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Predicting the consumption speed of a premixed flame subjected to an unsteady stretch rate

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Abstract—The stretched laminar flame model provides a convenient approach to embed realistic chemical kinetics when simulating turbulent premixed flames. When positive-only periodic strain rates are applied to a laminar flame there is a notable phase lag and diminished amplitude in heat release rate. Similar results have been observed with respect to the other component of stretch rate, namely the unsteady motion of a curved flame front when the stretch rates are periodic about zero. Both cases showed that the heat release rate or consumption speed of these laminar premixed flames can vary significantly from the quasi-steady flamelet model. Deviation from quasi-steady behaviour increases for conditions further from stoichiometric such that unsteady time scales of the flow are of the same magnitude as the chemistry. A challenge remains in how to use such results predictively for local and instantaneous consumption speed for small segments of turbulent flames where their stretch history is not periodic. This paper uses a frequency response analysis as a characterization tool to simplify the complex non-linear behaviour of premixed methane air flames for equivalence ratios from 1.0 down to 0.7, and frequencies from quasi-steady up to 2000 Hz using flame transfer functions. Various linear and nonlinear models were studied to identify appropriate flame transfer functions for low and higher frequency regimes, as well as to extend the predictive capabilities of these models. Linear models were only able to accurately predict the flame behaviour below a threshold of when the fluid and chemistry time scales are the same order of magnitude.

Keywords: Laminar Premixed Flames, Transient Response, Linear and Nonlinear Systems, Frequency Response Analysis

I. INTRODUCTION

Understanding turbulent combustion is important due to industrial applications such as internal combustion engines and furnaces. The challenges related to predicting turbulent combustion behavior have been discussed extensively in terms of their time-dependent and multidimensional nature, as well as having a large range of hydrodynamic time and length scales interacting with the time and length scales of the chemistry [1]. In this regard,, the formulation of these problems is well-posed by a system of partial differential equations and algebraic constraints that represent the conservation of mass and energy, as well as considerations of momentum and individual species while being subjected to convection, diffusion, and chemical reaction. All these phenomena are captured in direct numerical simulations with appropriate boundary conditions, but their solutions, due to these equations being highly nonlinear and strongly coupled, come at a significant computational cost [2], and thereby creates the need for model-level understandings.

A conceptual modeling approached that allows for estimation of local burning rates with pre-calculated complex chemistry is based on flamelets, which can collectively represent a turbulent flame. In their classical premixed form, flamelets provide a local consumption speed of the flame (referenced to their reactant state), and are generally assumed to be local planar structures subjected to a specified steady strain rate and of fixed reactant composition. This consumption speed, S_L, is the rate mass is converted from reactants to equilibrium products per unit area of flame and divided by the density of the reactants, and can readily be converted to the local heat release rate per unit flame area knowing the enthalpy of reaction. The validity of these assumptions has been challenged in terms of the response of laminar flames to changing positive strain rates [3], or mixture composition fluctuations [4]. Key observations for these planar flames included the flame responding in a quasi-steady manner at low frequencies, but at high frequencies the burning rate response becoming significantly attenuated, as well as having a phase lag.

Sahafzadeh et al. [5] showed the same results occur when flame stretch was created through the motion of a curved flame where both positive and negative transient stretch rates were applied. As a result, within an unsteady flow, classical flamelet models would predict the wrong magnitude of local burning and any expected maxima or minima events would occur at the wrong time. Lastly, an alternate approach to reduce the

computational load of complex chemistry is to use reduced chemistry and simple transport properties. It has been found that the transient response of a stretched flame is not necessarily captured accurately due to the change in the internal flame structure [6].

In the current work, the approach is to keep the full chemistry and then estimate the instantaneous local consumption speed by a frequency response analysis in the form of a flame transfer function using the local stretch history as the input.

The focus of this paper is on premixed combustion in the Damköhler and Karlovitz regimes where reaction occurs in identifiable flame structures that are locally subjected to unsteadiness in the flow. The objective of this paper is to further develop a model of a flame for the practical purpose of capturing the impact of unsteadiness on the rates of conversion from reactants to products. To be explicit, no consideration is given here to spatial variations along a flame, which is another important characteristic of turbulent flames.

