

ULTRASONIC FOULING MITIGATION FOR RENEWABLE ENERGY POWERED REVERSE OSMOSIS DESALINATION SYSTEMS

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Abstract

This thesis examines the use of ultrasound to mitigate the performance degradation of reverse osmosis membrane filtration systems due to the accumulation of contaminants on membrane surfaces known as fouling. Numerical models of the phenomena responsible for the fouling mitigation effects of ultrasound were produced. An approach by which ultrasound could be applied to fouling mitigation within commercially available reverse osmosis modules was developed. Relationships between the application of ultrasound and temperature distributions within the fluid contained in filtration modules were investigated for instrumentation and performance assessment purposes. A novel ultrasonic horn was developed and theoretically verified for enhancing the effectiveness of ultrasonic fouling mitigation within commercially available reverse osmosis modules. An experiment was also designed to assess the effectiveness of the approach developed, for which an experimental setup was developed and constructed. Preliminary experiments have been conducted. Future research will focus on detailed experimental analysis.

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List of Acronyms

CFD	Computational Fluid Dynamics
CP	Concentration Polarization
DWA	Drinking Water Advisory
FEA	Finite Element Analysis
MF	Microfiltration
PWM	Pulse Width Modulation
UF	Ultrafiltration
UFM	Ultrasonic Fouling Mitigation
RO	Reverse Osmosis
RRO	Renewable Reverse Osmosis
SEC	Specific Energy Consumption
SWRO	Spiral-Wound Reverse Osmosis
TDS	Total Dissolved Solids
VFD	Variable Frequency Drive
WHO	World Health Organization

List of Symbols

α	Attenuation Parameter
A	Area (m ²)
A_c	Cross-Sectional Area (m ²)
A_w	Solvent Transport Coefficient (m/sPa)
β	Bubble Volume Fraction or Ultrasonic Attenuation per Unit Length (m ⁻¹) (context dependent)
b	Darcy's Law Constant (Pas/m ⁴)
B_s	Solute Transfer Coefficient (m/s)
δ_{CP}	Concentration Polarization Layer Thickness (m)
C_F^B	Feed Bulk Concentration (mol/L)
C_F^S	Feed Surface Concentration (mol/L)
c	Speed of Sound (m/s) or Specific Heat Capacity (J/kgK) (context dependent)
C_P	Permeate Bulk Concentration (mol/L)
C_P^S	Permeate Surface Concentration (mol/L)
d	Diameter (m)
D_s	Solute Diffusion Coefficient (1/s)
$\Delta\Pi$	Osmotic Pressure Difference (Pa)
E	Elastic Modulus (Pa)
f	Cyclic Frequency (Hz)
f_f	Feed Spacer Volume Fraction
F	Flow Rate (m ³ /s) or Force (N) (context dependent)
γ	Polytropic Index
G	Gain
h_w	Convection Coefficient (W/m ² K)
I	Acoustic Intensity (W/m ²)
J_s	Solute Flux (kg/m ² s)
J_v	Solvent Flux (m/s)
k	Mass Transfer Coefficient (m/s), Stiffness (Pa), or Wave Number (context dependent)
k_{wall}	Thermal Conductivity (W/mK)
λ	Wavelength (m) or Attenuation Coefficient (m ⁻¹) (context dependent)
L	Length (m)
L_{th}	Thermal Power Loss (W)
L_v	Viscous Power Loss (W)
μ	Dynamic Viscosity (kg/ms) or Displacement (m) (context dependent)
ν	Kinematic Viscosity (m ² /s)
n	Moles or Material Index (context dependent)
N	Bubble Density (m ⁻¹³)
ω	Angular Frequency (1/s)
p_0	Hydrostatic Pressure (Pa)
P	Pressure (Pa)

p_{Cr}	Bubble Equilibrium Pressure (Pa)
p_h	Polyharmonic Pressure (Pa)
p_g	Gas Pressure (Pa)
p_I	Internal Bubble Size (Pa)
p_L	Liquid Pressure (Pa)
p_v	Vapour Pressure (Pa)
q	Heat Conducted per Unit Area (W/m ²)
ρ	Density (kg/m ³)
R	Radius (m)
R_{Cr}	Critical Bubble Radius (m)
r_{eq}	Equivalent Thermal Resistance (K/m ² W)
R_g	Ideal Gas Constant (J/Kmol)
σ	Surface Tension (N/m) or Stress (N/m ²)
t	Time (s)
T	Temperature (K) or Period (s) (context dependent)
t_f, h	Feed Channel Thickness (m)
t_{wall}	Wall Thickness (m)
U_i	Inlet Velocity (m/s)
u, v	Velocity (m/s) or displacement (context dependent)
$\mathbf{V}$	Velocity (m/s) or Volume Fraction (context dependent)
w	Feed Channel Width (m)
ξ	Energy Efficiency Coefficient
x, y, z	Position (m)

Subscripts:

a	Amplitude or Adjusted (context dependent)
f	Free Face
i	Initial, Index, or Imaginary (context dependent)
L	Liquid
o	Outlet
r	Real
s	Surface
S	Solid
t	Transducer Face
0	Initial or Equilibrium (context dependent)

Preamble: The Social Context of Canadian Water Research

This thesis focuses on research into improved technology for drinking water production in remote communities such as many of Canada’s Indigenous reserves. The work is motivated in part by the long-lived and widespread drinking water advisories (DWAs) on Indigenous reserves that are collectively described as the “First Nations drinking water crisis” [1–5]. Given this context, it is critical to first acknowledge that technical challenges are not fully responsible for the lack of adequate drinking water infrastructure in Indigenous communities [1, 6–8]. In fact, researchers focusing on the nature of the challenges faced by Indigenous populations around the world have explicitly stated that barriers for drinking water access in Indigenous communities including those faced by the Indigenous peoples of Canada are related to governance rather than technology [7, 8]. Supporting this point in the case of Indigenous peoples of Canada communities, a report by the Auditor General of Canada investigating the failure of the Federal Government to fulfill its 2015 promise regarding the elimination of all DWAs affecting Indigenous reserves repeatedly pointed to a lack of adequate funding from the Federal Government as a root cause of their failure to meet their commitments [1]. Financial constraints contribute to problems including an inability to recruit, train, and retain qualified system operators, difficulties around maintaining existing systems, and delays in construction of new water treatment infrastructure [1]. Funding deficiencies were traced back to a financial allocation model that was over 33 years out of date when the report was written [1]. Additionally, while regulations ensure safe drinking water in Canadian provinces and territories, no such regulations exist for Indigenous reserves, despite a previous report by the auditor general recommending their creation 15 years ago [1]. Scholars investigating the Indigenous drinking water crisis have also pointed to the difference between responses to DWAs within Indigenous communities and those in other Canadian communities, such as those issued in Walkerton, Ontario (2000) and North Battleford, Saskatchewan (2001) to highlight the existence of technology and resources to resolve drinking water availability interruptions [9, 10]. In these example cases, the DWAs were permanently resolved in a matter of days, and were followed by lengthy public inquiries that spurred provincial regulatory changes [9, 10].

The case of the Indigenous peoples of Canada is further complicated by the influence of mining and logging companies, whose interests often conflict directly with the needs of Indigenous stakeholders [6]. This conflict has motivated interested parties to re-frame the Indigenous drinking water crisis as a consequence of failures on the part of Indigenous communities [6]. Those presenting this narrative use it to justify dispossession of Indigenous land for purposes of extractive capitalist development, claiming that the jobs created by this development will improve the economic situation in Indigenous communities and fund improved infrastructure [6]. This narrative ignores the long and ongoing history of extractive capitalist development polluting water sources upon which Indigenous communities rely, as well as the fact that this development has not actually improved economic conditions for Indigenous communities in regions where it has occurred, but it is a convenient way for the Government to justify its constant prioritization of corporations above Indigenous communities [6]. Additionally, the perception that the Federal Government uses funding for water infrastructure as a strategic tool to pacify resistance to land dispossession associated with corporate activities fosters reluctance in some members of Indigenous communities to use the infrastructure provided [6, 7].

In light of this broader context, it becomes clear that the barriers preventing the resolution of the

Indigenous drinking water crisis have less to do with technology and more to do with socio-political issues and capital interests overshadowing Indigenous sovereignty. Therefore, as scholars in this field have already identified, improved technology will never resolve this crisis unless the Federal Government provides greater funding to its resolution and curtails the corporations that both contribute to and benefit from the crisis itself [6–8]. Many of the circumstances faced by Indigenous peoples of Canada with respect to drinking water access stem from colonial and capitalist practices that have impacted the development of every inhabited continent, suggesting that many of the rural communities that contribute to the global statistics on drinking water availability presented by organizations including the WHO face similarly complex challenges [6–8, 11]. This point is not meant to disparage the development of novel technologies geared towards drinking water infrastructure in rural communities, as these developments still have the potential to elevate the material conditions of rural populations worldwide and simplify the problems faced by Indigenous communities such as the Indigenous peoples of Canada [2]. Rather, this point is meant to warn readers of this thesis against the temptation to collapse a multidimensional problem such as water access into a simple technical challenge, and the confused frustration that inevitably follows this reduction.

Chapter 1

Introduction

1.1 Introduction

The overall goal of this research is to improve drinking water access for those who need it. Specifically, this research aims to do so by improving the practical utility of ultrasonic membrane cleaning technologies, thereby improving the effectiveness of membrane water filtration technologies. The sections below outline why this is important, and the specific problems that this research aims to address.

1.2 Motivation

A 2017 report from the World Health Organization (WHO) identified that 29% of the global population lacked access to readily available clean drinking water, with residents of rural communities comprising a disproportionate part of those affected by drinking water insecurity [11]. Demand for drinking water is projected to continue to increase as the world population grows, which will result in major increases in energy consumption associated with water filtration processes [12]. A need therefore exists for water purification technologies that can be deployed in rural environments while relying on renewable energy resources.

Many Indigenous peoples of Canada lack readily available clean drinking water [1]. Consistent failures on behalf of the Canadian Government to effectively provide for the construction, maintenance, and operation of adequate water infrastructure within Indigenous peoples of Canada reserves has produced the Indigenous drinking water crisis, characterized by widespread Drinking Water Advisories (DWAs) recommending that the water provided by the existing infrastructure be boiled prior to consumption or not consumed at all [1]. A characteristic example of these failures, identified in the preamble, is the Federal administration’s inability to meet their 2015 commitment to eliminate all long-term DWAs active within Indigenous peoples of Canada reserves by 2021 [1]. A 2021 report by the Auditor General of Canada points to a number of reasons for this failure: alongside the funding deficiencies identified previously is the fact that many of these reserves are small communities located in remote environs with limited transportation access, which renders many of the more traditional large-scale water infrastructure solutions that serve the more populated and accessible regions of Canada infeasible [1].

Despite the fact that global water access is largely a social problem, there do exist some technical barriers that can be removed by developing improved water infrastructure tailored to the unique challenges of small, remote communities [1]. In particular, the lack of energy and transportation infrastructure in many remote environs renders the operation of traditional water treatment systems unfeasible, motivating the development of systems that can operate using locally available energy sources with minimal reliance on consumables and maintenance [1, 2, 4, 13]. Reverse Osmosis (RO) is a water filtration technique that has been successfully implemented using renewable energy sources to treat brackish groundwater in small, remote rural communities [2]. Reverse Osmosis is a pressure-driven membrane filtration process that effectively removes organic, biological, and mineral contaminants from feed water to produce clean water known as “permeate” [13]. The use of locally available renewable energy sources allows sustainable operation of RO systems in isolated areas, termed Renewable Reverse Osmosis (RRO) systems [13].

Contaminants gradually obstruct membrane surfaces during operation in a process known as fouling [14]. Fluid boundary layers on membrane surfaces also experience high contaminant concentration known as Concentration Polarization (CP), increasing osmotic back-pressure [14]. These phenomena decrease permeate output and membrane service life while increasing power consumption, all of which jeopardize the viability of the technology in remote communities where energy, maintenance, and replacement components are difficult to obtain [1, 2, 14]. Experimental investigations have shown that intermittent operation (a common condition for RRO systems) exacerbates fouling, potentially due to bacterial growth occurring when the membrane surfaces are exposed to stagnant water for extended periods of time [2–4, 13]. Therefore, fouling mitigation is critical to the practical implementation of RRO systems.

Ultrasound has shown promise in simultaneously mitigating CP and fouling in membrane filtration contexts by producing microscopic cavitation bubbles which can erode solids and disrupt boundary layers [14]. Ultrasonic Fouling Mitigation (UFM) has been proven in microfiltration (MF) and ultrafiltration (UF) contexts; however, it has not been tested in RO applications beyond the lab-scale [13–15]. Nevertheless, its versatility with respect to filtration and fouling modalities, as well as its lack of dependence on consumables, make UFM an appealing technology for integration into RRO systems.

1.3 Problem Statement

The viability of RRO for remote communities would be significantly improved if membrane fouling could be effectively mitigated without greatly increasing energy requirements or relying upon consumables [2, 13]. Ultrasonic fouling mitigation has performed well at lab scale, and does not require consumables; however, its current implementations scale poorly to practical implementations due to their energy inefficiency, as well as challenges posed by the more complicated geometries used in practical membrane filtration modules [14]. Therefore, there exists a need for a scalable, energy-efficient implementation of UFM. This thesis is focused on satisfying this need.

1.4 Research Objective and Goals

This research endeavours to develop novel ultrasonic fouling mitigation technology for pilot-scale, RRO systems. The work will focus on brackish groundwater¹ filtration, as this is widely available globally (including within Indigenous peoples of Canada reserves) [2, 4, 17]. A method to effectively propagate ultrasonic energy through the industry-standard spiral-wound membrane structure must be developed and validated [2, 3]. Ultimately, the research endeavours to develop a retrofit for commercially available RO systems that gainfully incorporates ultrasonic agitation to minimize membrane fouling. It is worth noting that while RO is the focus of the research, the technology developed will likely be suitable for microfiltration (MF) and ultrafiltration (UF) applications with little to no modification.

1.5 Scope of Work

The work summarized in this thesis falls into two categories: 1) design, simulation, and modelling; and 2) experimental work. The design, simulation and modelling work focused on developing an effective

¹There is no universally accepted quantitative definition for brackish groundwater, but it is often considered to be water containing between 1000 and 10000 mg/L of Total Dissolved Solids (TDS) [16].

sonification approach for the UFM of SWRO modules, demonstrating its theoretical viability for a pilot-scale RRO system using numerical modelling, and optimizing the design of a novel SWRO sonification apparatus to demonstrate the superiority of these approaches in comparison to existing techniques. The experimental work focused specifically on demonstrating the effectiveness of UFM for partially reversing severe inorganic fouling.

Figure 1.1 illustrates the progression of the research conducted over the course of this thesis. Each of the elements contained therein is elaborated upon in more detail later on in the thesis.

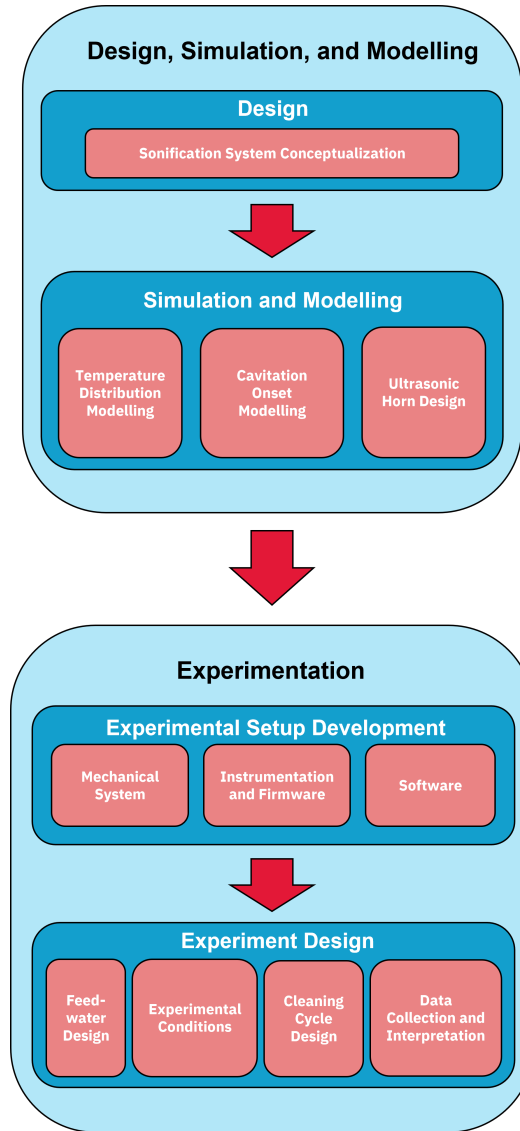


Figure 1.1: An illustration of the progression of research work conducted over the course of this thesis. Each of the sections included is elaborated upon in further detail below.

1.6 Contributions

This research made four primary contributions to the state of the art surrounding UFM in a RRO context, which are summarized below.

1.6.1 Temperature Distribution Modelling

The effects of ultrasonic sonification on temperatures within a representative RO module were estimated in order to investigate whether temperature increases due to sonification would negatively impact filtration performance and lay groundwork for the use of temperature differences between the inlet and outlet of the module for instrumentation purposes. Two numerical models of the module were developed, one of which included the effects of changing temperature on the mass transfer occurring within the module, and one of which neglected the effects of temperature on the mass transfer calculations in order to decouple the heat and mass transfer problems from one another. The two models predicted almost identical temperature distributions across a range of input parameters, and both predicted that sonification would have negligible impacts on filtration performance.

1.6.2 Cavitation Onset Modelling

A method to relocate the onset location of ultrasonic cavitation from the surface of the ultrasonic source located at the module inlet to a point further along the feed channel using the change in pressure along the flow direction of a RO module was hypothesized. To investigate its viability, a numerical model of the heat and mass transfer occurring within a representative pilot-scale RO module was synthesized with a numerical model of cavitation bubble dynamics to investigate ultrasonic attenuation within the context of a RO module. The resulting model was used to simulate a range of possible module operating parameters, and confirmed that the hypothetical technique was theoretically viable. A regime employing this technique to effectively propagate UFM through the modelled RO module was developed, and its expected total power consumption was shown to be similar to the power consumption of an RRO system employing the modelled RO module under standard operating conditions.

1.6.3 Ultrasonic Horn Design

A novel ultrasonic horn with segments inside and outside of the membrane module enclosure was designed to improve the transfer of vibrations across membrane module boundaries by minimizing the displacement amplitude at the membrane module boundary and maximizing the displacement amplitude at the free face of the submerged horn segment. An analytical model was used to calculate horn dimensions that would theoretically produce the desired behaviour, which were subsequently investigated using a FEA model. The FEA model showed reasonable agreement with the analytical dimensions, and greatly improved vibration transfer performance in comparison to an implementation where no ultrasonic horn was used.

1.6.4 Experimental Setup and Analysis of the Novel Ultrasonic Horn Design

An experimental setup for the investigation of UFM viability on pilot-scale RO modules was designed, constructed, and commissioned. An experiment to verify the effectiveness of UFM was investigated, and its theoretical results were hypothesized.

1.7 Thesis Organization

This thesis is structured into five chapters. The first chapter describes the motivation for the research compiled in this thesis, and outlines the work that was done. The second chapter provides a review of the literature relevant to the research conducted. The following two chapters contain the core contributions of this thesis, with Chapter 4 describing the contributions made in the design, simulation, and modelling space, and Chapter 5 discussing the work that was completed towards an experimental investigation of the technology developed. The sixth chapter summarizes the contents of the thesis, and outlines potential future research directions.

Chapter 2

Background

2.1 Introduction

This thesis builds off of a multidisciplinary literature base including elements of membrane science, fluid mechanics, heat transfer, and vibration analysis. This chapter summarizes the fundamental literature to describe the key methodologies employed and the basis that the research conducted in this thesis build upon. In the interest of synthesizing relevant concepts from different sources within the literature, this chapter also contains derivations of certain formulas not found within the prior art. This chapter begins by covering the fundamentals of RO and the modules used for its practical implementation. It then discusses the natures of the different fouling modalities that can occur within RO modules. Lastly, the underlying principles of UFM are discussed. These include the mechanics of ultrasonic cavitation and vibration transfer within solids.

2.2 Reverse Osmosis

Reverse Osmosis is a membrane-based separation process wherein a pressure differential across an osmotic membrane is used to remove organic, biological, and mineral contaminants from feed water to produce clean water known as permeate [13]. Industrial uptake of RO has been rapid since its initial commercialization in the 1960s, and it is now an industry standard for a wide variety of applications [18, 19]. Spiral-Wound Reverse Osmosis (SWRO) modules represent a common commercial implementation of RO technology [4, 14]. Pressures within these systems are on the order of 100 psi to 1000 psi, or 689 kpa to 6890 kpa (some “ultra-low energy” membranes operate at 100 psi, while certain seawater desalination membranes can operate at pressures of 1000 psi) [13, 20–22]. As shown in Figure 2.1, the permeable membrane elements are contained within a laminate structure composed of the following constituents:

- **Feed Spacer:** This is a polymer mesh designed to maintain separation of the spiral windings such that feed water can flow through the module.
- **Permeable Membrane:** This membrane allows osmotic diffusion of water while preventing or limiting the passage of other substances, thus allowing for filtration to occur. It is typically composed of a polyamide film with a thickness between $0.13 - 0.2 \mu\text{m}$ [23].
- **Porous Foam Membrane Backing:** Since the permeable membrane is extremely thin, it is bonded to a porous foam backing to prevent structural failure.
- **Permeate Spacer:** Placed within an envelope formed by foam-backed permeable membrane on all sides, this forms channels within the envelope through which permeate can flow.

This laminate structure is wound around a central collection tube into which the envelope formed by the permeable membrane, foam backing, and permeate spacer deposits permeate. Feed water flows axially along membrane surfaces. Water diffuses out of the feed flow through the membrane, and flows within the

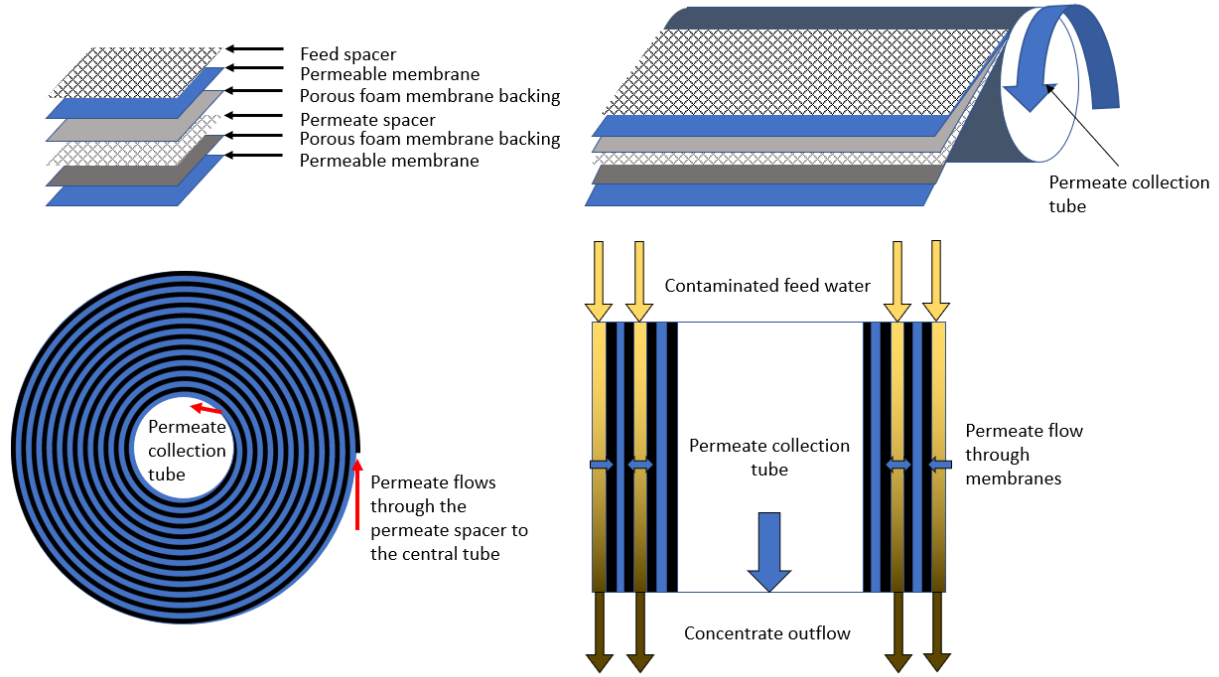


Figure 2.1: Clockwise, starting from the top left corner: laminate structure containing the permeable membrane; arrangement of this laminate in a spiral-wound configuration; radial cross-section of a SWRO module showing bulk flow directions and axial contaminant concentration gradient; axial cross-section of a SWRO module showing the flow of permeate within the spiral channel formed by the permeate spacer into the permeate collection tube.

spiral channel formed by the permeate spacer towards a central permeate collection tube. Contaminant concentration increases axially from the inlet to the outlet of the membrane, and varies throughout the cross-section of the membrane module such that fluid boundary layers near membrane surfaces have elevated contaminant concentration with respect to the bulk flow [19]. This elevated contaminant concentration towards membrane surfaces is known as Concentration Polarization, and reduces membrane performance by increasing the forward osmotic pressure that must be overcome to produce permeate [24]. High feed flow rates can help mitigate Concentration Polarization by promoting mixing due to increasing the turbulence produced by the feed spacer within boundary layers, while lower feed flow rates reduce energy consumption by reducing the pressure drop between the inlet and the outlet [14, 19].

2.3 Fouling

Membrane fouling refers to the progressive obstruction of a filtration membrane by contaminants suspended in the water fed to the system [25]. Fouling primarily occurs via the following four mechanisms, as illustrated in Figure 2.2 [14, 25]:

- **Biofouling:** Bacteria suspended within the feed water adhere to the membrane and reproduce using nutrients within the feed water, obstructing the membrane with a gel layer consisting of the organic

byproducts of their reproduction.

- **Organic fouling:** Organic molecules within the feed water (introduced by natural processes or human activity) adhere to and obstruct the membrane surface.
- **Inorganic fouling:** Ions dissolved within the feed water precipitate out of solution onto the membrane surface, forming an obstructive mineral scale.
- **Colloidal fouling:** Small particles suspended within the feed water are pressed into the membrane surface by the flow of permeate.

These fouling mechanisms can work separately or together, with variations in operating conditions resulting in different combinations of fouling modes [4, 14]. While inorganic, organic, and colloidal fouling only develop during operation due to their dependence on a continuous supply of fouling constituents (and, in the case of inorganic fouling, concentration gradients in the feed water within the module), biofouling flourishes at reduced flow rates, resulting in the development of severe multimodal fouling when intermittent operation alternately provides high and low flow rates [4, 14].

