77	1.732119E+16	89.833333	1.234286E-06	1.243314E-15	1.251688E-15	2.446678E-14	99.971127	2.999991
0.78	1.732106E+16	91.000000	1.234286E-06	1.289936E-15	1.267941E-15	2.510224E-14	99.970379	2.999991
0.79	1.732093E+16	92.166667	1.234286E-06	1.337706E-15	1.284193E-15	2.574585E-14	99.969622	2.999991
0.80	1.732079E+16	93.333333	1.234286E-06	1.386639E-15	1.300446E-15	2.639760E-14	99.968854	2.999991
0.81	1.732066E+16	94.500000	1.234286E-06	1.436748E-15	1.316698E-15	2.705750E-14	99.968076	2.999990
0.82	1.732052E+16	95.666667	1.234286E-06	1.488048E-15	1.332950E-15	2.772554E-14	99.967288	2.999990
0.83	1.732039E+16	96.833333	1.234286E-06	1.540551E-15	1.349202E-15	2.840173E-14	99.966491	2.999990
0.84	1.732025E+16	98.000000	1.234286E-06	1.594273E-15	1.365454E-15	2.908606E-14	99.965683	2.999990
0.85	1.732010E+16	99.166667	1.234286E-06	1.649226E-15	1.381705E-15	2.977854E-14	99.964865	2.999990
0.86	1.731996E+16	100.333333	1.234286E-06	1.705426E-15	1.397957E-15	3.047916E-14	99.964037	2.999989
0.87	1.731982E+16	101.500000	1.234286E-06	1.762885E-15	1.414208E-15	3.118792E-14	99.963199	2.999989
0.88	1.731967E+16	102.666667	1.234286E-06	1.821619E-15	1.430460E-15	3.190483E-14	99.962351	2.999989
0.89	1.731952E+16	103.833333	1.234286E-06	1.881640E-15	1.446711E-15	3.262989E-14	99.961493	2.999989
0.90	1.731937E+16	105.000000	1.234286E-06	1.942962E-15	1.462962E-15	3.336308E-14	99.960625	2.999988
0.91	1.731922E+16	106.166667	1.234286E-06	2.005601E-15	1.479213E-15	3.410443E-14	99.959747	2.999988
0.92	1.731906E+16	107.333333	1.234286E-06	2.069568E-15	1.495464E-15	3.485391E-14	99.958858	2.999988
0.93	1.731891E+16	108.500000	1.234286E-06	2.134880E-15	1.511714E-15	3.561154E-14	99.957959	2.999987
0.94	1.731875E+16	109.666667	1.234286E-06	2.201549E-15	1.527965E-15	3.637732E-14	99.957051	2.999987
0.95	1.731859E+16	110.833333	1.234286E-06	2.269589E-15	1.544215E-15	3.715123E-14	99.956131	2.999987
0.96	1.731843E+16	112.000000	1.234286E-06	2.339014E-15	1.560465E-15	3.793329E-14	99.955202	2.999987
0.97	1.731827E+16	113.166667	1.234286E-06	2.409839E-15	1.576715E-15	3.872350E-14	99.954263	2.999986
0.98	1.731810E+16	114.333333	1.234286E-06	2.482076E-15	1.592965E-15	3.952185E-14	99.953313	2.999986
0.99	1.731794E+16	115.500000	1.234286E-06	2.555741E-15	1.609215E-15	4.032834E-14	99.952353	2.999986
1.00	1.731777E+16	116.666667	1.234286E-06	2.630847E-15	1.625464E-15	4.114297E-14	99.951383	2.999986



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732619E+16	1.166667	3.509923E-07	2.024387E-20	1.342237E-17	6.727122E-18	99.999978	3.000000
0.02	1.732618E+16	2.333333	4.963779E-07	8.936079E-20	2.684474E-17	2.018136E-17	99.999950	3.000000
0.03	1.732618E+16	3.500000	6.079361E-07	2.280996E-19	4.026711E-17	4.036272E-17	99.999913	3.000000
0.04	1.732617E+16	4.666667	7.019839E-07	4.535724E-19	5.368947E-17	6.727120E-17	99.999870	3.000000
0.05	1.732616E+16	5.833333	7.848414E-07	7.806801E-19	6.711182E-17	1.009068E-16	99.999819	3.000000
0.06	1.732615E+16	7.000000	8.597502E-07	1.222796E-18	8.053417E-17	1.412695E-16	99.999761	3.000000
0.07	1.732614E+16	8.166667	9.286357E-07	1.792159E-18	9.395650E-17	1.883593E-16	99.999696	3.000000
0.08	1.732613E+16	9.333333	9.927526E-07	2.500118E-18	1.073788E-16	2.421762E-16	99.999623	3.000000
0.09	1.732611E+16	10.500000	1.052972E-06	3.357303E-18	1.208011E-16	3.027201E-16	99.999543	3.000000
0.10	1.732610E+16	11.666667	1.109929E-06	4.373747E-18	1.342235E-16	3.699912E-16	99.999455	3.000000
0.11	1.732608E+16	12.833333	1.164103E-06	5.558978E-18	1.476457E-16	4.439893E-16	99.999360	3.000000
0.12	1.732606E+16	14.000000	1.215864E-06	6.922083E-18	1.610680E-16	5.247145E-16	99.999258	3.000000
0.13	1.732604E+16	15.166667	1.234286E-06	8.473617E-18	1.744903E-16	6.121668E-16	99.999149	3.000000
0.14	1.732602E+16	16.333333	1.234286E-06	1.022509E-17	1.879125E-16	7.063461E-16	99.999031	3.000000
0.15	1.732600E+16	17.500000	1.234286E-06	1.218803E-17	2.013348E-16	8.072524E-16	99.998907	3.000000
0.16	1.732598E+16	18.666667	1.234286E-06	1.437393E-17	2.147570E-16	9.148858E-16	99.998775	3.000000
0.17	1.732595E+16	19.833333	1.234286E-06	1.679431E-17	2.281792E-16	1.029246E-15	99.998635	3.000000
0.18	1.732593E+16	21.000000	1.234286E-06	1.946069E-17	2.416014E-16	1.150334E-15	99.998489	3.000000
0.19	1.732590E+16	22.166667	1.234286E-06	2.238457E-17	2.550235E-16	1.278148E-15	99.998334	3.000000
0.20	1.732587E+16	23.333333	1.234286E-06	2.557748E-17	2.684457E-16	1.412689E-15	99.998172	3.000000
0.21	1.732585E+16	24.500000	1.234286E-06	2.905092E-17	2.818678E-16	1.553958E-15	99.998003	2.999999
0.22	1.732581E+16	25.666667	1.234286E-06	3.281641E-17	2.952899E-16	1.701953E-15	99.997826	2.999999
0.23	1.732578E+16	26.833333	1.234286E-06	3.688546E-17	3.087119E-16	1.856675E-15	99.997642	2.999999
0.24	1.732575E+16	28.000000	1.234286E-06	4.126958E-17	3.221340E-16	2.018124E-15	99.997450	2.999999
0.25	1.732571E+16	29.166667	1.234286E-06	4.598029E-17	3.355560E-16	2.186301E-15	99.997250	2.999999
0.26	1.732568E+16	30.333333	1.234286E-06	5.102909E-17	3.489780E-16	2.361204E-15	99.997043	2.999999
0.27	1.732564E+16	31.500000	1.234286E-06	5.642751E-17	3.623999E-16	2.542833E-15	99.996828	2.999999
0.28	1.732560E+16	32.666667	1.234286E-06	6.218705E-17	3.758219E-16	2.731190E-15	99.996606	2.999999
0.29	1.732556E+16	33.833333	1.234286E-06	6.831923E-17	3.892438E-16	2.926274E-15	99.996376	2.999999
0.30	1.732552E+16	35.000000	1.234286E-06	7.483556E-17	4.026656E-16	3.128084E-15	99.996139	2.999999
0.31	1.732548E+16	36.166667	1.234286E-06	8.174756E-17	4.160875E-16	3.336621E-15	99.995894	2.999999
0.32	1.732544E+16	37.333333	1.234286E-06	8.906672E-17	4.295093E-16	3.551885E-15	99.995641	2.999999
0.33	1.732539E+16	38.500000	1.234286E-06	9.680458E-17	4.429311E-16	3.773876E-15	99.995381	2.999999
0.34	1.732534E+16	39.666667	1.234286E-06	1.049726E-16	4.563528E-16	4.002593E-15	99.995113	2.999999
0.35	1.732530E+16	40.833333	1.234286E-06	1.135824E-16	4.697745E-16	4.238037E-15	99.994837	2.999999
0.36	1.732525E+16	42.000000	1.234286E-06	1.226454E-16	4.831961E-16	4.480208E-15	99.994553	2.999998
0.37	1.732520E+16	43.166667	1.234286E-06	1.321731E-16	4.966178E-16	4.729106E-15	99.994262	2.999998
0.38	1.732515E+16	44.333333	1.234286E-06	1.421771E-16	5.100394E-16	4.984730E-15	99.993964	2.999998
0.39	1.732509E+16	45.500000	1.234286E-06	1.526688E-16	5.234609E-16	5.247081E-15	99.993657	2.999998
0.40	1.732504E+16	46.666667	1.234286E-06	1.636598E-16	5.368824E-16	5.516158E-15	99.993343	2.999998
0.41	1.732498E+16	47.833333	1.234286E-06	1.751616E-16	5.503039E-16	5.791962E-15	99.993021	2.999998
0.42	1.732492E+16	49.000000	1.234286E-06	1.871857E-16	5.637253E-16	6.074493E-15	99.992691	2.999998
0.43	1.732487E+16	50.166667	1.234286E-06	1.997436E-16	5.771467E-16	6.363750E-15	99.992353	2.999998
0.44	1.732481E+16	51.333333	1.234286E-06	2.128468E-16	5.905680E-16	6.659733E-15	99.992008	2.999998
0.45	1.732475E+16	52.500000	1.234286E-06	2.265069E-16	6.039893E-16	6.962443E-15	99.991655	2.999998

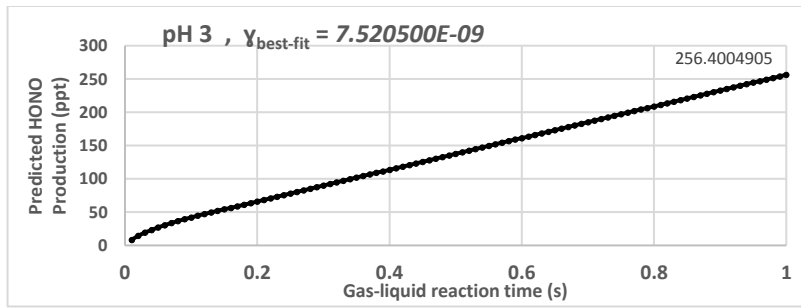
0.46	1.732468E+16	53.666667	1.234286E-06	2.407353E-16	6.174105E-16	7.271880E-15	99.991294	2.999997
0.47	1.732462E+16	54.833333	1.234286E-06	2.555435E-16	6.308317E-16	7.588043E-15	99.990925	2.999997
0.48	1.732455E+16	56.000000	1.234286E-06	2.709432E-16	6.442528E-16	7.910932E-15	99.990548	2.999997
0.49	1.732449E+16	57.166667	1.234286E-06	2.869457E-16	6.576739E-16	8.240547E-15	99.990164	2.999997
0.50	1.732442E+16	58.333333	1.234286E-06	3.035625E-16	6.710949E-16	8.576889E-15	99.989771	2.999997
0.51	1.732435E+16	59.500000	1.234286E-06	3.208053E-16	6.845159E-16	8.919957E-15	99.989371	2.999997
0.52	1.732428E+16	60.666667	1.234286E-06	3.386855E-16	6.979369E-16	9.269752E-15	99.988963	2.999997
0.53	1.732421E+16	61.833333	1.234286E-06	3.572146E-16	7.113577E-16	9.626272E-15	99.988547	2.999997
0.54	1.732413E+16	63.000000	1.234286E-06	3.764042E-16	7.247785E-16	9.989519E-15	99.988123	2.999996
0.55	1.732406E+16	64.166667	1.234286E-06	3.962657E-16	7.381993E-16	1.035949E-14	99.987691	2.999996
0.56	1.732398E+16	65.333333	1.234286E-06	4.168106E-16	7.516200E-16	1.073619E-14	99.987252	2.999996
0.57	1.732390E+16	66.500000	1.234286E-06	4.380506E-16	7.650407E-16	1.111962E-14	99.986804	2.999996
0.58	1.732383E+16	67.666667	1.234286E-06	4.599970E-16	7.784612E-16	1.150977E-14	99.986348	2.999996
0.59	1.732375E+16	68.833333	1.234286E-06	4.826613E-16	7.918818E-16	1.190664E-14	99.985885	2.999996
0.60	1.732366E+16	70.000000	1.234286E-06	5.060552E-16	8.053022E-16	1.231025E-14	99.985413	2.999996
0.61	1.732358E+16	71.166667	1.234286E-06	5.301901E-16	8.187226E-16	1.272058E-14	99.984933	2.999996
0.62	1.732350E+16	72.333333	1.234286E-06	5.550775E-16	8.321430E-16	1.313763E-14	99.984446	2.999995
0.63	1.732341E+16	73.500000	1.234286E-06	5.807289E-16	8.455632E-16	1.356141E-14	99.983950	2.999995
0.64	1.732332E+16	74.666667	1.234286E-06	6.071559E-16	8.589835E-16	1.399192E-14	99.983446	2.999995
0.65	1.732323E+16	75.833333	1.234286E-06	6.343699E-16	8.724036E-16	1.442915E-14	99.982935	2.999995
0.66	1.732314E+16	77.000000	1.234286E-06	6.623824E-16	8.858237E-16	1.487311E-14	99.982415	2.999995
0.67	1.732305E+16	78.166667	1.234286E-06	6.912051E-16	8.992437E-16	1.532379E-14	99.981887	2.999995
0.68	1.732296E+16	79.333333	1.234286E-06	7.208493E-16	9.126636E-16	1.578120E-14	99.981351	2.999994
0.69	1.732287E+16	80.500000	1.234286E-06	7.513266E-16	9.260835E-16	1.624534E-14	99.980807	2.999994
0.70	1.732277E+16	81.666667	1.234286E-06	7.826484E-16	9.395032E-16	1.671620E-14	99.980255	2.999994
0.71	1.732267E+16	82.833333	1.234286E-06	8.148264E-16	9.529230E-16	1.719379E-14	99.979695	2.999994
0.72	1.732257E+16	84.000000	1.234286E-06	8.478720E-16	9.663426E-16	1.767810E-14	99.979126	2.999994
0.73	1.732247E+16	85.166667	1.234286E-06	8.817967E-16	9.797622E-16	1.816913E-14	99.978550	2.999994
0.74	1.732237E+16	86.333333	1.234286E-06	9.166121E-16	9.931816E-16	1.866690E-14	99.977965	2.999993
0.75	1.732227E+16	87.500000	1.234286E-06	9.523295E-16	1.006601E-15	1.917138E-14	99.977372	2.999993
0.76	1.732217E+16	88.666667	1.234286E-06	9.889607E-16	1.020020E-15	1.968260E-14	99.976771	2.999993
0.77	1.732206E+16	89.833333	1.234286E-06	1.026517E-15	1.033440E-15	2.020054E-14	99.976162	2.999993
0.78	1.732195E+16	91.000000	1.234286E-06	1.065010E-15	1.046859E-15	2.072520E-14	99.975544	2.999993
0.79	1.732185E+16	92.166667	1.234286E-06	1.104451E-15	1.060278E-15	2.125659E-14	99.974919	2.999993
0.80	1.732174E+16	93.333333	1.234286E-06	1.144852E-15	1.073697E-15	2.179470E-14	99.974285	2.999992
0.81	1.732162E+16	94.500000	1.234286E-06	1.186224E-15	1.087116E-15	2.233954E-14	99.973643	2.999992
0.82	1.732151E+16	95.666667	1.234286E-06	1.228578E-15	1.100535E-15	2.289110E-14	99.972992	2.999992
0.83	1.732140E+16	96.833333	1.234286E-06	1.271927E-15	1.113953E-15	2.344939E-14	99.972334	2.999992
0.84	1.732128E+16	98.000000	1.234286E-06	1.316282E-15	1.127372E-15	2.401441E-14	99.971667	2.999992
0.85	1.732117E+16	99.166667	1.234286E-06	1.361654E-15	1.140791E-15	2.458614E-14	99.970991	2.999991
0.86	1.732105E+16	100.333333	1.234286E-06	1.408054E-15	1.154209E-15	2.516461E-14	99.970308	2.999991
0.87	1.732093E+16	101.500000	1.234286E-06	1.455495E-15	1.167628E-15	2.574980E-14	99.969616	2.999991
0.88	1.732081E+16	102.666667	1.234286E-06	1.503987E-15	1.181046E-15	2.634171E-14	99.968916	2.999991
0.89	1.732068E+16	103.833333	1.234286E-06	1.553543E-15	1.194464E-15	2.694034E-14	99.968207	2.999991
0.90	1.732056E+16	105.000000	1.234286E-06	1.604173E-15	1.207882E-15	2.754571E-14	99.967491	2.999990
0.91	1.732043E+16	106.166667	1.234286E-06	1.655890E-15	1.221300E-15	2.815779E-14	99.966765	2.999990
0.92	1.732031E+16	107.333333	1.234286E-06	1.708705E-15	1.234718E-15	2.877660E-14	99.966032	2.999990
0.93	1.732018E+16	108.500000	1.234286E-06	1.762628E-15	1.248136E-15	2.940214E-14	99.965290	2.999990
0.94	1.732005E+16	109.666667	1.234286E-06	1.817673E-15	1.261554E-15	3.003440E-14	99.964539	2.999989
0.95	1.731992E+16	110.833333	1.234286E-06	1.873850E-15	1.274971E-15	3.067338E-14	99.963781	2.999989
0.96	1.731978E+16	112.000000	1.234286E-06	1.931170E-15	1.288389E-15	3.131909E-14	99.963013	2.999989
0.97	1.731965E+16	113.166667	1.234286E-06	1.989646E-15	1.301806E-15	3.197152E-14	99.962238	2.999989
0.98	1.731951E+16	114.333333	1.234286E-06	2.049289E-15	1.315224E-15	3.263068E-14	99.961454	2.999989
0.99	1.731938E+16	115.500000	1.234286E-06	2.110109E-15	1.328641E-15	3.329656E-14	99.960661	2.999988
1.00	1.731924E+16	116.666667	1.234286E-06	2.172120E-15	1.342058E-15	3.396916E-14	99.959860	2.999988