II. Frequency Response Analysis

To create a useful transfer function from a frequency response analysis, consideration needs to be given to its input and output. Within the context of premixed turbulent flame modeling in the flamelet regime, a goal is often to represent the flame as an interface with burning rates that vary over the surface depending on local conditions. For example, basic flamelet libraries are used to assign a consumption speed to an element of the flame depending on its equivalence ratio and stretch rate. Since one of the goals of the current work is to better account for the unsteadiness in turbulent flames, which includes unsteadiness in stretch rate, the input to the transfer function was chosen to be the varying stretch rate and the output is the varying local consumption speed. By choosing stretch rate, the transfer function could be seen as independent of the geometry that creates it, and therefore applicable to flamelets of a turbulent flame.

The numerically modeled flame used to produce the results for this frequency response analysis has been previously reported in the combustion literature [5], and is therefore only briefly described here. Reactants of methane and air of a specifiable equivalence ratio flow radially outward from the inlet boundary (r = 5 cm) and through the outlet boundary (r = 11 cm). The mean and fluctuating components of the inlet mass flow rate were specified so that all the chemical reactions occur within the domain and are well removed from the boundaries. The model is based on a finite volume approach for solving the discretized equations for mass, momentum, energy, and species. The thermodynamic and transport properties come from CHEMKIN, and the reaction mechanism is based on GRI 3.0 [7] involving 36 species and 219 reactions.

For the simulations, the mass flow rate was changed sinusoidally with time (Eq. 1) at the inlet boundary.

$$\dot{m}(t) = \dot{m}_0 + BSin(\omega t) \qquad (1)$$

In Eq. 1, $\dot{m}$ is the mass flow rate at the inlet boundary, $\dot{m}_0$ the mean mass flow rate at steady state, B represents the amplitude of the oscillation, and ω is the angular frequency. The frequency was varied between 20 Hz and 2000 Hz. The reason to consider frequencies up to 2000 Hz is for the relevance to turbulent flows. For example, in the middle of a premixed turbulent duct flame stabilized by a backward facing step, mean frequency of the flame motion across a fixed point was observed to be in this range [8]. In the present study, the equivalence ratio was varied from 1.0 to 0.7 in order to compare the stoichiometric condition to lean flames, which are usually of interest due to their applicability to low-emission combustion systems.

The geometry studied herein has unique features of flame dynamics relative to the counter-flow configuration, which is usually used to generate flamelet libraries. The steady flame is unstretched due to the balance of curvature and flow divergence (*i.e.*, strain). However, when the flame is exposed to a flow field fluctuation, the expanding flame is subjected to positive stretch, whereas the contracting flame generates negative stretch, which has generally been ignored in the literature. The magnitude of the stretch rate could be changed by varying mean flame curvature, amplitude and frequency of oscillations, equivalence ratio, and fuel type. The choice of the marker, usually associated with a scalar field, to convert a flame with internal structure spread over space to an interface affects the magnitude of the stretch rate. To reduce this sensitivity, it is common to choose a marker that is on the trailing edge of the flame structure [9]. The flame marker used in this work is an iso-therm based on the temperature field with a value of 90% of the maximum temperature. Once calculated, this changing stretch rate becomes the input for the response analysis to create the transfer function.

The output for the response analysis is related to the total heat release, which is the chemical energy source term integrated for all species and in all control volumes in the domain, and is defined by Eq. 2.

$$\dot{E}_b = \sum_{i=1}^{N_{cv}} \sum_{k=1}^{N_{sp}} h_k \, \dot{\omega}_k \, \mathbb{V}(i) \qquad (2)$$

In Eq. 2, $\dot{E}_b$ is referred to here as the rate of enthalpy conversion from chemical to sensible sources for the whole flame, otherwise known as the burning rate, $\mathbb{V}(i)$ represents the volume of cell i, h_k is the molar specific enthalpy of species k, and $\dot{\omega}_k$ is the molar rate of creation of species k per unit volume.

Fig. 1 shows this instantaneous consumption speed as a phase plot with respect to the corresponding instantaneous stretch rate. The quasi-steady response is a point (not shown in the figure) located on $\kappa = 0$ and $S_L = 0.2$, which is essentially the steady state value and would be referred to as S_L^0. At very low frequencies (20 Hz), the relationship between local flame speed and stretch rate is almost linear. By further increasing the frequency, the line becomes an ellipse. The slope of the ellipses are negative which has been shown in other works for

methane-air flames in the same range of equivalence ratio [1]. The sensitivity of the local flame speed to the stretch rate first increases (*i.e.*, the vertical amplitude of the ellipse) in low the frequency regime and then decreases in the high frequency regime. For the case of $\varphi = 0.8$, this changing behaviour is seen in the variation from 100 to 200 Hz where the consumption speed increases, and from 200 to 500 Hz where the consumption speed decreases. Hence, there seems to be separate low and high frequency responses.