The effectiveness of fouling mitigation strategies also vary with operating conditions [4]. In particular, the commonly-adopted approach of utilizing chemicals known as anti-scalants to combat inorganic fouling can exacerbate biofouling by providing bacteria with additional sources of nutrients [4, 14, 26]. This not only stresses the need for novel, generally applicable fouling mitigation strategies, but also provides an example of the high contextual sensitivity of existing fouling mitigation technologies. In commercial systems, less selective filtration technologies are often installed prior to membrane filtration modules to pre-treat the feed water, mitigating membrane fouling by removing some of the more easily excluded contaminants prior to the membrane module [2, 3, 14]. This approach increases the size, cost, and power demand of a typical filtration plant, and may require large quantities of consumables depending on the pretreatment technologies used; as such, RRO installations often only employ minimal pretreatment stages [2, 3, 13, 14].

The effect of fouling in intermittently operated RO systems has been experimentally evaluated in the literature [4]. One such experimental evaluation, using groundwater sampled from Nobleton Ontario as feed water for a lab-scale RO filtration system, showed that unmitigated fouling would reduce permeate output by over 50% within a week of operation, with the use of anti-scalants and a clean water rinse at the end of the daily operating cycle reducing the degradation to 30% [4]. Fouling remains a topic of keen interest within the membrane filtration industry, and considerable research efforts have gone into advancing technologies for its modelling, prediction, diagnosis, and mitigation in recent years [25–28].

2.4 Flow Within SWRO Modules

Flow within SWRO modules is impacted by a combination of classical fluid-mechanical effects (turbulence and pressure gradients due to viscous losses) as well as the effects of solvent diffusion through the membrane [19, 28, 29]. An accurate picture of the flow within an SWRO membrane cannot be drawn by considering these effects in isolation of one another [19, 29, 30]. The problem is further confounded by the addition of ultrasound, whose introduction of heat into the system affects diffusive behaviours [19, 31, 32]. The problem quickly becomes analytically intractable; however, an understanding of the individual mechanics at play is critical to understanding some of the numerical solutions developed in this thesis.

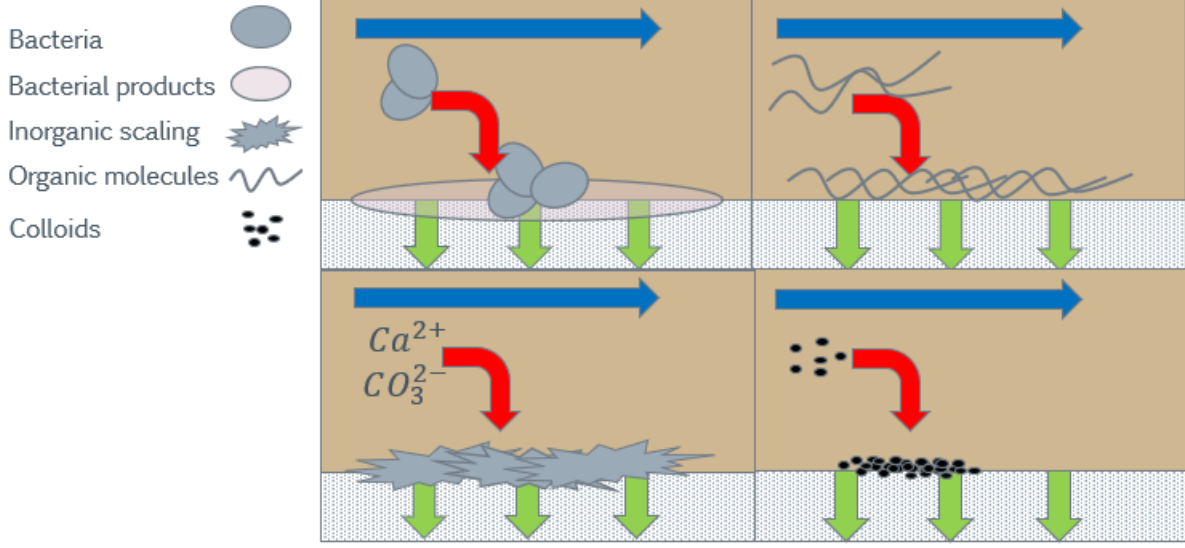


Figure 2.2: (Clockwise from top left) Biofouling, organic fouling, inorganic fouling, and colloidal fouling.

2.4.1 Diffusion

Based on the solution-diffusion model, solvent flux J_v (m/s) through a RO membrane can be described in terms of the solvent transport coefficient A_w (m/s/Pa) of the membrane as well as the transmembrane and osmotic pressure differences ΔP (Pa) and $\Delta \Pi$ (Pa) as shown in equation (2.1) [31]:

$$J_v = A_w(\Delta P - \Delta \Pi) \quad (2.1)$$

The transmembrane pressure difference is simply the difference in hydraulic pressures between the feed and permeate sides of the membrane. The osmotic pressure difference is proportionally related to the difference in solute concentration at its feed surface C_F^S (mol/L) and permeate surface C_P^S (mol/L) by the temperature T (K) and the ideal gas constant R_g (J/Kmol) as shown in equation (2.2) [19]:

$$\Delta \Pi = R_g T (C_F^S - C_P^S) \quad (2.2)$$

Flux of solute through the membrane can also be expressed in terms of these concentrations and a solute transfer coefficient B_s (m/s) as shown in equation (2.3) [19, 29, 31]:

$$J_s = B_s (C_F^S - C_P^S) \quad (2.3)$$

The transport coefficients A_w and B_s are related such that if C_P^S is small in comparison to C_F^S , the approximation $J_s \approx J_v C_P^S$ can be used [19, 29]. Collecting equations (2.1), (2.2), and (2.3) produces equation (2.4), which allows for the direct calculation of solvent flux through an RO membrane from measurable parameters [19]:

$$J_v = \frac{A_w \Delta P}{1 + \frac{A_w R_g T C_P^S}{B_s}} \quad (2.4)$$

As water diffuses through the membrane, the solute concentration within the layer of fluid adjacent to the feed-facing membrane surface increases [29]. The relationship between the concentration at this surface

in relation to the concentration within the bulk flow C_F^B and the concentration at the permeate-facing membrane surface is shown in equation (2.5) [19, 29]:

$$\frac{C_F^S - C_P^S}{C_F^B - C_P^S} = e^{\left(\frac{J_v}{k}\right)} \quad (2.5)$$

Here, k (m/s) is referred to as the mass transfer coefficient defined in terms of Concentration Polarization layer thickness δ_{CP} and diffusion coefficient of the solute D_s (1/s) as $k = \frac{D}{\delta_{CP}}$.

2.4.2 Flow Behaviours

Figure 2.3 illustrates a simplified RO module feed channel. When discussing the flow behaviours within SWRO modules, it is helpful to separate the discussion into two parts: bulk flow effects and small-scale effects. In this context, those relationships that can be effectively approximated by reducing the system to a single dimension running from inlet to outlet are considered to be bulk flow effects, while those changes involving multidimensional expressions are defined as small-scale.

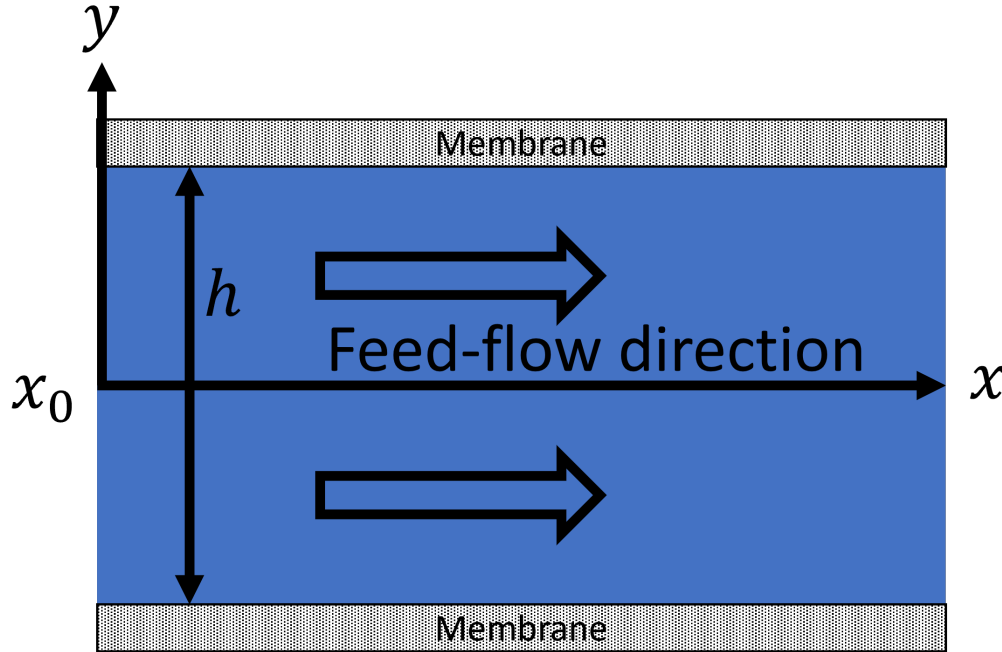


Figure 2.3: Feed channel illustration including coordinates. The feed channel width w (m) describes the dimension perpendicular to the cross-section illustrated.

2.4.2.1 Bulk Flow

A mass conservation argument can be used to express the bulk flow rate $F(x)$ (m^3/s) in terms of membrane flux in a rectangular feed channel of width w (m), thickness t_f (m), and length running from x_0 to x as shown in equation (2.6) [19]:

$$\rho F(x_0) - \rho F(x) - \rho w \int_{x_0}^x J_v(a) da = 0 \quad (2.6)$$

Here, ρ is the density of the water. Dividing density out of the equation and differentiating with respect to x gives equation (2.7):

$$-\frac{dF(x)}{dx} - wJ_v(x) = 0 \quad (2.7)$$

Therefore, equation (2.8) can be derived to express the relationship between J_v and $F(x)$ as follows:

$$\frac{dF(x)}{dx} = -wJ_v(x) \quad (2.8)$$

The cross-sectional area $A_c = wt_f$ (m^2) of the feed channel remains constant along the length of the channel [19]. The feed flow velocity averaged across the feed channel cross-section, expressed as $\bar{u}(x)$ (m/s), can then be expressed by recognizing that $F = A_c \bar{u}$, producing the result shown in equation (2.9):

$$\frac{d\bar{u}(x)}{dx} = -\frac{w}{A_c} J_v(x) \quad (2.9)$$

The pressure drop along the length of a RO module is often approximated using Darcy's law such that an experimentally-determined constant b can be used to relate bulk pressure $p_b(x)$ (Pa) to flow rate as follows in equation (2.10) [19, 33]:

$$\frac{dp_b(x)}{dx} = -bF(x) \quad (2.10)$$

With a suitable expression for J_v (such as that shown in equation (2.1)) and a description of the channel geometry, equations (2.10), (2.9), and (2.8) can be used to develop an expression for the change in bulk flow properties within the module.

2.4.2.2 Small-Scale Effects

The Navier Stokes equations can be used to describe local flow geometries. For illustrative purposes, consider the simplified case illustrated by Figure 2.3 in which a feed channel lacking a feed spacer is bounded on both sides by parallel permeable RO membranes of infinite width admitting flux J_v under steady-state, incompressible conditions. The set of two dimensional Cartesian Navier-Stokes (equations (2.11) and (2.12)) and continuity (equation (2.13)) equations can be assembled as follows:

$$u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{1}{\rho} \frac{\partial P}{\partial x} + \nu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) \quad (2.11)$$

$$u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = -\frac{1}{\rho} \frac{\partial P}{\partial y} + \nu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) \quad (2.12)$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \quad (2.13)$$

Here, u (m/s) and v (m/s) are the velocities in directions x and y , where x is aligned with the feed channel and y runs perpendicular to its boundaries, P (Pa) is pressure, ρ (kg/m^3) is density, and ν (m^2/s) is the kinematic viscosity. Setting the origin of the channel at the center of its inlet, halfway between the

bounding membranes, and expressing the separation of the two membranes as h (m), the following boundary conditions can be assembled at the upper membrane:

$$v|_{y=\frac{h}{2}} = J_v \quad (2.14)$$

$$u|_{y=\frac{h}{2}} = \frac{\partial u}{\partial x}|_{y=\frac{h}{2}} = \frac{\partial^2 u}{\partial x^2}|_{y=\frac{h}{2}} = 0 \quad (2.15)$$

Symmetry, in turn, produces the following boundary conditions:

$$v|_{y=0} = \frac{\partial v}{\partial x}|_{y=0} = \frac{\partial^2 v}{\partial x^2}|_{y=0} = 0 \quad (2.16)$$

$$\frac{\partial u}{\partial y}|_{y=0} = 0 \quad (2.17)$$

From continuity and equation (2.17), it can also be shown that:

$$\frac{\partial^2 v}{\partial y^2} = \frac{\partial}{\partial x} \frac{\partial u}{\partial y} = 0 \quad (2.18)$$

Since J_v is a function of the difference in hydraulic pressure across the membrane, it will vary with x ; however, it can be assumed for simplicity that pressure variations along the feed channel are small in comparison to the hydraulic pressure difference, making $v|_{y=\frac{h}{2}} = J_v$ approximately constant for the purposes of this analysis.

Applying the boundary conditions and evaluating at $y = 0$, equations (2.11)-(2.13) reduce to:

$$u \frac{\partial u}{\partial x} = -\frac{1}{\rho} \frac{\partial P}{\partial x} + \nu \frac{\partial^2 u}{\partial x^2} \quad (2.19)$$

$$0 = \frac{1}{\rho} \frac{\partial P}{\partial y} \quad (2.20)$$

By a similar process to that demonstrated in equation (2.18), it can be shown using equation (2.19) that $\frac{\partial^2 u}{\partial x^2} = 0$. This produces the following expression for $u|_{y=0}$:

$$u|_{y=0} = Ax + C \quad (2.21)$$

Here, the constant C is simply the velocity at the inlet, and will be defined as U_i . The value A is another constant, equal to $\frac{\partial u}{\partial x}|_{y=0}$. Continuity therefore requires that $\frac{\partial v}{\partial y}|_{y=0} = -A$.

Compiling the conditions on $\frac{\partial u}{\partial x}$ and $\frac{\partial v}{\partial y}$, it becomes clear that a quadratic relationship for $\frac{\partial u}{\partial x}$ and $\frac{\partial v}{\partial y}$ satisfies all requirements. The following relationships can therefore be defined:

$$\frac{\partial v}{\partial y} = \frac{4A}{h^2} \left(y^2 - \frac{h^2}{4} \right) \quad (2.22)$$

$$\frac{\partial u}{\partial x} = -\frac{4A}{h^2} \left(y^2 - \frac{h^2}{4} \right) \quad (2.23)$$

When integrated, these produce:

$$v = \frac{4A}{h^2} \left(\frac{y^3}{3} - \frac{h^2}{4} y \right) + f(x) \quad (2.24)$$

$$u = -\frac{4A}{h^2}(y^2 - \frac{h^2}{4})x + f(y) \quad (2.25)$$

The generic function $f(x)$ can be shown to be necessarily constant by differentiating equation (2.24) by x . From equations (2.16) and (2.21), it can be shown that $f(x) = 0$. The generic function $f(y)$ is simply the flow profile at the inlet, and must satisfy the conditions $f(0) = U_i$ as well as all other conditions placed on u . A quadratic solution $f(y) = U_i - \frac{4U_i y^2}{h^2}$ satisfies the conditions. Finally, since $v|_{y=\frac{h}{2}} = J_v$, the constant A becomes:

$$A = -3\frac{J_v}{h} \quad (2.26)$$

As such, the velocity field can finally be expressed as shown in equation (2.27):

$$\mathbf{V} = (\frac{12J_v y^2}{h^3}x - 3\frac{J_v}{h}x + U_i - \frac{4U_i y^2}{h^2})\mathbf{i} - \frac{12J_v}{h^3}(\frac{y^3}{3} - \frac{h^2}{4}y)\mathbf{j} \quad (2.27)$$

The stream function for this flow is shown in Figure 2.4. Analytical solutions to the Navier-Stokes equations describing RO modules quickly become analytically intractable as varying membrane flux and feed spacer effects come into consideration. Computational Fluid Dynamics (CFD) programs are sometimes used to develop clearer pictures of the local flow behaviours in these systems [28, 34].

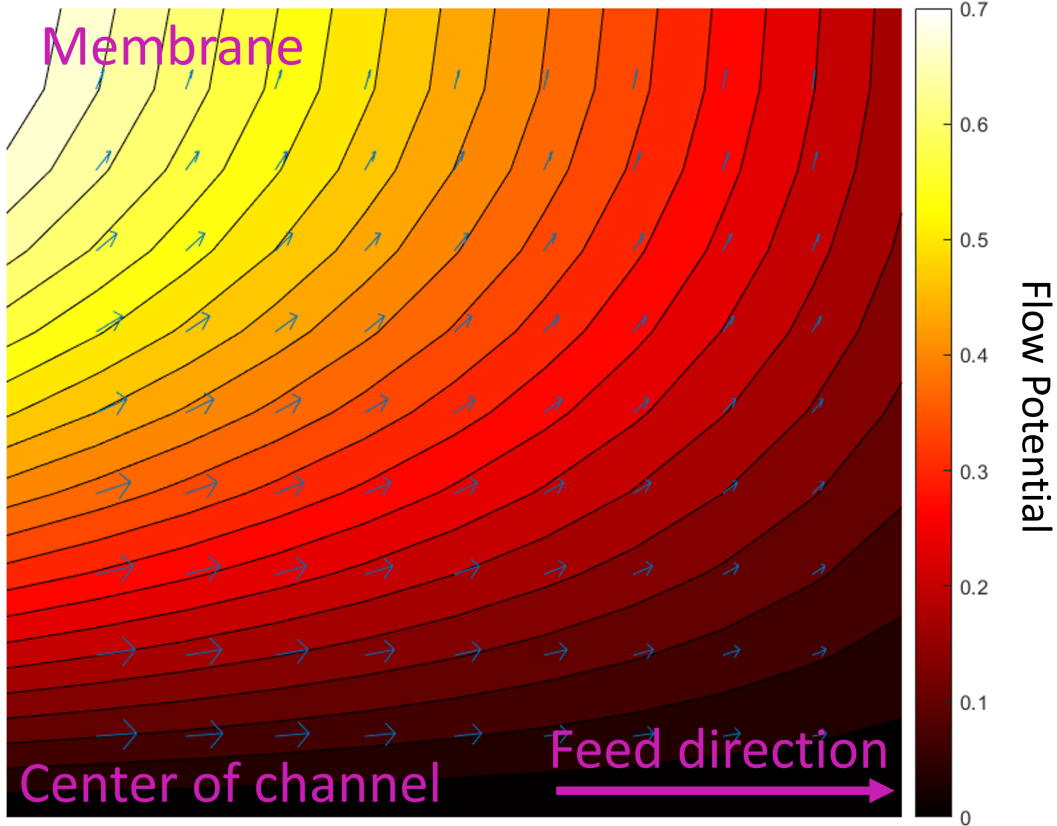


Figure 2.4: Stream function of idealized flow within an SWRO module.

2.4.2.3 Model Synthesis

Efforts have been made to predict RO module performance by combining diffusion models with models for bulk flow behaviour [19, 30, 35–38]. An analytical example of this approach is developed in [19] and validated in [30] for a rectangular feed channel with uniform properties in axes except the one aligned with the flow direction, where pressure and solute concentration in the permeate channel is uniform. When diffusion is assumed to vary only with pressure, the following equations describe the bulk flow rate F (m³/s), pressure P (Pa), and concentration C_F^B (mol/L) in the feed channel [19]:

$$F(x) = F_i - \frac{1}{\sinh \phi} (F_i \sinh(\phi(1 - \frac{x}{L})) + F_o \sinh \frac{\phi x}{L}) \quad (2.28)$$

$$P(x) = P_i - \frac{bL}{\phi \sinh \phi} (F_o (\cosh \frac{\phi x}{L} - 1) - F_i (\cosh(\phi(1 - \frac{x}{L})) - \cosh \phi)) \quad (2.29)$$

$$C_F^B = C_{Fi}^B + \frac{F_i(C_{Fi}^B - C_P)}{F(x)} \quad (2.30)$$

The subscripts i and o denote "inlet" and "outlet", and L (m) denotes the length of the RO module. The uniform permeate solute concentration is C_P . In these equations, the dimensionless coefficient ϕ is expressed as [19]:

$$\phi = L \sqrt{\frac{wbA_w}{1 + A_w(\frac{R_g}{B_s})TC_P}} \quad (2.31)$$

In the above, w (m) is the width of the rectangular feed channel, equivalent to h in Figure 2.3. While the assumptions that facilitate this analytical solution may not always hold true, the trends described (decreasing temperature and pressure as well as increasing concentration along the length of the module) are qualitatively useful. The decreasing pressure and increasing concentration are especially noteworthy, as both of these facilitate transient cavitation [32, 39, 40]. Numerical solutions relaxing the assumptions used can also be developed.

These models serve to effectively model the variation in bulk parameters along the length of SWRO modules, which plays an important role in the modelling of ultrasonic effects within SWRO modules.

2.5 Ultrasonic Fouling Mitigation

Ultrasonic Fouling Mitigation (UFM) is a technique wherein membrane filtration modules are exposed to high intensity sonification at a frequency beyond 20 kHz [14]. Under the correct conditions, sonification can produce the rapid expansion and violent collapse of microscopic bubbles within a fluid medium, a phenomenon known as inertial cavitation [41]. The violent collapse of these bubbles produces flow effects that are capable of scouring surfaces, allowing ultrasonic cavitation to have a restorative effect on filtration membrane performance [14].

While UFM has shown promising experimental results, it has proven difficult to upscale for industrial use [14]. This is largely due to the energy consumption associated with sonification, which is compounded by inefficiencies associated with the traditional means by which ultrasound is delivered to membrane modules [14]. Typically, the module is sonified via ultrasonic bath, a method that results in ultrasonic intensity reduction

of up to 90% between the emitters and the target [42]. When translating this technology from research to practice, the problem is additionally confounded by the overlapping membrane layers in SWRO modules [19]. Experimental studies involving ultrasonic fouling mitigation with SWRO modules are not available within the literature; however, multiple overlapping layers of membrane will likely have an attenuating effect on ultrasonic excitation, further limiting the effectiveness of ultrasonic bath-based excitation for industrial applications [14].

2.5.1 Cavitation Mechanics

Cavitation occurs when the thermodynamic equilibrium of a liquid medium is disturbed, causing bounded gaseous regions to change in volume or spontaneously develop [43]. The volumetric changes in these gaseous regions can occur due to [32]:

- Compression and expansion of gaseous regions;
- Dissolution and diffusion of gases into and out of solution within the liquid; and
- Partial evaporation of the liquid.

Several phenomena can disturb the thermodynamic equilibrium within a liquid medium such that cavitation occurs, including the introduction of thermal energy or chemically reactive substances; however, this work is specifically focused on cavitation generated by temporal and spatial pressure variations within a liquid medium [32]. There are two processes by which pressure fluctuations suitable for the generation of cavitation can occur [43]. Velocity gradients within a liquid medium can produce large variations in pressure within the medium, causing gaseous regions to expand in regions of low pressure and contract in regions of high pressure [43]. This process is known as hydrodynamic cavitation [43]. Alternatively, variations in the pressures applied to the boundaries of a fluid medium can cause temporal pressure variations within the liquid medium, resulting in corresponding expansion and contraction of gaseous regions therein [43]. It is this second process that occurs in response to ultrasonic signals when UFM is employed.

In order to understand cavitation in the context of UFM, the dynamics of individual gaseous bubbles responding to ultrasonic acoustic perturbations must first be described. These single-bubble cavitation dynamics models can then be used to estimate the net transfer of energy from the acoustic wave to the liquid during a harmonic cycle, which can then be used to describe the attenuation of the acoustic waves within the fluid medium. Combining these two models allows the acoustic pressure amplitude, and corresponding cavitation phenomena, to be estimated throughout a liquid medium undergoing sonification.

2.5.1.1 Single-Bubble Cavitation Dynamics

Cavitation dynamics in response to a given periodic pressure fluctuation at a defined fluid boundary depend on the properties and concentrations of the constituents of the medium, as well as the conditions of the medium in the absence of pressure fluctuations. Analyzing the effects of all of these parameters simultaneously becomes overwhelming. Instead, some of these parameters can become latent variables within composite parameters that are assumed to remain constant in a broader analysis of a given scenario. Care must be taken to identify the appropriate composite parameters in order to confirm that they truly do

remain approximately constant in a given context. Using this approach, analytical models for the dynamics surrounding the formation and growth of a single cavitation bubble can be developed.

As shown in Figure 2.5b, there are three distinct forms of cavitation. In quasi-static cavitation, the size of gas bubbles within the liquid is such that equilibrium is almost achieved at the boundary of the bubble [41]. This model can be used to predict changes in bubble size in response to slow, small changes in pressure when fluid velocities at the boundary of the bubble are negligible. Stable cavitation refers to bubbles whose sizes change in relation to oscillating pressures, but whose radii remain in the stable region of the plot shown in Figure 2.5a for the entire range of pressure oscillations. In this stable region, velocity effects can no longer be neglected when modelling bubble dynamics. Bubble sizes will change over the course of a pressure cycle; however, the average size of a bubble taken over the period of a pressure cycle will remain constant as long as the pressure oscillations are purely periodic. The third form of cavitation is inertial cavitation [41]. Here, the pressure oscillations produce liquid pressures for which no equilibrium solution exists for bubble radii. Bubbles grow uncontrollably for the part of the pressure cycle where the liquid pressure is below the lower limit of equilibrium p_{Cr} as shown in Figure 2.5 [41]. This allows bubbles to grow from cycle to cycle, until they eventually reach an untenable size and implode [14]. It is this implosion that is of use in ultrasonic fouling mitigation [14].

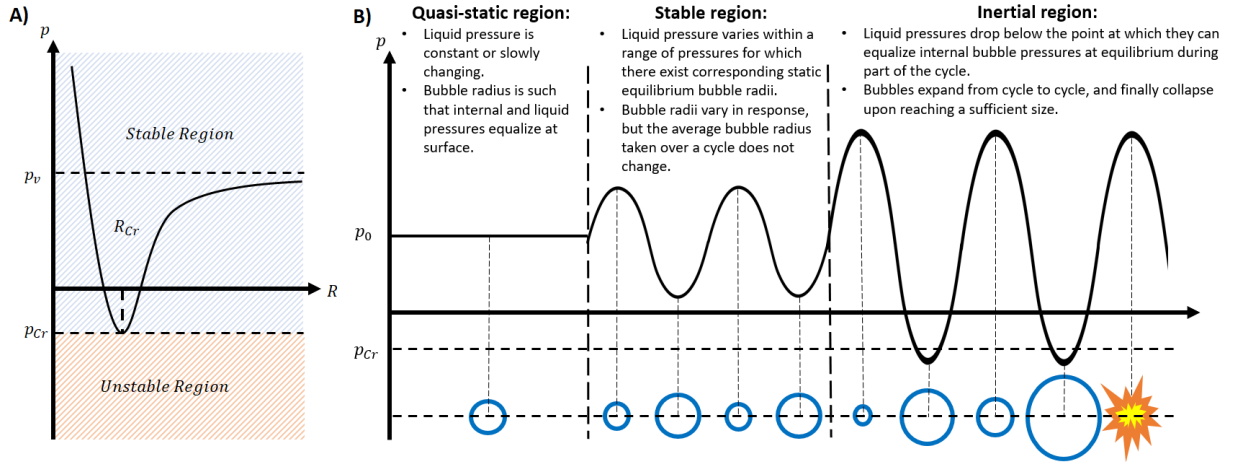


Figure 2.5: **A)**: Liquid pressure relative to its corresponding equilibrium bubble radius. As bubble radius increases, the corresponding equilibrium liquid pressure asymptotically approaches the vapour pressure p_v of the liquid. More importantly, there exists a pressure p_{Cr} below which no equilibrium bubble radius exists. The bubble radius at this point is R_{Cr} . **B)**: The three phases of cavitation in a fluid medium, described by pressure fluctuations and corresponding bubble size behaviours. The label p_0 represents the hydrostatic pressure.