## FOUR LAMPS



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO2}}$ (mol)	$\Phi_{\text{NO2}}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732615E+16	1.166667	3.509915E-07	2.402137E-19	1.592695E-16	7.982380E-17	99.999744	3.000000
0.02	1.732609E+16	2.333333	4.963752E-07	1.060355E-18	3.185384E-16	2.394711E-16	99.999401	3.000000
0.03	1.732601E+16	3.500000	6.079304E-07	2.706629E-18	4.778066E-16	4.789415E-16	99.998973	3.000000
0.04	1.732592E+16	4.666667	7.019739E-07	5.382088E-18	6.370741E-16	7.982345E-16	99.998457	3.000000
0.05	1.732582E+16	5.833333	7.848260E-07	9.263547E-18	7.963406E-16	1.197350E-15	99.997855	2.999999
0.06	1.732570E+16	7.000000	8.597279E-07	1.450970E-17	9.556060E-16	1.676286E-15	99.997166	2.999999
0.07	1.732557E+16	8.166667	9.286050E-07	2.126576E-17	1.114870E-15	2.235044E-15	99.996390	2.999999
0.08	1.732542E+16	9.333333	9.927120E-07	2.966639E-17	1.274133E-15	2.873621E-15	99.995526	2.999999
0.09	1.732525E+16	10.500000	1.052920E-06	3.983775E-17	1.433395E-15	3.592018E-15	99.994576	2.999999
0.10	1.732507E+16	11.666667	1.109864E-06	5.189888E-17	1.592654E-15	4.390233E-15	99.993537	2.999998
0.11	1.732488E+16	12.833333	1.164022E-06	6.596282E-17	1.751912E-15	5.268265E-15	99.992412	2.999998
0.12	1.732467E+16	14.000000	1.215766E-06	8.213743E-17	1.911168E-15	6.226113E-15	99.991198	2.999998
0.13	1.732444E+16	15.166667	1.234286E-06	1.005479E-16	2.070422E-15	7.263776E-15	99.989897	2.999997
0.14	1.732420E+16	16.333333	1.234286E-06	1.213307E-16	2.229674E-15	8.381253E-15	99.988507	2.999997
0.15	1.732394E+16	17.500000	1.234286E-06	1.446225E-16	2.388924E-15	9.578542E-15	99.987029	2.999997
0.16	1.732367E+16	18.666667	1.234286E-06	1.705599E-16	2.548171E-15	1.085564E-14	99.985464	2.999996
0.17	1.732339E+16	19.833333	1.234286E-06	1.992795E-16	2.707416E-15	1.221255E-14	99.983809	2.999996
0.18	1.732308E+16	21.000000	1.234286E-06	2.309178E-16	2.866658E-15	1.364927E-14	99.982066	2.999995
0.19	1.732277E+16	22.166667	1.234286E-06	2.656115E-16	3.025897E-15	1.516579E-14	99.980235	2.999995
0.20	1.732243E+16	23.333333	1.234286E-06	3.034970E-16	3.185133E-15	1.676211E-14	99.978314	2.999994
0.21	1.732209E+16	24.500000	1.234286E-06	3.447109E-16	3.344366E-15	1.843824E-14	99.976304	2.999994
0.22	1.732172E+16	25.666667	1.234286E-06	3.893898E-16	3.503595E-15	2.019417E-14	99.974206	2.999993
0.23	1.732134E+16	26.833333	1.234286E-06	4.376703E-16	3.662821E-15	2.202990E-14	99.972018	2.999992
0.24	1.732095E+16	28.000000	1.234286E-06	4.896889E-16	3.822044E-15	2.394542E-14	99.969740	2.999992
0.25	1.732054E+16	29.166667	1.234286E-06	5.455821E-16	3.981263E-15	2.594074E-14	99.967373	2.999991
0.26	1.732011E+16	30.333333	1.234286E-06	6.054864E-16	4.140478E-15	2.801584E-14	99.964916	2.999990
0.27	1.731967E+16	31.500000	1.234286E-06	6.695385E-16	4.299690E-15	3.017074E-14	99.962369	2.999989
0.28	1.731921E+16	32.666667	1.234286E-06	7.378747E-16	4.458897E-15	3.240543E-14	99.959733	2.999989
0.29	1.731874E+16	33.833333	1.234286E-06	8.106317E-16	4.618100E-15	3.471989E-14	99.957006	2.999988
0.30	1.731825E+16	35.000000	1.234286E-06	8.879459E-16	4.777298E-15	3.711414E-14	99.954189	2.999987
0.31	1.731775E+16	36.166667	1.234286E-06	9.699537E-16	4.936492E-15	3.958817E-14	99.951281	2.999986
0.32	1.731723E+16	37.333333	1.234286E-06	1.056792E-15	5.095681E-15	4.214197E-14	99.948283	2.999985
0.33	1.731670E+16	38.500000	1.234286E-06	1.148597E-15	5.254866E-15	4.477555E-14	99.945194	2.999984
0.34	1.731614E+16	39.666667	1.234286E-06	1.245505E-15	5.414045E-15	4.748889E-14	99.942014	2.999983
0.35	1.731558E+16	40.833333	1.234286E-06	1.347652E-15	5.573220E-15	5.028201E-14	99.938743	2.999982
0.36	1.731500E+16	42.000000	1.234286E-06	1.455176E-15	5.732389E-15	5.315488E-14	99.935381	2.999981
0.37	1.731440E+16	43.166667	1.234286E-06	1.568212E-15	5.891553E-15	5.610752E-14	99.931927	2.999980
0.38	1.731378E+16	44.333333	1.234286E-06	1.686897E-15	6.050711E-15	5.913991E-14	99.928382	2.999979
0.39	1.731315E+16	45.500000	1.234286E-06	1.811368E-15	6.209864E-15	6.225206E-14	99.924746	2.999978
0.40	1.731251E+16	46.666667	1.234286E-06	1.941760E-15	6.369011E-15	6.544396E-14	99.921018	2.999977
0.41	1.731184E+16	47.833333	1.234286E-06	2.078211E-15	6.528152E-15	6.871560E-14	99.917198	2.999976
0.42	1.731117E+16	49.000000	1.234286E-06	2.220856E-15	6.687286E-15	7.206699E-14	99.913286	2.999975
0.43	1.731047E+16	50.166667	1.234286E-06	2.369832E-15	6.846415E-15	7.549812E-14	99.909281	2.999973
0.44	1.730976E+16	51.333333	1.234286E-06	2.525276E-15	7.005537E-15	7.900898E-14	99.905185	2.999972
0.45	1.730904E+16	52.500000	1.234286E-06	2.687323E-15	7.164653E-15	8.259957E-14	99.900996	2.999971

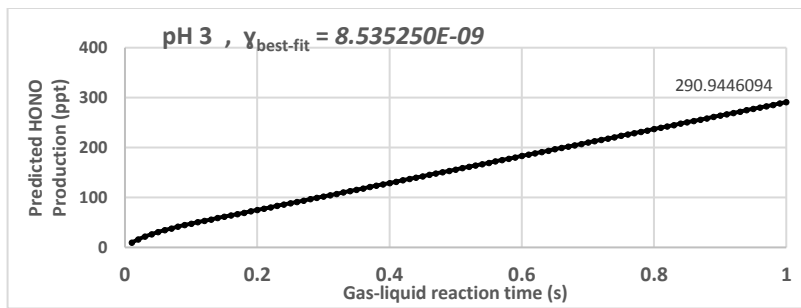
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0.47	1.730754E+16	54.833333	1.234286E-06	3.031775E-15	7.482864E-15	9.001993E-14	99.892340	2.999968
0.48	1.730676E+16	56.000000	1.234286E-06	3.214451E-15	7.641960E-15	9.384969E-14	99.887873	2.999967
0.49	1.730597E+16	57.166667	1.234286E-06	3.404277E-15	7.801048E-15	9.775917E-14	99.883312	2.999966
0.50	1.730517E+16	58.333333	1.234286E-06	3.601388E-15	7.960129E-15	1.017484E-13	99.878659	2.999964
0.51	1.730434E+16	59.500000	1.234286E-06	3.805921E-15	8.119202E-15	1.058172E-13	99.873912	2.999963
0.52	1.730351E+16	60.666667	1.234286E-06	4.018012E-15	8.278268E-15	1.099658E-13	99.869072	2.999961
0.53	1.730265E+16	61.833333	1.234286E-06	4.237797E-15	8.437327E-15	1.141941E-13	99.864139	2.999960
0.54	1.730178E+16	63.000000	1.234286E-06	4.465413E-15	8.596377E-15	1.185021E-13	99.859111	2.999958
0.55	1.730089E+16	64.166667	1.234286E-06	4.700996E-15	8.755420E-15	1.228898E-13	99.853990	2.999957
0.56	1.729999E+16	65.333333	1.234286E-06	4.944681E-15	8.914454E-15	1.273571E-13	99.848775	2.999955
0.57	1.729907E+16	66.500000	1.234286E-06	5.196606E-15	9.073481E-15	1.319042E-13	99.843465	2.999954
0.58	1.729813E+16	67.666667	1.234286E-06	5.456906E-15	9.232498E-15	1.365309E-13	99.838062	2.999952
0.59	1.729718E+16	68.833333	1.234286E-06	5.725717E-15	9.391508E-15	1.412372E-13	99.832564	2.999950
0.60	1.729621E+16	70.000000	1.234286E-06	6.003177E-15	9.550508E-15	1.460232E-13	99.826971	2.999949
0.61	1.729523E+16	71.166667	1.234286E-06	6.289420E-15	9.709500E-15	1.508889E-13	99.821284	2.999947
0.62	1.729422E+16	72.333333	1.234286E-06	6.584583E-15	9.868483E-15	1.558343E-13	99.815501	2.999945
0.63	1.729321E+16	73.500000	1.234286E-06	6.888803E-15	1.002746E-14	1.608592E-13	99.809624	2.999943
0.64	1.729217E+16	74.666667	1.234286E-06	7.202215E-15	1.018642E-14	1.659639E-13	99.803652	2.999942
0.65	1.729112E+16	75.833333	1.234286E-06	7.524955E-15	1.034538E-14	1.711481E-13	99.797585	2.999940
0.66	1.729005E+16	77.000000	1.234286E-06	7.857159E-15	1.050432E-14	1.764120E-13	99.791422	2.999938
0.67	1.728897E+16	78.166667	1.234286E-06	8.198964E-15	1.066326E-14	1.817555E-13	99.785163	2.999936
0.68	1.728787E+16	79.333333	1.234286E-06	8.550506E-15	1.082218E-14	1.871786E-13	99.778809	2.999934
0.69	1.728675E+16	80.500000	1.234286E-06	8.911921E-15	1.098110E-14	1.926813E-13	99.772359	2.999932
0.70	1.728562E+16	81.666667	1.234286E-06	9.283343E-15	1.114000E-14	1.982637E-13	99.765813	2.999930
0.71	1.728446E+16	82.833333	1.234286E-06	9.664911E-15	1.129890E-14	2.039256E-13	99.759171	2.999928
0.72	1.728330E+16	84.000000	1.234286E-06	1.005676E-14	1.145778E-14	2.096671E-13	99.752433	2.999926
0.73	1.728211E+16	85.166667	1.234286E-06	1.045902E-14	1.161666E-14	2.154882E-13	99.745598	2.999924
0.74	1.728091E+16	86.333333	1.234286E-06	1.087184E-14	1.177552E-14	2.213889E-13	99.738667	2.999922
0.75	1.727969E+16	87.500000	1.234286E-06	1.129535E-14	1.193437E-14	2.273691E-13	99.731639	2.999920
0.76	1.727846E+16	88.666667	1.234286E-06	1.172968E-14	1.209321E-14	2.334290E-13	99.724515	2.999918
0.77	1.727721E+16	89.833333	1.234286E-06	1.217497E-14	1.225204E-14	2.395683E-13	99.717294	2.999916
0.78	1.727594E+16	91.000000	1.234286E-06	1.263135E-14	1.241086E-14	2.457873E-13	99.709975	2.999914
0.79	1.727466E+16	92.166667	1.234286E-06	1.309897E-14	1.256967E-14	2.520857E-13	99.702559	2.999911
0.80	1.727335E+16	93.333333	1.234286E-06	1.357795E-14	1.272846E-14	2.584637E-13	99.695046	2.999909
0.81	1.727204E+16	94.500000	1.234286E-06	1.406844E-14	1.288725E-14	2.649213E-13	99.687436	2.999907
0.82	1.727070E+16	95.666667	1.234286E-06	1.457057E-14	1.304602E-14	2.714583E-13	99.679728	2.999904
0.83	1.726935E+16	96.833333	1.234286E-06	1.508447E-14	1.320478E-14	2.780749E-13	99.671922	2.999902
0.84	1.726798E+16	98.000000	1.234286E-06	1.561029E-14	1.336352E-14	2.847710E-13	99.664018	2.999900
0.85	1.726659E+16	99.166667	1.234286E-06	1.614815E-14	1.352226E-14	2.915466E-13	99.656016	2.999897
0.86	1.726519E+16	100.333333	1.234286E-06	1.669819E-14	1.368098E-14	2.984017E-13	99.647916	2.999895
0.87	1.726377E+16	101.500000	1.234286E-06	1.726055E-14	1.383969E-14	3.053362E-13	99.639718	2.999893
0.88	1.726233E+16	102.666667	1.234286E-06	1.783536E-14	1.399839E-14	3.123503E-13	99.631421	2.999890
0.89	1.726088E+16	103.833333	1.234286E-06	1.842277E-14	1.415707E-14	3.194438E-13	99.623026	2.999888
0.90	1.725940E+16	105.000000	1.234286E-06	1.902290E-14	1.431574E-14	3.266167E-13	99.614532	2.999885
0.91	1.725792E+16	106.166667	1.234286E-06	1.963588E-14	1.447440E-14	3.338691E-13	99.605939	2.999883
0.92	1.725641E+16	107.333333	1.234286E-06	2.026187E-14	1.463304E-14	3.412010E-13	99.597248	2.999880
0.93	1.725489E+16	108.500000	1.234286E-06	2.090098E-14	1.479167E-14	3.486123E-13	99.588457	2.999877
0.94	1.725335E+16	109.666667	1.234286E-06	2.155336E-14	1.495028E-14	3.561030E-13	99.579567	2.999875
0.95	1.725179E+16	110.833333	1.234286E-06	2.221915E-14	1.510888E-14	3.636732E-13	99.570577	2.999872
0.96	1.725021E+16	112.000000	1.234286E-06	2.289847E-14	1.526747E-14	3.713228E-13	99.561488	2.999869
0.97	1.724862E+16	113.166667	1.234286E-06	2.359147E-14	1.542605E-14	3.790517E-13	99.552299	2.999867
0.98	1.724701E+16	114.333333	1.234286E-06	2.429827E-14	1.558460E-14	3.868601E-13	99.543011	2.999864
0.99	1.724539E+16	115.500000	1.234286E-06	2.501902E-14	1.574315E-14	3.947478E-13	99.533622	2.999861
1.00	1.724374E+16	116.666667	1.234286E-06	2.575385E-14	1.590168E-14	4.027149E-13	99.524134	2.999858