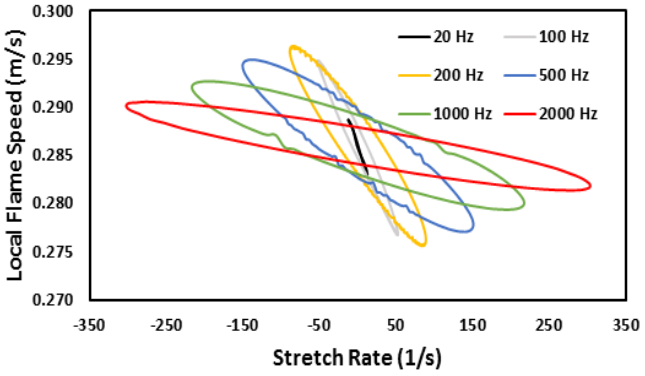

Figure 1. Local flame speed versus stretch rate for the equivalence ratio of φ=0.8 and quasi-steady response for the frequencies between 20 Hz and 2000 Hz

From this analysis, it is obvious that the flame response to a changing stretch rate depends on parameters such as equivalence ratio and the frequency of oscillation. Therefore, it would seem desirable to find a describing function to replace the cumbersome complex chemistry computations of transient response of turbulent and laminar premixed flames.

III. Linear Higher Order Analysis

In this section of the paper, in order to include flame behavior to a flow change upstream of the flame front, one needs to simulate each case for a wide range of frequencies and various input functions such as step, ramp, pulse, etc. This time consuming process can be replaced by one or more transfer functions to define the overall behavior of the flame. With regard to the application of this study, the input to the transfer functions are converted to stretch rate. The calculation of stretch rate is adopted from [5]. Therefore, the relationship between the stretch rate and local flame speed, which has been ignored in the current approach to flamelet modeling, reveals how flamelets respond to the time-dependent motion of a curved flame front. In order to have a better prediction of the transfer functions, a Polynomial Discrete-Time ARX (Autoregressive Exogenous) Model [10], which is a generalized transfer function, has been used. Equation (5) shows the general form of linear (due to the linear relationship between input and output) higher order (more than one term) transfer functions.

$$C(z^{-1})y(t) = \sum_{i=1}^{nu} D_i(z^{-1})u_i(t - nk_i) \quad (3)$$

In this equation, $u(t)$ is the input, $y(t)$ is the output, C and D are polynomials expressed in the time-shift operator z^{-1}, u_i is the i^{th} input, *nu*, the total number of inputs, and nk_i, the i^{th} input delay that characterizes the transport delay. In the present study, the system is SISO (single input/single output), therefore the transfer function takes a more familiar form wherein *i*=1. A Z-transform (Time-Discrete Fourier Transformation) can be used to convert the discrete-time form of the transfer function (Eq. 3) into a complex frequency domain representation.

This approach was first used to estimate the transfer function of the flame (with equivalence ratio of 0.8) response at 20 Hz fluctuations in mass flow rate. Then, the flame response to higher frequencies has been predicted using this transfer function. It has been observed that the accuracy of predictions decreases with increasing frequency. Increasing error in prediction of the transient response in the low frequency regime confirms that nonlinearity of the system increases with increasing frequency at each equivalence ratio. However, it could be considered insignificant until the oscillation reaches the high frequency regime, where the intrinsic structure of the flame may be changed locally. In the next step, the whole range of low frequencies (frequencies less than 200 Hz, which is the cut-off frequency for equivalence ratio of 0.8) has been used to generate the transfer function (Eq. 6). Figure 5 shows that the average accuracy of the predictions is ~ 88% for frequencies up to 200 Hz; however, the flame response experiences a significant drop in accuracy after 200 Hz (not shown in the figure).

$$\begin{aligned} C(z) &= 1 + 0.9623z^{-1} + 0.636z^{-2} + 0.2826z^{-3} + 0.122z^{-4} \\ D(z) &= -0.6376z^{-1} + 0.6915z^{-2} + 0.5377z^{-3} - 0.5923z^{-4} \end{aligned} \quad (4)$$

C(z) and D(z) are the expressions represented in Eq. 3. The fourth order transfer function results indicate that a minimum of the first four terms on each side of Eq. 3 is required to have the most accurate predictions. It should be noted that C(z) and D(z) are usually referred to as the *poles* and *zeros* of a transfer function in the literature.