2.5.1.1.1 Quasi-Static Single Bubble System

The simplest cavitation model is the quasi-static single bubble system model. By examining a bubble within a liquid medium, its internal pressure p_I (Pa) can be expressed as shown in equation (2.32) [41]:

$$p_I = p_L + \frac{2\sigma}{R} \quad (2.32)$$

Here, R (m) is the radius of the gas bubble, p_L (Pa) is the pressure within the medium, and σ (N/m)

is the surface tension at the surface of the bubble. Under static conditions, equation (2.32) can provide the expression for equilibrium conditions shown in equation (2.33):

$$p_{I0} = p_0 + \frac{2\sigma}{R_0} \quad (2.33)$$

Here, R_0 (m) is the radius of the gas bubble at equilibrium and p_0 (Pa) is the static pressure within the medium. The radius R_0 of the bubble at equilibrium is a composite parameter, containing within it information on the solubility of the gas, the temperature of the system, and the pressure within the system [32, 44]. The same is true of the surface tension σ , as it can vary due to the concentration of dissolved constituents and other impurities as well as temperature [39, 40].

The pressure within the bubble is also expressed by equation (2.34):

$$p_I = p_g + p_v \quad (2.34)$$

Here, p_g (Pa) and p_v (Pa) are the pressures produced by dissolved gas and vapour from the evaporation of the liquid medium within the bubble, respectively. The vapour pressure is often considered to be negligible in this simplified analysis [40]. However, a more general assumption is that p_v only varies with temperature, which renders it constant in this analysis [41].

Changes in the gas pressure within the bubble can be related to the bubble size through equation (2.35):

$$p_g = p_{g0} \left(\frac{R_0}{R} \right)^{3\gamma} \quad (2.35)$$

Here, γ is the polytropic index of the gas (which is equal to the ratio of the constant pressure and constant volume heat capacities under adiabatic conditions) and p_{g0} (Pa) is the gas pressure within the bubble under static equilibrium at p_0 . Assuming quasi-static conditions and conducting some algebra produces equation (2.36) [41]:

$$p_L = (p_0 - p_v + \frac{2\sigma}{R_0}) \left(\frac{R_0}{R} \right)^{3\gamma} + p_v - \frac{2\sigma}{R} \quad (2.36)$$

This provides the relationship between fluid pressure and bubble size in the general case. The isothermal limiting case ($\gamma = 1$) can be expressed as equation (2.37) [41]:

$$p_L = (p_0 - p_v + \frac{2\sigma}{R_0}) \left(\frac{R_0}{R} \right)^3 + p_v - \frac{2\sigma}{R} \quad (2.37)$$

2.5.1.1.2 Stable Single Bubble Dynamic System

Now that the basic equations governing the relationships between liquid and gas pressure in a quasi-static medium have been developed, the analysis can now consider the propagation of motion within the medium. First, the dynamics of a stable cavitation bubble (which oscillate for many acoustic cycles while maintaining the same mean characteristics) must be investigated [45]. This analysis starts with the derivation of the Rayleigh-Plesset equation shown as equation (2.38), a derivation of which can be found in Appendix A [46]:

$$R\ddot{R} + \frac{3\dot{R}^2}{2} = \frac{p_L(t) - p_0 - p(t)}{\rho} \quad (2.38)$$

Here, $p_L(t)$ (Pa) is the pressure at the boundary of the bubble. Dots over variables are used to denote their derivatives with respect to time. A dynamic form of equation (2.33) can be determined by including

the effects of viscous shear (with viscosity μ (kg/ms)). Since velocity in the field is exclusively radial and varies only with radius, the viscous shear can be expressed using equation (2.39) [47, 48]:

$$\sigma_{rr} = -2\mu \frac{\partial u_r}{\partial r} \quad (2.39)$$

Viscosity is another composite parameter, varying with fluid composition and temperature [39].

The derivation in Appendix B produces the dynamic form of equation (2.33) as shown in equation (2.40) [32, 45]:

$$p_I = p_L + \frac{4\mu\dot{R}}{R} + \frac{2\sigma}{R} \quad (2.40)$$

Rearranging equation (2.40) and substituting into equation (2.38) gives equation (2.63):

$$R\ddot{R} + \frac{3\dot{R}^2}{2} = \frac{1}{\rho}(p_I - \frac{4\mu\dot{R}}{R} - \frac{2\sigma}{R} - p_0 - p(t)) \quad (2.41)$$

Recalling equations (2.34) and (2.35), and acknowledging the implicit relationship for equilibrium gas pressure within the bubble p_{g0} within equation (2.36), equation (2.63) becomes equation (2.66):

$$R\ddot{R} + \frac{3\dot{R}^2}{2} = \frac{1}{\rho}((p_0 - p_v + \frac{2\sigma}{R_0})(\frac{R_0}{R})^{3\gamma} + p_v - \frac{4\mu\dot{R}}{R} - \frac{2\sigma}{R} - p_0 - p(t)) \quad (2.42)$$

When vapour pressures and viscous damping are neglected and $p(t) = P_A \sin(\omega t)$, this system oscillates at a natural frequency ω_r (1/s) defined by equation (2.43) [45]:

$$\omega_r^2 = \frac{1}{\rho R_0^2} (3\gamma(p_0 + \frac{2\sigma}{R_0}) - \frac{2\sigma}{R_0}) \quad (2.43)$$

2.5.1.1.3 Inertial Cavitation

The violent flow effects that are of relevance to UFM occur during inertial cavitation [14, 32]. The conditions that produce inertial cavitation are therefore of interest, as are the conditions produced by the collapse of an inertial cavitation bubble.

Understanding the onset of inertial cavitation requires a return to the quasi-static analysis. Differentiating equation (2.37) with respect to R gives equation (2.44):

$$\frac{dp_L}{dR} = -3(p_0 - p_v + \frac{2\sigma}{R_0}) \frac{R_0^3}{R^4} + \frac{2\sigma}{R^2} \quad (2.44)$$

Figure 2.5 A) shows that there exists a pressure below which there does not exist a stable radius for gas bubbles suspended within a liquid. Setting $\frac{dp_L}{dR}$ equal to zero returns a single admissible solution for the bubble radius R_{Cr} (m) at this pressure, which is given by equation (2.45):

$$R_{Cr} = R_0 \sqrt{\frac{3R_0}{2\sigma}(p_0 - p_v) + 3} \quad (2.45)$$

The pressure corresponding to equation (2.45) is calculated using equation (2.46):

$$p_{Cr} = p_v - \sqrt{\frac{32\sigma^3}{27R_0^2(R_0(p_0 - p_v) + 2\sigma)}} \quad (2.46)$$

The pressure expressed in equation (2.46) corresponds to the lowest liquid pressure at which the pressure within a cavitation bubble can be at equilibrium with its surroundings. Therefore, cavitation bubbles become unstable when the pressure drops below this threshold, leading to inertial cavitation. This pressure is therefore the threshold below which cavitation develops [41]. For approximation purposes, the vapour pressure p_v is often ignored, and surface tension effects are assumed to dominate the effects of external pressure ($p_\infty \ll \frac{2\sigma}{R_0}$). The result is equation (2.47):

$$p_{Cr} = -\sqrt{\frac{16}{27}} \frac{\sigma}{R_0} \quad (2.47)$$

For analysis of ultrasonic cavitation, it is necessary to know the magnitude of perturbation from the static pressure p_∞ (Pa) that is required to produce pressures lower than p_{Cr} (Pa). This perturbation will represent the minimum amplitude of a pressure wave passing through the fluid medium that will produce cavitation. Termed the Blake threshold (p_{Blake}), this is expressed using equation (2.48):

$$\begin{aligned} p_{Blake} &= p_0 - p_{Cr} \\ &= p_0 + \sqrt{\frac{16}{27}} \frac{\sigma}{R_0} \end{aligned} \quad (2.48)$$

It is well known that ultrasonic agitation of fluids raises their temperatures, and that inertial cavitation in particular is known for producing very high temperatures during bubble collapses, showing that acoustic cavitation cannot in general be considered to be isothermal [14, 45, 49–52]. Additionally, literature investigating cavitation in response to high frequency impulses, such as ultrasound, has demonstrated the importance of accounting for inertial effects, showing that the process is not truly quasi-static [32, 41, 46, 48, 49, 53]. Nevertheless, the Blake threshold has been shown to correlate reasonably well with experimental data investigating inertial cavitation brought on by ultrasonic excitation [49, 50, 53]. Therefore, it will also be considered as the criteria for the onset of inertial cavitation within this work.

The equations used to simulate cavitation dynamics presuppose a nominal bubble radius that a bubble will possess under static conditions. Experimentally validated literature on the subject has used a default bubble radius of 2 μm for air bubbles in water at ambient conditions, with a bubble density of $3.6 \times 10^{11} \text{ m}^{-3}$. In the research conducted throughout this thesis, bubbles are also assumed to be composed of air, but the pressure within the system is much higher than ambient pressure [14, 20]. Diffusion is neglected in the models used to approximate bubble dynamics, meaning that the molar quantity of air within the bubbles can be treated as a constant n regardless of system pressure. This constant can be found based on the values under ambient conditions by substituting equation (2.33) into the ideal gas law and solving as shown in equation (2.49):

$$n = \frac{P_0 4\pi R_0^3 + 8\pi\sigma R_0^2}{3R_g T_0} \quad (2.49)$$

Where T_0 and P_0 are the temperature and pressure at which R_0 has been reported in the literature, and R is the ideal gas constant. Bubble density N can then be calculated based on the molar concentration of air within the fluid medium. Since RO membranes admit the passage of dissolved gases, this concentration is considered to be constant along the length of the module. The actual size of the bubble at a given pressure comes from the solution of equation (2.49) for R_0 at differing values of P_0 and T_0 .

2.5.1.2 Attenuation

In a cavitation field, kinetic energy dissipates [44]. To predict the effectiveness of UFM, it is critical to understand how this dissipation will affect cavitation throughout the filtration module.

There is a fairly detailed mathematical analysis of the dynamics of waves passing through a bounded fluid volume in [44], the relevant parts of which the following section attempts to summarize. Assuming that only waves of a single frequency ω exist within the volume allows for the expression of the driving pressure $p_L(x, y, z, t)$ and velocity $\mathbf{V}(x, y, z, t)$ within the liquid medium in terms of oscillation amplitudes p_a and $\mathbf{V}_a$ as shown in equations (2.50) and (2.51):

$$p_L = p_a(x, y, z) \cos(\omega t) \quad (2.50)$$

$$\mathbf{V} = \mathbf{V}_a(x, y, z) \cos(\omega t) \quad (2.51)$$

Note that both $p_a(x, y, z)$ and $\mathbf{V}_a(x, y, z)$ are complex fields. Recognizing that wave intensity I is equal to $\Re(p|\mathbf{V}|)$, the synthesis shown in equation (2.52) can occur:

$$I = \Re(p_a|\mathbf{V}_a|) \cos^2(\omega t) \quad (2.52)$$

The average intensity at any point is then shown by equation (2.53):

$$I_{avg} = \frac{1}{2} \Re(p_a|\mathbf{V}_a|) \quad (2.53)$$

For a plane travelling wave, average ultrasonic intensity can be expressed as shown in equation (2.54):

$$I = \frac{p_a^2}{2\rho c} \quad (2.54)$$

If p_a and $\mathbf{V}_a$ are real and $\mathbf{V}_a$ is only non-zero in one direction (as is the case in a plane travelling wave) equation (2.53) becomes equation (2.55):

$$I = \frac{p_a V_a}{2} \quad (2.55)$$

Note that the variable expressing the velocity amplitude within the fluid is no longer bold, as it is treated as a scalar under these circumstances. The relationship shown in equation (2.56) between pressure and amplitude can then be constructed [43]:

$$p_a = \rho c V_a \quad (2.56)$$

Consider now a system wherein the fluid is sonified by a spatially uniform, oscillating boundary condition described by amplitudes p_s and $\mathbf{V}_s$ occurring on region $S_{Sonified}$ with unsonified boundaries $S_{Boundaries}$. If no dissipation occurs within the system, an energy balance can be constructed as shown in equation (2.57):

$$\iint_{S_{Sonified}} \frac{1}{2} \Re(p_s|\mathbf{V}_s|) \cdot dS_{Sonified} = \iint_{S_{Boundaries}} \frac{1}{2} \Re(p_a|\mathbf{V}_a|) \cdot dS_{Boundaries} \quad (2.57)$$

Dissipation can be approximated by defining a complex wave number k in terms of a real part k_r and attenuation parameter α introduced by the presence of bubbles as equation (2.58) [44]:

$$k = k_r + \alpha i \quad (2.58)$$

Adding this dissipation to equation (2.57) gives equation (2.59):

$$\iint_{S_{Sonified}} \frac{1}{2} \Re(p_s |\mathbf{V}_s|) \cdot dS_{Sonified} = \iint_{S_{Boundaries}} \frac{1}{2} \Re(p_a |\mathbf{V}_a|) \cdot dS_{Boundaries} + \iiint_V \alpha \frac{|p_a|^2}{\rho_L c_L} \quad (2.59)$$

Here, c_L is the speed of sound within the medium, and ρ_L is the density of the medium. Assuming now that one-dimensional, plane waves are entering and leaving a system of constant cross-sectional area A and length L in the axis along which the waves travel, equation (2.59) becomes equation (2.60):

$$\frac{p_a(0)^2}{2\rho c} A = \frac{p_a(L)^2}{2\rho c} A + \int_0^L \alpha \frac{p_a(x)^2}{\rho_L c_L} A dx \quad (2.60)$$

In the above, $p_a(0)$ refers to the pressure amplitude at point $x = 0$. Rearranging to solve for p_a at point L gives equation (2.61):

$$p_a(L) = \sqrt{p_a(0)^2 - 2\rho c \int_0^L \alpha \frac{p_a(x)^2}{\rho_L c_L} A dx} \quad (2.61)$$

When (2.61) is linearized for small $L = \Delta x$, the argument of the integral becomes effectively constant such that equation (2.62) holds true:

$$p_a(\Delta x) = \sqrt{p_a(0)^2 - 2\rho c \alpha \frac{p_a(0)^2}{\rho_L c_L} A \Delta x} \quad (2.62)$$

The determination of k in equation (2.58) requires a detailed investigation of the physical mechanisms by which kinetic energy dissipates within a cavitating system. In particular, linear approximations grossly underestimate wave energy attenuation due to inertial cavitation, which is of keen interest to this investigation [49]. An analysis accounting for the non-linear energy dissipation behaviours is contained within [49], and outlined below.

The Rayleigh-Plesset equation, used to describe bubble dynamics, is shown in equation (2.63) [32, 45–48]:

$$R\ddot{R} + \frac{3\dot{R}^2}{2} = \frac{1}{\rho}(p_I - \frac{4\mu\dot{R}}{R} - \frac{2\sigma}{R} - p_0 - p(t)) \quad (2.63)$$

Multiplying the expanded form of the Rayleigh-Plesset equation shown in equation (2.63) by the partial derivative of bubble volume with respect to time ($\frac{\partial V}{\partial t}$) produces equation (2.64) [49]:

$$\frac{\partial}{\partial t}(2\pi\rho_L R^3 \dot{R}^2 + 4\pi R^2 \sigma) = -16\pi\mu R \dot{R}^2 - p \frac{\partial V}{\partial t} + p_g \frac{\partial V}{\partial t} \quad (2.64)$$

Assuming periodic oscillation, a time average of equation (2.64) reduces to equation (2.65) [49]:

$$\langle -p \frac{\partial V}{\partial t} \rangle = \frac{1}{T} \int_0^T -p_g \frac{\partial V}{\partial t} dt + \frac{1}{T} \int_0^T 16\pi\mu_L R \dot{R}^2 dt \quad (2.65)$$

The two terms on the right hand side of the equation are the average power dissipation due to thermal and viscous factors over a cycle of period T , and are hereafter referred to as $L_{th} = \frac{1}{T} \int_0^T -p_g \frac{\partial V}{\partial t} dt$ and $L_v = \frac{1}{T} \int_0^T 16\pi\mu_L R \dot{R}^2 dt$. The numerical solution of these integrals can be found by solving the bubble dynamics equation expressed by equation (2.63) for a sinusoidal forcing pressure to give an approximation

of the energy losses associated with cavitation. Assuming polytropic conditions, equation (2.63) becomes equation (2.66):

$$R\ddot{R} + \frac{3\dot{R}^2}{2} = \frac{1}{\rho}((p_0 - p_v + \frac{2\sigma}{R_0})(\frac{R_0}{R})^{3\gamma} + p_v - \frac{4\mu\dot{R}}{R} - \frac{2\sigma}{R} - p_0 - p(t)) \quad (2.66)$$

It is critical to note here that phenomena such as water evaporation, gaseous diffusion, and chemical reactions between the various compounds contained within the water become important when considering inertial cavitation, thereby invalidating some of the assumptions used to develop the bubble dynamics model in equation (2.66) [49, 54–56]. To more accurately model inertial cavitation, a non-polytropic model for gas pressure accounting for diffusion of material and heat can be substituted into equation (2.63) in order to close the equation [49, 54–56]. However, development of such a model for gas pressure is itself a non-trivial pursuit, and renders the cavitation model sensitive to fluid domain composition parameters for which insufficient data exists in a SWRO context [54–56]. For this reason, detailed attenuation models developed in this work will only be able to reliably estimate attenuation within regions of the fluid medium that are not actively undergoing inertial cavitation. While this does impose limitations on the broader applicability of the attenuation models developed, the estimation of ultrasonic attenuation outside of the regions of the fluid medium undergoing inertial cavitation is ultimately an important part of the research presented within this thesis.

The Caflisch equations, which are governing equations for a liquid continuum containing bubbles subjected to pressure waves of arbitrary amplitude, are then utilized to develop an expression for wave energy dissipation [49]. They are expressed in terms of velocity and pressure fields within the continuum as equations (2.67) and (2.68) [57]:

$$\frac{1}{\rho_L c_L^2} \frac{\partial p}{\partial t} + \nabla \cdot \mathbf{V} = \frac{\partial \beta}{\partial t} \quad (2.67)$$

$$\rho_L \frac{\partial \mathbf{V}}{\partial t} = -\nabla p \quad (2.68)$$

In this equation, β is the fraction of the medium composed of bubbles, and can be expressed as equation (2.69) [49]:

$$\beta = N(x, y, z) \frac{4}{3} \pi R(x, y, z, t)^3 \quad (2.69)$$

Here, $N(x, y, z)$ is the bubble density at a point (x, y, z) in the continuum, and $R(x, y, z, t)$ is the radius of a bubble at that same point and the current instant in time t . Equations (2.67) and (2.68) can be combined to eliminate $\mathbf{V}$ as follows in equation (2.70) [57]:

$$\nabla^2 p = \frac{1}{c_L^2} \frac{\partial^2 p}{\partial t^2} - \rho_L \frac{\partial^2 \beta}{\partial t^2} \quad (2.70)$$

Linearizing equations (2.50) and (2.70) allows for the expressing of $p_a(x, y, z)$ in the form of the Helmholtz equation shown in equation (2.71):

$$\nabla^2 p_a + k^2 p_a = 0 \quad (2.71)$$

While equation (2.71) assumes linear oscillation, equation (2.65) only assumes periodic oscillation. As such, a formulation for α in terms of L_{th} and L_v can be developed using equation (2.71) [49]. To start

with, the pressure field p within the medium is defined as the sum of a mean value p_0 , the driving pressure p_L , and a term p_h accounting for polyharmonic pressure oscillations introduced by the nonlinearity of the system (whose frequencies will all be some multiple of the driving frequency ω) [49]. The antiderivative W of equation (2.50) is given by equation (2.72):

$$W = \frac{1}{\omega} p_a \sin(\omega t) \quad (2.72)$$

Taking a single-period time average of the product of equations (2.70) and (2.72) and recognizing the periodic nature of all properties gives equation (2.73):

$$\langle W \nabla^2 p \rangle = \frac{1}{c_L^2} \langle p_L \frac{\partial p}{\partial t} \rangle - \rho \langle p_L \frac{\partial \beta}{\partial t} \rangle \quad (2.73)$$

Deducing from the composition of p that $\langle W \nabla^2 p \rangle = \langle W \nabla^2 p_L \rangle$ and that $\langle p_L \frac{\partial p}{\partial t} \rangle = 0$, the remaining term $\langle p_L \frac{\partial \beta}{\partial t} \rangle$ is now considered. Again referring to the composition of p , it is clear that $\langle p_L \frac{\partial \beta}{\partial t} \rangle = \langle p \frac{\partial \beta}{\partial t} \rangle - \langle p_h \frac{\partial \beta}{\partial t} \rangle$. The authors of [49] decided to neglect $p_h \frac{\partial \beta}{\partial t}$, a decision justified by experimental data indicating that its effects are an order of magnitude less than those of $\langle p_L \frac{\partial \beta}{\partial t} \rangle$. This simplification of equation (2.73) produces equation (2.74):

$$\langle W \nabla^2 p \rangle = \langle p \frac{\partial \beta}{\partial t} \rangle \quad (2.74)$$

This allows for an equivalence to be drawn with equation (2.65) as shown in equation (2.75):

$$\langle W \nabla^2 p \rangle = \rho_L N (L_{th} + L_v) \quad (2.75)$$

In complex form, equation (2.72) can be given as equation (2.76) [49]:

$$W = \frac{1}{2i\omega} (p_a e^{i\omega t} - \bar{p}_a e^{-i\omega t}) \quad (2.76)$$

Here, the overline denotes the complex conjugate. Substituting in equations (2.50) and (2.72) gives equation (2.77):

$$\frac{1}{4\omega} (\bar{p}_a \nabla^2 p_a - p_a \nabla^2 \bar{p}_a) = \rho_L N (L_{th} + L_v) \quad (2.77)$$

A division of both sides by $|p_a|^2$ gives equation (2.78) [49]:

$$\Im\left(\frac{\nabla^2 p_a}{|p_a|}\right) = -\frac{2\omega \rho_L N (L_{th} + L_v)}{|p_a|^2} \quad (2.78)$$

Which, returning to the relationship between p_a and k expressed in equation (2.71), yields equation (2.79):

$$\Im(k^2) = -\frac{2\omega \rho_L N (L_{th} + L_v)}{|p_a|^2} \quad (2.79)$$

Coupling equation (2.79) with an expression for $\Re(k^2)$ and the definition of k allows for a derivation of α that can be utilized with equation (2.59) in order to successfully capture the large energy dissipations due to non-linear behaviour of inertial cavitation. An example of such an expression used in the literature is the linear dispersion relationship in equation (2.80) [49]:

$$\Re(k^2) = \frac{\omega^2}{C_L^2} + \frac{4\pi R_0 \omega^2 N}{\omega_r^2 - \omega^2} \quad (2.80)$$

Recalling equation (2.58) allows the following relationships to be expressed by equations (2.81)-(2.83):

$$k^2 = k_r^2 - \alpha^2 + 2\alpha k_r i \quad (2.81)$$

$$\Re(k^2) = k_r^2 - \alpha^2 \quad (2.82)$$

$$\Im(k^2) = 2\alpha k_r i \quad (2.83)$$

A quadratic relationship can be established and solved for α^2 as expressed by equation (2.84):

$$\alpha^2 = \frac{-\Re(k^2) \pm \sqrt{(\Re(k^2))^2 + \Im(k^2)^2}}{2} \quad (2.84)$$

The value determined for α can be substituted into the discretization in equation (2.62) to complete this equation.

The value for α calculated in equation (2.84) applies to ultrasonic attenuation within the fluid volume in the SWRO module feed channel. However, the feed channel also contains a solid feed spacer whose effects on ultrasonic attenuation should not be neglected. To account for these effects, the attenuation per unit length α_S (dB/m) is calculated for the desired frequency using the formula shown in equation (2.85) [58]:

$$\alpha_L = k(f)^n \quad (2.85)$$

Where k is a constant, f is the frequency of the applied sonification, and n is the material index of the solid. The attenuation in dB can then be calculated by multiplying α_L by the same Δx used in equation (2.62). From there, the change ΔI_S in W/m² can be calculated from the initial ultrasonic intensity I_0 using equation (2.86):

$$\Delta I_S = I_0 - I_0(10^{-\frac{\alpha_L \Delta x}{10}}) \quad (2.86)$$

The effects of feed spacer attenuation on the pressure amplitude reduction for a length Δx can be incorporated as a modification to equation (2.62) by a weighted average using solid and liquid volume fractions V_S and V_L as shown by equation (2.87):

$$p_a(\Delta x) = \sqrt{p_a(0)^2 - V_L 2\rho c \alpha \frac{p_a(0)^2}{\rho_L c_L} A \Delta x - V_S \Delta I} \quad (2.87)$$

Equation (2.87) can be generalized to a discrete space of N elements as shown in equation (2.88):

$$p_a(i) = \sqrt{(p_a(i-1))^2 - V_L 2\rho c \alpha \frac{(p_a(i-1))^2}{\rho_L c_L} A \Delta x - V_S (I(i-1) - I(i-1)(10^{-\frac{\alpha_L \Delta x}{10}}))} \quad (2.88)$$

2.5.2 Sonification

Fluid media are typically sonified by transferring vibrations from some form of electromechanical system known as an ultrasonic transducer to the fluid [14, 15, 42, 59]. Typically, the ultrasonic transducer uses piezoelectric materials to convert periodic electric fields into pressure waves through strain induced within the materials by the changing electric fields [60–63]. These waves are then transferred to the fluid via mechanisms such as horns or baths [14]. Ultrasonic baths are typical within literature on UFM, but exhibit poor energy efficiency, motivating the decision to investigate ultrasonic horns in this research [14, 42].