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732615E+16	1.166667	3.509916E-07	2.173844E-19	1.441329E-16	7.223756E-17	99.999768	3.000000
0.02	1.732610E+16	2.333333	4.963755E-07	9.595811E-19	2.882654E-16	2.167124E-16	99.999458	3.000000
0.03	1.732603E+16	3.500000	6.079310E-07	2.449397E-18	4.323973E-16	4.334243E-16	99.999070	3.000000
0.04	1.732595E+16	4.666667	7.019750E-07	4.870587E-18	5.765286E-16	7.223727E-16	99.998604	3.000000
0.05	1.732585E+16	5.833333	7.848276E-07	8.383162E-18	7.206590E-16	1.083557E-15	99.998059	2.999999
0.06	1.732575E+16	7.000000	8.597302E-07	1.313073E-17	8.647887E-16	1.516978E-15	99.997435	2.999999
0.07	1.732563E+16	8.166667	9.286082E-07	1.924471E-17	1.008917E-15	2.022633E-15	99.996733	2.999999
0.08	1.732549E+16	9.333333	9.927162E-07	2.684697E-17	1.153045E-15	2.600523E-15	99.995952	2.999999
0.09	1.732534E+16	10.500000	1.052925E-06	3.605166E-17	1.297171E-15	3.250646E-15	99.995091	2.999999
0.10	1.732518E+16	11.666667	1.109870E-06	4.696653E-17	1.441296E-15	3.973003E-15	99.994152	2.999998
0.11	1.732500E+16	12.833333	1.164030E-06	5.969387E-17	1.585420E-15	4.767592E-15	99.993133	2.999998
0.12	1.732481E+16	14.000000	1.215776E-06	7.433129E-17	1.729542E-15	5.634412E-15	99.992035	2.999998
0.13	1.732461E+16	15.166667	1.234286E-06	9.099204E-17	1.873662E-15	6.573462E-15	99.990857	2.999998
0.14	1.732439E+16	16.333333	1.234286E-06	1.097997E-16	2.017780E-15	7.584742E-15	99.989599	2.999997
0.15	1.732416E+16	17.500000	1.234286E-06	1.308780E-16	2.161897E-15	8.668249E-15	99.988262	2.999997
0.16	1.732391E+16	18.666667	1.234286E-06	1.543504E-16	2.306012E-15	9.823984E-15	99.986845	2.999997
0.17	1.732365E+16	19.833333	1.234286E-06	1.803406E-16	2.450124E-15	1.105194E-14	99.985348	2.999996
0.18	1.732338E+16	21.000000	1.234286E-06	2.089722E-16	2.594235E-15	1.235213E-14	99.983771	2.999996
0.19	1.732309E+16	22.166667	1.234286E-06	2.403687E-16	2.738343E-15	1.372454E-14	99.982113	2.999995
0.20	1.732279E+16	23.333333	1.234286E-06	2.746538E-16	2.882448E-15	1.516916E-14	99.980375	2.999995
0.21	1.732248E+16	24.500000	1.234286E-06	3.119511E-16	3.026551E-15	1.668601E-14	99.978556	2.999994
0.22	1.732215E+16	25.666667	1.234286E-06	3.523841E-16	3.170651E-15	1.827508E-14	99.976657	2.999994
0.23	1.732180E+16	26.833333	1.234286E-06	3.960763E-16	3.314749E-15	1.993636E-14	99.974677	2.999993
0.24	1.732145E+16	28.000000	1.234286E-06	4.431515E-16	3.458843E-15	2.166986E-14	99.972616	2.999992
0.25	1.732108E+16	29.166667	1.234286E-06	4.937331E-16	3.602935E-15	2.347557E-14	99.970474	2.999992
0.26	1.732069E+16	30.333333	1.234286E-06	5.479448E-16	3.747023E-15	2.535349E-14	99.968250	2.999991
0.27	1.732029E+16	31.500000	1.234286E-06	6.059100E-16	3.891109E-15	2.730362E-14	99.965945	2.999990
0.28	1.731988E+16	32.666667	1.234286E-06	6.677523E-16	4.035191E-15	2.932596E-14	99.963559	2.999990
0.29	1.731945E+16	33.833333	1.234286E-06	7.335953E-16	4.179269E-15	3.142050E-14	99.961091	2.999989
0.30	1.731901E+16	35.000000	1.234286E-06	8.035625E-16	4.323344E-15	3.358725E-14	99.958542	2.999988
0.31	1.731855E+16	36.166667	1.234286E-06	8.777775E-16	4.467415E-15	3.582619E-14	99.955911	2.999987
0.32	1.731808E+16	37.333333	1.234286E-06	9.563638E-16	4.611482E-15	3.813734E-14	99.953197	2.999987
0.33	1.731760E+16	38.500000	1.234286E-06	1.039445E-15	4.755545E-15	4.052068E-14	99.950402	2.999986
0.34	1.731710E+16	39.666667	1.234286E-06	1.127144E-15	4.899605E-15	4.297621E-14	99.947524	2.999985
0.35	1.731659E+16	40.833333	1.234286E-06	1.219585E-15	5.043660E-15	4.550394E-14	99.944564	2.999984
0.36	1.731606E+16	42.000000	1.234286E-06	1.316892E-15	5.187710E-15	4.810385E-14	99.941521	2.999983
0.37	1.731552E+16	43.166667	1.234286E-06	1.419187E-15	5.331757E-15	5.077595E-14	99.938396	2.999982
0.38	1.731496E+16	44.333333	1.234286E-06	1.526595E-15	5.475799E-15	5.352023E-14	99.935188	2.999981
0.39	1.731439E+16	45.500000	1.234286E-06	1.639238E-15	5.619836E-15	5.633669E-14	99.931897	2.999980
0.40	1.731381E+16	46.666667	1.234286E-06	1.757241E-15	5.763869E-15	5.922533E-14	99.928523	2.999979
0.41	1.731321E+16	47.833333	1.234286E-06	1.880727E-15	5.907896E-15	6.218614E-14	99.925066	2.999978
0.42	1.731259E+16	49.000000	1.234286E-06	2.009818E-15	6.051919E-15	6.521913E-14	99.921525	2.999977
0.43	1.731197E+16	50.166667	1.234286E-06	2.144640E-15	6.195936E-15	6.832428E-14	99.917901	2.999976
0.44	1.731132E+16	51.333333	1.234286E-06	2.285314E-15	6.339949E-15	7.150160E-14	99.914194	2.999975
0.45	1.731067E+16	52.500000	1.234286E-06	2.431965E-15	6.483956E-15	7.475108E-14	99.910403	2.999974

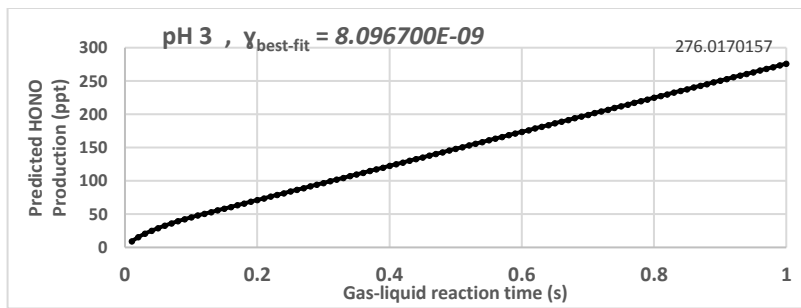
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0.47	1.730931E+16	54.833333	1.234286E-06	2.743689E-15	6.771953E-15	8.146651E-14	99.902569	2.999971
0.48	1.730861E+16	56.000000	1.234286E-06	2.909010E-15	6.915944E-15	8.493245E-14	99.898526	2.999970
0.49	1.730789E+16	57.166667	1.234286E-06	3.080801E-15	7.059928E-15	8.847054E-14	99.894399	2.999969
0.50	1.730716E+16	58.333333	1.234286E-06	3.259185E-15	7.203907E-15	9.208078E-14	99.890188	2.999968
0.51	1.730642E+16	59.500000	1.234286E-06	3.444286E-15	7.347879E-15	9.576316E-14	99.885892	2.999966
0.52	1.730566E+16	60.666667	1.234286E-06	3.636228E-15	7.491845E-15	9.951767E-14	99.881512	2.999965
0.53	1.730489E+16	61.833333	1.234286E-06	3.835133E-15	7.635805E-15	1.033443E-13	99.877047	2.999964
0.54	1.730410E+16	63.000000	1.234286E-06	4.041125E-15	7.779759E-15	1.072431E-13	99.872497	2.999962
0.55	1.730330E+16	64.166667	1.234286E-06	4.254327E-15	7.923706E-15	1.112140E-13	99.867862	2.999961
0.56	1.730248E+16	65.333333	1.234286E-06	4.474862E-15	8.067647E-15	1.152570E-13	99.863142	2.999959
0.57	1.730165E+16	66.500000	1.234286E-06	4.702855E-15	8.211580E-15	1.193722E-13	99.858337	2.999958
0.58	1.730080E+16	67.666667	1.234286E-06	4.938427E-15	8.355507E-15	1.235594E-13	99.853447	2.999957
0.59	1.729994E+16	68.833333	1.234286E-06	5.181703E-15	8.499427E-15	1.278188E-13	99.848471	2.999955
0.60	1.729906E+16	70.000000	1.234286E-06	5.432806E-15	8.643340E-15	1.321502E-13	99.843410	2.999954
0.61	1.729817E+16	71.166667	1.234286E-06	5.691859E-15	8.787245E-15	1.365538E-13	99.838262	2.999952
0.62	1.729726E+16	72.333333	1.234286E-06	5.958985E-15	8.931143E-15	1.410295E-13	99.833029	2.999950
0.63	1.729634E+16	73.500000	1.234286E-06	6.234307E-15	9.075034E-15	1.455772E-13	99.827710	2.999949
0.64	1.729540E+16	74.666667	1.234286E-06	6.517949E-15	9.218917E-15	1.501971E-13	99.822305	2.999947
0.65	1.729445E+16	75.833333	1.234286E-06	6.810033E-15	9.362792E-15	1.548890E-13	99.816814	2.999946
0.66	1.729349E+16	77.000000	1.234286E-06	7.110684E-15	9.506659E-15	1.596530E-13	99.811236	2.999944
0.67	1.729250E+16	78.166667	1.234286E-06	7.420024E-15	9.650519E-15	1.644891E-13	99.805572	2.999942
0.68	1.729151E+16	79.333333	1.234286E-06	7.738177E-15	9.794370E-15	1.693972E-13	99.799821	2.999940
0.69	1.729050E+16	80.500000	1.234286E-06	8.065264E-15	9.938213E-15	1.743774E-13	99.793984	2.999939
0.70	1.728947E+16	81.666667	1.234286E-06	8.401411E-15	1.008205E-14	1.794297E-13	99.788059	2.999937
0.71	1.728843E+16	82.833333	1.234286E-06	8.746739E-15	1.022587E-14	1.845540E-13	99.782048	2.999935
0.72	1.728737E+16	84.000000	1.234286E-06	9.101372E-15	1.036969E-14	1.897503E-13	99.775950	2.999933
0.73	1.728630E+16	85.166667	1.234286E-06	9.465434E-15	1.051350E-14	1.950187E-13	99.769764	2.999931
0.74	1.728521E+16	86.333333	1.234286E-06	9.839046E-15	1.065730E-14	2.003592E-13	99.763491	2.999930
0.75	1.728411E+16	87.500000	1.234286E-06	1.022233E-14	1.080109E-14	2.057716E-13	99.757130	2.999928
0.76	1.728299E+16	88.666667	1.234286E-06	1.061542E-14	1.094487E-14	2.112561E-13	99.750682	2.999926
0.77	1.728186E+16	89.833333	1.234286E-06	1.101842E-14	1.108865E-14	2.168126E-13	99.744146	2.999924
0.78	1.728071E+16	91.000000	1.234286E-06	1.143147E-14	1.123241E-14	2.224412E-13	99.737523	2.999922
0.79	1.727955E+16	92.166667	1.234286E-06	1.185468E-14	1.137616E-14	2.281417E-13	99.730811	2.999920
0.80	1.727837E+16	93.333333	1.234286E-06	1.228818E-14	1.151991E-14	2.339142E-13	99.724011	2.999918
0.81	1.727718E+16	94.500000	1.234286E-06	1.273210E-14	1.166364E-14	2.397588E-13	99.717123	2.999916
0.82	1.727597E+16	95.666667	1.234286E-06	1.318655E-14	1.180737E-14	2.456753E-13	99.710147	2.999914
0.83	1.727475E+16	96.833333	1.234286E-06	1.365165E-14	1.195108E-14	2.516638E-13	99.703082	2.999911
0.84	1.727351E+16	98.000000	1.234286E-06	1.412754E-14	1.209479E-14	2.577243E-13	99.695928	2.999909
0.85	1.727225E+16	99.166667	1.234286E-06	1.461433E-14	1.223848E-14	2.638568E-13	99.688686	2.999907
0.86	1.727098E+16	100.333333	1.234286E-06	1.511215E-14	1.238217E-14	2.700612E-13	99.681355	2.999905
0.87	1.726970E+16	101.500000	1.234286E-06	1.562112E-14	1.252584E-14	2.763376E-13	99.673935	2.999903
0.88	1.726840E+16	102.666667	1.234286E-06	1.614136E-14	1.266951E-14	2.826859E-13	99.666425	2.999901
0.89	1.726708E+16	103.833333	1.234286E-06	1.667300E-14	1.281316E-14	2.891062E-13	99.658827	2.999898
0.90	1.726575E+16	105.000000	1.234286E-06	1.721615E-14	1.295680E-14	2.955984E-13	99.651139	2.999896
0.91	1.726440E+16	106.166667	1.234286E-06	1.777095E-14	1.310043E-14	3.021626E-13	99.643362	2.999894
0.92	1.726304E+16	107.333333	1.234286E-06	1.833751E-14	1.324405E-14	3.087987E-13	99.635495	2.999891
0.93	1.726166E+16	108.500000	1.234286E-06	1.891595E-14	1.338766E-14	3.155067E-13	99.627538	2.999889
0.94	1.726026E+16	109.666667	1.234286E-06	1.950640E-14	1.353126E-14	3.222866E-13	99.619491	2.999887
0.95	1.725885E+16	110.833333	1.234286E-06	2.010899E-14	1.367484E-14	3.291384E-13	99.611355	2.999884
0.96	1.725743E+16	112.000000	1.234286E-06	2.072383E-14	1.381842E-14	3.360622E-13	99.603128	2.999882
0.97	1.725599E+16	113.166667	1.234286E-06	2.135105E-14	1.396198E-14	3.430578E-13	99.594811	2.999879
0.98	1.725453E+16	114.333333	1.234286E-06	2.199076E-14	1.410553E-14	3.501253E-13	99.586404	2.999877
0.99	1.725306E+16	115.500000	1.234286E-06	2.264310E-14	1.424907E-14	3.572647E-13	99.577907	2.999874
1.00	1.725157E+16	116.666667	1.234286E-06	2.330819E-14	1.439260E-14	3.644759E-13	99.569318	2.999872