Based on the higher order linear model, a transfer function (Eq. 5) is generated for predicting the high frequency regime transient response. Figure 3 illustrates the accuracy of this model for frequencies higher than 200 Hz.

$$\begin{aligned} C(z) &= 1 + 0.2641z^{-1} - 0.2513z^{-2} - 0.3054z^{-3} - 0.2756z^{-4} \\ D(z) &= 0.0012z^{-1} - 0.0044z^{-2} + 0.0051z^{-3} - 0.0019z^{-4} \end{aligned} \quad (5)$$

In order to study the effect of the amplitude on flame behavior and the transfer function, the ratio of the oscillations to the mean value was doubled. The results depict a fourth order transfer function similar to the previous cases, which

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predicts the high frequency responses (70% for 500 Hz, 84% for 1000 Hz, and 91% for 2000 Hz), with different coefficients.

The fourth order equation is the effective transfer function for various equivalence ratios. For example, a stoichiometric flame was tested with different flame curvature and amplitude. The optimum transfer function has the same format as it does with the other cases. The accuracies for the high range of frequencies is 83% for 500 Hz, 93% for 1000 Hz, and 94% for 2000 Hz. The higher accuracy at the same frequencies was expected due to the faster burning rate at the stoichiometric condition compared to the lean flames.

As can be concluded from the recent results in this section, the whole range of frequencies is divided in two regimes based on the cut-off frequency obtained from numerical simulations of transient response of laminar premixed flames for each equivalence ratio, and a separate transfer function is defined for each section. Although the accuracies are in an acceptable range, there may be considerable improvement using nonlinear models to predict the output. Therefore, in order to study the capability of nonlinear models to predict the flame response more accurately, different nonlinear transfer functions were analyzed in the next section.

IV. NONLINEAR SYSTEM ANALYSIS

As shown in the previous section, although linear transfer functions can achieve accurate prediction in the low frequency range of flame response to changes in stretch rate, they are not able to predict the response at some high frequencies. As mentioned in the introduction, in analyzing flame instabilities, flow velocity perturbations (as the input to the system) change the heat release rate (as the output) by influencing the flame surface area. Therefore, flame transfer functions are studied using the flame response to velocity fluctuations. The heat release rate modulations result in acoustic pressure perturbations, and could be linked to inlet flow velocity oscillations. Therefore, in order to capture the nonlinearities in the thermos-acoustic coupling, the flame transfer function has been replaced by the flame-describing function [11]. It has been reported that in premixed combustion systems, the relationship between velocity and heat release makes the system nonlinear, whereas gas dynamic processes generally stay in the linear regime [12].

Among these predictive models, using NARX (Nonlinear Autoregressive Exogenous) led to better results in estimating the transient response of the flame for the whole range of frequencies, including both low and high frequency regimes. Figure 3 illustrates the NARX predictions in comparison to the complex chemistry numerical results for the flame with an equivalence ratio of 0.8 at different frequencies. NARX models (which are an extension of ARX in polynomial transfer functions) are flexible nonlinear functions that are able to capture the complex behavior in nonlinear systems such as the current data set. Eq. (6) illustrates the structure of a linear Single Input/Single Output ARX model:

$$y(t) + a_1 y(t-1) + a_2 y(t-2) + \cdots + a_{na} y(t-na) = b_1 u(t) + b_2 u(t-1) + \cdots + b_{nb} u(t-nb+1) + e(t) \qquad (6)$$

Where u, y and e are the input, output, and noise, respectively. This structure implies that the output $y(t)$ is predicted as a weighted sum of past output values and current and past input values. na is the number of past output terms, and nb is the number of past input terms used to predict the current output. It has been shown that the surface wrinkling in turbulent flames at one location, in addition to the local velocity perturbation, also depends on the flame surface fluctuations at previous times upstream of the flame front [13]. Therefore, an ARX model could capture this memory effect occurring in turbulent flames by modifying the laminar flamelet response to a change in upstream flowrate.

After applying the nonlinear ARX model to predict the flame response, the results need to be validated by comparing the estimations with time series datasets obtained from complex chemistry numerical simulations. The nonlinear ARX model has been applied to three different datasets including, the low frequency regime (nonlinear ARX 2 in Fig. 2), the high frequency regime (nonlinear ARX 2 in Fig. 3), and the whole range of frequencies (nonlinear ARX 1 in Fig. 2 and 3). Therefore, three different nonlinear transfer functions were generated and tested against the numerical computations. As can be concluded from Figs. 2 and 3, nonlinear ARX model 2 based on two different frequency regimes, shows accurate predictions for each frequency compared to the linear higher order ARX model and nonlinear ARX model 1. It should be noted that these models are all capable of predicting the transient responses due to their storing of time histories in their structures. However, because of the nonlinear relationship between the input and output at high frequencies, nonlinear models are more accurate in general.