2.5.2.1 Vibrations in Solids

Displacement within an isotropic solid body in response to one-dimensional, longitudinal pressure waves can be modelled using the differential equation shown in equation (2.89) [61]:

$$\frac{\partial(A_c \sigma)}{\partial t^2} = A \rho \frac{\partial^2 \mu}{\partial t^2} dx \quad (2.89)$$

Here, σ (N/m²) is the stress at a point x along the length of the body, A_c (m²) is the cross-sectional area of the body, μ (m) is the displacement of the particles at position x , and E (Pa) is the elastic modulus of the body. In the case of one-dimensional, longitudinal, harmonic vibrations in members of uniform or conical cross-section, equation (2.89) can be reduced to the second order ordinary differential equation for the displacement amplitude u (m) shown in equation (2.90) [64]:

$$\frac{d^2 u}{dx^2} + \frac{1}{A_c} \frac{dA_c}{dx} \frac{du}{dx} + k u^2 = 0 \quad (2.90)$$

In equation (2.90), k is the wave number and is expressed in terms of the longitudinal speed of sound c (m/s) and the angular vibration frequency ω by equation (2.91) [64]:

$$k = \frac{\omega}{c} \quad (2.91)$$

The speed of sound c within a vibrating column can be calculated using equation (2.92) [62]:

$$c = \sqrt{\frac{E}{\rho}} \quad (2.92)$$

The wavelength λ (m) of a given cyclic frequency f to be calculated using equation (2.93):

$$\lambda = \frac{c}{f} \quad (2.93)$$

The general solution of equation (2.90) can express the displacement of particles undergoing longitudinal vibration within a column of constant cross-section with respect to position x as shown in equation (2.94) [64]:

$$u = A \cos(kx) + B \sin(kx) \quad (2.94)$$

In the above, A and B are constants to be solved for via boundary conditions, k is the wave number of the column material, and x is the position along the length of the column with respect to some origin where $x = 0$. If the cross-section of the column is conical, the general solution to (2.90) becomes equation (2.95) [64]:

$$u = S(A \cos(kx) + B \sin(kx)) \quad (2.95)$$

Here, S is an expression of the diameter d (m) of the column at point x outlined in equation (2.96) [64]:

$$S = \frac{2}{d} \quad (2.96)$$

Boundary conditions at the terminal faces of vibrating columns can be expressed in terms of both displacement u and force F (N) at these faces [65]. Force can be related to the spatial derivative of displacement as shown in equation (2.97) [64]:

$$F = EA \frac{du}{dx} \quad (2.97)$$

This condition can be used to constrain the derivatives of (2.94) and (2.95) as shown in equations (2.98) and (2.99), respectively:

$$\frac{du}{dx} = -Ak \sin(kx) + Bk \cos(kx) \quad (2.98)$$

$$\frac{du}{dx} = S(-Ak \sin(kx) + Bk \cos(kx)) + \frac{dS}{dx}(A \cos(kx) + B \sin(kx)) \quad (2.99)$$

Equations (2.94) and (2.95) are sinusoidal in nature; therefore, there are points along the length of the system described at which the longitudinal displacement within a body will be equal to 0 at all times, as well as points where the displacement amplitude reaches a local maximum or minimum. Regions that remain stationary are termed nodes, while regions that reach a local maximum or minimum displacement amplitude are termed antinodes [66]. Nodes and antinodes are separated by half a wavelength [62, 66]. Since nodes and antinodes represent critical points in terms of harmonic displacement amplitude, controlling the location of these points is an important part of designing systems for fluid sonification.

2.5.2.2 Ultrasonic Transducers

Ultrasonic transducers convert between electrical signals and mechanical frequencies with cyclic frequencies greater than 20 kHz [14, 65]. They rely on piezoelectric materials, within which gradients in electric charge are coupled to mechanical strain [14]. Power ultrasonic transducers are specifically meant to produce mechanical vibrations from electrical signals, and are used in UFM to generate the ultrasonic vibrations by which ultrasonic cavitation is induced [14, 60, 65].

The form of transducer used in this research is known as a Langevin transducer, and is shown in Figure 2.6 [60, 65]. The Langevin transducer is the most common power ultrasonic transducer available [60, 65, 67]. The key components of a Langevin ultrasonic transducer are described below:

- **Piezoelectric Disks:** These components are responsible for converting the electrical signal provided to the transducer into motion [65]. They are typically aligned with opposing polarities such that they can share a common ground electrode at their interface [65].
- **Front Mass:** This part of the transducer transmits the vibrations generated by the piezoelectric disks to the system to which the ultrasonic transducer is attached [65].
- **Back Mass:** This provides an inertial balance for the front mass such that the transducer nominally oscillates around the piezoelectric disks [65]. It is usually made of a denser material than the front mass [65].
- **Clamp Bolt:** Piezoelectric materials are ceramics that are typically weak in tension [65]. Because of this, they must be pre-stressed in compression to avoid reaching their tensile limit when producing high-amplitude vibrations [65].

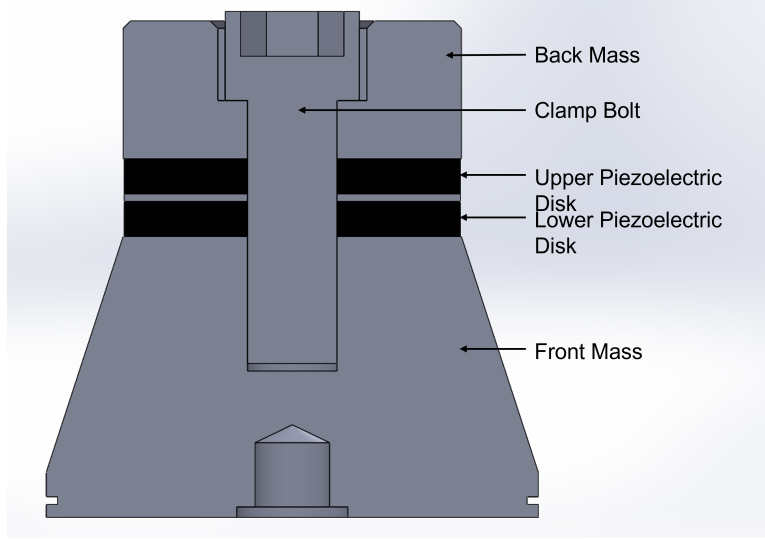


Figure 2.6: Cross-section of a typical Langevin ultrasonic transducer.

2.5.2.3 Ultrasonic Horns

Ultrasonic horns are commonly attached to ultrasonic transducers to assist in transferring the mechanical vibrations generated by the transducer to the object or medium within which the vibrations are to be absorbed [62, 64, 65]. Often, the surface area of the free end of the horn will be less than the transducer output surface area to increase the vibration amplitude at the output [64]. The ratio of input to output displacement amplitude is described as the amplitude gain, denoted as G . To assess the effectiveness of the design of a horn, the amplitude gain can be adjusted with respect to the ratio between the transducer output area and the free end, as shown in equation (2.100) [64]:

$$G_a = G \frac{A_f}{A_t} = \frac{u_f}{u_t} \frac{A_f}{A_t} \quad (2.100)$$

In equation (2.100), G_a is the adjusted gain, u_i (m) and A_i (m^2) are the displacement amplitude and cross sectional area of the horn at location i , and subscripts t and f denote the output end of the transducer and the free end of the horn, respectively.

Transducers are designed to resonate at their specified operating frequencies with an antinode at their emitter [62, 64, 65]. Therefore, ultrasonic horns made out of a homogeneous material typically have a length of half the wavelength of the operating frequency within their material [62, 64, 65].

2.6 Summary and Research Needs

This chapter represents a review of the relevant literature describing the fundamentals of RO, membrane fouling, ultrasonic cavitation, and vibrations in solids as they relate to the investigation of UFM. Attempts to investigate the prospective effectiveness of UFM on SWRO modules were not found within the literature, nor were any attempts to improve the energy efficiency of UFM. The research within this thesis sought therefore to fill this gap in the literature by designing and simulating UFM technologies with enhanced energy efficiency and applicability to industrial-scale RO applications.

Chapter 3

Design, Simulation and Modelling Towards the Novel Ultrasonic Horn Design

3.1 Introduction

First, the principles outlined in the previous chapter were used to define the qualitative features of the sonification system to be further developed in this thesis. Numerical modelling and simulation techniques were then used to defend the theoretical viability of UFM for SWRO systems in the context of the hypothetical apparatus, and to inform the design of the experiments and the apparatus to be used in experimental investigations. The modelling work associated with this investigation can be separated into three distinct efforts: first, the modelling of the temperature distributions expected within SWRO modules undergoing sonification; second, the prediction of inertial cavitation onset location within SWRO modules under varying inlet conditions; and third, the efficiency optimization of the novel ultrasonic horn using Finite Element Analysis (FEA). The following sections will discuss each investigation in detail, including their findings and contribution to the broader work.

3.2 Sonification System

The literature makes it clear that the scalability of UFM is limited by the tendency of the membrane housing to prevent ultrasonic energy from reaching its intended target [14, 42]. The flat-sheet membrane housings, which include pressure vessels, have already been demonstrated to attenuate ultrasound too rapidly for effective UFM at scale [14, 42]. Researchers have also hypothesized that overlapping membrane windings, such as those found in the Spiral-wound membrane elements of interest in this work, would also contribute further to this rapid attenuation of the ultrasonic energy [14]. In order to counteract this effect, the ultrasonic apparatus investigated within this research has two distinct features. Firstly, rather than submerging the membrane module in a sonified body of water (ultrasonic bath), the emitter itself is immersed within the membrane pressure vessel in order to reduce attenuation of the ultrasound. Secondly, the ultrasonic emitter is aligned axially with the feed channel of the membrane module, such that the ultrasonic waves need not pass through the membrane windings or the membrane housing in order to reach any part of the feed channel. The sonification apparatus does not interfere with RO module operation as designed, allowing it to be installed in existing RO systems for online membrane cleaning purposes. The diagram shown in Figure 3.1 illustrates the difference between the conventional ultrasonic baths used in the majority of the studies reviewed in [14] and the novel orientation of the ultrasonic emitter developed in this research.

3.3 Temperature Distribution Modelling

The following section contains material that has been published previously in the journal “Desalination” (full citation: L. Horrigan and M. Freire-Gormaly. “Modelling the effects of ultrasonic sonification on reverse osmosis feed channel temperature”. In: Desalination 521.1 (2022). DOI: <https://doi.org/10.1016/j.desal.2021.115332>). It has been reproduced here in accordance with the rights afforded to authors by the publisher of “Desalination”, Elsevier [68].

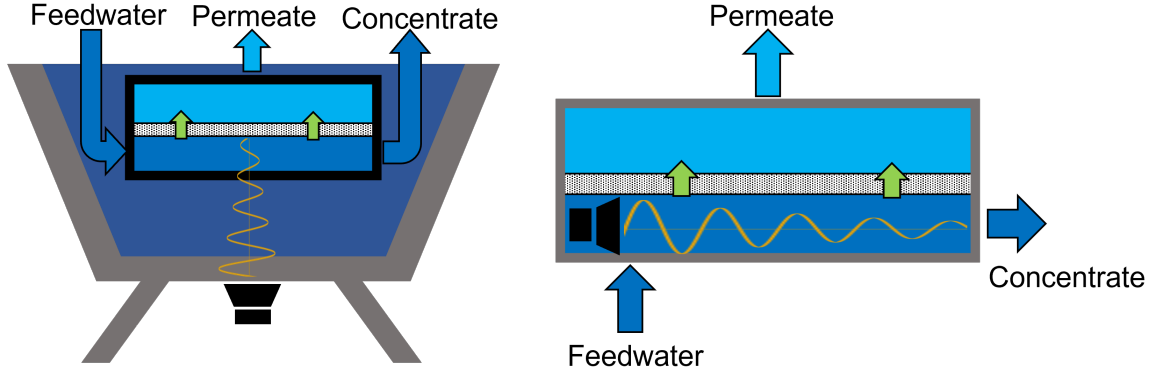


Figure 3.1: Left: Propagation perpendicular to membrane surfaces from outside of the module via ultrasonic bath, as is typically done in current UFM research. Right: novel apparatus for propagation of ultrasound axially within the module. Immersion of the ultrasonic emitter avoids attenuation from module structural components, providing an opportunity for improved energy efficiency. In SWRO configurations, axial sonification can prevent attenuation effects caused by the membranes themselves, improving the radial uniformity and efficiency of membrane sonification.

One of the drawbacks of ultrasonic baths, the primary technology used for UFM in research, is energy inefficiency in this application [14, 42]. In order to argue the merits of the proposed immersed horn approach in comparison to ultrasonic baths, a measure of its energy efficiency would be useful. Additionally, elevated temperatures can negatively impact membrane filtration performance by decreasing membrane permeability and encouraging certain fouling modes [19, 69]. To investigate these potential drawbacks, numerical models of the temperature distribution within a standard SWRO subjected to sonification were developed, and a proposed instrumentation system by which these models could be used to estimate the energy efficiency of the sonification approach was outlined.

3.3.1 Mathematical Model

The following section outlines the various components of the mathematical models developed to predict temperature distributions within the RO module.

3.3.1.1 System Description

Consider a rectangular flow channel with width w (m), thickness t_f (m) and length L (m), where the bulk fluid flow is in a direction perpendicular to the plane formed by w and t_f . Such a channel is illustrated in Figure 3.2. The walls dimensionally described by t_f are perfectly thermally insulated and impermeable. One wall described by w is a permeable membrane, allowing water to pass through it with a flux of J_v (m/s). The channel into which the permeate water passes is considered to be perfectly thermally insulated and is sealed at one end. The other wall described by w is impermeable, but conducts heat according to $q = \frac{T(x) - T_{ambient}}{r_{eq}}$; here, q (W/m²) is the heat flux per unit area, $T(x)$ (K) is the temperature within the flow channel at distance x from the inlet, $T_{ambient}$ (K) is the temperature outside of the system, and r_{eq} (K/m²W) is the thermal resistance per unit area of the wall. One example of the formulation of this thermal resistance could be a combination of conductive resistance through the wall (described by thickness t_{wall} (m) and thermal

conductivity k_{wall} (W/mK)) and convective heat transfer between the outer surface of the wall and the ambient air (described by convection coefficient h_w (W/m²K)). Temperature gradients within the fluid in any direction other than that of flow are neglected, as are the effects of viscous friction upon flow behaviours near walls; that is to say, temperature $T(x)$ and flow rate $F(x)$ at a distance x from the inlet are considered to be uniform in the wt_f plane. This model endeavours to determine $T(x)$ in terms of the inlet temperature of the water, the flow rate F (m³/s), the pressure P (Pa), and the solute concentration C_s at the inlet of the flow channel, as well as a function $U(x)$ (W/m³) describing the conversion of ultrasonic energy into heat within the flow channel. Given the shape of $U(x)$, this temperature gradient prediction will allow estimation of its parameters, allowing approximation of ultrasonic intensity within the flow channel. The relationships used to couple J_v and $F(x)$ are established in equations (2.6), (2.7), and (2.8).

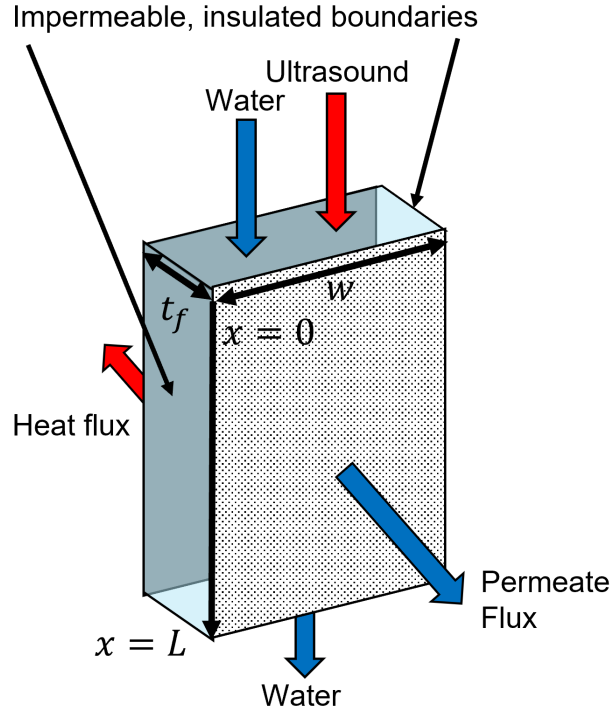


Figure 3.2: A visualization of the system used to develop the mathematical temperature distribution models.

3.3.1.2 Ultrasonic Intensity Formulation

Ultrasonic attenuation depends on the cavitation regime, which is itself coupled to the heat and mass transfer problems [49]. However, the solution of this problem remains beyond the scope of investigation, so an analytical approximation for the ultrasonic attenuation was developed. Literature suggests that ultrasonic intensity decays roughly exponentially with distance from its emitter in fluid media [70]. Therefore, the general form of $U(x)$ will be assumed to be an exponential described as $U(x) = \xi \beta I_0 e^{(-\lambda x)}$; here, I_0 describes the intensity of ultrasonic energy in W/m² at the emitter surface, ξ is a dimensionless efficiency coefficient describing the ratio of energy absorbed by the water to total power attenuation, β (m⁻¹) is a constant

describing total ultrasonic intensity attenuation per unit length, and λ (m^{-1}) is a constant included to describe the shape of exponential decay of the ultrasonic intensity curve. The resulting units are W/m^3 ; therefore, this function can be treated as an expression of thermal energy generation density. The ultrasonic intensity $I(x) = I_0 e^{(-\lambda x)}$ is measurable at the inlet ($x = 0$) and outlet ($x = L$) of the flow channel, which allows for the construction of the equation $\lambda = -\ln(\frac{I(L)}{I_0})$.

To determine β , an energy balance can be constructed. The power emitted from the ultrasonic transducer must eventually be absorbed by the environment; as such, equation (3.1) can be expressed as:

$$P_{emitter} = \int_0^\infty \beta w t_f I_0 e^{(-\lambda x)} dx \quad (3.1)$$

Integrating and solving for β gives equation (3.2):

$$\beta = \frac{P_{emitter} \lambda}{I_0 w t_f} \quad (3.2)$$

Initial intensity I_0 and emitter power $P_{emitter}$ are related through the channel cross-sectional area by equation (3.3):

$$I_0 = \frac{P_{emitter}}{w t_f} \quad (3.3)$$

Therefore, equation (3.4) can be produced:

$$\beta = \lambda \quad (3.4)$$

This gives the thermal energy generation function described in equation (3.5):

$$U(x) = \xi \lambda I_0 e^{(-\lambda x)} \quad (3.5)$$

The above analysis can also be used to estimate the maximum temperature attainable in the system, by assessing the limit of power absorbed by the system as λ approaches infinity, assuming perfect conversion of ultrasonic energy to heat within the fluid ($\xi = 1$), and neglecting both permeate and heat flux. To assess the maximum temperature attainable in the system, the analysis starts with the integral shown in equation (3.6):

$$P_{absorbed} = \int_0^L w t_f \lambda I_0 e^{(-\lambda x)} dx \quad (3.6)$$

Evaluating the integral gives equation (3.7):

$$P_{absorbed} = -w t_f I_0 (e^{(-\lambda L)} - 1) \quad (3.7)$$

The limit of equation (3.7) as λ approaches infinity is expressed in equation (3.8):

$$\begin{aligned} P_{absorbed} &= w t_f I_0 \\ &= P_{emitter} \end{aligned} \quad (3.8)$$

Assuming steady-state conditions in the time domain and neglecting heat and permeate flux, the maximum bulk temperature increase must therefore be constrained by equation (3.9):

$$\Delta T = \frac{P_{emitter}}{F \rho c} \quad (3.9)$$

In equation (3.9), F is the flow rate through the system which, when permeate flux is neglected, will remain constant across the length of the channel. The parameters ρ and c are the density and specific heat capacity of water, respectively.

In the system outlined above, a method for the determination of ξ is sufficient to allow for calorimetric estimation of ultrasonic energy absorption in a dynamic fluid medium with steady-state flow properties. This can be found by relating $T(L)$ to ξ .

3.3.1.3 Energy Balance

Under steady-state conditions, an energy balance within a control volume such as that shown within Figure 3.2 comprising the entire area of the flow channel and running from the inlet to a distance x along the length of the channel can be constructed in the form of equation (3.10):

$$\begin{aligned} wt_f \lambda \int_0^x \xi I_0 e^{(-\lambda a)} da - c\rho(F(x)T(x) - F(0)T(0)) - c\rho \int_0^x T(a)wJ_v(a)da \\ - \frac{w}{r_{eq}} \int_0^x (T(a) - T_{ambient})da + k_{water}(\frac{dT(x)}{dx} - \frac{dT(0)}{dx}) = 0 \end{aligned} \quad (3.10)$$

The terms above are described in the order they appear as follows:

- Energy introduced to the system by ultrasonic excitation.
- The difference between thermal energy leaving and entering the system due to axial flow.
- Energy leaving the system due to diffusion through the membrane.
- Energy leaving the system through heat transfer to the ambient environment.
- The difference between energy entering and leaving the system due to thermal conduction within the medium at the ends of the flow channel.

Differentiating with respect to x gives equation (3.11):

$$\begin{aligned} wt_f \lambda \xi I_0 e^{(-\lambda x)} - c\rho(F(x)\frac{dT(x)}{dx} + T(x)\frac{dF(x)}{dx}) - c\rho T(x)wJ_v(x) \\ - \frac{w(T(x) - T_{ambient})}{r_{eq}} + k_{water}(\frac{d^2T(x)}{dx^2} - \frac{d^2T(0)}{dx^2}) = 0 \end{aligned} \quad (3.11)$$

Since $T_{ambient}$ is a known constant, substituting $\Delta T(x) = T(x) - T_{ambient}$ simplifies the equation without removing any information from it. This, along with the substitution of equation (2.8), produces equation (3.12):

$$wt_f \lambda \xi I_0 e^{(-\lambda x)} - c\rho(F(x)\frac{dT(x)}{dx} + T(x)\frac{dF(x)}{dx}) + c\rho T(x)\frac{dF(x)}{dx} - \frac{w\Delta T(x)}{r_{eq}} + k_{water}\frac{d^2T(x)}{dx^2} = 0 \quad (3.12)$$

Simplifying and rearranging for $\frac{dT(x)}{dx}$ gives equation (3.13):

$$\frac{dT(x)}{dx} = \frac{k_{water}}{c\rho F(x)} \frac{d^2T(x)}{dx^2} + \frac{wt_f \lambda \xi I_0 e^{(-\lambda x)}}{c\rho F(x)} - \frac{w\Delta T(x)}{c\rho F(x)r_{eq}} \quad (3.13)$$

To approximate this formula, $\Delta T(x)$ is assumed to be linear over small intervals Δx . This allows for the approximation $\Delta T(x) \approx \Delta x \sum_{i=1}^N D_i + \Delta T(0)$, where N is the number of intervals such that $\Delta x = \frac{L}{N}$. Expressing equation (3.13) in terms of this approximation gives equation (3.14):

$$D_i \approx \frac{wt_f r_{eq} \xi \lambda I_0 e^{(-\lambda i \Delta x)} - w \Delta x \sum_{j=1}^{i-1} D_j - w \Delta T(0)}{c \rho F(i \Delta x) r_{eq}} \quad (3.14)$$

The formula for $\Delta T(x)$ then becomes equation (3.15):

$$\begin{aligned} \Delta T(x) &= \Delta T(N \Delta x) \\ &\approx \Delta x \sum_{i=1}^N \left(\frac{wt_f r_{eq} \xi \lambda I_0 e^{(-\lambda i \Delta x)} - w \Delta x \sum_{j=1}^{i-1} D_j - w \Delta T(0)}{c \rho F(i \Delta x) r_{eq}} \right) \end{aligned} \quad (3.15)$$

To simplify notation, the substitutions in equations (3.16), (3.17), and (3.18) were made as follows:

$$a_i = t_f r_{eq} \xi \lambda I_0 e^{(-\lambda i \Delta x)} - \Delta T(0) \quad (3.16)$$

$$B_i = \frac{w}{c \rho r_{eq}} \quad (3.17)$$

$$F_i = F(i \Delta x) \quad (3.18)$$

If the flow rate can be assumed to be independent of temperature, equation (3.19) can be developed:

$$D_i \approx B_i \frac{1}{F_i} (a_i) - \Delta x (B_i)^2 \frac{1}{F_i} \sum_{j=0}^{i-1} \frac{a_j}{F_j} + \frac{1}{F_i} \sum_{k=2}^{i-1} (-\Delta x)^k (B_i)^{(k+1)} \sum_{m=1}^{i-k+1} \frac{a_m \sum_{y=m+1}^{i-1} \frac{\prod_{z=m+1}^{i-1} F_z}{F_y}}{\prod_{p=m}^{i-1} F_p} \quad (3.19)$$

In this case, $\Delta T(N \Delta x)$ becomes equation (3.20):

$$\Delta T(N \Delta x) \approx \Delta x \sum_{i=0}^N \left(B_i \frac{1}{F_i} (a_i) - \Delta x (B_i)^2 \frac{1}{F_i} \sum_{j=0}^{i-1} \frac{a_j}{F_j} + \frac{1}{F_i} \sum_{k=2}^{i-1} (-\Delta x)^k (B_i)^{(k+1)} \sum_{m=1}^{i-k+1} \frac{a_m \sum_{y=m+1}^{i-1} \frac{\prod_{z=m+1}^{i-1} F_z}{F_y}}{\prod_{p=m}^{i-1} F_p} \right) \quad (3.20)$$

3.3.1.4 Temperature Independent Flow Modelling

The mass conservation expression in equation (2.6) yields equation (3.21) which describes the flow rate at a distance x from the inlet:

$$F(x) = F(0) - w \int_0^X J_v(a) da \quad (3.21)$$

The literature contains a derivation and experimental validation of an analytical model for bulk flow parameters within a flow channel possessing the characteristics discussed in [19], which uses equation (2.1) to describe water flux through a RO membrane. This model also assumes the applicability of Darcy's law as described in equation (2.10).

$$\frac{d^2 F(x)}{dx^2} = -w \frac{dJ_v(x)}{dx} \quad (3.22)$$

Differentiating equation (2.1) with the constant temperature assumption gives equation (3.23):

$$\frac{dJ_v(x)}{dx} = \frac{A_w}{1 + (\frac{A_w R_g}{B_s})T(0)C_p} \frac{dP(x)}{dx} \quad (3.23)$$

Combining equations (2.10), (3.22), and (3.23) gives equation (3.24):

$$\frac{d^2 F(x)}{dx^2} = \frac{wbA_w}{1 + (\frac{A_w R_g}{B_s})T(0)C_p} F(x) \quad (3.24)$$

Putting the equation in terms of pressure instead of flow rate gives equation (3.25):

$$\frac{d^3 P(x)}{dx^3} = \frac{wbA_w}{1 + (\frac{A_w R_g}{B_s})T(0)C_p} \frac{dP(x)}{dx} \quad (3.25)$$

To simplify the solution of this equation, a coefficient ϕ is defined by equation (3.26):

$$\phi = L \sqrt{\frac{wbA_w}{1 + (\frac{A_w R_g}{B_s})T(0)C_p}} \quad (3.26)$$

This simplifies equation (3.25) to equation (3.27):

$$\frac{d^3 P(x)}{dx^3} = \frac{\phi^2}{L^2} \frac{dP(x)}{dx} \quad (3.27)$$

The pressure and flow rate are known at the inlet, and the flux at the inlet can be calculated from the pressure. As such, the boundary conditions shown in equations (3.28), (3.29), and (3.30) can be applied:

$$P(0) = P_i \quad (3.28)$$

$$\frac{dP(0)}{dx} = -bF(0) \quad (3.29)$$

$$\frac{d^2 P(x)}{dx^2} = -b \frac{dF(0)}{dx} = bwJ_v(0) = \frac{A_w P_i}{1 + (\frac{A_w R_g}{B_s})T(0)C_p} \quad (3.30)$$

The solution to the differential equation in equation (3.27) is equation (3.31):

$$P(x) = P_i + \frac{L^2 bwJ_v(0)}{\phi^2} (\cosh \frac{\phi x}{L} - 1) - \frac{LbF(0)}{\phi} \sinh \frac{\phi x}{L} \quad (3.31)$$

Using the relationship in equation (2.10), equation (3.32) can be formed from equation (3.31):

$$\begin{aligned} F(x) &= \frac{-1}{b} \frac{dP(x)}{dx} \\ &= -\frac{LwJ_v(0)}{\phi} \sinh \frac{\phi x}{L} + F(0) \cosh \frac{\phi x}{L} \end{aligned} \quad (3.32)$$

Equation (3.32) can be directly substituted into equations (3.10)-(3.20) for simulation purposes.