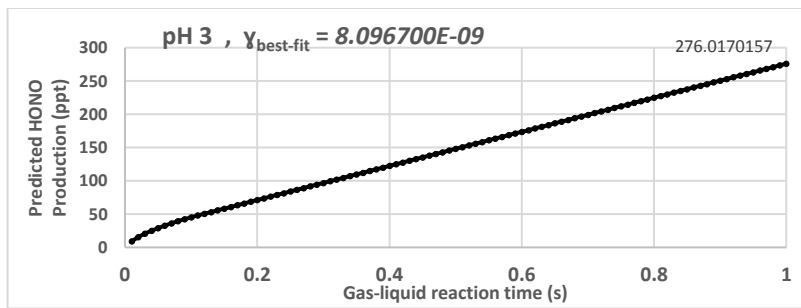
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO2}}$ (mol)	$\Phi_{\text{NO2}}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732615E+16	1.166667	3.509915E-07	2.467163E-19	1.635809E-16	8.198463E-17	99.999737	3.000000
0.02	1.732608E+16	2.333333	4.963751E-07	1.089059E-18	3.271612E-16	2.459536E-16	99.999385	3.000000
0.03	1.732601E+16	3.500000	6.079302E-07	2.779897E-18	4.907408E-16	4.919064E-16	99.998945	3.000000
0.04	1.732592E+16	4.666667	7.019736E-07	5.527782E-18	6.543196E-16	8.198426E-16	99.998415	2.999999
0.05	1.732581E+16	5.833333	7.848255E-07	9.514312E-18	8.178973E-16	1.229762E-15	99.997797	2.999999
0.06	1.732569E+16	7.000000	8.597272E-07	1.490248E-17	9.814740E-16	1.721663E-15	99.997089	2.999999
0.07	1.732555E+16	8.166667	9.286041E-07	2.184142E-17	1.145049E-15	2.295546E-15	99.996292	2.999999
0.08	1.732540E+16	9.333333	9.927108E-07	3.046946E-17	1.308623E-15	2.951409E-15	99.995405	2.999999
0.09	1.732523E+16	10.500000	1.052918E-06	4.091616E-17	1.472196E-15	3.689252E-15	99.994429	2.999998
0.10	1.732504E+16	11.666667	1.109862E-06	5.330379E-17	1.635766E-15	4.509074E-15	99.993363	2.999998
0.11	1.732484E+16	12.833333	1.164019E-06	6.774844E-17	1.799335E-15	5.410873E-15	99.992206	2.999998
0.12	1.732462E+16	14.000000	1.215763E-06	8.436090E-17	1.962902E-15	6.394650E-15	99.990960	2.999998
0.13	1.732439E+16	15.166667	1.234286E-06	1.032697E-16	2.126467E-15	7.460401E-15	99.989623	2.999997
0.14	1.732415E+16	16.333333	1.234286E-06	1.246151E-16	2.290029E-15	8.608126E-15	99.988196	2.999997
0.15	1.732388E+16	17.500000	1.234286E-06	1.485375E-16	2.453589E-15	9.837824E-15	99.986678	2.999997
0.16	1.732360E+16	18.666667	1.234286E-06	1.751770E-16	2.617146E-15	1.114949E-14	99.985070	2.999996
0.17	1.732331E+16	19.833333	1.234286E-06	2.046740E-16	2.780701E-15	1.254313E-14	99.983371	2.999996
0.18	1.732300E+16	21.000000	1.234286E-06	2.371687E-16	2.944253E-15	1.401874E-14	99.981581	2.999995
0.19	1.732267E+16	22.166667	1.234286E-06	2.728015E-16	3.107801E-15	1.557631E-14	99.979699	2.999995
0.20	1.732233E+16	23.333333	1.234286E-06	3.117125E-16	3.271347E-15	1.721584E-14	99.977727	2.999994
0.21	1.732197E+16	24.500000	1.234286E-06	3.540420E-16	3.434889E-15	1.893734E-14	99.975663	2.999993
0.22	1.732160E+16	25.666667	1.234286E-06	3.999304E-16	3.598428E-15	2.074079E-14	99.973507	2.999993
0.23	1.732121E+16	26.833333	1.234286E-06	4.495177E-16	3.761964E-15	2.262621E-14	99.971260	2.999992
0.24	1.732081E+16	28.000000	1.234286E-06	5.029443E-16	3.925495E-15	2.459358E-14	99.968921	2.999991
0.25	1.732039E+16	29.166667	1.234286E-06	5.603504E-16	4.089023E-15	2.664290E-14	99.966490	2.999991
0.26	1.731995E+16	30.333333	1.234286E-06	6.218762E-16	4.252546E-15	2.877417E-14	99.963967	2.999990
0.27	1.731949E+16	31.500000	1.234286E-06	6.876620E-16	4.416066E-15	3.098739E-14	99.961351	2.999989
0.28	1.731903E+16	32.666667	1.234286E-06	7.578479E-16	4.579581E-15	3.328255E-14	99.958643	2.999988
0.29	1.731854E+16	33.833333	1.234286E-06	8.325742E-16	4.743092E-15	3.565966E-14	99.955842	2.999987
0.30	1.731804E+16	35.000000	1.234286E-06	9.119810E-16	4.906598E-15	3.811871E-14	99.952949	2.999987
0.31	1.731752E+16	36.166667	1.234286E-06	9.962086E-16	5.070099E-15	4.065970E-14	99.949962	2.999986
0.32	1.731699E+16	37.333333	1.234286E-06	1.085397E-15	5.233595E-15	4.328262E-14	99.946883	2.999985
0.33	1.731644E+16	38.500000	1.234286E-06	1.179687E-15	5.397086E-15	4.598747E-14	99.943710	2.999984
0.34	1.731587E+16	39.666667	1.234286E-06	1.279217E-15	5.560572E-15	4.877424E-14	99.940444	2.999983
0.35	1.731529E+16	40.833333	1.234286E-06	1.384130E-15	5.724053E-15	5.164295E-14	99.937085	2.999982
0.36	1.731469E+16	42.000000	1.234286E-06	1.494563E-15	5.887528E-15	5.459357E-14	99.933632	2.999981
0.37	1.731408E+16	43.166667	1.234286E-06	1.610659E-15	6.050998E-15	5.762611E-14	99.930085	2.999980
0.38	1.731345E+16	44.333333	1.234286E-06	1.732556E-15	6.214461E-15	6.074057E-14	99.926444	2.999979
0.39	1.731280E+16	45.500000	1.234286E-06	1.860396E-15	6.377919E-15	6.393693E-14	99.922709	2.999978
0.40	1.731214E+16	46.666667	1.234286E-06	1.994317E-15	6.541371E-15	6.721520E-14	99.918880	2.999976
0.41	1.731146E+16	47.833333	1.234286E-06	2.134460E-15	6.704816E-15	7.057538E-14	99.914957	2.999975
0.42	1.731076E+16	49.000000	1.234286E-06	2.280966E-15	6.868255E-15	7.401746E-14	99.910939	2.999974
0.43	1.731005E+16	50.166667	1.234286E-06	2.433974E-15	7.031687E-15	7.754143E-14	99.906826	2.999973
0.44	1.730932E+16	51.333333	1.234286E-06	2.593624E-15	7.195113E-15	8.114729E-14	99.902619	2.999971
0.45	1.730857E+16	52.500000	1.234286E-06	2.760057E-15	7.358531E-15	8.483504E-14	99.898316	2.999970

0.46	1.730781E+16	53.666667	1.234286E-06	2.933412E-15	7.521943E-15	8.860467E-14	99.893919	2.999969
0.47	1.730703E+16	54.833333	1.234286E-06	3.113830E-15	7.685348E-15	9.245618E-14	99.889426	2.999967
0.48	1.730624E+16	56.000000	1.234286E-06	3.301450E-15	7.848745E-15	9.638956E-14	99.884838	2.999966
0.49	1.730543E+16	57.166667	1.234286E-06	3.496412E-15	8.012134E-15	1.004048E-13	99.880155	2.999965
0.50	1.730460E+16	58.333333	1.234286E-06	3.698857E-15	8.175516E-15	1.045019E-13	99.875375	2.999963
0.51	1.730375E+16	59.500000	1.234286E-06	3.908925E-15	8.338891E-15	1.086809E-13	99.870500	2.999962
0.52	1.730289E+16	60.666667	1.234286E-06	4.126755E-15	8.502257E-15	1.129417E-13	99.865529	2.999960
0.53	1.730201E+16	61.833333	1.234286E-06	4.352487E-15	8.665615E-15	1.172844E-13	99.860462	2.999959
0.54	1.730112E+16	63.000000	1.234286E-06	4.586262E-15	8.828965E-15	1.217090E-13	99.855299	2.999957
0.55	1.730021E+16	64.166667	1.234286E-06	4.828219E-15	8.992307E-15	1.262153E-13	99.850039	2.999956
0.56	1.729928E+16	65.333333	1.234286E-06	5.078498E-15	9.155640E-15	1.308035E-13	99.844683	2.999954
0.57	1.729834E+16	66.500000	1.234286E-06	5.337239E-15	9.318964E-15	1.354736E-13	99.839230	2.999952
0.58	1.729737E+16	67.666667	1.234286E-06	5.604581E-15	9.482279E-15	1.402254E-13	99.833680	2.999951
0.59	1.729640E+16	68.833333	1.234286E-06	5.880666E-15	9.645586E-15	1.450591E-13	99.828033	2.999949
0.60	1.729540E+16	70.000000	1.234286E-06	6.165632E-15	9.808883E-15	1.499746E-13	99.822289	2.999947
0.61	1.729439E+16	71.166667	1.234286E-06	6.459620E-15	9.972171E-15	1.549719E-13	99.816448	2.999945
0.62	1.729336E+16	72.333333	1.234286E-06	6.762769E-15	1.013545E-14	1.600510E-13	99.810509	2.999944
0.63	1.729231E+16	73.500000	1.234286E-06	7.075219E-15	1.029872E-14	1.652119E-13	99.804473	2.999942
0.64	1.729125E+16	74.666667	1.234286E-06	7.397109E-15	1.046198E-14	1.704546E-13	99.798339	2.999940
0.65	1.729017E+16	75.833333	1.234286E-06	7.728580E-15	1.062523E-14	1.757790E-13	99.792108	2.999938
0.66	1.728907E+16	77.000000	1.234286E-06	8.069772E-15	1.078846E-14	1.811853E-13	99.785778	2.999936
0.67	1.728796E+16	78.166667	1.234286E-06	8.420824E-15	1.095169E-14	1.866733E-13	99.779350	2.999934
0.68	1.728683E+16	79.333333	1.234286E-06	8.781875E-15	1.111491E-14	1.922431E-13	99.772824	2.999932
0.69	1.728568E+16	80.500000	1.234286E-06	9.153066E-15	1.127812E-14	1.978946E-13	99.766200	2.999930
0.70	1.728452E+16	81.666667	1.234286E-06	9.534536E-15	1.144132E-14	2.036279E-13	99.759477	2.999928
0.71	1.728334E+16	82.833333	1.234286E-06	9.926425E-15	1.160450E-14	2.094430E-13	99.752655	2.999926
0.72	1.728214E+16	84.000000	1.234286E-06	1.032887E-14	1.176768E-14	2.153397E-13	99.745735	2.999924
0.73	1.728092E+16	85.166667	1.234286E-06	1.074202E-14	1.193084E-14	2.213183E-13	99.738716	2.999922
0.74	1.727969E+16	86.333333	1.234286E-06	1.116600E-14	1.209399E-14	2.273785E-13	99.731597	2.999920
0.75	1.727844E+16	87.500000	1.234286E-06	1.160096E-14	1.225713E-14	2.335204E-13	99.724379	2.999918
0.76	1.727717E+16	88.666667	1.234286E-06	1.204704E-14	1.242026E-14	2.397441E-13	99.717062	2.999916
0.77	1.727588E+16	89.833333	1.234286E-06	1.250437E-14	1.258338E-14	2.460495E-13	99.709645	2.999913
0.78	1.727458E+16	91.000000	1.234286E-06	1.297310E-14	1.274648E-14	2.524366E-13	99.702129	2.999911
0.79	1.727326E+16	92.166667	1.234286E-06	1.345336E-14	1.290958E-14	2.589053E-13	99.694513	2.999909
0.80	1.727192E+16	93.333333	1.234286E-06	1.394530E-14	1.307266E-14	2.654558E-13	99.686797	2.999907
0.81	1.727057E+16	94.500000	1.234286E-06	1.444906E-14	1.323573E-14	2.720879E-13	99.678980	2.999904
0.82	1.726920E+16	95.666667	1.234286E-06	1.496476E-14	1.339878E-14	2.788017E-13	99.671064	2.999902
0.83	1.726781E+16	96.833333	1.234286E-06	1.549256E-14	1.356182E-14	2.855971E-13	99.663047	2.999900
0.84	1.726640E+16	98.000000	1.234286E-06	1.603260E-14	1.372485E-14	2.924742E-13	99.654930	2.999897
0.85	1.726498E+16	99.166667	1.234286E-06	1.658500E-14	1.388787E-14	2.994329E-13	99.646712	2.999895
0.86	1.726354E+16	100.333333	1.234286E-06	1.714992E-14	1.405087E-14	3.064733E-13	99.638393	2.999892
0.87	1.726208E+16	101.500000	1.234286E-06	1.772748E-14	1.421386E-14	3.135953E-13	99.629973	2.999890
0.88	1.726060E+16	102.666667	1.234286E-06	1.831784E-14	1.437684E-14	3.207989E-13	99.621452	2.999887
0.89	1.725911E+16	103.833333	1.234286E-06	1.892112E-14	1.453980E-14	3.280841E-13	99.612830	2.999885
0.90	1.725760E+16	105.000000	1.234286E-06	1.953748E-14	1.470275E-14	3.354510E-13	99.604106	2.999882
0.91	1.725607E+16	106.166667	1.234286E-06	2.016704E-14	1.486569E-14	3.428994E-13	99.595281	2.999879
0.92	1.725452E+16	107.333333	1.234286E-06	2.080994E-14	1.502861E-14	3.504294E-13	99.586355	2.999877
0.93	1.725296E+16	108.500000	1.234286E-06	2.146634E-14	1.519151E-14	3.580410E-13	99.577326	2.999874
0.94	1.725138E+16	109.666667	1.234286E-06	2.213636E-14	1.535440E-14	3.657341E-13	99.568196	2.999871
0.95	1.724978E+16	110.833333	1.234286E-06	2.282014E-14	1.551728E-14	3.735088E-13	99.558963	2.999869
0.96	1.724816E+16	112.000000	1.234286E-06	2.351782E-14	1.568014E-14	3.813651E-13	99.549629	2.999866
0.97	1.724652E+16	113.166667	1.234286E-06	2.422955E-14	1.584299E-14	3.893029E-13	99.540192	2.999863
0.98	1.724487E+16	114.333333	1.234286E-06	2.495546E-14	1.600582E-14	3.973222E-13	99.530652	2.999860
0.99	1.724320E+16	115.500000	1.234286E-06	2.569569E-14	1.616863E-14	4.054231E-13	99.521010	2.999857
1.00	1.724151E+16	116.666667	1.234286E-06	2.645038E-14	1.633143E-14	4.136054E-13	99.511265	2.999854