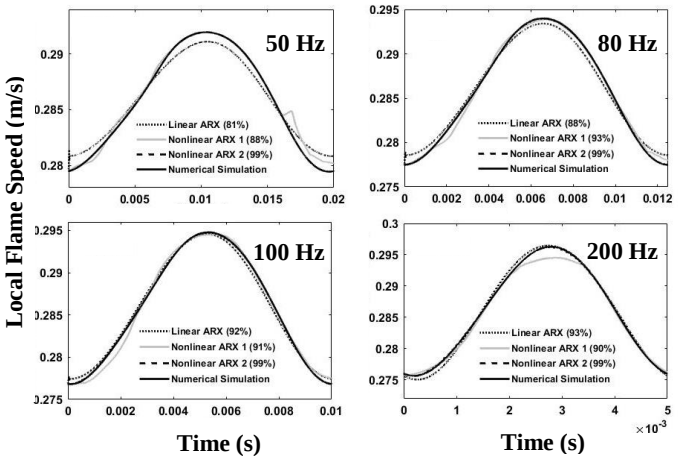

Figure 2. Estimation of transient response of a laminar premixed flame for φ=0.8 using a higher order linear ARX model and a nonlinear ARX model in the low frequency regime

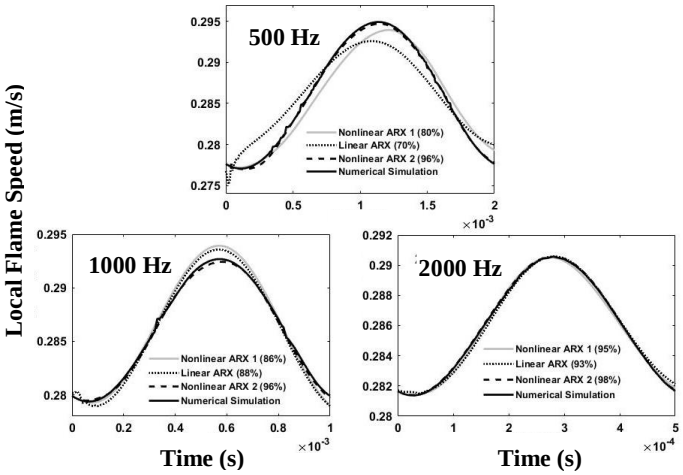

Figure 3. Estimation of transient response of a laminar premixed flame for φ=0.8 using the higher order linear ARX model and nonlinear ARX model in the high frequency regime

V. CONCLUSIONS

In this paper, the transient response data on the rate of conversion of chemical to sensible enthalpy, and the local flame speed for a laminar premixed flame that was exposed to periodic flow conditions, was analyzed in order to estimate a transfer function between these inputs and outputs. The study of the transient response analysis of a curved flame could be a potential modification to the quasi-steady assumption used in laminar flamelet libraries in order to improve premixed turbulent combustion modeling. The transient response dataset was taken from a previous study, which was a complex chemistry simulation of an inwardly burning laminar premixed (lean methane/air) flame in a cylindrically-symmetric geometry for different equivalence ratios (0.7 – 1.0) with cyclic exposure to positive and negative stretch rates at different frequencies (0 – 2000 Hz). In this paper, the higher order linear and nonlinear analyses have been performed for equivalence ratio of 0.8 only, to show the capability of transfer functions to capture the flame behavior when exposed to a flow perturbation upstream of the flame front.

A linear first order model was applied to the data and it fit the low frequency results for each flame. However, the flame behavior deviates from that of a linear first order system as the frequency increased and approached conditions where the chemical and flow time scales were similar. Applying higher order linear transfer functions improved the predictions (except for in the high frequency regime) due to the capability of the transfer function to store the time histories in its structure.

Nonlinear models, such as the nonlinear ARX model, could correctly predict the transient local flame speed over the whole range of frequencies and changing flow conditions. This transfer function could also reconstruct the local flame speed response for any arbitrary flow input, which enables the model to capture the transient effects of a flame in any conditions. Therefore, estimating a flame transfer function for laminar premixed flames could yield a better understanding of flame dynamics and could be used in order to modify the quasi-steady assumption in laminar flamelet models of turbulent combustion. Using the generated transfer functions based on the simulation datasets, the transient complex chemistry results were predicted with an accuracy over 70%.

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