3.3.1.5 Temperature Dependent Flow Modelling

To determine the validity of the temperature independence assumption, a model accounting for the change of J_v in terms of $T(x)$ was also developed. Discretizing equation (3.21) produces equation (3.33) for flow rate at element i in terms of membrane flux:

$$F(i) = F(0) - w\Delta x \sum_{j=0}^{i-1} J_v(j\Delta x) \quad (3.33)$$

Equation (2.1) expresses the flux through the membrane in terms of temperature and pressure across the membrane. Equation (2.10) expresses a relationship between flow rate and pressure; therefore, pressure must also be discretized in the same manner as flow rate as shown by equation (3.34):

$$P(i) = P(0) - b\Delta x \sum_{j=0}^{i-1} F(j) \quad (3.34)$$

Collecting equations (2.1), (3.33), and (3.34) produces the discrete flow rate expression in equation (3.35):

$$F(i) = F(0) - w\Delta x \sum_{j=0}^{i-1} \frac{A_w(P(0) - b\Delta x \sum_{k=0}^j F(k))}{1 + (\frac{A_w R_g}{B_s})T(j)C_p} \quad (3.35)$$

Equations (3.14) and (3.15) can directly accept equation (3.35) in place of the continuous flow rate expression for modelling purposes.

3.3.2 Results and Discussion

In order to evaluate the models in a RO context, parameters representative of a typical RO module (FILMTEC[®] TW30-2514) were curated from literature [20, 60, 71], as shown in Table 3.4 .

Table 3.1: Reverse Osmosis Module Properties

Parameter	Symbol	Value	Units
Initial flow rate	$F(0)$	1.759×10^{-4}	m ³ /s
Inlet pressure (gauge)	$P(0)$	1.551×10^6	Pa
Permeate channel pressure (gauge)	P_p	0	Pa
Inlet temperature	$T(0)$	298	K
Ambient temperature	T_a	298	K
Water transport coefficient	A_w	8.041×10^{-12}	m/s/Pa
Solute transport coefficient	B_s	4.578×10^{-7}	m/s
Ideal gas constant	R_g	8.314	J/molK
Channel width	w	2.203	m
Channel thickness	t_f	1×10^{-3}	m
Darcy's law constant	b	3.95×10^5	Pas/m ⁴
Permeate channel solute concentration	C_p	3.422×10^{-5}	mol/m ³
Water specific heat capacity	c	4184	J/kgK
Water density	ρ	1000	kg/m ³
Module length	L	0.3556	m

Table 3.2: Variable Parameter Ranges

Parameter	Symbol	Minimum Value	Maximum Value	Default Value	Units
Thermal resistance	r_{eq}	1×10^{-3}	1×10^{-2}	5×10^{-3}	K/m ² W
Initial intensity	I_0	7×10^{-2}	7×10^4	3.5×10^4	W/m ²
Attenuation constant	λ	0.5	100	50	None

To demonstrate that the numerical models both converge to a consistent output with increasing discretization resolution, each model was run iteratively with the number of discrete elements used to represent the module increasing by one with each iteration. The temperatures predicted at the module outlets were compared after each iteration. The models were considered to have converged when the temperatures reported at the outlets changed by less than 1×10^{-6} K between iterations.

To verify that the models produce reasonable results, the case of a perfectly insulated module with no permeate flux and complete absorption of emitted ultrasound was modelled using both approaches. Since this is the case where the water in the feed channel would reach the highest possible temperature for a given flow rate and ultrasonic emitter power, agreement between the model predictions and the maximum limiting temperature increase along the length of the module calculated using equation (3.9) was used to verify the legitimacy of the model results. Immediate attenuation and perfect insulation (λ and r_{eq} set to infinity) could not be modelled due to computational instability, so these conditions were approximated by setting λ to 100 m⁻¹ and r_{eq} to 100 K/m²W. Permeate flux was eliminated by assigning to the membrane a membrane permeability (A_w) of zero, and all other parameters remained at their default values as assigned in Tables 3.4 and 3.2. The models were run repetitively until the convergence criterion, described above, was reached. As shown in Table 3.3, both models converged after 1333 iterations to a predicted outlet temperature value of 298.1061 K, which represented an increase in temperature of 0.1061 K from the modelled inlet temperature of 298 K. Bearing in mind that $P_{emitter} = I_0 w t_f$, equation (3.9) predicts a maximum temperature of $\Delta T = \frac{(3.5 \times 10^4 \text{ W/m}^2)(1 \times 10^{-3} \text{ m})(2.203 \text{ m})}{(1.759 \times 10^{-4} \text{ m}^3/\text{s})(1000 \text{ kg/m}^3)(4184 \text{ J/kgK})} = 0.1048 \text{ K}$. Figure 3.3 shows that the temperatures quickly reached a plateau due to the sufficiently rapid absorption of ultrasound near the module inlet, and did not decline towards the outlet as they would if the selected value for r_{eq} were insufficient to prevent heat flux out of the system. The error in comparison to the analytical calculation for both models was 1.24%, indicating good agreement between the models and the analytical analysis in this specific scenario.

Table 3.3: Legitimacy Assessment Results

Model	Value	Error
Analytical	0.1048K	-
Temperature Dependent	0.1061 K	1.24%
Temperature Independent	0.1061 K	1.24%

The effects of variations in the parameters r_{eq} , λ , and I_0 were evaluated by varying one parameter across a specified range while holding the others constant. The parameter ξ was kept at a constant value of 1, as varying ξ has the same modelling effect as varying I_0 . Table 3.2 specifies the ranges and default values.

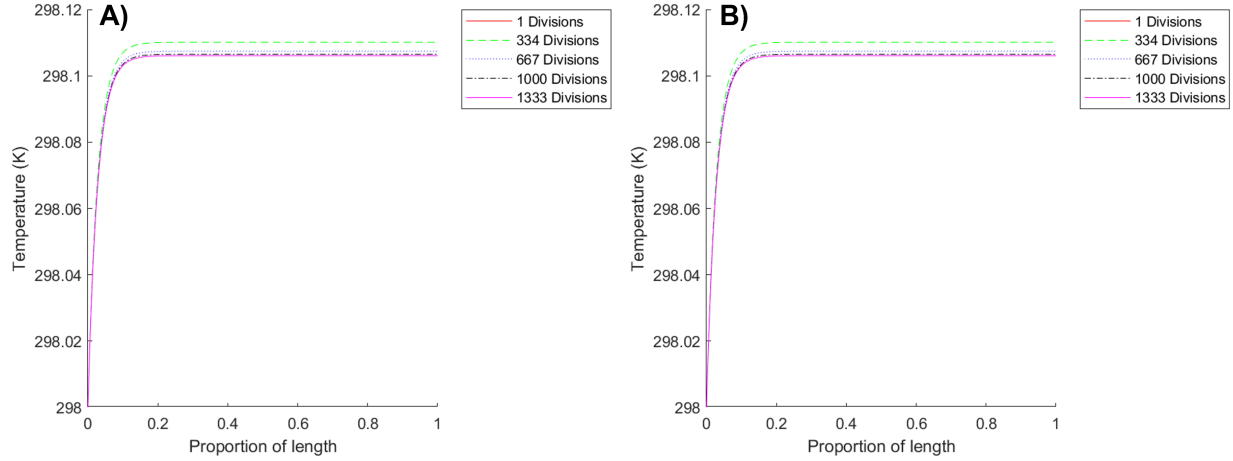


Figure 3.3: Temperature distributions predicted when assessing result legitimacy by the temperature dependent (A)) and temperature independent (B)) models. The temperatures quickly reach a plateau that persists for the length of the module, showing that the selected thermal resistance and attenuation constant values are sufficient for approximating immediate attenuation and perfect insulation for the purposes of this comparison.

Figure 3.4 shows the results generated by the two models. Applying the convergence criteria to the models with default values resulted in convergence after 837 and 841 iterations (corresponding to Δx values of 4.25×10^{-4} and 4.23×10^{-4}) for the temperature independent and temperature dependent models, respectively. The parameter ranges in Table 3.2 were then assessed using a Δx of 4.23×10^{-4} to produce the remaining results.

As can be seen in the graphs (Figure 3.3 - Figure 3.5), accounting for the temperature changes along the length of the module had negligible impact on the results. Both models predicted a pronounced temperature peak, the location of which corresponds with the rate of attenuation of the ultrasound. Maximum temperature values for the default value cases were 298.1005 K with both models.

The negligible effects of temperature changes along the length of the membrane on overall results is supported by Figure 3.5, which shows permeate flux and flow rate along the length of the membrane calculated using the temperature dependent and independent models. The decline of permeate flux over the length of the module was slightly more pronounced when temperature changes were taken into account, and the rate at which the temperature flux decreases did not decrease as significantly over the length of the module as it did in the temperature independent case. That being said, the differences between the two models are on the order of 1×10^{-10} m/s, which is negligible in the context of flow rates on the order of 1×10^{-4} m³/s.

Increasing the initial intensity (I_0) of the ultrasonic intensity predictably resulted in increased peak temperatures. Alterations in the thermal resistance of the outside module showed diminishing impact with increasing value, as the heat transferred out of the system via the uninsulated wall vanishes in comparison to the heat transferred out via mass transfer with increasing thermal resistance. This vanishing effect renders heat loss through the uninsulated wall of the system negligible for thermal resistances above $r_{eq} = 1 \times 10^{-2}$ K/m²W. Temperature increases along the length of the module were on the order of 1×10^{-2} K to 1×10^{-1} K (Figure 3.4).

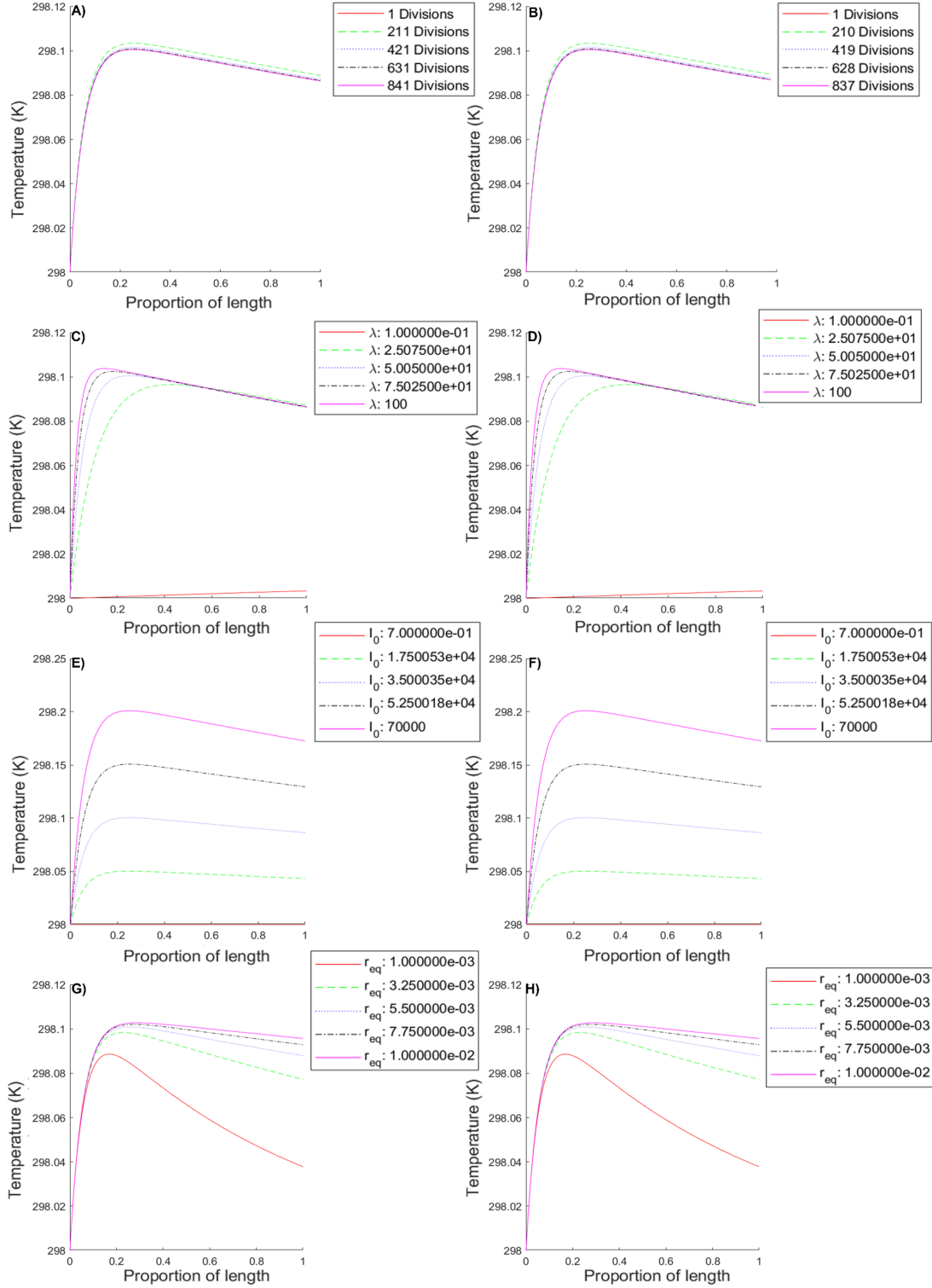


Figure 3.4: Temperature with respect to proportion of module length for the temperature dependent (left) and temperature independent (right) models. Graphs **A)** and **B)** show the models converging with progressively refined discretizations of the module length; graphs **C)** and **D)** show the models assessed across λ values; graphs **E)** and **F)** show the models assessed across I_0 values; and graphs **G)** and **H)** show the models assessed across r_{eq} values.

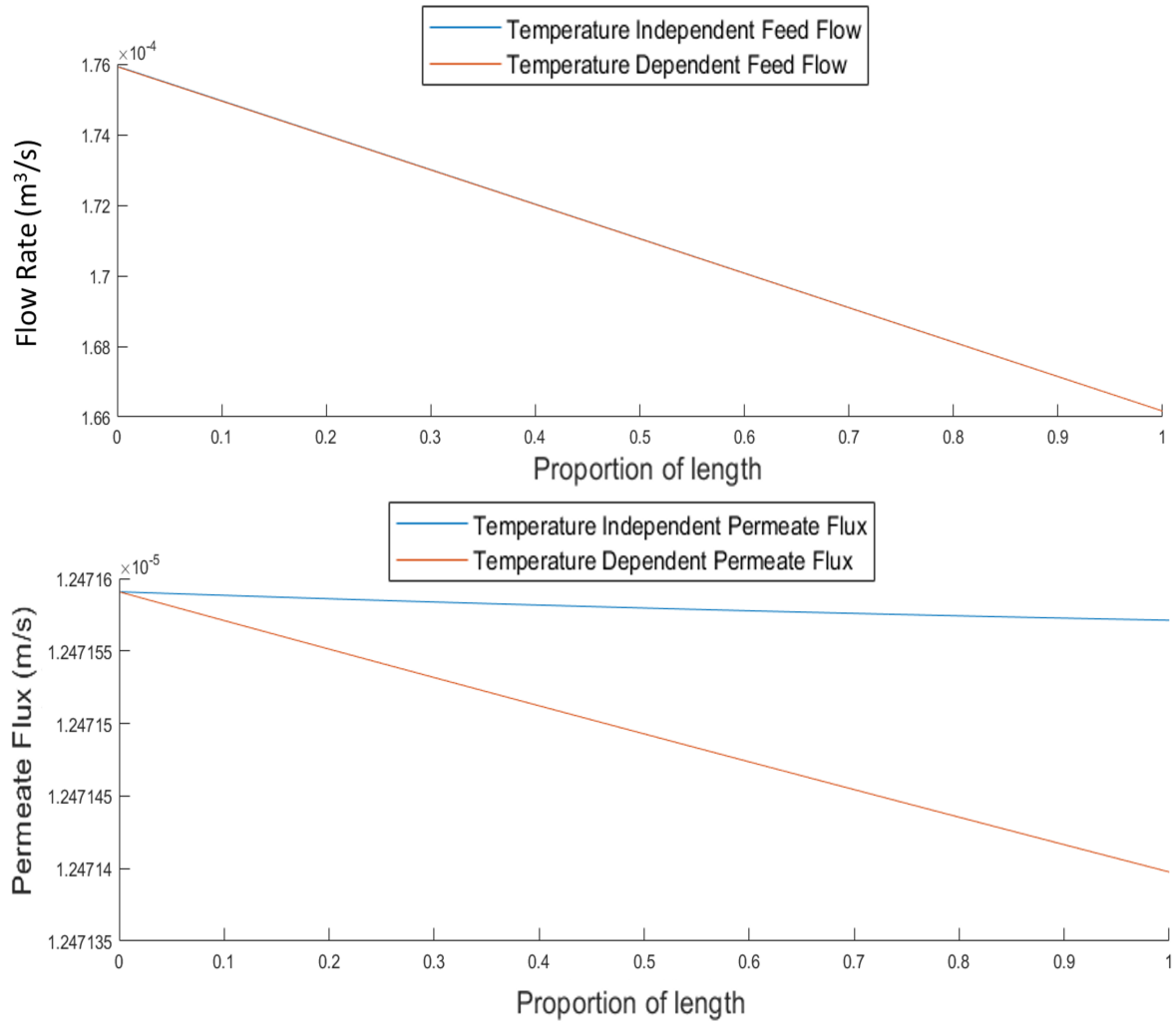


Figure 3.5: Flow rate (A) and permeate flux (B) distributions along the length of the module with default parameters for the temperature dependent and independent models. A comparison of these graphs shows that incorporating temperature into the models has a negligible impact on the results.

3.4 Cavitation Onset Modelling

In order to justify the experimental investigation of UFM, it was first necessary to demonstrate its theoretical viability in a SWRO context. In order to do this, a numerical model was constructed to determine flow properties throughout a typical SWRO module, which were compared against simulated ultrasonic attenuation curves in order to determine where inertial cavitation would occur within the module under different flow regimes. By determining this information, flow regimes could be constructed by which the entire module could be exposed to inertial cavitation, thus producing effective UFM.

3.4.1 Model Development

Salient qualitative elements of the mathematical and numerical derivations from the background section of this thesis can be summarized as follows:

- Inertial cavitation occurs in regions within which the sonification pressure amplitude is high relative to the hydraulic pressure, and is therefore encouraged by low hydraulic pressures.
- Permeate yield is directly proportional to hydraulic pressure.
- Both hydraulic pressure and pressure amplitude monotonically decrease along the length of the module when sonification is applied axially along the feed channel from the inlet.
- The rate at which hydraulic pressure decreases is proportional to the flow rate through the feed channel.
- Inertial cavitation attenuates ultrasound much more quickly than other forms of cavitation.
- Bubble dynamics associated with inertial cavitation cannot be accurately modelled from the existing information characterizing feed water in SWRO modules.

These items suggest that UFM may not be effective at the elevated pressures required for RO, and that sustaining inertial cavitation simultaneously throughout the entire module is likely not feasible. They also present the specific mechanisms by which to control the onset location of inertial cavitation within the module by taking advantage of hydrodynamic effects. Recalling the proportionality between the Blake threshold and the pressure within the medium expressed in equation (2.48) as well as the pressure drop caused by flow within the module expressed in equation (2.10), it is clear that the Blake threshold will decrease along the length of the module. This means that inertial cavitation could be produced at distances removed from the ultrasonic emitter, as opposed to directly adjacent to it (which is what occurs in constant pressure media) [45]. While the reduction in Blake threshold is accompanied by a reduction in pressure amplitude due to ultrasonic attenuation as described by equation (2.62), the proportional relationship between the rate at which pressure decreases along the length of the module and the flow rate within the module means that sufficiently high flow rates could reduce the pressure along the length of the module at a rate that exceeds the reduction in ultrasonic pressure amplitude due to attenuation.

To test this approach, a linear discretization of the system similar to that developed for the purposes of temperature distribution modelling was implemented. The energy balance described in equation (3.10) was discretized as shown in equation (3.36):

$$0 = wt_f \Delta I - c_p \rho_L (F(i)T(i) - F(i-1)T(i-1)) - c_p \rho_L (wT(i)J_v(i)\Delta x) - \frac{w(T(i) - T_a)}{r_{eq}} + k_{water} \left(\frac{dT(i)}{dx} - \frac{dT(i-1)}{dx} \right) \quad (3.36)$$

Here, ΔI is a discrete generalization of the exponential attenuation function used in the temperature distribution model, to allow for the more nuanced ultrasonic attenuation modelling occurring in this portion of the work. Solving equation (3.36) for temperature yields:

$$T(i) = \frac{c_p \rho_L F(i-1)T(i-1) + wt_f \Delta I + \frac{w}{r_{eq}} T_a}{c_p \rho_L F(i) + c_p \rho_L w J_v(i) + \frac{w}{r_{eq}}} \quad (3.37)$$

The procedure for calculating parameters throughout the system was as follows:

1. Set system parameters:
 - Module length L
 - Step size Δx
 - Feed channel area A
 - Volume fractions V_L and V_S
 - Moles per bubble n
 - Ambient temperature and initial fluid temperature T_a and $T(0)$
 - Surface tension σ
 - Viscosity μ
2. Set operating parameters:
 - Initial pressure $P(0)$
 - Initial flow rate $F(0)$
 - Initial ultrasonic intensity $I(0)$
 - Calculate initial pressure amplitude $p_a(0)$ from initial intensity using equation (2.54)
3. For values of i from 0 to $\frac{L}{\Delta x}$:
 - (a) Using pressure $P(i)$ as the pressure in the feed channel:
 - Calculate permeate flux $J_v(i)$ using equation (2.1)
 - Calculate stable bubble size R_0 from equation (2.49)
 - Check if the pressure amplitude is greater than the Blake threshold calculated using 2.48
 - If the pressure amplitude is greater than the Blake threshold, terminate iterations here
 - Calculate the pressure amplitude $p_a(i)$ using equation (2.88)
 - Calculate the new ultrasonic intensity using equation (2.54)
 - (b) Using the change in intensity, calculate the temperature $T(i+1)$ using equation (3.37)
 - (c) Calculate $F(i+1)$ to $P(i+1)$ from equations 3.35 and 3.34

This approach couples the cavitation and flow analyses by passing information on the hydrodynamic pressure from the flow model to the cavitation model and passing information on energy dissipation from the cavitation model to the flow model (via the energy balance in equation (3.36)).

3.4.2 Discussion

The following sections will discuss how the simulations were conducted, as well as the simulation results as they relate to the feasibility of inertial cavitation generation, parameter estimation, and energy efficiency. The section will end with a discussion of how the model limitations might impact the breadth of its applicability.

3.4.2.1 Simulation conditions

A set of parameters representative of a typical RRO system employing a Filmtec TW30-2514™ was compiled in table 3.4 [20, 58, 60, 71–73].

Table 3.4: System properties used within the simulation for determining the cavitation onset within SWRO modules

Parameter	Symbol	Value	Units
Sonification power	NA	1.2×10^2	W
Sonification frequency	ω	2.8×10^4	Hz
Initial flow rate	$F(0)$	3.889×10^{-4}	m^3/s
Permeate channel pressure	P_p	101300	Pa
Inlet temperature	$T(0)$	298	K
Ambient temperature	T_a	298	K
Solvent transport coefficient	A_w	8.041×10^{-12}	$\text{m}/\text{s}/\text{Pa}$
Solute transport coefficient	B_s	4.578×10^{-7}	m/s
Ideal gas constant	R_g	8.314	J/molK
Specific heat ratio of air	γ	1.4	NA
Module length	L	0.2951	m
Thermal resistance	r_{eq}	∞	K/Wm^2
Channel width	w	2.203	m
Channel thickness	t_f	1×10^{-3}	m
Feed spacer volume fraction	f_f	7.76×10^{-2}	NA
Darcy's law constant	b	3.95×10^5	Pas/m^4
Permeate channel solute concentration	C_p	3.422×10^{-5}	mol/m^3
Water specific heat capacity	c	4184	J/kgK
Water density	ρ_L	998	kg/m^3
Water surface tension	σ	7.286×10^{-2}	N/m
Water viscosity	μ	8.9×10^{-4}	kg/ms
Water bulk modulus	B	2.15×10^9	Pa
Bubble radius at ambient conditions	R_0	2×10^{-6}	m
Feed channel air concentration	C_a	4.84×10^2	mol/m^3
Sonification power	P_s	1.2×10^2	W
Sonification frequency	f	2.8×10^4	Hz

It is worth noting that, while inlet pressure, inlet flow rate, and sonification power are all controllable variables, analysis here is simplified by only considering the case where the ultrasonic transducer operates at maximum power. This is because maintaining high operating pressures while UFM occurs minimizes reductions in permeate yield, which is an important practical consideration for this technology [4, 19]. Equation (2.48) shows that higher operating pressures require greater sonification pressure amplitudes in order to produce inertial cavitation, so the ultrasonic power must be maximized to achieve maximum operating

pressures during UFM.

Convergence in terms of step size was investigated by repeatedly running the simulation on a truncated length of the module while halving the step size with each iteration and observing the average relative error in the values returned for feed channel pressure, feed channel flow rate, permeate flux, sonification pressure amplitude, temperature, and Blake threshold. As Figure 3.6 shows, the error diminishes as the step sizes are halved, at a rate that diminishes towards a step size of approximately 5×10^{-4} m. Therefore, the remaining simulations use a step size of 5×10^{-4} m.