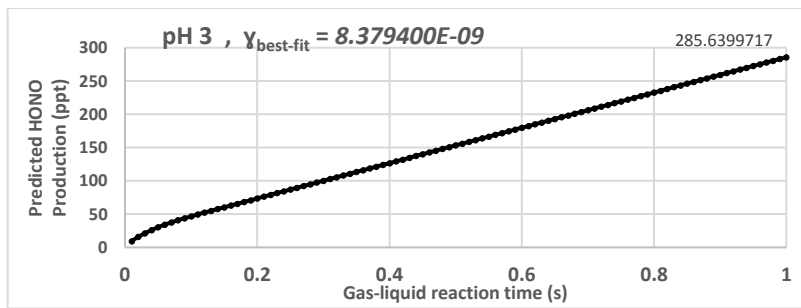
$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% $\text{NO}_2$ left	film pH
0.01	1.732615E+16	1.166667	3.509915E-07	2.340398E-19	1.551759E-16	7.777218E-17	99.999750	3.000000
0.02	1.732609E+16	2.333333	4.963753E-07	1.033102E-18	3.103514E-16	2.333163E-16	99.999417	3.000000
0.03	1.732602E+16	3.500000	6.079306E-07	2.637063E-18	4.655262E-16	4.666319E-16	99.998999	3.000000
0.04	1.732593E+16	4.666667	7.019742E-07	5.243758E-18	6.207002E-16	7.777185E-16	99.998497	3.000000
0.05	1.732583E+16	5.833333	7.848264E-07	9.025456E-18	7.758734E-16	1.166576E-15	99.997910	2.999999
0.06	1.732571E+16	7.000000	8.597285E-07	1.413677E-17	9.310455E-16	1.633203E-15	99.997239	2.999999
0.07	1.732558E+16	8.166667	9.286059E-07	2.071919E-17	1.086216E-15	2.177600E-15	99.996483	2.999999
0.08	1.732544E+16	9.333333	9.927131E-07	2.890391E-17	1.241386E-15	2.799765E-15	99.995641	2.999999
0.09	1.732528E+16	10.500000	1.052922E-06	3.881384E-17	1.396554E-15	3.499698E-15	99.994715	2.999999
0.10	1.732510E+16	11.666667	1.109865E-06	5.056498E-17	1.551721E-15	4.277398E-15	99.993704	2.999998
0.11	1.732491E+16	12.833333	1.164024E-06	6.426745E-17	1.706886E-15	5.132863E-15	99.992607	2.999998
0.12	1.732471E+16	14.000000	1.215769E-06	8.002635E-17	1.862050E-15	6.066094E-15	99.991424	2.999998
0.13	1.732449E+16	15.166667	1.234286E-06	9.796359E-17	2.017211E-15	7.077089E-15	99.990156	2.999998
0.14	1.732425E+16	16.333333	1.234286E-06	1.182123E-16	2.172370E-15	8.165846E-15	99.988802	2.999997
0.15	1.732400E+16	17.500000	1.234286E-06	1.409055E-16	2.327527E-15	9.332364E-15	99.987363	2.999997
0.16	1.732374E+16	18.666667	1.234286E-06	1.661763E-16	2.482682E-15	1.057664E-14	99.985837	2.999996
0.17	1.732346E+16	19.833333	1.234286E-06	1.941577E-16	2.637834E-15	1.189868E-14	99.984225	2.999996
0.18	1.732316E+16	21.000000	1.234286E-06	2.249829E-16	2.792984E-15	1.329847E-14	99.982527	2.999995
0.19	1.732285E+16	22.166667	1.234286E-06	2.587849E-16	2.948131E-15	1.477602E-14	99.980742	2.999995
0.20	1.732253E+16	23.333333	1.234286E-06	2.956967E-16	3.103275E-15	1.633132E-14	99.978871	2.999994
0.21	1.732219E+16	24.500000	1.234286E-06	3.358514E-16	3.258417E-15	1.796437E-14	99.976913	2.999994
0.22	1.732184E+16	25.666667	1.234286E-06	3.793821E-16	3.413555E-15	1.967518E-14	99.974869	2.999993
0.23	1.732147E+16	26.833333	1.234286E-06	4.264217E-16	3.568690E-15	2.146373E-14	99.972737	2.999992
0.24	1.732108E+16	28.000000	1.234286E-06	4.771034E-16	3.723821E-15	2.333002E-14	99.970518	2.999992
0.25	1.732068E+16	29.166667	1.234286E-06	5.315601E-16	3.878949E-15	2.527406E-14	99.968211	2.999991
0.26	1.732027E+16	30.333333	1.234286E-06	5.899250E-16	4.034074E-15	2.729584E-14	99.965818	2.999990
0.27	1.731984E+16	31.500000	1.234286E-06	6.523309E-16	4.189194E-15	2.939537E-14	99.963337	2.999990
0.28	1.731939E+16	32.666667	1.234286E-06	7.189110E-16	4.344311E-15	3.157262E-14	99.960768	2.999989
0.29	1.731893E+16	33.833333	1.234286E-06	7.897981E-16	4.499424E-15	3.382762E-14	99.958111	2.999988
0.30	1.731846E+16	35.000000	1.234286E-06	8.651254E-16	4.654532E-15	3.616034E-14	99.955366	2.999987
0.31	1.731797E+16	36.166667	1.234286E-06	9.450258E-16	4.809637E-15	3.857079E-14	99.952533	2.999986
0.32	1.731746E+16	37.333333	1.234286E-06	1.029632E-15	4.964737E-15	4.105897E-14	99.949612	2.999986
0.33	1.731694E+16	38.500000	1.234286E-06	1.119078E-15	5.119832E-15	4.362488E-14	99.946602	2.999985
0.34	1.731640E+16	39.666667	1.234286E-06	1.213496E-15	5.274922E-15	4.626850E-14	99.943504	2.999984
0.35	1.731585E+16	40.833333	1.234286E-06	1.313018E-15	5.430008E-15	4.898984E-14	99.940317	2.999983
0.36	1.731528E+16	42.000000	1.234286E-06	1.417779E-15	5.585089E-15	5.178890E-14	99.937041	2.999982
0.37	1.731470E+16	43.166667	1.234286E-06	1.527910E-15	5.740165E-15	5.466567E-14	99.933677	2.999981
0.38	1.731410E+16	44.333333	1.234286E-06	1.643546E-15	5.895235E-15	5.762015E-14	99.930223	2.999980
0.39	1.731349E+16	45.500000	1.234286E-06	1.764818E-15	6.050300E-15	6.065233E-14	99.926680	2.999979
0.40	1.731286E+16	46.666667	1.234286E-06	1.891859E-15	6.205360E-15	6.376222E-14	99.923047	2.999978
0.41	1.731221E+16	47.833333	1.234286E-06	2.024804E-15	6.360414E-15	6.694981E-14	99.919325	2.999976
0.42	1.731155E+16	49.000000	1.234286E-06	2.163784E-15	6.515462E-15	7.021509E-14	99.915514	2.999975
0.43	1.731088E+16	50.166667	1.234286E-06	2.308932E-15	6.670504E-15	7.355806E-14	99.911613	2.999974
0.44	1.731019E+16	51.333333	1.234286E-06	2.460381E-15	6.825540E-15	7.697872E-14	99.907621	2.999973
0.45	1.730948E+16	52.500000	1.234286E-06	2.618265E-15	6.980570E-15	8.047706E-14	99.903540	2.999972

0.46	1.730876E+16	53.666667	1.234286E-06	2.782716E-15	7.135594E-15	8.405309E-14	99.899368	2.999970
0.47	1.730802E+16	54.833333	1.234286E-06	2.953866E-15	7.290611E-15	8.770679E-14	99.895106	2.999969
0.48	1.730726E+16	56.000000	1.234286E-06	3.131849E-15	7.445622E-15	9.143816E-14	99.890754	2.999968
0.49	1.730649E+16	57.166667	1.234286E-06	3.316798E-15	7.600626E-15	9.524721E-14	99.886311	2.999966
0.50	1.730571E+16	58.333333	1.234286E-06	3.508845E-15	7.755623E-15	9.913391E-14	99.881777	2.999965
0.51	1.730491E+16	59.500000	1.234286E-06	3.708123E-15	7.910613E-15	1.030983E-13	99.877152	2.999964
0.52	1.730409E+16	60.666667	1.234286E-06	3.914764E-15	8.065596E-15	1.071403E-13	99.872436	2.999962
0.53	1.730326E+16	61.833333	1.234286E-06	4.128903E-15	8.220571E-15	1.112600E-13	99.867630	2.999961
0.54	1.730241E+16	63.000000	1.234286E-06	4.350671E-15	8.375539E-15	1.154573E-13	99.862731	2.999959
0.55	1.730154E+16	64.166667	1.234286E-06	4.580201E-15	8.530500E-15	1.197323E-13	99.857742	2.999958
0.56	1.730066E+16	65.333333	1.234286E-06	4.817626E-15	8.685453E-15	1.240849E-13	99.852660	2.999956
0.57	1.729977E+16	66.500000	1.234286E-06	5.063079E-15	8.840398E-15	1.285151E-13	99.847487	2.999955
0.58	1.729885E+16	67.666667	1.234286E-06	5.316692E-15	8.995335E-15	1.330230E-13	99.842222	2.999953
0.59	1.729793E+16	68.833333	1.234286E-06	5.578598E-15	9.150264E-15	1.376084E-13	99.836866	2.999952
0.60	1.729698E+16	70.000000	1.234286E-06	5.848929E-15	9.305185E-15	1.422715E-13	99.831417	2.999950
0.61	1.729602E+16	71.166667	1.234286E-06	6.127820E-15	9.460097E-15	1.470123E-13	99.825875	2.999948
0.62	1.729505E+16	72.333333	1.234286E-06	6.415401E-15	9.615001E-15	1.518306E-13	99.820242	2.999947
0.63	1.729405E+16	73.500000	1.234286E-06	6.711806E-15	9.769896E-15	1.567265E-13	99.814515	2.999945
0.64	1.729305E+16	74.666667	1.234286E-06	7.017167E-15	9.924782E-15	1.617000E-13	99.808696	2.999943
0.65	1.729202E+16	75.833333	1.234286E-06	7.331617E-15	1.007966E-14	1.667511E-13	99.802785	2.999941
0.66	1.729098E+16	77.000000	1.234286E-06	7.655289E-15	1.023453E-14	1.718798E-13	99.796780	2.999940
0.67	1.728992E+16	78.166667	1.234286E-06	7.988314E-15	1.038939E-14	1.770861E-13	99.790682	2.999938
0.68	1.728885E+16	79.333333	1.234286E-06	8.330827E-15	1.054424E-14	1.823700E-13	99.784491	2.999936
0.69	1.728776E+16	80.500000	1.234286E-06	8.682958E-15	1.069908E-14	1.877314E-13	99.778207	2.999934
0.70	1.728666E+16	81.666667	1.234286E-06	9.044841E-15	1.085391E-14	1.931704E-13	99.771829	2.999932
0.71	1.728554E+16	82.833333	1.234286E-06	9.416609E-15	1.100873E-14	1.986869E-13	99.765358	2.999930
0.72	1.728440E+16	84.000000	1.234286E-06	9.798393E-15	1.116354E-14	2.042810E-13	99.758793	2.999928
0.73	1.728325E+16	85.166667	1.234286E-06	1.019033E-14	1.131834E-14	2.099527E-13	99.752133	2.999926
0.74	1.728208E+16	86.333333	1.234286E-06	1.059254E-14	1.147313E-14	2.157019E-13	99.745380	2.999924
0.75	1.728089E+16	87.500000	1.234286E-06	1.100517E-14	1.162791E-14	2.215286E-13	99.738533	2.999922
0.76	1.727969E+16	88.666667	1.234286E-06	1.142835E-14	1.178268E-14	2.274328E-13	99.731591	2.999920
0.77	1.727847E+16	89.833333	1.234286E-06	1.186220E-14	1.193744E-14	2.334146E-13	99.724555	2.999918
0.78	1.727723E+16	91.000000	1.234286E-06	1.230687E-14	1.209218E-14	2.394738E-13	99.717425	2.999916
0.79	1.727598E+16	92.166667	1.234286E-06	1.276248E-14	1.224692E-14	2.456106E-13	99.710199	2.999914
0.80	1.727471E+16	93.333333	1.234286E-06	1.322916E-14	1.240165E-14	2.518249E-13	99.702879	2.999911
0.81	1.727343E+16	94.500000	1.234286E-06	1.370706E-14	1.255636E-14	2.581167E-13	99.695464	2.999909
0.82	1.727213E+16	95.666667	1.234286E-06	1.419629E-14	1.271106E-14	2.644859E-13	99.687954	2.999907
0.83	1.727081E+16	96.833333	1.234286E-06	1.469700E-14	1.286576E-14	2.709327E-13	99.680348	2.999905
0.84	1.726947E+16	98.000000	1.234286E-06	1.520931E-14	1.302044E-14	2.774569E-13	99.672647	2.999902
0.85	1.726812E+16	99.166667	1.234286E-06	1.573336E-14	1.317510E-14	2.840586E-13	99.664851	2.999900
0.86	1.726676E+16	100.333333	1.234286E-06	1.626928E-14	1.332976E-14	2.907377E-13	99.656959	2.999898
0.87	1.726537E+16	101.500000	1.234286E-06	1.681721E-14	1.348440E-14	2.974943E-13	99.648971	2.999895
0.88	1.726397E+16	102.666667	1.234286E-06	1.737726E-14	1.363904E-14	3.043283E-13	99.640887	2.999893
0.89	1.726255E+16	103.833333	1.234286E-06	1.794958E-14	1.379366E-14	3.112398E-13	99.632707	2.999891
0.90	1.726112E+16	105.000000	1.234286E-06	1.853431E-14	1.394826E-14	3.182286E-13	99.624432	2.999888
0.91	1.725967E+16	106.166667	1.234286E-06	1.913156E-14	1.410286E-14	3.252949E-13	99.616059	2.999886
0.92	1.725820E+16	107.333333	1.234286E-06	1.974147E-14	1.425744E-14	3.324387E-13	99.607590	2.999883
0.93	1.725672E+16	108.500000	1.234286E-06	2.036418E-14	1.441201E-14	3.396598E-13	99.599025	2.999881
0.94	1.725522E+16	109.666667	1.234286E-06	2.099982E-14	1.456656E-14	3.469583E-13	99.590363	2.999878
0.95	1.725370E+16	110.833333	1.234286E-06	2.164851E-14	1.472110E-14	3.543342E-13	99.581604	2.999875
0.96	1.725216E+16	112.000000	1.234286E-06	2.231040E-14	1.487563E-14	3.617875E-13	99.572748	2.999873
0.97	1.725061E+16	113.166667	1.234286E-06	2.298560E-14	1.503015E-14	3.693182E-13	99.563796	2.999870
0.98	1.724905E+16	114.333333	1.234286E-06	2.367427E-14	1.518465E-14	3.769262E-13	99.554745	2.999867
0.99	1.724746E+16	115.500000	1.234286E-06	2.437652E-14	1.533913E-14	3.846116E-13	99.545598	2.999865
1.00	1.724586E+16	116.666667	1.234286E-06	2.509248E-14	1.549361E-14	3.923743E-13	99.536353	2.999862