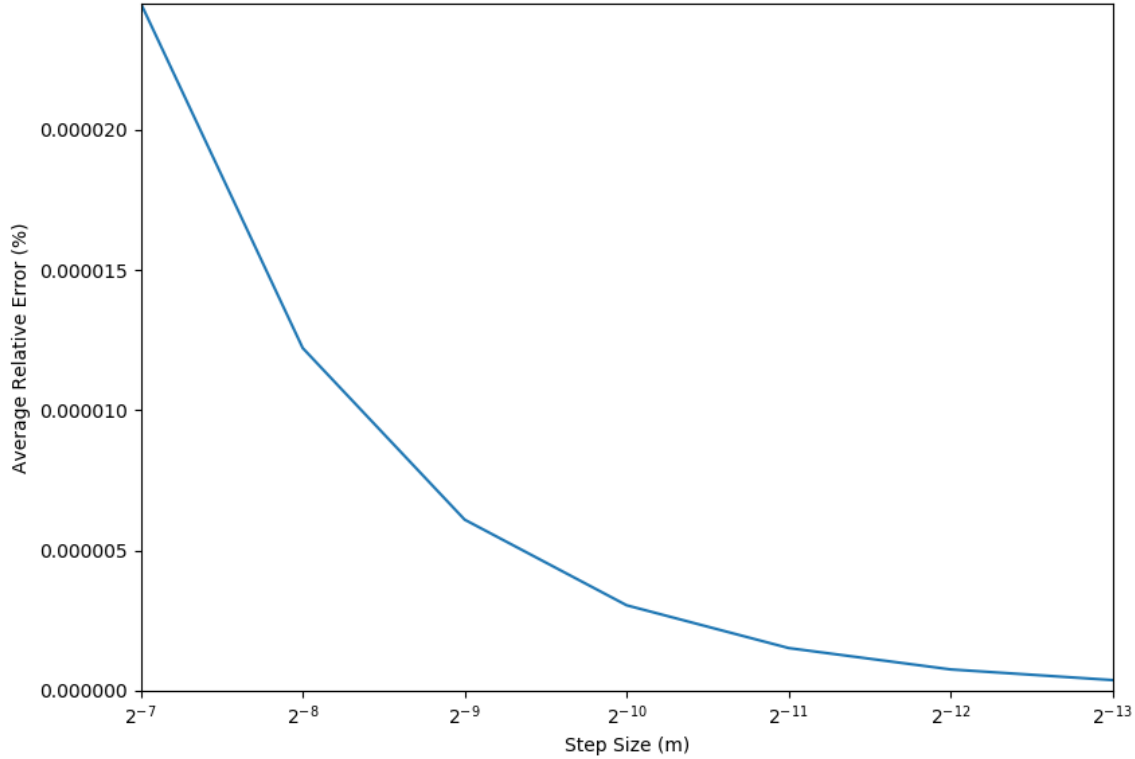


Figure 3.6: Average relative error of selected element properties as a function of step size. Reductions of step size to below 5×10^{-4} m (approx. 2^{-11} m) have minimal effect on the error observed. Average error is calculated from the relative errors in feed channel pressure, feed channel flow rate, permeate flux, sonification pressure amplitude, temperature, and Blake threshold

3.4.2.2 Feasibility of Inertial Cavitation Generation

Figure 3.7 plots the results of an analysis seeking the cavitation onset location for inlet pressures of 270 kPa, 340 kPa, 400 kPa, and 1618.3 kPa, with an inlet flow rate of 3.889×10^{-4} m³/s. The flow rate was set to the maximum rated flow rate for the TW30-2514 module, to produce the maximum possible change in Blake threshold across the length of the module [20]. The four inlet pressure cases illustrated were selected out

of a broader set of inlet pressures analyzed due to their effective illustration of the variation in cavitation onset location with inlet pressure. The upper and lower bounds of the inlet pressure range correspond (respectively) to the recommended operating pressure of the TW30-2514 module and the minimum inlet pressure to drive flow at the specified rate through the module assuming that the outlet experiences atmospheric pressure [20]. In the case with the lowest inlet pressure, the sonification pressure amplitude immediately surpasses the Blake threshold. At the maximum inlet pressure, the sonification pressure amplitude never approaches the Blake threshold. Of interest, however, are the cases of the two more moderate inlet pressure values. At an inlet pressure of 340 kPa, the model predicts an inertial cavitation onset position of 0.02 m away from the inlet. This occurs because the pressure amplitude, which is initially lower than the Blake threshold, reduces minimally under conditions of stable cavitation, while the Blake threshold drops comparatively quickly due to head losses. The case of a 400 kPa inlet pressure, where the onset of inertial cavitation approaches the outlet of the module, shows that the Blake threshold diminishes faster than the pressure amplitude under conditions of stable cavitation throughout the module, and produces an inertial cavitation onset position that is 0.21 m away from the inlet.

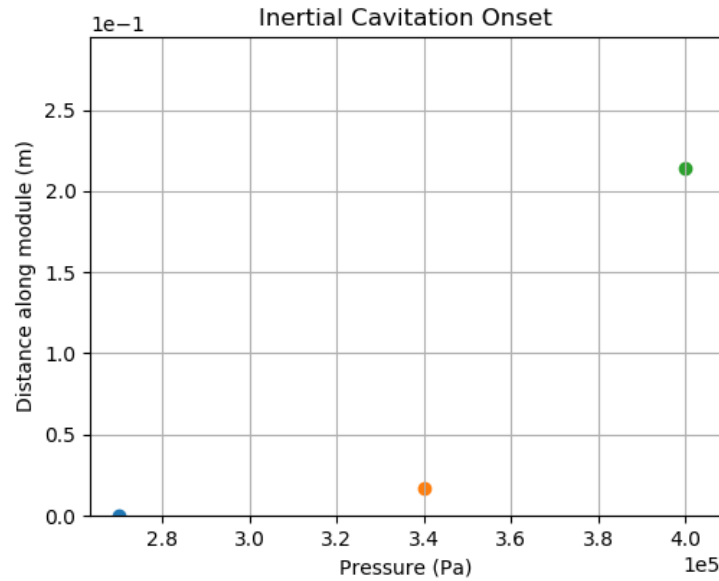


Figure 3.7: Results of an analysis comprising four inlet pressure cases (270 kPa, 340 kPa, 400 kPa, and 1618.3 kPa) and the corresponding positions of inertial cavitation onset. At an inlet pressure of 270 kPa, inertial cavitation is achieved immediately at the inlet of the module, whereas the sonification pressure amplitude never approaches the Blake threshold with an inlet pressure of 1618.3 kPa (hence the absence of a corresponding point on the plot). With an inlet pressure of 340 kPa, the sonification pressure is achieved slightly after the inlet. For an inlet pressure of 400 kPa, the pressure amplitude starts below the Blake threshold, but surpasses it due to the pressure drop within the module, ultimately attaining inertial cavitation further towards the outlet of the module.

3.4.2.3 Parameter estimation

Now that the viability of this approach has been verified in principle, an approximate relationship must be established between inlet conditions and the location of inertial cavitation onset. Figure 3.8 a) shows that an approximately linear relationship exists between the location of inertial cavitation onset and the inlet

pressure, as long as the inlet pressure produces a Blake threshold higher than the initial pressure amplitude. Figure 3.8 b) shows the relationship between flow rate and the onset location of inertial cavitation with a fixed inlet pressure, which shows an approximately inverse relationship between flow rate and inertial cavitation onset position. The origin of these relationships is the assumed applicability of Darcy's law in the correlation of feed pressure and flow rate.

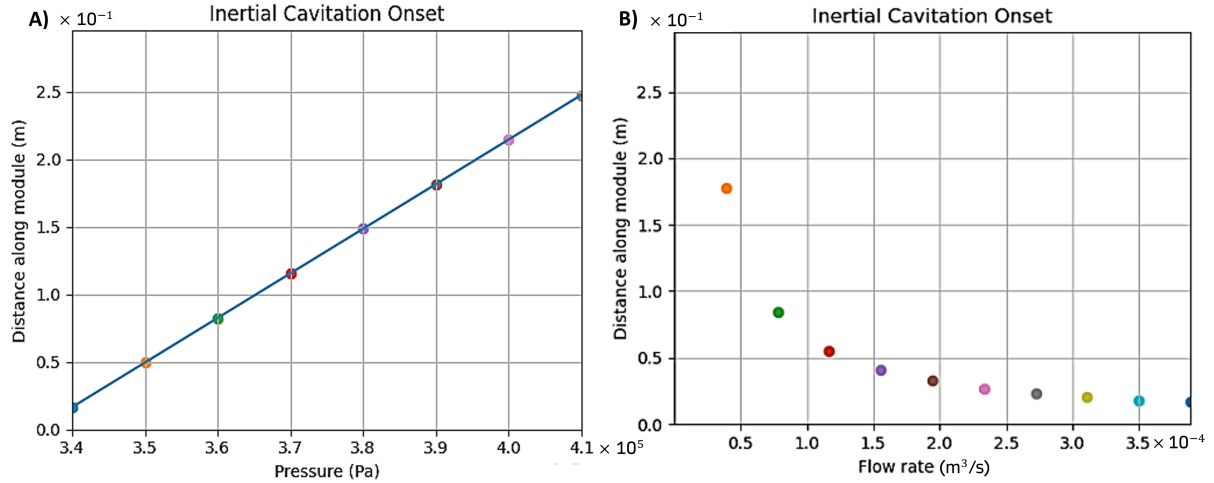


Figure 3.8: Inertial cavitation onset position relative to the SWRO module inlet as a function of A) inlet pressure (with a constant flow rate of $3.889 \times 10^{-4} \text{ m}^3/\text{s}$) and B) flow rate (with a constant inlet pressure of 330 kPa. The relationship in A) is approximately linear, as shown by the line of best fit (slope of 3.3×10^{-6} , intercept of -1.1055 , and standard error of 1.31×10^{-17}). The relationship in Figure B) appears to be approximately inversely proportional.

3.4.2.4 Energy Efficiency

The remaining questions surrounding the estimation of UFM viability within SWRO modules pertain to the holistic system performance under conditions conducive to UFM. System performance can be assessed in terms of three parameters: bulk permeate production rate of the system during operation, measured in m^3/s ; total system power consumption, measured in Watts; and Specific Energy Consumption (SEC), defined as the total module permeate production rate divided by the module power consumption and expressed in terms of kJ/m^3 . Permeate production and total power consumption provide information on the specifications required to successfully meet a certain drinking water demand while operating UFM (either continuously to mitigate fouling or intermittently within a periodic cleaning program), while SEC gives an idea of system efficiency. The approximately linear relationship between inertial cavitation onset position and inlet pressure with a fixed inlet flow rate makes this approach, hereafter referred to as fixed-flow UFM, more practical than the variable flow fixed pressure approach. Therefore, only fixed-flow UFM will be examined going forward.

Figure 3.9 a) illustrates the average permeate produced across the range of inlet parameters under four conditions: fixed-flow UFM at the maximum flow rate specified prior, fixed-flow UFM at a more typical flow rate of $8.796 \times 10^{-5} \text{ m}^3/\text{s}$, manufacturer-recommended operating pressure at maximum flow rate, and manufacturer-recommended operating pressure at a flow rate of $8.796 \times 10^{-5} \text{ m}^3/\text{s}$. Since inlet pressure varies during UFM conditions, representative values were produced by averaging outputs procured from a

range of inlet pressures for both flow rates. These ranges were calculated by conducting linear regression to determine the relationship between inlet pressure and inertial cavitation onset position for both flow rates, calculating the pressures that produce cavitation at the inlet and the outlet of the module using the linear relationships developed, and taking a sample of ten evenly-distributed points from between these two values for both cases (including the boundaries). The pressure ranges were 335-424 kPa for the maximum flow rate case and 335-355 kPa for the typical flow rate case.

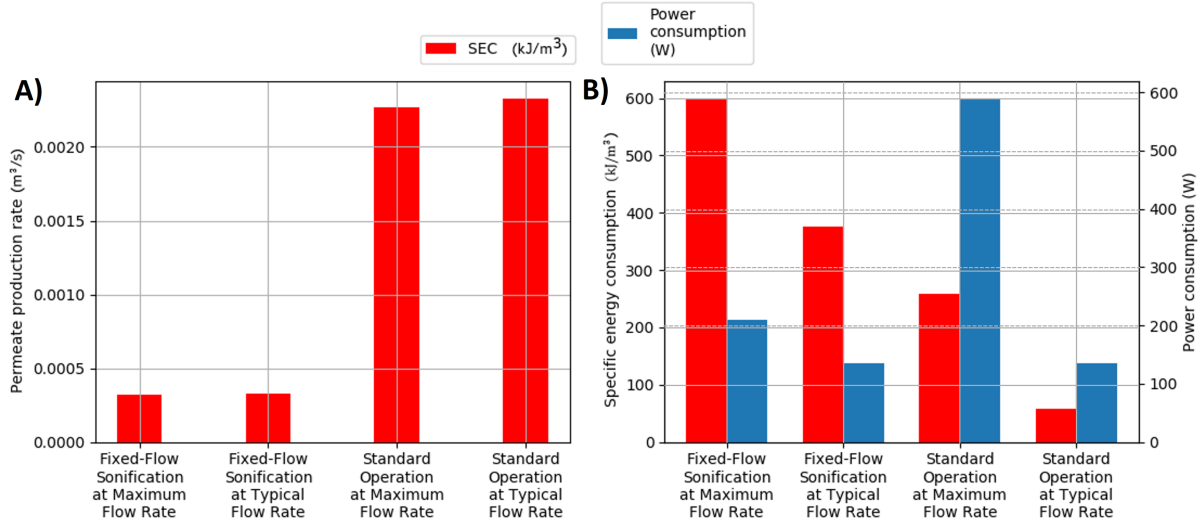


Figure 3.9: a) Permeate production rates and b) power consumption and SEC for UFM conditions compared to manufacturer-recommended operating conditions. Permeate production and total power consumption provide information on the specifications required to successfully meet a certain drinking water demand while operating UFM (either continuously to mitigate fouling or intermittently within a periodic cleaning program), while SEC gives an idea of system efficiency. While comparable in terms of overall power demand, UFM conditions compare poorly to manufacturer recommended conditions in terms of SEC and permeate production, suggesting that UFM is not suitable for online operation in a SWRO context.

Permeate production under UFM conditions is an order of magnitude less than that produced during standard operation, meaning that UFM could only be viably implemented in an offline capacity. Remarkably, the system power consumption for UFM at the typical flow rate is almost identical to the system power consumption at the manufacturer-recommended operating pressure with the same flow rate (134.8 W and 134.3 W, respectively). This shows that UFM can be implemented within an RRO system without necessitating an increase in energy generation capacity, improving the prospective economic viability of the technology. Fixed-flow UFM could be implemented as a periodic cleaning method for installed SWRO membranes, with cleaning events triggered based on a fixed schedule or in response to module performance degradation.

3.4.2.5 Limitation Assessment

The assumptions made within the model derivation present some limitations around the applicability of the model. In particular, the domain is reduced to a single dimension. This makes it impossible to fully account for the effects of the feed spacer on both the flow and the ultrasonic problems [14, 28, 34, 43, 45]. The model also cannot account for ultrasonic scattering or Bjerknes forces generated by the cavitation bubbles

themselves [14, 43, 45, 53]. The potential discrepancies that this assumption could cause between the results produced by the model and those that a physical experiment might generate are discussed below in terms of both flow parameter estimation and effective ultrasonic intensity estimation.

3.4.2.5.1 Feed Spacer Geometry

The effects of a typical feed spacer on the flow through SWRO modules have been studied through Computational Fluid Dynamics (CFD) [28, 34]. While substantial multidimensional variations in flow velocities can be seen, it is clear from the available literature that any pressure variations perpendicular to the flow axis are eclipsed by the axial pressure drop [28]. Based on this, the one dimensional approximation is likely acceptable for the prediction of flow properties.

Solids immersed in fluids contribute to the scattering of ultrasound within the fluid [14, 43]. This generally reduces cavitation by defocusing the ultrasonic energy within the fluid medium [14, 43]. Because of this, the model may underestimate the rate of ultrasonic attenuation within the medium, potentially requiring a reduction in the maximum pressure identified for the cleaning regime. Solids immersed in fluids are also known to provide sites that facilitate the nucleation of cavitation bubbles by trapping gas pockets within surface imperfections, reducing the effective Blake threshold in their vicinity [43]. In the scenario being investigated, this might result in a more gradual transition into inertial cavitation along the length of the module, led by the boundary layers around solid surfaces and beginning closer to the ultrasonic emitter than anticipated by the model.

Since the feed spacer is a solid plastic mesh, cavitation cannot occur within it; therefore, ultrasound passing through the feed spacer may not attenuate as quickly as it does within inertially cavitating fluid, which may result in the formation of phenomena such as standing waves within the feed spacer [66]. This may allow the feed spacer to transmit some ultrasonic energy back into the fluid after the ultrasonic energy carried by the fluid has largely attenuated, potentially expanding the region of inertial cavitation beyond the immediate vicinity of the inertial cavitation onset location predicted by the model.

3.4.2.5.2 Cavitation bubble effects

Cavitation bubbles themselves can scatter ultrasound, contributing to its rapid attenuation in regions of inertial cavitation [43]. While this scattering is most significant in regions undergoing inertial cavitation, bubbles of any size can contribute to scattering, which may result in the model underestimating the rate of ultrasonic attenuation within the fluid [43].

Cavitation bubbles can also move through a fluid spontaneously in the direction of wave propagation, due to phenomena such as Bjerknes forces and acoustic streaming [14, 43, 53]. As cavitation bubbles travel in the direction of wave propagation, they may extend the effective region of inertial cavitation beyond the immediate vicinity of the inertial cavitation onset location predicted by the model [14, 43, 53].

While these limitations introduced some uncertainty around the specific numbers predicted by the model, they did not challenge the essential result of this investigation: the viability of delaying the onset of inertial cavitation using variations in SWRO operating parameters. Therefore, the research focus shifted to the next challenge: improving vibration transfer across membrane module boundaries.

3.5 Ultrasonic Horn Design

To be effective, UFM requires ultrasonic intensities in the range of $1 \times 10^0 - 1 \times 10^1 \text{ W/cm}^2$ [15]. Therefore, care must be taken to prevent inefficiencies in the transfer of ultrasonic energy from the generator to the fluid medium. To do this, an ultrasonic horn was designed with dimensions carefully selected to reduce parasitic losses and interference produced by the pressure vessel enclosing the membrane module.

3.5.1 System Configuration

Ideally, the ultrasonic transducer used to generate cavitation would simply be immersed within the membrane pressure vessel, thus eliminating the need to pass ultrasound through the boundaries of the pressure vessel and the associated reduction in effective ultrasonic intensity within the membrane module [42]. However, there are a limited number of submersible transducers that are commercially available [74], and the form factors are not conducive to this application. Insulating enclosures for non-submersible transducers could theoretically be designed to allow them to be used within membrane module pressure vessels; however, the insulation would have to be carefully designed to avoid interfering with the vibration of the transducer [65]. Additionally, high power transducers operate at voltages in excess of 1 kV, further limiting the room for error in the design of these enclosures [75]. Therefore, while the ultrasonic emitter was immersed within the membrane module, it was decided that the transducer generating the ultrasonic waves would be located outside of the module.

Figure 3.10 shows a cross-section of the proposed novel ultrasonic horn, referred to hereafter as the SWRO sonification apparatus. The objective of this phase of the work was to determine suitable values for lengths L_1 and L_2 such that the emitter would vibrate in longitudinal vibration at the operating frequency of the transducer and the transfer of vibrations to the pressure vessel would be reduced relative to the default implementation wherein the transducer is directly affixed to the exterior of the pressure vessel.

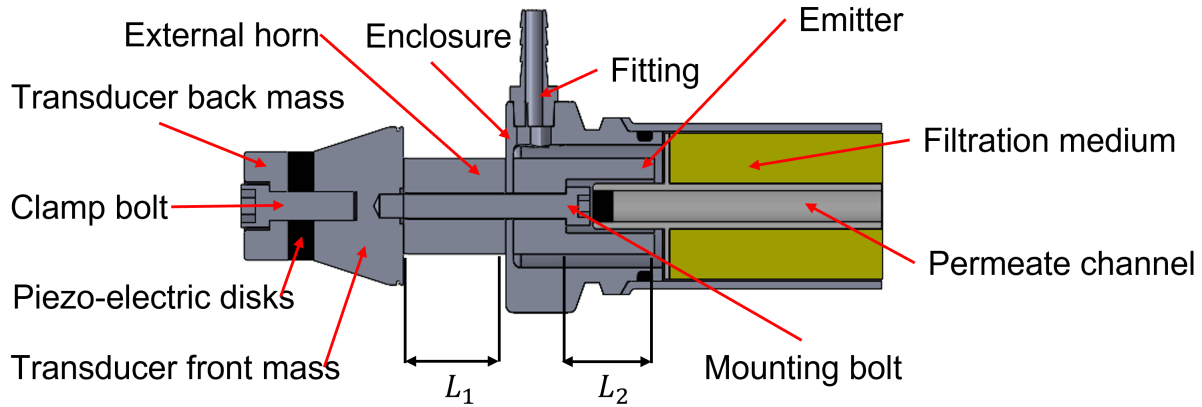


Figure 3.10: SWRO module with integrated SWRO sonification apparatus.

3.5.2 Methodology

The analysis was conducted in two parts. Firstly, a first principles model was constructed to try to predict the behaviours of the vibrating horn. Second, a Finite Element Analysis (FEA) model was produced to simulate the behaviour of the system. Suitable dimensions were calculated using the analytical model and tested in the FEA model to gauge improvement over the default case, where the transducer is affixed directly to the outside of the pressure vessel with no internal or external horn segment.

3.5.2.1 First Principles Analysis

The objective of the first principles analysis was to determine the dimensions of the ultrasonic horn that would theoretically transfer as little vibration as possible to the pressure vessel enclosing the membrane module. Intuitively, placing the node of the longitudinally vibrating system at the interface between the column and the enclosure will transfer a minimum of vibrations to the enclosure, allowing maximum vibration transfer to the immersed horn segment and the fluid medium beyond. As such, this was the express goal of the analysis.

To conduct the modelling, the vibrating column was divided into two segments at the middle of its passage through the pressure vessel wall, as illustrated in Figure 3.11. The part outside of the enclosure was bounded on its other end by the surface of the transducer, and the immersed segment was bounded by the emitting face. Both segments were independently modelled using equations (2.94) and (2.98).

The first segment consisted of two sets of equations, modelling the external segment and the external half of the pressure vessel wall. For analysis purposes, the diameter of the pressure vessel wall was not considered to extend beyond the diameter of the vibrating column. This decision was supported by the fact that the purpose of the analysis was to find conditions under which the longitudinal movement within this boundary would be negligible, suggesting that the effects of its geometry on the behaviour of the system should not be insignificant.

Transducers are typically designed such that they achieve longitudinal resonance in free space at their designed frequencies [62, 64, 65]. For an object vibrating longitudinally in free space, the force acting on its ends is assumed to be negligible [64, 65]. If the horn is designed correctly, the entire vibrating system should achieve resonance [62, 64, 65]. Therefore, since the transducer can be expected to resonate at the selected operating frequency with no force acting on its output surface, it was assumed that no force would act on the transducer interface surface of the external horn segment. A displacement amplitude D_I was considered to occur at this interface, which was left undefined since the dimensions calculated should be independent of this value. The displacement at the end of this segment was constrained to be equal to 0 at all times.

The conditions described above produced the system of equations shown in equations (3.38)-(3.42):

$$D_I = A_1 \quad (3.38)$$

$$A_2 \cos(L_1 k_2) + B_2 \sin(L_1 k_2) = A_1 \cos(L_1 k_1) + B_1 \sin(L_1 k_1) \quad (3.39)$$

$$0 = -B_1 E_1 k_1 \quad (3.40)$$

$$0 = E_1(-A_1 k_1 \sin(L_1 k_1) + B_1 k_1 \cos(L_1 k_1)) - E_2(-A_2 k_2 \sin(L_1 k_2) + B_2 k_2 \cos(L_1 k_2)) \quad (3.41)$$

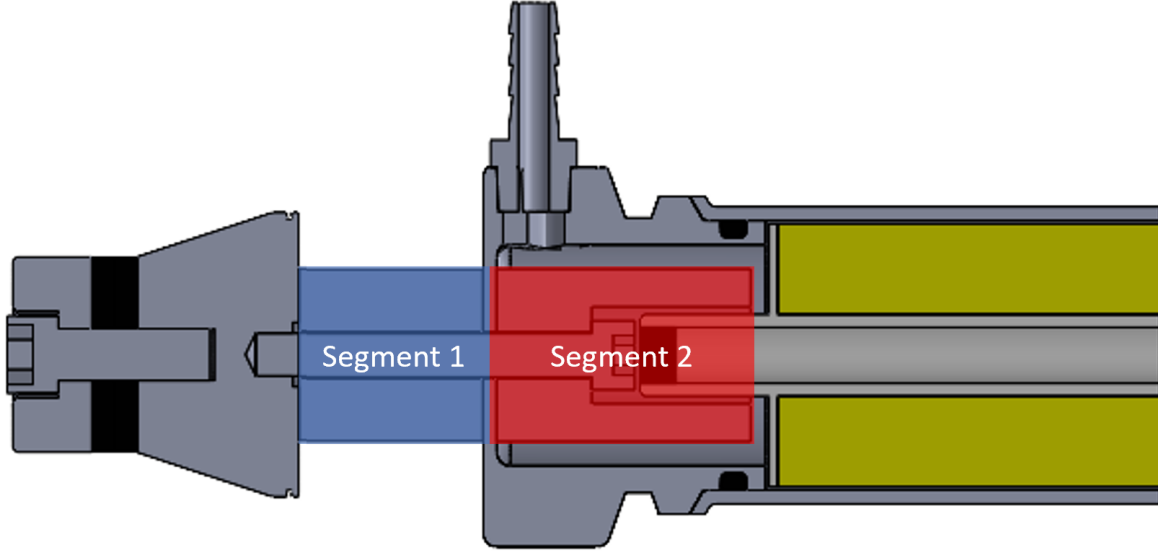


Figure 3.11: Illustration of the division between the modelled segments.

$$0 = A_2 \cos(k_2(L_1 + \frac{w}{2})) + B_2 \sin(k_2(L_1 + \frac{w}{2})) \quad (3.42)$$

These five equations fully constrain the four constants (A_1, B_1, A_2, B_2) within the general solutions and the unknown length L_1 . Substituting equations (2.91) and (2.92) into equations (3.38)-(3.41) and solving for the constants produced equations (3.43)-(3.46):

$$A_1 = D_I \quad (3.43)$$

$$A_2 = \frac{D_I(E_1 \sin(\frac{2L_1\omega\pi}{\sqrt{\frac{E_1}{\rho_1}}})\sqrt{\frac{E_2}{\rho_2}} \sin(\frac{2L_1\omega\pi}{\sqrt{\frac{E_2}{\rho_2}}}) + E_2\sqrt{\frac{E_1}{\rho_1}} \cos(\frac{2L_1\omega\pi}{\sqrt{\frac{E_1}{\rho_1}}}) \cos(\frac{2L_1\omega\pi}{\sqrt{\frac{E_2}{\rho_2}}}))}{E_2\sqrt{\frac{E_1}{\rho_1}}(\sin^2(\frac{2L_1\omega\pi}{\sqrt{\frac{E_2}{\rho_2}}}) + \cos^2(\frac{2L_1\omega\pi}{\sqrt{\frac{E_2}{\rho_2}}}))} \quad (3.44)$$

$$B_1 = 0 \quad (3.45)$$

$$B_2 = -\frac{D_I(E_1 \sin(\frac{2L_1\omega\pi}{\sqrt{\frac{E_1}{\rho_1}}})\sqrt{\frac{E_2}{\rho_2}} \cos(\frac{2L_1\omega\pi}{\sqrt{\frac{E_2}{\rho_2}}}) - E_2\sqrt{\frac{E_1}{\rho_1}} \sin(\frac{2L_1\omega\pi}{\sqrt{\frac{E_2}{\rho_2}}}) \cos(\frac{2L_1\omega\pi}{\sqrt{\frac{E_1}{\rho_1}}}))}{E_2\sqrt{\frac{E_1}{\rho_1}}(\sin^2(\frac{2L_1\omega\pi}{\sqrt{\frac{E_2}{\rho_2}}}) + \cos^2(\frac{2L_1\omega\pi}{\sqrt{\frac{E_2}{\rho_2}}}))} \quad (3.46)$$

Equation (3.47) can then be produced by substituting 3.44 and 3.46 into equation (3.42):

$$\begin{aligned}
0 = & \frac{D_I(E_1 \sin(\frac{2L_1 \omega p i}{\sqrt{\frac{E_1}{\rho_1}}}) \sqrt{\frac{E_2}{\rho_2}} \sin(\frac{2L_1 \omega p i}{\sqrt{\frac{E_2}{\rho_2}}}) + E_2 \sqrt{\frac{E_1}{\rho_1}} \cos(\frac{2L_1 \omega p i}{\sqrt{\frac{E_1}{\rho_1}}}) \cos(\frac{2L_1 \omega p i}{\sqrt{\frac{E_2}{\rho_2}}})) \cos(\frac{2\omega p i(L_1 + w/2)}{\sqrt{\frac{E_2}{\rho_2}}})}{E_2 \sqrt{\frac{E_1}{\rho_1}} (\sin(\frac{2L_1 \omega p i}{\sqrt{\frac{E_2}{\rho_2}}})^2 + \cos(\frac{2L_1 \omega p i}{\sqrt{\frac{E_2}{\rho_2}}})^2)} \\
& - \frac{D_I(E_1 \sin(\frac{2L_1 \omega p i}{\sqrt{\frac{E_1}{\rho_1}}}) \sqrt{\frac{E_2}{\rho_2}} \cos(\frac{2L_1 \omega p i}{\sqrt{\frac{E_2}{\rho_2}}}) - E_2 \sqrt{\frac{E_1}{\rho_1}} \sin(\frac{2L_1 \omega p i}{\sqrt{\frac{E_2}{\rho_2}}}) \cos(\frac{2L_1 \omega p i}{\sqrt{\frac{E_1}{\rho_1}}})) \sin(\frac{2\omega p i(L_1 + w/2)}{\sqrt{\frac{E_2}{\rho_2}}})}{E_2 \sqrt{\frac{E_1}{\rho_1}} (\sin(\frac{2L_1 \omega p i}{\sqrt{\frac{E_2}{\rho_2}}})^2 + \cos(\frac{2L_1 \omega p i}{\sqrt{\frac{E_2}{\rho_2}}})^2)}
\end{aligned} \tag{3.47}$$

No attempt was made to solve (3.47) analytically for L_1 ; rather, L_1 was solved numerically.

The second segment was divided into three sections: the internal half of the pressure vessel wall section, the fixed-length solid section, and the hollow section of variable length. The hollow section was made hollow for two reasons: first, to accommodate the end of the filtration module permeate tube, and second, to avoid wasting energy by transferring vibrations to the permeate tube and its contents. A force of arbitrary amplitude F_I was assumed to act at the boundary with the first segment (modelled above), while the displacement at this boundary was constrained to equal 0. Modelling the system in this way produced equations (3.48)-(3.53):

$$0 = -A_3 \tag{3.48}$$

$$0 = A_3 \cos(\frac{w}{2}k_3) - A_4 \cos(\frac{w}{2}k_4) + B_3 \sin(\frac{w}{2}k_3) - B_4 \sin(\frac{w}{2}k_4) \tag{3.49}$$

$$0 = A_4 \cos(k_4(L_{solid} + \frac{w}{2})) - A_5 \cos(k_5(L_{solid} + \frac{w}{2})) + B_4 \sin(k_4(L_{solid} + \frac{w}{2})) - B_5 \sin(k_5(L_{solid} + \frac{w}{2})) \tag{3.50}$$

$$0 = -B_3 E_3 k_3 - \frac{F_I}{A_{c3} E_3} \tag{3.51}$$

$$0 = E_3(-A_3 k_3 \sin(\frac{w}{2}k_3) + B_3 k_3 \cos(\frac{w}{2}k_3)) - E_4(-A_4 k_4 \sin(\frac{w}{2}k_4) + B_4 k_4 \cos(\frac{w}{2}k_4)) \tag{3.52}$$

$$\begin{aligned}
0 = & E_4(-A_4 k_4 \sin(k_4(L_{solid} + \frac{w}{2})) + B_4 k_4 \cos(k_4(L_{solid} + \frac{w}{2}))) \\
& - E_5(-A_5 k_5 \sin(k_5(L_{solid} + \frac{w}{2})) + B_5 k_5 \cos(k_5(L_{solid} + \frac{w}{2})))
\end{aligned} \tag{3.53}$$

Equations (3.54)-(3.59) were produced using the same procedure as that implemented to solve for the parameters of the first segment.

$$0 = A_3 \tag{3.54}$$

$$A_4 = \frac{F_I(E_3 \cos(\frac{w\omega\pi}{\sqrt{\frac{E_3}{\rho_3}}}) \sin(\frac{w\omega\pi}{\sqrt{\frac{E_4}{\rho_4}}}) \sqrt{\frac{E_4}{\rho_4}} - E_4 \cos(\frac{w\omega\pi}{\sqrt{\frac{E_4}{\rho_4}}}) \sin(\frac{w\omega\pi}{\sqrt{\frac{E_3}{\rho_3}}}) \sqrt{\frac{E_3}{\rho_3}})}{2E_4\omega\pi(\cos^2(\frac{w\omega\pi}{\sqrt{\frac{E_4}{\rho_4}}}) + \sin^2(\frac{w\omega\pi}{\sqrt{\frac{E_4}{\rho_4}}}))E_3^2 A_{c3}} \tag{3.55}$$

$$\begin{aligned}
A_5 = \frac{F_I}{2\sqrt{\frac{E_4}{\rho_4}} E_5 \omega \pi \rho_4 A_{c3} E_3^2} & (-E_5(\rho_4 \sqrt{\frac{E_3}{\rho_3}} \sqrt{\frac{E_4}{\rho_4}} \sin(\frac{w\omega\pi}{\sqrt{\frac{E_3}{\rho_3}}}) \cos(\frac{2\omega\pi L_{solid}}{\sqrt{\frac{E_4}{\rho_4}}}) \\
& + E_3 \cos(\frac{w\omega\pi}{\sqrt{\frac{E_3}{\rho_3}}}) \sin(\frac{2\omega\pi L_{solid}}{\sqrt{\frac{E_4}{\rho_4}}})) \cos(\frac{2\omega\pi(L_{solid} + \frac{w}{2})}{\sqrt{\frac{E_5}{\rho_5}}}) \\
& + \rho_4 \sqrt{\frac{E_5}{\rho_5}} \sin(\frac{2\omega\pi(L_{solid} + \frac{w}{2})}{\sqrt{\frac{E_5}{\rho_5}}}) (E_3 \sqrt{\frac{E_4}{\rho_4}} \cos(\frac{w\omega\pi}{\sqrt{\frac{E_3}{\rho_3}}}) \cos(\frac{2\omega\pi L_{solid}}{\sqrt{\frac{E_4}{\rho_4}}}) \\
& - \sqrt{\frac{E_3}{\rho_3}} E_4 \sin(\frac{w\omega\pi}{\sqrt{\frac{E_3}{\rho_3}}}) \sin(\frac{2\omega\pi L_{solid}}{\sqrt{\frac{E_4}{\rho_4}}}))
\end{aligned} \tag{3.56}$$

$$B_3 = -\frac{F_I \sqrt{\frac{E_3}{\rho_3}}}{2A_{c3} E_3^2 \omega \pi} \tag{3.57}$$

$$B_4 = -\frac{F_I (E_3 \cos(\frac{w\omega\pi}{\sqrt{\frac{E_3}{\rho_3}}}) \cos(\frac{w\omega\pi}{\sqrt{\frac{E_4}{\rho_4}}}) \sqrt{\frac{E_4}{\rho_4}} + E_4 \sin(\frac{w\omega\pi}{\sqrt{\frac{E_3}{\rho_3}}}) \sqrt{\frac{E_3}{\rho_3}} \sin(\frac{w\omega\pi}{\sqrt{\frac{E_4}{\rho_4}}}))}{2E_4 \omega \pi (\cos^2(\frac{w\omega\pi}{\sqrt{\frac{E_4}{\rho_4}}}) + \sin^2(\frac{w\omega\pi}{\sqrt{\frac{E_4}{\rho_4}}})) E_3^2 A_{c3}} \tag{3.58}$$

$$\begin{aligned}
B_5 = -\frac{F_I}{2\sqrt{\frac{E_4}{\rho_4}} E_5 \omega \pi \rho_4 A_{c1} E_3^2} & (\rho_4 \sqrt{\frac{E_5}{\rho_5}} (E_3 \sqrt{\frac{E_4}{\rho_4}} \cos(\frac{w\omega\pi}{\sqrt{\frac{E_3}{\rho_3}}}) \cos(\frac{2\omega\pi L_{solid}}{\sqrt{\frac{E_4}{\rho_4}}}) \\
& - \sqrt{\frac{E_3}{\rho_3}} E_4 \sin(\frac{w\omega\pi}{\sqrt{\frac{E_3}{\rho_3}}}) \sin(\frac{2\omega\pi L_{solid}}{\sqrt{\frac{E_4}{\rho_4}}})) \cos(\frac{2\omega\pi(L_{solid} + \frac{w}{2})}{\sqrt{\frac{E_5}{\rho_5}}}) \\
& + \sin(\frac{2\omega\pi(L_{solid} + \frac{w}{2})}{\sqrt{\frac{E_5}{\rho_5}}}) E_5 (\rho_4 \sqrt{\frac{E_3}{\rho_3}} \sqrt{\frac{E_4}{\rho_4}} \sin(\frac{w\omega\pi}{\sqrt{\frac{E_3}{\rho_3}}}) \cos(\frac{2\omega\pi L_{solid}}{\sqrt{\frac{E_4}{\rho_4}}}) + E_3 \cos(\frac{w\omega\pi}{\sqrt{\frac{E_3}{\rho_3}}}) \sin(\frac{2\omega\pi L_{solid}}{\sqrt{\frac{E_4}{\rho_4}}}))
\end{aligned} \tag{3.59}$$

To find the value for L_2 that would maximize the displacement amplitude at the emitter surface, the displacement general solution was differentiated with respect to L_2 and set equal to 0 at the emitter position, producing equation (3.60):

$$0 = -\frac{2A_5 \omega \pi \sin(\frac{2\omega\pi(L_2 + L_{solid} + \frac{w}{2})}{\sqrt{\frac{E_5}{\rho_5}}})}{\sqrt{\frac{E_5}{\rho_5}}} + \frac{2B_5 \omega \pi \cos(\frac{2\omega\pi(L_2 + L_{solid} + \frac{w}{2})}{\sqrt{\frac{E_5}{\rho_5}}})}{\sqrt{\frac{E_5}{\rho_5}}} \tag{3.60}$$

Solving equation (3.60) using the solutions from equations (3.56) and (3.59) produces equation (3.61):

$$(3.61)$$

The derivation described above allowed L_1 and L_2 to be estimated based on a first-principles approach. Equations (3.47) and (3.61), while not reduced to closed-form solutions for L_1 and L_2 , allowed for the solution of these lengths via a trivial numerical estimation step, saving time in comparison to a naive search using more computationally intensive numerical tools such as FEA.

To validate the effectiveness of the first principles approach, an FEA analysis of the first principles solution for L_1 and L_2 was conducted. Figure 3.12 shows a cross-section of the FEA model constructed to verify the analytically produced dimensions. The simulation was conducted using the Harmonic Acoustic model in Ansys version 20.1, and the geometry was developed in Solidworks 2021. To simulate the motion of the transducer, harmonic pressures of equal magnitudes and opposite directions were applied to the outer surfaces of the piezoelectric disks. The model was constrained using fixed supports on the surfaces where the surface of the enclosure is designed to make contact with the surrounding pressure vessel. Since the ultrasonic energy is expected to be entirely converted to heat through cavitation, radiation boundary conditions were assigned to the open surfaces of the fluid domain in order to prevent any reflection effects.

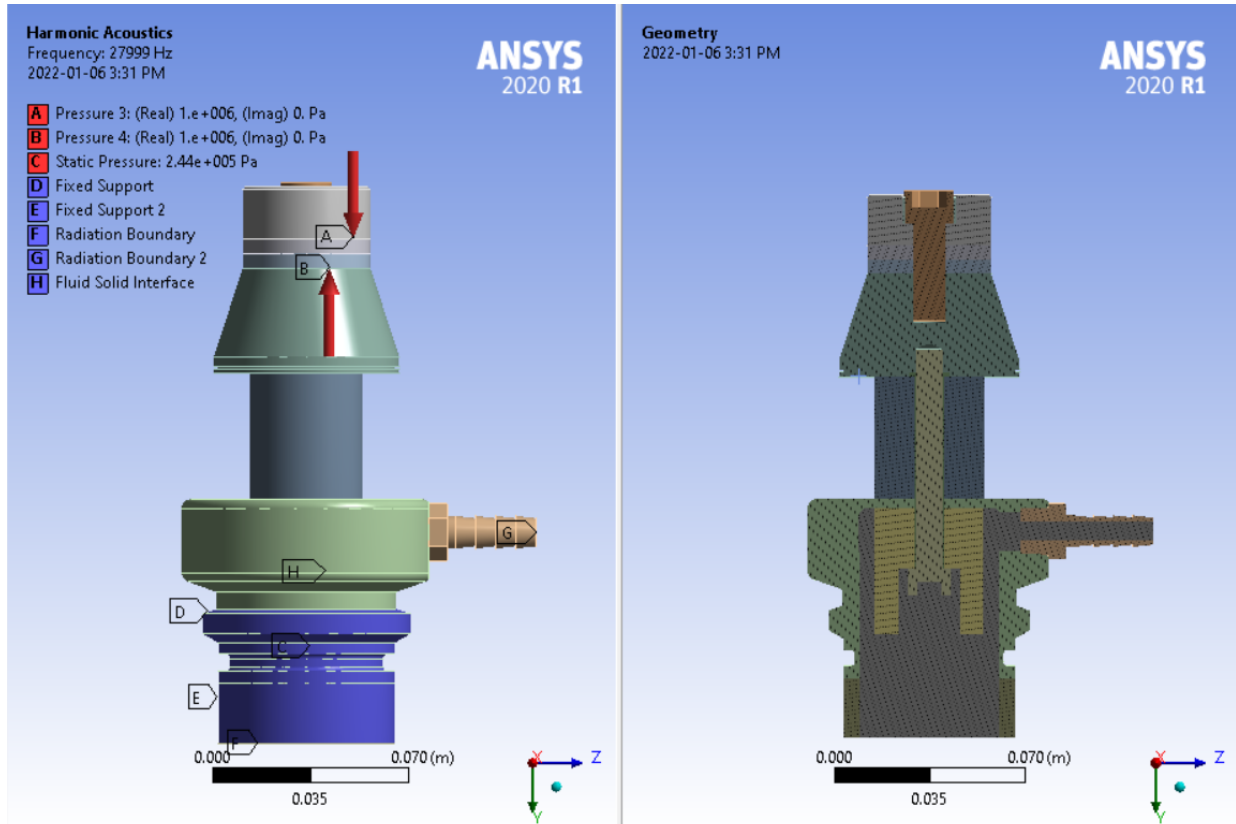


Figure 3.12: Full system FEA analysis with boundary conditions shown with arrows (left), and a cross-section of the geometry (right).

To provide a point of comparison, a default implementation where the transducer was simply affixed to the outside of the enclosure was also modelled in Ansys, as shown in Figure 3.13. All boundary conditions and materials are the same as in the simulation described above.

Since the analytical model assumed that the transducer would resonate at its specified operating frequency, the transducer model was investigated on its own before the full system simulations were conducted. Figure 3.14 shows the model developed for these purposes, which consisted of a modal analysis as well as a harmonic analysis with the same driving conditions as the full system model. All visible dimensions were measured manually from an ultrasonic transducer purchased from Beijing Ultrasonics, and dimensions that could not be measured (such as the length of the clamp bolt) were estimated based on mechanical design best practices. Materials were assigned based on a combination of data provided by the supplier and common practices discussed in the literature [60, 65].

To minimize the computational intensity of the FEA work, a mesh independence study was conducted on the isolated transducer model instead of the entire system. A mesh subjected to an Ansys “multizone” mesh control was compared against a default mesh at various resolutions to examine the consistency of the solution.

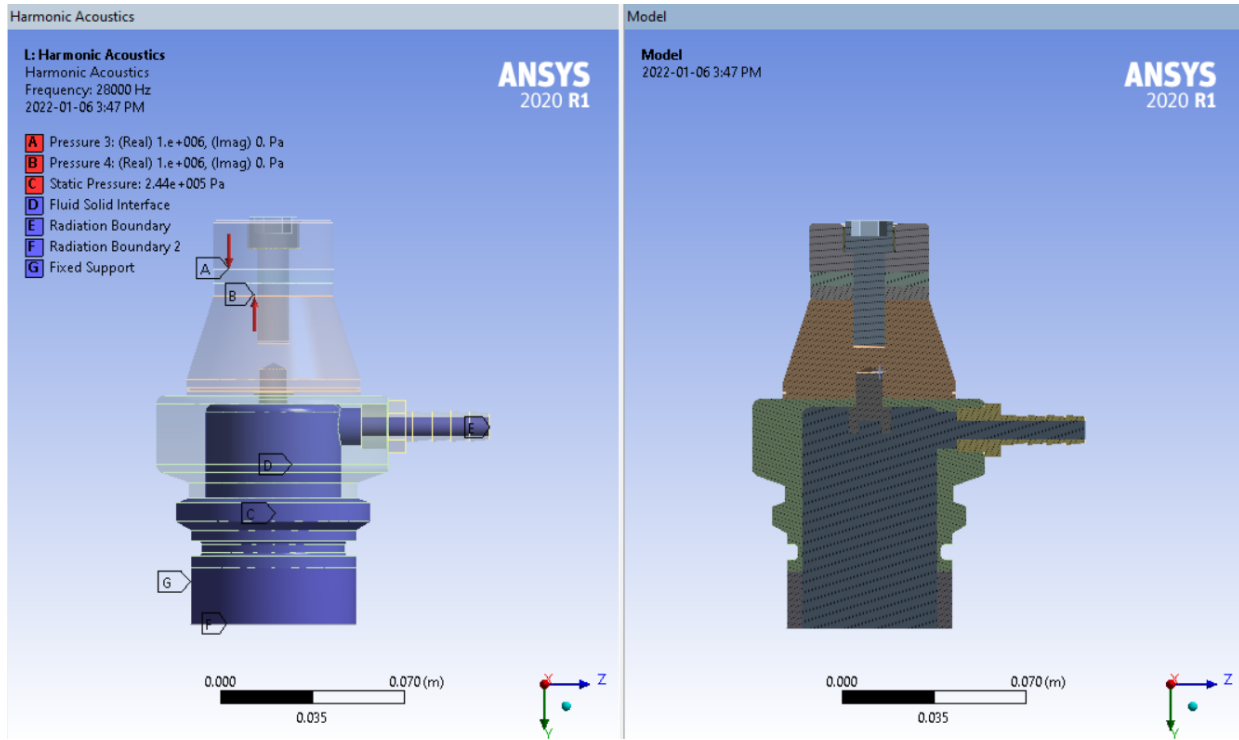


Figure 3.13: Default implementation FEA analysis with boundary conditions shown with arrows (left), and a cross-section of the geometry (right).

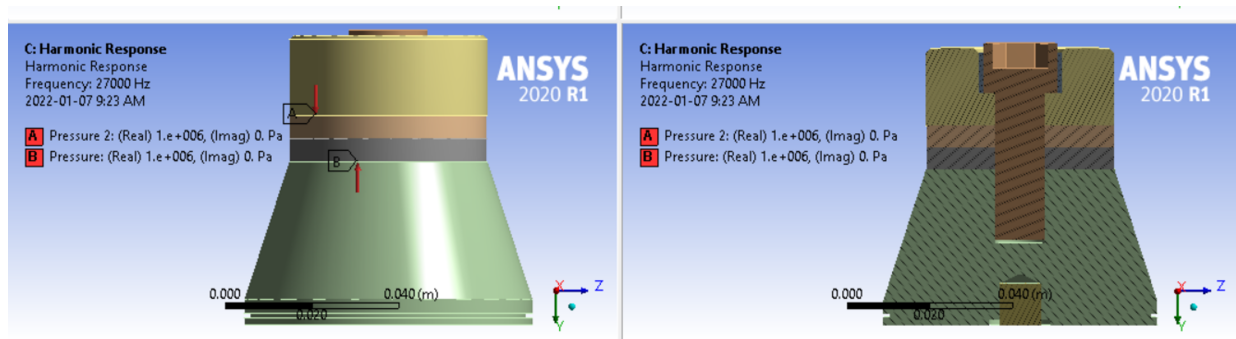


Figure 3.14: Simulation conditions (left) and cross-section (right) for the transducer FEA analysis. Before the simulations were conducted on the full system, modal and harmonic analyses were conducted on the transducer in isolation to investigate mesh convergence and verify the reasonableness of the simulation results.

3.5.3 Results

The analytical process was conducted first, in order to inform the dimensions tested within the FEA simulation. The transducer model was then constructed in order to test mesh independence and tune the transducer materials. Then, the default case and the dimensions calculated analytically were both tested.

Table 3.5 shows the material and material properties assigned to each part of the system as illustrated in Figure 3.10. To account for the possibility that the mounting bolt running through the center of the system could be a different material from that of the external horn and the enclosure, the effective material properties of the segments were treated as an average of the properties of the bolt material and the enclosure or horn material, weighted based on their relative cross-sectional areas. This approach was also used to factor in the effect of filling all gaps and clearances within the system with epoxy.

Table 3.5: Material properties of the Ultrasonic Horn for fouling mitigation

Component	Material	Density (kg/m ³)	Elastic Modulus/Stiffness Matrix (Pa)	Source
Transducer back mass	Stainless steel	7750	1.93×10^{11}	[76]
Clamp bolt	High Strength Low Alloy Steel	7850	2.1×10^{11}	[76]
Piezo-electric disks	PZT 4	7500	$k_{11} = \begin{bmatrix} 1.39 \times 10^{11} & 7.43 \times 10^{10} & 7.78 \times 10^{10} \\ 7.43 \times 10^{10} & 1.15 \times 10^{11} & 7.78 \times 10^{10} \\ 7.78 \times 10^{10} & 7.43 \times 10^{10} & 1.39 \times 10^{11} \end{bmatrix}$ $k_{22} = \begin{bmatrix} 2.56 \times 10^{10} & 0 & 0 \\ 0 & 3.06 \times 10^{10} & 0 \\ 0 & 0 & 2.56 \times 10^{10} \end{bmatrix}$	[77]
Transducer front mass	Aluminum Alloy (tuned)	2810	7.1395×10^{10}	[76]
Epoxy filling	Resin Epoxy	1160	3.78×10^9	[76]
Mounting bolt	High Strength Low Alloy Steel	7850	2.1×10^{11}	[76]
External horn	Aluminum Alloy	2770	7.1×10^{10}	[76]
Enclosure	Stainless steel	7750	1.93×10^{11}	[76]
Fitting	Stainless steel	7750	1.93×10^{11}	[76]
Emitter	Aluminum Alloy	2770	7.1×10^{10}	[76]
Fluid medium	Water	998.2	-	[76]

3.5.3.1 First Principles Results

Table 3.6 describes the dimensions and material properties used for each segment within the analytical model. Numerical solving of equations 3.47 and 3.61 using the values included in Table 3.6 yielded lengths

of $L_1 = 44.72\text{mm}$ and $L_2 = 24.08\text{mm}$. These values represented the solution of the first principles approach, which went on to be examined in the FEA simulation and used for the experimental setup.

Table 3.6: Parameters used for analytical calculations

Section	Length (mm)	Outer Diameter (mm)	Inner Diameter (mm)	Density (kg/m ³)	Elastic Modulus (Pa)
1	L_1	40	0	3050.74375	78805237500
2	1.5875	40	0	7654.13125	191578987500
3	1.5875	40	0	7654.13125	191578987500
4	22	40	0	3050.74375	78805237500
5	L_2	40	22.5	2700	71000000000

3.5.3.2 Finite Element Analysis Results

Figure 3.15 shows the results of the mesh independence analysis. Explicitly defining the maximum element size within the mesh settings was determined to be ineffective due to meshing failures at many maximum mesh sizes. The exact source of these errors was unclear, but they seemed to stem from the Ansys meshing software struggling to discretize the model geometry into elements complying with the constraints produced by assigning specific values to the maximum mesh size parameter. Therefore, the mesh was refined by adjusting the “resolution” parameter within the Ansys meshing settings. The number of elements produced by each meshing resolution was recorded in order to provide a more effective comparison between the two approaches.

Figure 3.15 shows consistency in the uncontrolled mesh results from element counts of 8214 to 37602, whereas the multizone mesh results continued to vary relatively significantly throughout this range and did not show a convincing degree of consistency even with a mesh consisting of 69225 elements. Therefore, an uncontrolled meshing approach was selected for the ensuing analysis. The meshing settings that produced the 27202 element uncontrolled mesh were selected for use in the remainder of the analysis, as this configuration produced the results that most closely resembled the expected results (27999 Hz produced by the simulation, in comparison to an expected frequency of 28000 Hz). This mesh was produced by setting the Ansys meshing Resolution parameter to a value of 6.

Figure 3.16 shows the results of the modal and harmonic analyses conducted on the transducer with the selected meshing criteria. It is worth noting that the manufacturer specifications for the transducer modelled include a tolerance of ± 1 kHz on the nominal transducer frequency, so all the results obtained by this FEA model were reasonable [60, 62].