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO2}}$ (mol)	$\Phi_{\text{NO2}}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732615E+16	1.166667	3.509915E-07	2.340398E-19	1.551759E-16	7.777218E-17	99.999750	3.000000
0.02	1.732609E+16	2.333333	4.963753E-07	1.033102E-18	3.103514E-16	2.333163E-16	99.999417	3.000000
0.03	1.732602E+16	3.500000	6.079306E-07	2.637063E-18	4.655262E-16	4.666319E-16	99.998999	3.000000
0.04	1.732593E+16	4.666667	7.019742E-07	5.243758E-18	6.207002E-16	7.777185E-16	99.998497	3.000000
0.05	1.732583E+16	5.833333	7.848264E-07	9.025456E-18	7.758734E-16	1.166576E-15	99.997910	2.999999
0.06	1.732571E+16	7.000000	8.597285E-07	1.413677E-17	9.310455E-16	1.633203E-15	99.997239	2.999999
0.07	1.732558E+16	8.166667	9.286059E-07	2.071919E-17	1.086216E-15	2.177600E-15	99.996483	2.999999
0.08	1.732544E+16	9.333333	9.927131E-07	2.890391E-17	1.241386E-15	2.799765E-15	99.995641	2.999999
0.09	1.732528E+16	10.500000	1.052922E-06	3.881384E-17	1.396554E-15	3.499698E-15	99.994715	2.999999
0.10	1.732510E+16	11.666667	1.109865E-06	5.056498E-17	1.551721E-15	4.277398E-15	99.993704	2.999998
0.11	1.732491E+16	12.833333	1.164024E-06	6.426745E-17	1.706886E-15	5.132863E-15	99.992607	2.999998
0.12	1.732471E+16	14.000000	1.215769E-06	8.002635E-17	1.862050E-15	6.066094E-15	99.991424	2.999998
0.13	1.732449E+16	15.166667	1.234286E-06	9.796359E-17	2.017211E-15	7.077089E-15	99.990156	2.999998
0.14	1.732425E+16	16.333333	1.234286E-06	1.182123E-16	2.172370E-15	8.165846E-15	99.988802	2.999997
0.15	1.732400E+16	17.500000	1.234286E-06	1.409055E-16	2.327527E-15	9.332364E-15	99.987363	2.999997
0.16	1.732374E+16	18.666667	1.234286E-06	1.661763E-16	2.482682E-15	1.057664E-14	99.985837	2.999996
0.17	1.732346E+16	19.833333	1.234286E-06	1.941577E-16	2.637834E-15	1.189868E-14	99.984225	2.999996
0.18	1.732316E+16	21.000000	1.234286E-06	2.249829E-16	2.792984E-15	1.329847E-14	99.982527	2.999995
0.19	1.732285E+16	22.166667	1.234286E-06	2.587849E-16	2.948131E-15	1.477602E-14	99.980742	2.999995
0.20	1.732253E+16	23.333333	1.234286E-06	2.956967E-16	3.103275E-15	1.633132E-14	99.978871	2.999994
0.21	1.732219E+16	24.500000	1.234286E-06	3.358514E-16	3.258417E-15	1.796437E-14	99.976913	2.999994
0.22	1.732184E+16	25.666667	1.234286E-06	3.793821E-16	3.413555E-15	1.967518E-14	99.974869	2.999993
0.23	1.732147E+16	26.833333	1.234286E-06	4.264217E-16	3.568690E-15	2.146373E-14	99.972737	2.999992
0.24	1.732108E+16	28.000000	1.234286E-06	4.771034E-16	3.723821E-15	2.333002E-14	99.970518	2.999992
0.25	1.732068E+16	29.166667	1.234286E-06	5.315601E-16	3.878949E-15	2.527406E-14	99.968211	2.999991
0.26	1.732027E+16	30.333333	1.234286E-06	5.899250E-16	4.034074E-15	2.729584E-14	99.965818	2.999990
0.27	1.731984E+16	31.500000	1.234286E-06	6.523309E-16	4.189194E-15	2.939537E-14	99.963337	2.999990
0.28	1.731939E+16	32.666667	1.234286E-06	7.189110E-16	4.344311E-15	3.157262E-14	99.960768	2.999989
0.29	1.731893E+16	33.833333	1.234286E-06	7.897981E-16	4.499424E-15	3.382762E-14	99.958111	2.999988
0.30	1.731846E+16	35.000000	1.234286E-06	8.651254E-16	4.654532E-15	3.616034E-14	99.955366	2.999987
0.31	1.731797E+16	36.166667	1.234286E-06	9.450258E-16	4.809637E-15	3.857079E-14	99.952533	2.999986
0.32	1.731746E+16	37.333333	1.234286E-06	1.029632E-15	4.964737E-15	4.105897E-14	99.949612	2.999986
0.33	1.731694E+16	38.500000	1.234286E-06	1.119078E-15	5.119832E-15	4.362488E-14	99.946602	2.999985
0.34	1.731640E+16	39.666667	1.234286E-06	1.213496E-15	5.274922E-15	4.626850E-14	99.943504	2.999984
0.35	1.731585E+16	40.833333	1.234286E-06	1.313018E-15	5.430008E-15	4.898984E-14	99.940317	2.999983
0.36	1.731528E+16	42.000000	1.234286E-06	1.417779E-15	5.585089E-15	5.178890E-14	99.937041	2.999982
0.37	1.731470E+16	43.166667	1.234286E-06	1.527910E-15	5.740165E-15	5.466567E-14	99.933677	2.999981
0.38	1.731410E+16	44.333333	1.234286E-06	1.643546E-15	5.895235E-15	5.762015E-14	99.930223	2.999980
0.39	1.731349E+16	45.500000	1.234286E-06	1.764818E-15	6.050300E-15	6.065233E-14	99.926680	2.999979
0.40	1.731286E+16	46.666667	1.234286E-06	1.891859E-15	6.205360E-15	6.376222E-14	99.923047	2.999978
0.41	1.731221E+16	47.833333	1.234286E-06	2.024804E-15	6.360414E-15	6.694981E-14	99.919325	2.999976
0.42	1.731155E+16	49.000000	1.234286E-06	2.163784E-15	6.515462E-15	7.021509E-14	99.915514	2.999975
0.43	1.731088E+16	50.166667	1.234286E-06	2.308932E-15	6.670504E-15	7.355806E-14	99.911613	2.999974
0.44	1.731019E+16	51.333333	1.234286E-06	2.460381E-15	6.825540E-15	7.697872E-14	99.907621	2.999973
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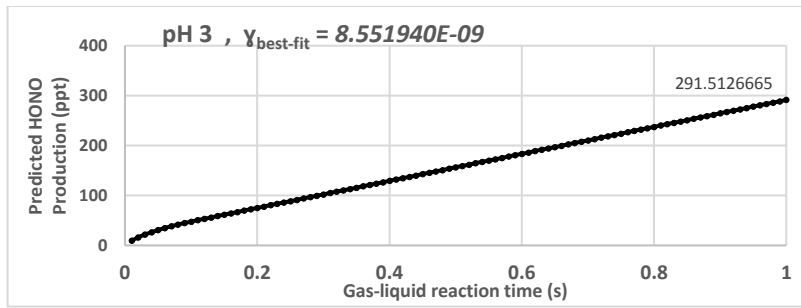
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0.47	1.730802E+16	54.833333	1.234286E-06	2.953866E-15	7.290611E-15	8.770679E-14	99.895106	2.999969
0.48	1.730726E+16	56.000000	1.234286E-06	3.131849E-15	7.445622E-15	9.143816E-14	99.890754	2.999968
0.49	1.730649E+16	57.166667	1.234286E-06	3.316798E-15	7.600626E-15	9.524721E-14	99.886311	2.999966
0.50	1.730571E+16	58.333333	1.234286E-06	3.508845E-15	7.755623E-15	9.913391E-14	99.881777	2.999965
0.51	1.730491E+16	59.500000	1.234286E-06	3.708123E-15	7.910613E-15	1.030983E-13	99.877152	2.999964
0.52	1.730409E+16	60.666667	1.234286E-06	3.914764E-15	8.065596E-15	1.071403E-13	99.872436	2.999962
0.53	1.730326E+16	61.833333	1.234286E-06	4.128903E-15	8.220571E-15	1.112600E-13	99.867630	2.999961
0.54	1.730241E+16	63.000000	1.234286E-06	4.350671E-15	8.375539E-15	1.154573E-13	99.862731	2.999959
0.55	1.730154E+16	64.166667	1.234286E-06	4.580201E-15	8.530500E-15	1.197323E-13	99.857742	2.999958
0.56	1.730066E+16	65.333333	1.234286E-06	4.817626E-15	8.685453E-15	1.240849E-13	99.852660	2.999956
0.57	1.729977E+16	66.500000	1.234286E-06	5.063079E-15	8.840398E-15	1.285151E-13	99.847487	2.999955
0.58	1.729885E+16	67.666667	1.234286E-06	5.316692E-15	8.995335E-15	1.330230E-13	99.842222	2.999953
0.59	1.729793E+16	68.833333	1.234286E-06	5.578598E-15	9.150264E-15	1.376084E-13	99.836866	2.999952
0.60	1.729698E+16	70.000000	1.234286E-06	5.848929E-15	9.305185E-15	1.422715E-13	99.831417	2.999950
0.61	1.729602E+16	71.166667	1.234286E-06	6.127820E-15	9.460097E-15	1.470123E-13	99.825875	2.999948
0.62	1.729505E+16	72.333333	1.234286E-06	6.415401E-15	9.615001E-15	1.518306E-13	99.820242	2.999947
0.63	1.729405E+16	73.500000	1.234286E-06	6.711806E-15	9.769896E-15	1.567265E-13	99.814515	2.999945
0.64	1.729305E+16	74.666667	1.234286E-06	7.017167E-15	9.924782E-15	1.617000E-13	99.808696	2.999943
0.65	1.729202E+16	75.833333	1.234286E-06	7.331617E-15	1.007966E-14	1.667511E-13	99.802785	2.999941
0.66	1.729098E+16	77.000000	1.234286E-06	7.655289E-15	1.023453E-14	1.718798E-13	99.796780	2.999940
0.67	1.728992E+16	78.166667	1.234286E-06	7.988314E-15	1.038939E-14	1.770861E-13	99.790682	2.999938
0.68	1.728885E+16	79.333333	1.234286E-06	8.330827E-15	1.054424E-14	1.823700E-13	99.784491	2.999936
0.69	1.728776E+16	80.500000	1.234286E-06	8.682958E-15	1.069908E-14	1.877314E-13	99.778207	2.999934
0.70	1.728666E+16	81.666667	1.234286E-06	9.044841E-15	1.085391E-14	1.931704E-13	99.771829	2.999932
0.71	1.728554E+16	82.833333	1.234286E-06	9.416609E-15	1.100873E-14	1.986869E-13	99.765358	2.999930
0.72	1.728440E+16	84.000000	1.234286E-06	9.798393E-15	1.116354E-14	2.042810E-13	99.758793	2.999928
0.73	1.728325E+16	85.166667	1.234286E-06	1.019033E-14	1.131834E-14	2.099527E-13	99.752133	2.999926
0.74	1.728208E+16	86.333333	1.234286E-06	1.059254E-14	1.147313E-14	2.157019E-13	99.745380	2.999924
0.75	1.728089E+16	87.500000	1.234286E-06	1.100517E-14	1.162791E-14	2.215286E-13	99.738533	2.999922
0.76	1.727969E+16	88.666667	1.234286E-06	1.142835E-14	1.178268E-14	2.274328E-13	99.731591	2.999920
0.77	1.727847E+16	89.833333	1.234286E-06	1.186220E-14	1.193744E-14	2.334146E-13	99.724555	2.999918
0.78	1.727723E+16	91.000000	1.234286E-06	1.230687E-14	1.209218E-14	2.394738E-13	99.717425	2.999916
0.79	1.727598E+16	92.166667	1.234286E-06	1.276248E-14	1.224692E-14	2.456106E-13	99.710199	2.999914
0.80	1.727471E+16	93.333333	1.234286E-06	1.322916E-14	1.240165E-14	2.518249E-13	99.702879	2.999911
0.81	1.727343E+16	94.500000	1.234286E-06	1.370706E-14	1.255636E-14	2.581167E-13	99.695464	2.999909
0.82	1.727213E+16	95.666667	1.234286E-06	1.419629E-14	1.271106E-14	2.644859E-13	99.687954	2.999907
0.83	1.727081E+16	96.833333	1.234286E-06	1.469700E-14	1.286576E-14	2.709327E-13	99.680348	2.999905
0.84	1.726947E+16	98.000000	1.234286E-06	1.520931E-14	1.302044E-14	2.774569E-13	99.672647	2.999902
0.85	1.726812E+16	99.166667	1.234286E-06	1.573336E-14	1.317510E-14	2.840586E-13	99.664851	2.999900
0.86	1.726676E+16	100.333333	1.234286E-06	1.626928E-14	1.332976E-14	2.907377E-13	99.656959	2.999898
0.87	1.726537E+16	101.500000	1.234286E-06	1.681721E-14	1.348440E-14	2.974943E-13	99.648971	2.999895
0.88	1.726397E+16	102.666667	1.234286E-06	1.737726E-14	1.363904E-14	3.043283E-13	99.640887	2.999893
0.89	1.726255E+16	103.833333	1.234286E-06	1.794958E-14	1.379366E-14	3.112398E-13	99.632707	2.999891
0.90	1.726112E+16	105.000000	1.234286E-06	1.853431E-14	1.394826E-14	3.182286E-13	99.624432	2.999888
0.91	1.725967E+16	106.166667	1.234286E-06	1.913156E-14	1.410286E-14	3.252949E-13	99.616059	2.999886
0.92	1.725820E+16	107.333333	1.234286E-06	1.974147E-14	1.425744E-14	3.324387E-13	99.607590	2.999883
0.93	1.725672E+16	108.500000	1.234286E-06	2.036418E-14	1.441201E-14	3.396598E-13	99.599025	2.999881
0.94	1.725522E+16	109.666667	1.234286E-06	2.099982E-14	1.456656E-14	3.469583E-13	99.590363	2.999878
0.95	1.725370E+16	110.833333	1.234286E-06	2.164851E-14	1.472110E-14	3.543342E-13	99.581604	2.999875
0.96	1.725216E+16	112.000000	1.234286E-06	2.231040E-14	1.487563E-14	3.617875E-13	99.572748	2.999873
0.97	1.725061E+16	113.166667	1.234286E-06	2.298560E-14	1.503015E-14	3.693182E-13	99.563796	2.999870
0.98	1.724905E+16	114.333333	1.234286E-06	2.367427E-14	1.518465E-14	3.769262E-13	99.554745	2.999867
0.99	1.724746E+16	115.500000	1.234286E-06	2.437652E-14	1.533913E-14	3.846116E-13	99.545598	2.999865
1.00	1.724586E+16	116.666667	1.234286E-06	2.509248E-14	1.549361E-14	3.923743E-13	99.536353	2.999862



$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO2}}$ (mol)	$\Phi_{\text{NO2}}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732615E+16	1.166667	3.509915E-07	2.422114E-19	1.605940E-16	8.048763E-17	99.999742	3.000000
0.02	1.732609E+16	2.333333	4.963752E-07	1.069173E-18	3.211874E-16	2.414626E-16	99.999396	3.000000
0.03	1.732601E+16	3.500000	6.079303E-07	2.729137E-18	4.817801E-16	4.829244E-16	99.998964	3.000000
0.04	1.732592E+16	4.666667	7.019738E-07	5.426847E-18	6.423721E-16	8.048727E-16	99.998444	3.000000
0.05	1.732582E+16	5.833333	7.848259E-07	9.340584E-18	8.029631E-16	1.207307E-15	99.997837	2.999999
0.06	1.732570E+16	7.000000	8.597277E-07	1.463036E-17	9.635529E-16	1.690226E-15	99.997142	2.999999
0.07	1.732556E+16	8.166667	9.286048E-07	2.144261E-17	1.124142E-15	2.253630E-15	99.996360	2.999999
0.08	1.732541E+16	9.333333	9.927116E-07	2.991310E-17	1.284729E-15	2.897518E-15	99.995489	2.999999
0.09	1.732524E+16	10.500000	1.052920E-06	4.016905E-17	1.445315E-15	3.621889E-15	99.994531	2.999999
0.10	1.732506E+16	11.666667	1.109863E-06	5.233048E-17	1.605899E-15	4.426742E-15	99.993484	2.999998
0.11	1.732487E+16	12.833333	1.164021E-06	6.651138E-17	1.766481E-15	5.312076E-15	99.992349	2.999998
0.12	1.732465E+16	14.000000	1.215765E-06	8.282051E-17	1.927061E-15	6.277889E-15	99.991125	2.999998
0.13	1.732443E+16	15.166667	1.234286E-06	1.013840E-16	2.087640E-15	7.324181E-15	99.989813	2.999997
0.14	1.732418E+16	16.333333	1.234286E-06	1.223397E-16	2.248216E-15	8.450951E-15	99.988411	2.999997
0.15	1.732393E+16	17.500000	1.234286E-06	1.458252E-16	2.408790E-15	9.658196E-15	99.986922	2.999997
0.16	1.732365E+16	18.666667	1.234286E-06	1.719783E-16	2.569361E-15	1.094592E-14	99.985343	2.999996
0.17	1.732336E+16	19.833333	1.234286E-06	2.009368E-16	2.729930E-15	1.231411E-14	99.983675	2.999996
0.18	1.732306E+16	21.000000	1.234286E-06	2.328382E-16	2.890496E-15	1.376277E-14	99.981917	2.999995
0.19	1.732274E+16	22.166667	1.234286E-06	2.678203E-16	3.051059E-15	1.529190E-14	99.980070	2.999995
0.20	1.732240E+16	23.333333	1.234286E-06	3.060209E-16	3.211619E-15	1.690150E-14	99.978134	2.999994
0.21	1.732205E+16	24.500000	1.234286E-06	3.475775E-16	3.372175E-15	1.859157E-14	99.976107	2.999993
0.22	1.732168E+16	25.666667	1.234286E-06	3.926280E-16	3.532729E-15	2.036210E-14	99.973991	2.999993
0.23	1.732130E+16	26.833333	1.234286E-06	4.413100E-16	3.693279E-15	2.221309E-14	99.971785	2.999992
0.24	1.732090E+16	28.000000	1.234286E-06	4.937611E-16	3.853825E-15	2.414454E-14	99.969488	2.999992
0.25	1.732049E+16	29.166667	1.234286E-06	5.501191E-16	4.014368E-15	2.615645E-14	99.967102	2.999991
0.26	1.732006E+16	30.333333	1.234286E-06	6.105216E-16	4.174907E-15	2.824881E-14	99.964624	2.999990
0.27	1.731962E+16	31.500000	1.234286E-06	6.751062E-16	4.335442E-15	3.042162E-14	99.962057	2.999989
0.28	1.731916E+16	32.666667	1.234286E-06	7.440107E-16	4.495972E-15	3.267489E-14	99.959398	2.999989
0.29	1.731868E+16	33.833333	1.234286E-06	8.173726E-16	4.656498E-15	3.500860E-14	99.956648	2.999988
0.30	1.731819E+16	35.000000	1.234286E-06	8.953297E-16	4.817020E-15	3.742276E-14	99.953808	2.999987
0.31	1.731768E+16	36.166667	1.234286E-06	9.780195E-16	4.977537E-15	3.991735E-14	99.950876	2.999986
0.32	1.731716E+16	37.333333	1.234286E-06	1.065580E-15	5.138050E-15	4.249239E-14	99.947853	2.999985
0.33	1.731662E+16	38.500000	1.234286E-06	1.158148E-15	5.298558E-15	4.514786E-14	99.944738	2.999984
0.34	1.731606E+16	39.666667	1.234286E-06	1.255862E-15	5.459060E-15	4.788377E-14	99.941532	2.999983
0.35	1.731549E+16	40.833333	1.234286E-06	1.358858E-15	5.619557E-15	5.070010E-14	99.938233	2.999982
0.36	1.731490E+16	42.000000	1.234286E-06	1.467276E-15	5.780050E-15	5.359686E-14	99.934843	2.999981
0.37	1.731430E+16	43.166667	1.234286E-06	1.581252E-15	5.940536E-15	5.657405E-14	99.931361	2.999980
0.38	1.731368E+16	44.333333	1.234286E-06	1.700924E-15	6.101017E-15	5.963165E-14	99.927787	2.999979
0.39	1.731304E+16	45.500000	1.234286E-06	1.826430E-15	6.261492E-15	6.276967E-14	99.924120	2.999978
0.40	1.731239E+16	46.666667	1.234286E-06	1.957906E-15	6.421962E-15	6.598811E-14	99.920361	2.999977
0.41	1.731173E+16	47.833333	1.234286E-06	2.095491E-15	6.582425E-15	6.928695E-14	99.916509	2.999976
0.42	1.731104E+16	49.000000	1.234286E-06	2.239322E-15	6.742882E-15	7.266620E-14	99.912565	2.999974
0.43	1.731034E+16	50.166667	1.234286E-06	2.389537E-15	6.903333E-15	7.612584E-14	99.908527	2.999973
0.44	1.730963E+16	51.333333	1.234286E-06	2.546273E-15	7.063777E-15	7.966589E-14	99.904396	2.999972
0.45	1.730889E+16	52.500000	1.234286E-06	2.709668E-15	7.224215E-15	8.328633E-14	99.900173	2.999971

0.46	1.730815E+16	53.666667	1.234286E-06	2.879859E-15	7.384646E-15	8.698716E-14	99.895855	2.999969
0.47	1.730738E+16	54.833333	1.234286E-06	3.056983E-15	7.545070E-15	9.076837E-14	99.891445	2.999968
0.48	1.730660E+16	56.000000	1.234286E-06	3.241178E-15	7.705487E-15	9.462997E-14	99.886940	2.999967
0.49	1.730581E+16	57.166667	1.234286E-06	3.432582E-15	7.865896E-15	9.857194E-14	99.882342	2.999965
0.50	1.730499E+16	58.333333	1.234286E-06	3.631332E-15	8.026299E-15	1.025943E-13	99.877650	2.999964
0.51	1.730416E+16	59.500000	1.234286E-06	3.837565E-15	8.186693E-15	1.066970E-13	99.872864	2.999962
0.52	1.730332E+16	60.666667	1.234286E-06	4.051419E-15	8.347081E-15	1.108801E-13	99.867984	2.999961
0.53	1.730246E+16	61.833333	1.234286E-06	4.273031E-15	8.507460E-15	1.151435E-13	99.863009	2.999959
0.54	1.730158E+16	63.000000	1.234286E-06	4.502539E-15	8.667831E-15	1.194873E-13	99.857940	2.999958
0.55	1.730068E+16	64.166667	1.234286E-06	4.740080E-15	8.828195E-15	1.239114E-13	99.852776	2.999956
0.56	1.729977E+16	65.333333	1.234286E-06	4.985791E-15	8.988550E-15	1.284159E-13	99.847518	2.999955
0.57	1.729884E+16	66.500000	1.234286E-06	5.239810E-15	9.148896E-15	1.330007E-13	99.842164	2.999953
0.58	1.729790E+16	67.666667	1.234286E-06	5.502273E-15	9.309235E-15	1.376659E-13	99.836716	2.999952
0.59	1.729694E+16	68.833333	1.234286E-06	5.773319E-15	9.469564E-15	1.424113E-13	99.831172	2.999950
0.60	1.729596E+16	70.000000	1.234286E-06	6.053085E-15	9.629884E-15	1.472371E-13	99.825533	2.999948
0.61	1.729497E+16	71.166667	1.234286E-06	6.341707E-15	9.790196E-15	1.521433E-13	99.819798	2.999946
0.62	1.729396E+16	72.333333	1.234286E-06	6.639324E-15	9.950498E-15	1.571297E-13	99.813968	2.999945
0.63	1.729293E+16	73.500000	1.234286E-06	6.946072E-15	1.011079E-14	1.621964E-13	99.808042	2.999943
0.64	1.729189E+16	74.666667	1.234286E-06	7.262089E-15	1.027108E-14	1.673435E-13	99.802020	2.999941
0.65	1.729083E+16	75.833333	1.234286E-06	7.587511E-15	1.043135E-14	1.725708E-13	99.795902	2.999939
0.66	1.728975E+16	77.000000	1.234286E-06	7.922477E-15	1.059161E-14	1.778784E-13	99.789688	2.999937
0.67	1.728866E+16	78.166667	1.234286E-06	8.267122E-15	1.075187E-14	1.832663E-13	99.783377	2.999936
0.68	1.728755E+16	79.333333	1.234286E-06	8.621586E-15	1.091211E-14	1.887345E-13	99.776970	2.999934
0.69	1.728642E+16	80.500000	1.234286E-06	8.986003E-15	1.107235E-14	1.942829E-13	99.770467	2.999932
0.70	1.728528E+16	81.666667	1.234286E-06	9.360513E-15	1.123257E-14	1.999116E-13	99.763867	2.999930
0.71	1.728412E+16	82.833333	1.234286E-06	9.745251E-15	1.139278E-14	2.056206E-13	99.757169	2.999928
0.72	1.728294E+16	84.000000	1.234286E-06	1.014036E-14	1.155299E-14	2.114098E-13	99.750375	2.999926
0.73	1.728175E+16	85.166667	1.234286E-06	1.054596E-14	1.171318E-14	2.172793E-13	99.743484	2.999924
0.74	1.728054E+16	86.333333	1.234286E-06	1.096221E-14	1.187336E-14	2.232290E-13	99.736495	2.999921
0.75	1.727931E+16	87.500000	1.234286E-06	1.138923E-14	1.203353E-14	2.292589E-13	99.729409	2.999919
0.76	1.727806E+16	88.666667	1.234286E-06	1.182717E-14	1.219369E-14	2.353691E-13	99.722225	2.999917
0.77	1.727680E+16	89.833333	1.234286E-06	1.227616E-14	1.235383E-14	2.415594E-13	99.714944	2.999915
0.78	1.727552E+16	91.000000	1.234286E-06	1.273634E-14	1.251397E-14	2.478300E-13	99.707565	2.999913
0.79	1.727423E+16	92.166667	1.234286E-06	1.320784E-14	1.267409E-14	2.541808E-13	99.700087	2.999911
0.80	1.727292E+16	93.333333	1.234286E-06	1.369081E-14	1.283421E-14	2.606118E-13	99.692512	2.999908
0.81	1.727159E+16	94.500000	1.234286E-06	1.418537E-14	1.299431E-14	2.671230E-13	99.684838	2.999906
0.82	1.727024E+16	95.666667	1.234286E-06	1.469167E-14	1.315439E-14	2.737143E-13	99.677066	2.999904
0.83	1.726888E+16	96.833333	1.234286E-06	1.520984E-14	1.331447E-14	2.803858E-13	99.669195	2.999901
0.84	1.726749E+16	98.000000	1.234286E-06	1.574003E-14	1.347453E-14	2.871375E-13	99.661226	2.999899
0.85	1.726610E+16	99.166667	1.234286E-06	1.628235E-14	1.363458E-14	2.939694E-13	99.653158	2.999897
0.86	1.726468E+16	100.333333	1.234286E-06	1.683697E-14	1.379462E-14	3.008814E-13	99.644990	2.999894
0.87	1.726325E+16	101.500000	1.234286E-06	1.740400E-14	1.395464E-14	3.078735E-13	99.636724	2.999892
0.88	1.726180E+16	102.666667	1.234286E-06	1.798359E-14	1.411465E-14	3.149458E-13	99.628359	2.999889
0.89	1.726033E+16	103.833333	1.234286E-06	1.857587E-14	1.427465E-14	3.220982E-13	99.619894	2.999887
0.90	1.725885E+16	105.000000	1.234286E-06	1.918098E-14	1.443464E-14	3.293307E-13	99.611329	2.999884
0.91	1.725735E+16	106.166667	1.234286E-06	1.979906E-14	1.459461E-14	3.366434E-13	99.602665	2.999882
0.92	1.725583E+16	107.333333	1.234286E-06	2.043024E-14	1.475456E-14	3.440361E-13	99.593901	2.999879
0.93	1.725429E+16	108.500000	1.234286E-06	2.107467E-14	1.491451E-14	3.515089E-13	99.585037	2.999876
0.94	1.725274E+16	109.666667	1.234286E-06	2.173247E-14	1.507444E-14	3.590619E-13	99.576073	2.999874
0.95	1.725117E+16	110.833333	1.234286E-06	2.240378E-14	1.523435E-14	3.666949E-13	99.567009	2.999871
0.96	1.724958E+16	112.000000	1.234286E-06	2.308874E-14	1.539425E-14	3.744079E-13	99.557845	2.999868
0.97	1.724798E+16	113.166667	1.234286E-06	2.378750E-14	1.555414E-14	3.822010E-13	99.548580	2.999866
0.98	1.724635E+16	114.333333	1.234286E-06	2.450017E-14	1.571401E-14	3.900742E-13	99.539214	2.999863
0.99	1.724471E+16	115.500000	1.234286E-06	2.522690E-14	1.587387E-14	3.980274E-13	99.529748	2.999860
1.00	1.724306E+16	116.666667	1.234286E-06	2.596783E-14	1.603371E-14	4.060607E-13	99.520181	2.999857





$t_{\text{reac}}$ (s)	$Z_{\text{collisions}}$ (/mol)	$t_{\text{diffusion}}$ (s)	$V_{\text{film,diff}}$ (L)	$\Phi_{\text{HONO}}$ (mol)	$\Phi_{\text{HNO}_2}$ (mol)	$\Phi_{\text{NO}_2}$ (mol)	% NO <sub>2</sub> left	film pH
0.01	1.732615E+16	1.166667	3.509915E-07	2.471988E-19	1.639007E-16	8.214494E-17	99.999736	3.000000
0.02	1.732608E+16	2.333333	4.963751E-07	1.091188E-18	3.278009E-16	2.464345E-16	99.999384	3.000000
0.03	1.732601E+16	3.500000	6.079302E-07	2.785333E-18	4.917004E-16	4.928683E-16	99.998943	3.000000
0.04	1.732592E+16	4.666667	7.019736E-07	5.538591E-18	6.555990E-16	8.214457E-16	99.998412	2.999999
0.05	1.732581E+16	5.833333	7.848255E-07	9.532916E-18	8.194967E-16	1.232166E-15	99.997793	2.999999
0.06	1.732569E+16	7.000000	8.597272E-07	1.493162E-17	9.833932E-16	1.725029E-15	99.997084	2.999999
0.07	1.732555E+16	8.166667	9.286041E-07	2.188413E-17	1.147288E-15	2.300034E-15	99.996285	2.999999
0.08	1.732539E+16	9.333333	9.927107E-07	3.052904E-17	1.311182E-15	2.957180E-15	99.995396	2.999999
0.09	1.732522E+16	10.500000	1.052918E-06	4.099617E-17	1.475074E-15	3.696466E-15	99.994418	2.999998
0.10	1.732504E+16	11.666667	1.109862E-06	5.340802E-17	1.638965E-15	4.517891E-15	99.993350	2.999998
0.11	1.732484E+16	12.833333	1.164019E-06	6.788092E-17	1.802853E-15	5.421454E-15	99.992191	2.999998
0.12	1.732462E+16	14.000000	1.215763E-06	8.452586E-17	1.966740E-15	6.407154E-15	99.990942	2.999998
0.13	1.732439E+16	15.166667	1.234286E-06	1.034716E-16	2.130625E-15	7.474989E-15	99.989603	2.999997
0.14	1.732414E+16	16.333333	1.234286E-06	1.248588E-16	2.294507E-15	8.624958E-15	99.988173	2.999997
0.15	1.732388E+16	17.500000	1.234286E-06	1.488279E-16	2.458386E-15	9.857060E-15	99.986652	2.999997
0.16	1.732360E+16	18.666667	1.234286E-06	1.755195E-16	2.622264E-15	1.117129E-14	99.985041	2.999996
0.17	1.732330E+16	19.833333	1.234286E-06	2.050742E-16	2.786138E-15	1.256766E-14	99.983338	2.999996
0.18	1.732299E+16	21.000000	1.234286E-06	2.376325E-16	2.950009E-15	1.404615E-14	99.981545	2.999995
0.19	1.732267E+16	22.166667	1.234286E-06	2.733349E-16	3.113878E-15	1.560676E-14	99.979660	2.999995
0.20	1.732232E+16	23.333333	1.234286E-06	3.123220E-16	3.277743E-15	1.724950E-14	99.977683	2.999994
0.21	1.732197E+16	24.500000	1.234286E-06	3.547343E-16	3.441605E-15	1.897436E-14	99.975615	2.999993
0.22	1.732159E+16	25.666667	1.234286E-06	4.007124E-16	3.605464E-15	2.078135E-14	99.973456	2.999993
0.23	1.732120E+16	26.833333	1.234286E-06	4.503967E-16	3.769319E-15	2.267045E-14	99.971204	2.999992
0.24	1.732080E+16	28.000000	1.234286E-06	5.039277E-16	3.933170E-15	2.464166E-14	99.968860	2.999991
0.25	1.732037E+16	29.166667	1.234286E-06	5.614461E-16	4.097017E-15	2.669499E-14	99.966424	2.999991
0.26	1.731994E+16	30.333333	1.234286E-06	6.230922E-16	4.260861E-15	2.883043E-14	99.963896	2.999990
0.27	1.731948E+16	31.500000	1.234286E-06	6.890066E-16	4.424700E-15	3.104798E-14	99.961275	2.999989
0.28	1.731901E+16	32.666667	1.234286E-06	7.593297E-16	4.588535E-15	3.334763E-14	99.958562	2.999988
0.29	1.731853E+16	33.833333	1.234286E-06	8.342021E-16	4.752365E-15	3.572939E-14	99.955756	2.999987
0.30	1.731802E+16	35.000000	1.234286E-06	9.137642E-16	4.916190E-15	3.819324E-14	99.952857	2.999987
0.31	1.731750E+16	36.166667	1.234286E-06	9.981564E-16	5.080011E-15	4.073919E-14	99.949864	2.999986
0.32	1.731697E+16	37.333333	1.234286E-06	1.087519E-15	5.243827E-15	4.336724E-14	99.946779	2.999985
0.33	1.731642E+16	38.500000	1.234286E-06	1.181993E-15	5.407638E-15	4.607738E-14	99.943600	2.999984
0.34	1.731585E+16	39.666667	1.234286E-06	1.281719E-15	5.571443E-15	4.886960E-14	99.940328	2.999983
0.35	1.731527E+16	40.833333	1.234286E-06	1.386836E-15	5.735243E-15	5.174391E-14	99.936962	2.999982
0.36	1.731467E+16	42.000000	1.234286E-06	1.497486E-15	5.899038E-15	5.470031E-14	99.933502	2.999981
0.37	1.731405E+16	43.166667	1.234286E-06	1.613808E-15	6.062827E-15	5.773878E-14	99.929948	2.999980
0.38	1.731342E+16	44.333333	1.234286E-06	1.735944E-15	6.226610E-15	6.085932E-14	99.926300	2.999979
0.39	1.731277E+16	45.500000	1.234286E-06	1.864033E-15	6.390387E-15	6.406193E-14	99.922558	2.999977
0.40	1.731211E+16	46.666667	1.234286E-06	1.998216E-15	6.554158E-15	6.734661E-14	99.918722	2.999976
0.41	1.731143E+16	47.833333	1.234286E-06	2.138633E-15	6.717923E-15	7.071336E-14	99.914790	2.999975
0.42	1.731073E+16	49.000000	1.234286E-06	2.285426E-15	6.881681E-15	7.416216E-14	99.910765	2.999974
0.43	1.731002E+16	50.166667	1.234286E-06	2.438733E-15	7.045432E-15	7.769302E-14	99.906644	2.999973
0.44	1.730929E+16	51.333333	1.234286E-06	2.598695E-15	7.209177E-15	8.130593E-14	99.902428	2.999971
0.45	1.730854E+16	52.500000	1.234286E-06	2.765453E-15	7.372915E-15	8.500089E-14	99.898118	2.999970

0.46	1.730778E+16	53.666667	1.234286E-06	2.939147E-15	7.536646E-15	8.877789E-14	99.893712	2.999969
0.47	1.730700E+16	54.833333	1.234286E-06	3.119917E-15	7.700370E-15	9.263692E-14	99.889210	2.999967
0.48	1.730620E+16	56.000000	1.234286E-06	3.307904E-15	7.864086E-15	9.657799E-14	99.884613	2.999966
0.49	1.730539E+16	57.166667	1.234286E-06	3.503248E-15	8.027795E-15	1.006011E-13	99.879920	2.999965
0.50	1.730456E+16	58.333333	1.234286E-06	3.706089E-15	8.191496E-15	1.047062E-13	99.875132	2.999963
0.51	1.730371E+16	59.500000	1.234286E-06	3.916567E-15	8.355189E-15	1.088934E-13	99.870247	2.999962
0.52	1.730285E+16	60.666667	1.234286E-06	4.134823E-15	8.518875E-15	1.131625E-13	99.865266	2.999960
0.53	1.730197E+16	61.833333	1.234286E-06	4.360996E-15	8.682552E-15	1.175137E-13	99.860189	2.999959
0.54	1.730107E+16	63.000000	1.234286E-06	4.595228E-15	8.846221E-15	1.219469E-13	99.855016	2.999957
0.55	1.730016E+16	64.166667	1.234286E-06	4.837657E-15	9.009881E-15	1.264620E-13	99.849746	2.999956
0.56	1.729923E+16	65.333333	1.234286E-06	5.088425E-15	9.173533E-15	1.310592E-13	99.844379	2.999954
0.57	1.729828E+16	66.500000	1.234286E-06	5.347672E-15	9.337176E-15	1.357384E-13	99.838915	2.999952
0.58	1.729732E+16	67.666667	1.234286E-06	5.615537E-15	9.500811E-15	1.404995E-13	99.833355	2.999951
0.59	1.729634E+16	68.833333	1.234286E-06	5.892162E-15	9.664436E-15	1.453426E-13	99.827697	2.999949
0.60	1.729534E+16	70.000000	1.234286E-06	6.177685E-15	9.828052E-15	1.502677E-13	99.821942	2.999947
0.61	1.729433E+16	71.166667	1.234286E-06	6.472247E-15	9.991658E-15	1.552748E-13	99.816089	2.999945
0.62	1.729330E+16	72.333333	1.234286E-06	6.775988E-15	1.015526E-14	1.603638E-13	99.810139	2.999944
0.63	1.729225E+16	73.500000	1.234286E-06	7.089049E-15	1.031884E-14	1.655348E-13	99.804091	2.999942
0.64	1.729118E+16	74.666667	1.234286E-06	7.411569E-15	1.048242E-14	1.707877E-13	99.797945	2.999940
0.65	1.729010E+16	75.833333	1.234286E-06	7.743688E-15	1.064599E-14	1.761226E-13	99.791701	2.999938
0.66	1.728900E+16	77.000000	1.234286E-06	8.085546E-15	1.080955E-14	1.815394E-13	99.785359	2.999936
0.67	1.728789E+16	78.166667	1.234286E-06	8.437284E-15	1.097309E-14	1.870381E-13	99.778919	2.999934
0.68	1.728675E+16	79.333333	1.234286E-06	8.799040E-15	1.113663E-14	1.926188E-13	99.772380	2.999932
0.69	1.728560E+16	80.500000	1.234286E-06	9.170957E-15	1.130016E-14	1.982814E-13	99.765743	2.999930
0.70	1.728444E+16	81.666667	1.234286E-06	9.553172E-15	1.146367E-14	2.040259E-13	99.759007	2.999928
0.71	1.728325E+16	82.833333	1.234286E-06	9.945826E-15	1.162717E-14	2.098523E-13	99.752172	2.999926
0.72	1.728205E+16	84.000000	1.234286E-06	1.034906E-14	1.179067E-14	2.157606E-13	99.745238	2.999924
0.73	1.728083E+16	85.166667	1.234286E-06	1.076301E-14	1.195415E-14	2.217508E-13	99.738205	2.999922
0.74	1.727960E+16	86.333333	1.234286E-06	1.118782E-14	1.211762E-14	2.278229E-13	99.731073	2.999920
0.75	1.727834E+16	87.500000	1.234286E-06	1.162363E-14	1.228108E-14	2.339768E-13	99.723841	2.999918
0.76	1.727707E+16	88.666667	1.234286E-06	1.207058E-14	1.244453E-14	2.402126E-13	99.716509	2.999915
0.77	1.727579E+16	89.833333	1.234286E-06	1.252881E-14	1.260796E-14	2.465303E-13	99.709078	2.999913
0.78	1.727448E+16	91.000000	1.234286E-06	1.299845E-14	1.277138E-14	2.529299E-13	99.701547	2.999911
0.79	1.727316E+16	92.166667	1.234286E-06	1.347966E-14	1.293480E-14	2.594113E-13	99.693916	2.999909
0.80	1.727182E+16	93.333333	1.234286E-06	1.397256E-14	1.309819E-14	2.659745E-13	99.686185	2.999906
0.81	1.727046E+16	94.500000	1.234286E-06	1.447729E-14	1.326158E-14	2.726196E-13	99.678353	2.999904
0.82	1.726909E+16	95.666667	1.234286E-06	1.499401E-14	1.342495E-14	2.793465E-13	99.670421	2.999902
0.83	1.726770E+16	96.833333	1.234286E-06	1.552284E-14	1.358831E-14	2.861552E-13	99.662389	2.999899
0.84	1.726629E+16	98.000000	1.234286E-06	1.606393E-14	1.375166E-14	2.930457E-13	99.654255	2.999897
0.85	1.726486E+16	99.166667	1.234286E-06	1.661741E-14	1.391500E-14	3.000180E-13	99.646021	2.999894
0.86	1.726342E+16	100.333333	1.234286E-06	1.718343E-14	1.407832E-14	3.070721E-13	99.637686	2.999892
0.87	1.726195E+16	101.500000	1.234286E-06	1.776212E-14	1.424162E-14	3.142080E-13	99.629250	2.999889
0.88	1.726048E+16	102.666667	1.234286E-06	1.835363E-14	1.440492E-14	3.214257E-13	99.620712	2.999887
0.89	1.725898E+16	103.833333	1.234286E-06	1.895809E-14	1.456820E-14	3.287252E-13	99.612073	2.999884
0.90	1.725746E+16	105.000000	1.234286E-06	1.957565E-14	1.473146E-14	3.361064E-13	99.603333	2.999882
0.91	1.725593E+16	106.166667	1.234286E-06	2.020644E-14	1.489471E-14	3.435693E-13	99.594491	2.999879
0.92	1.725438E+16	107.333333	1.234286E-06	2.085060E-14	1.505795E-14	3.511140E-13	99.585546	2.999876
0.93	1.725281E+16	108.500000	1.234286E-06	2.150828E-14	1.522118E-14	3.587405E-13	99.576500	2.999874
0.94	1.725123E+16	109.666667	1.234286E-06	2.217961E-14	1.538438E-14	3.664486E-13	99.567352	2.999871
0.95	1.724963E+16	110.833333	1.234286E-06	2.286472E-14	1.554758E-14	3.742385E-13	99.558102	2.999868
0.96	1.724801E+16	112.000000	1.234286E-06	2.356377E-14	1.571076E-14	3.821101E-13	99.548749	2.999866
0.97	1.724637E+16	113.166667	1.234286E-06	2.427689E-14	1.587392E-14	3.900634E-13	99.539294	2.999863
0.98	1.724471E+16	114.333333	1.234286E-06	2.500422E-14	1.603707E-14	3.980984E-13	99.529735	2.999860
0.99	1.724304E+16	115.500000	1.234286E-06	2.574589E-14	1.620020E-14	4.062151E-13	99.520075	2.999857
1.00	1.724135E+16	116.666667	1.234286E-06	2.650206E-14	1.636332E-14	4.144134E-13	99.510311	2.999854