Figure 3.17 shows the deformation in the longitudinal axis of the default implementation of the system, and Figure 3.18 shows the total deformation of the system. Clearly, this design did a poor job of transferring vibrations through the enclosure and into the fluid medium; instead, the enclosure resisted the motion of the transducer face. The vibrations produced by the piezoelectric disks remain largely confined to the transducer itself, and longitudinal deformation does not exceed an order of magnitude of 10^{-8} m within the enclosure.

Figure 3.19 and 3.20 shows the longitudinal and total deformation of the horn design (respectively) using the dimensions calculated from the analytical approach. As can be seen, the emitter experienced

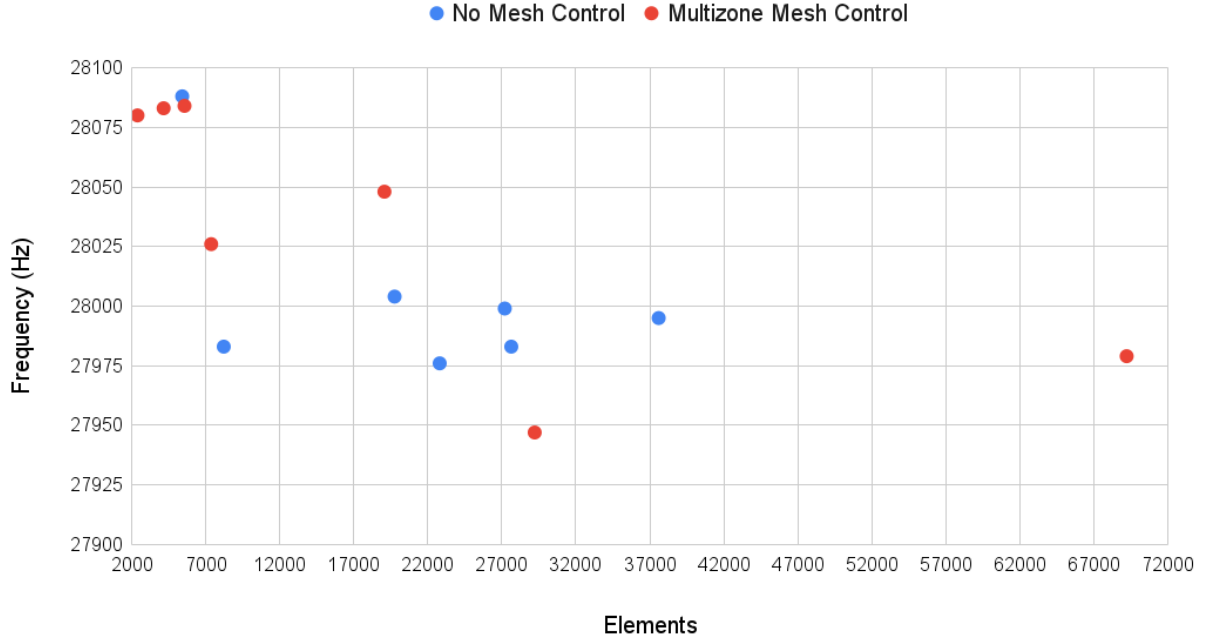


Figure 3.15: Mesh independence study comparing a Multizone mesh control against a default Ansys mesh at various resolutions. The figure shows good agreement among the results produced with an uncontrolled mesh past 8214 elements. The results produced by the most refined mesh, which was a mesh produced with multizone mesh control, also agreed well with the uncontrolled mesh results. The resonant frequency predicted by an uncontrolled mesh comprised of 27202 elements agreed particularly well with the expected results, returning a resonant frequency of 27999 Hz in comparison to the expected 28000 Hz; therefore, the resolution settings that produced this mesh were used for the rest of the analysis. This mesh was produced by setting the Ansys meshing Resolution parameter to a value of 6.

substantial longitudinal deformation, reaching an order of magnitude of 10^{-6} m at its greatest deformation. Figure 3.20 shows that the enclosure did not experience significant longitudinal deformation in comparison to the vibrating column; rather, the deformation produced within the enclosure came primarily from the radial expansion and contraction of the vibrating column. The emitter also experienced significant radial deformation.

To highlight the differences in the vibratory behaviours of the different implementations, a compilation of all of the FEA results associated with the comparative FEA analysis is included in Figure 3.21.

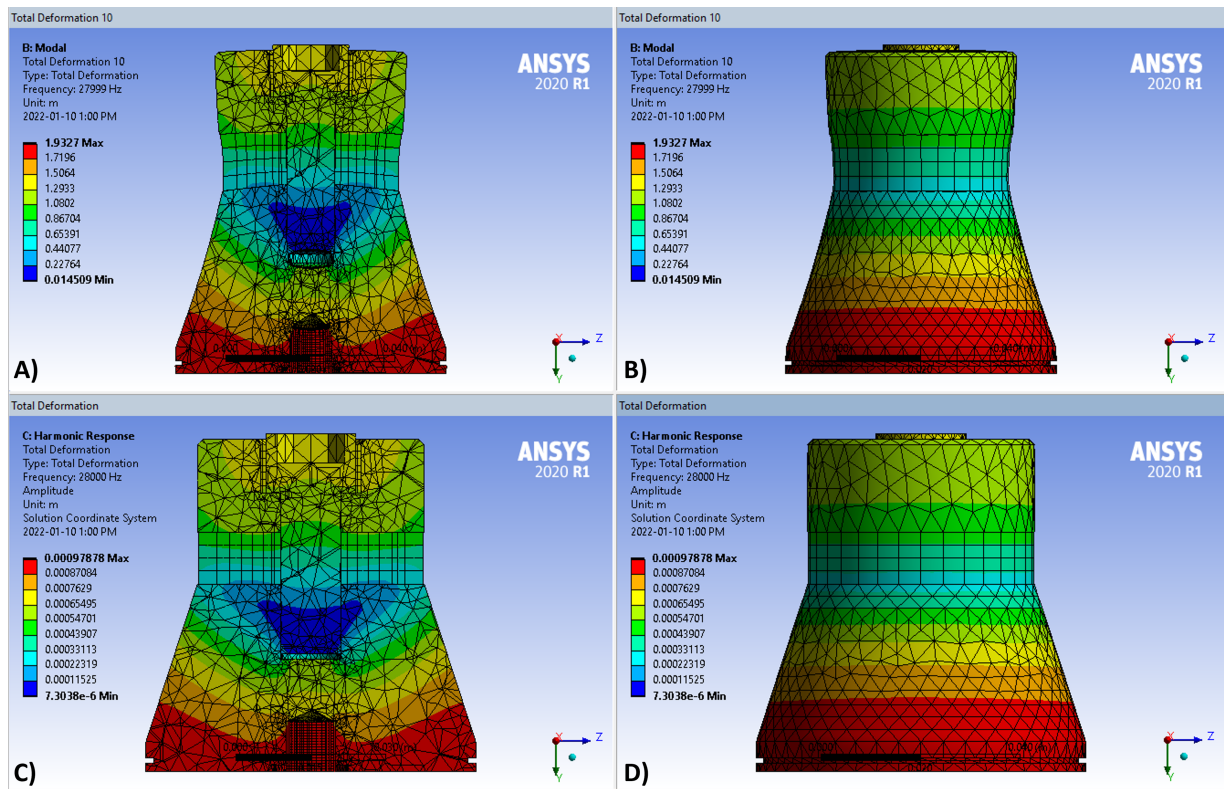


Figure 3.16: Modal (A,B) and harmonic (C,D) analysis results for the isolated transducer model. The legend values for plots C) and D) have units of meters (m).

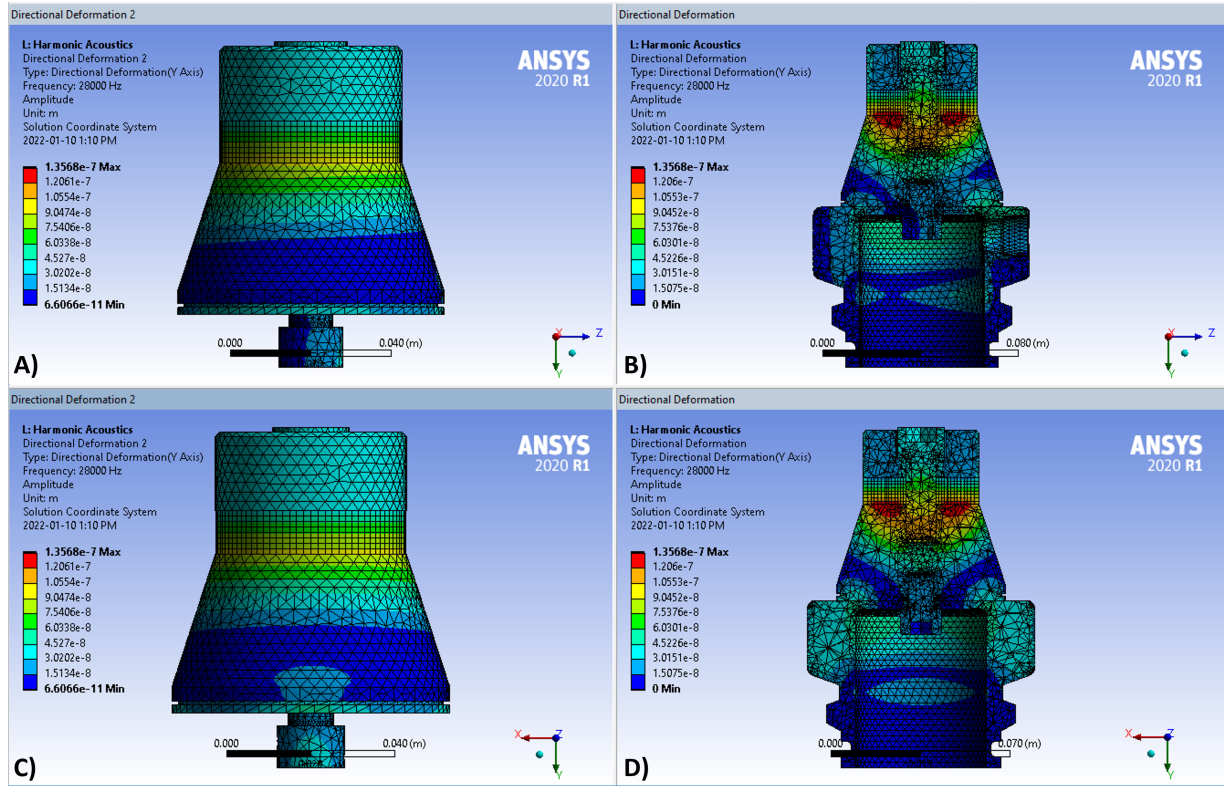


Figure 3.17: Directional deformation of the default transducer installation. Panels B and D show that the maximum deformation occurs within the transducer itself, with other regions of high deformation amplitude occurring within the sides of the membrane module enclosure end cap. A region of minimum deformation appears near the enclosure end cap boundary. The enclosure was excluded from panels A and C to avoid obstructing relevant elements of the system in the other figures. All legend values have units of meters (m).

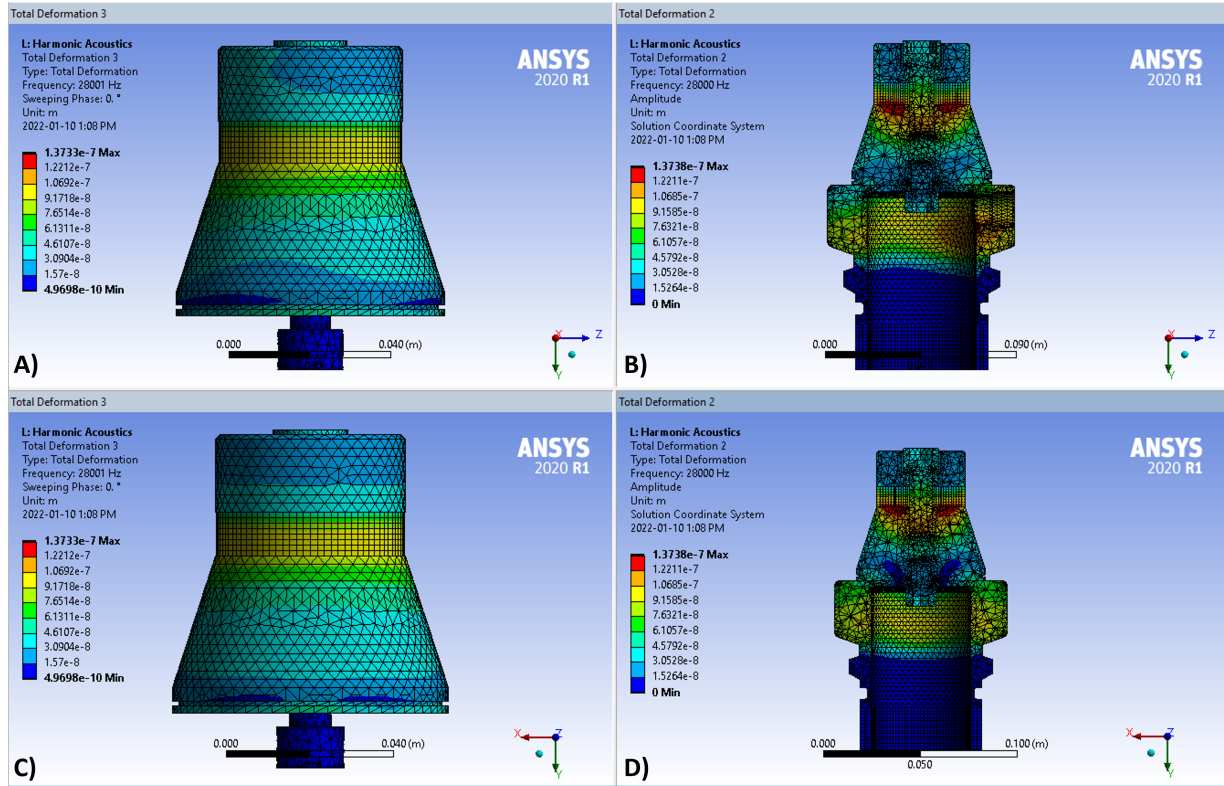


Figure 3.18: Total deformation of the default transducer installation. Panels B and D show that the maximum deformation occurs within the transducer itself, with other regions of high deformation amplitude occurring within the sides of the membrane module enclosure end cap. A region of minimum deformation appears near the enclosure end cap boundary. The enclosure was excluded from panels A and C to avoid obstructing relevant elements of the system in the other figures. All legend values have units of meters (m).

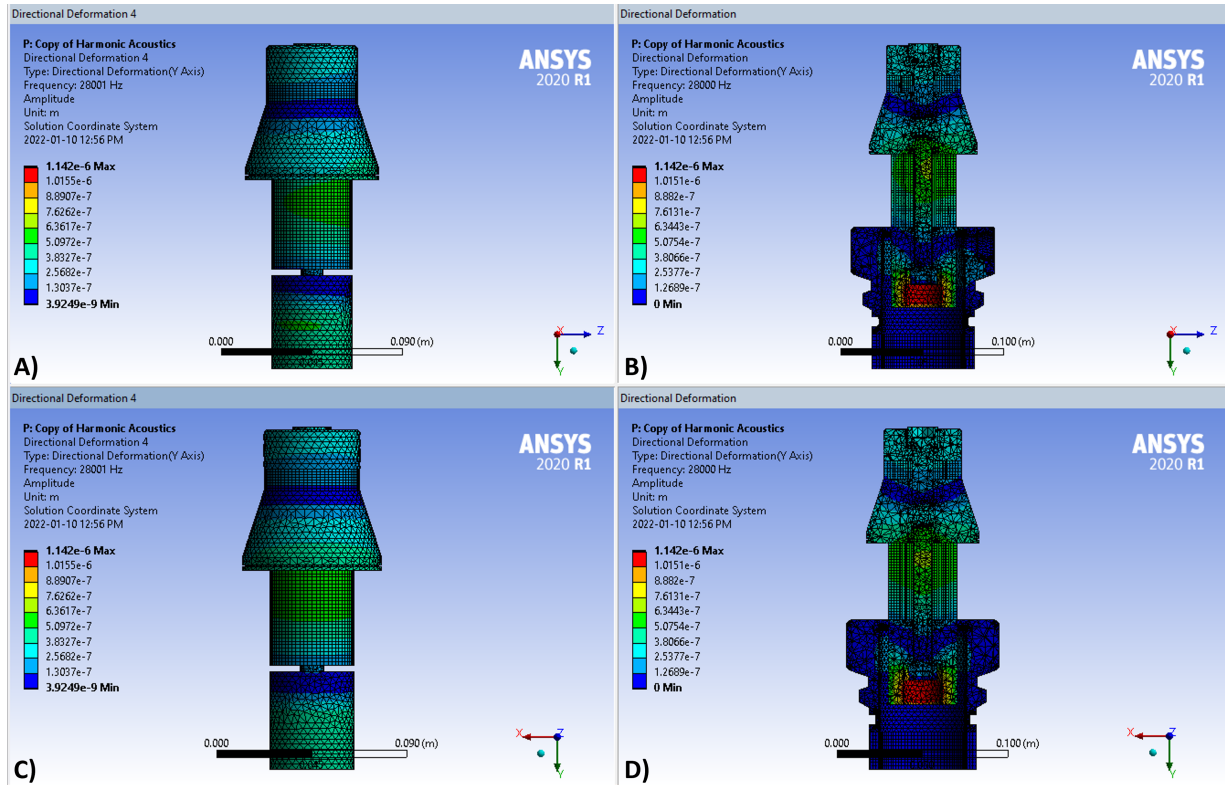


Figure 3.19: Directional deformation of the actual transducer installation. Panels B and D show that the maximum deformation occurs near the free face of the emitter, with other regions of high deformation amplitude occurring within the external horn. A region of minimum deformation appears near the enclosure end cap boundary. The enclosure was excluded from panels A and C to avoid obstructing relevant elements of the system in the other figures. All legend values have units of meters (m).

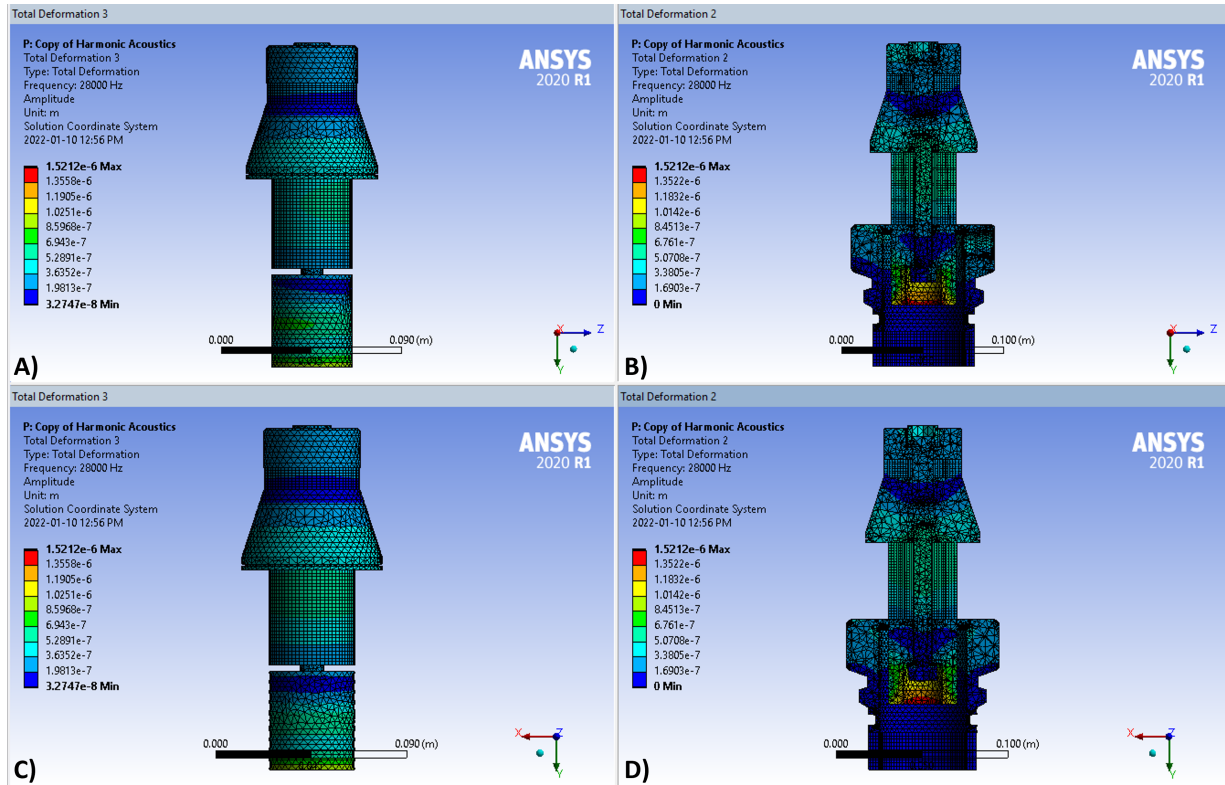


Figure 3.20: Total deformation of the actual transducer installation. Panels B and D show that the maximum deformation occurs near the free face of the emitter, with other regions of high deformation amplitude occurring within the external horn. A region of minimum deformation appears near the enclosure end cap boundary. The enclosure was excluded from panels A and C to avoid obstructing relevant elements of the system in the other figures. All legend values have units of meters (m).

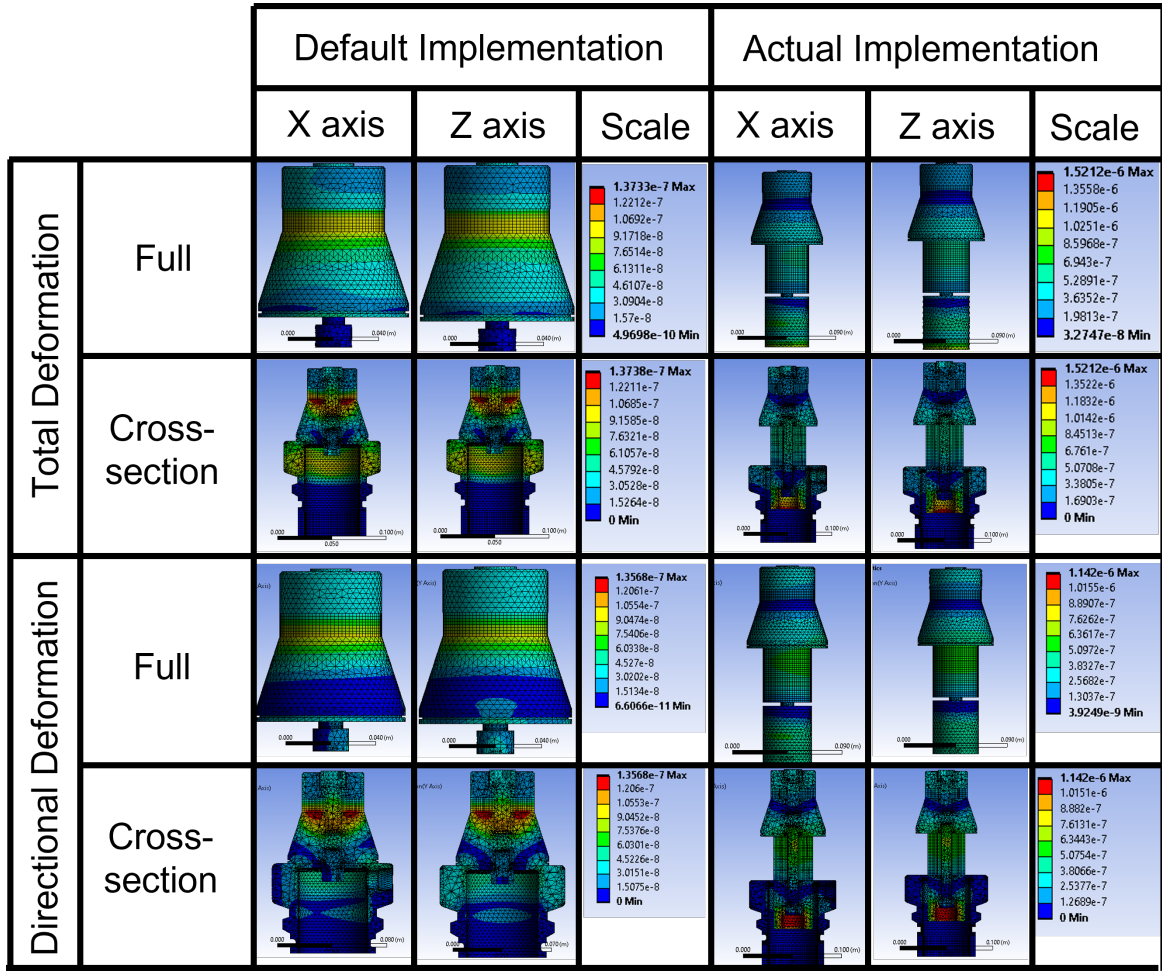


Figure 3.21: Compilation of all the FEA results generated, provided for comparison purposes. All legend values have units of meters (m).

3.5.4 Discussion

The results above show that the dimensions produced by the first principles analysis achieved reasonable effectiveness with regards to producing longitudinal vibrations at the emitter while limiting the transfer of vibrations to the enclosure, which were the express purposes of this investigation. Figures 3.19 and 3.20 show that the deformation within the actual system is close to its minimum value near the interface between the horn and the enclosure, while its maximum deformation occurs close to the free end of the emitter. These results suggest the existence of a displacement node in the proximity of the enclosure boundary and an anti-node at the free face of the emitter, as predicted by the first principles analysis. By comparison, Figures 3.17 and 3.18 show that the maximum deformation within the system occurs within the transducer, and that the vibrations are largely distributed throughout the enclosure end cap. The maximum deformations recorded for the actual system exceed those of the default implementation by an order of magnitude. Therefore, the horn design using the recommended dimensions will outperform the default implementation in terms of transferring longitudinal vibrations to the fluid within the membrane module.

However, some aspects of the of the results suggest that the performance of the system could be further optimized. Firstly, the nodal regions shown by the areas of minimum deformation in Figures 3.19 and 3.20 are not perfectly perpendicular to the direction of vibration, as they would be were the system vibrating in perfect longitudinal vibration. There are two factors that could contribute to this. First, the emitter face of the transducer is wider than a quarter wavelength, which is considered to be the threshold beyond which one-dimensional approximations such as those made within the first principles analysis fail to apply [64, 65]. Second, the fact that the last segment of the emitter horn is hollow may have contributed to this irregularity. Horns with discontinuities in their cross-sectional areas are not uncommon; however, the change in cross-sectional area is typically accomplished by changing the outer diameter of the horn as opposed to the inner diameter [62, 63, 65].

Secondly, the maximum longitudinal deformation in the external system does not occur precisely at the emitter face of the transducer, but in fact occurs within the external horn. Similarly, the region of minimum deformation nearest the enclosure wall is within the immersed horn segment. This suggests that the assumption of a deformation anti-node at the transducer face is not necessarily valid, and that the first principles analysis may have to include the transducer itself in order to better approximate an optimal solution. Preliminary attempts were made to develop such a model; however, initial results were poor, and further efforts were curtailed due to time constraints around the experimental portions of the investigation. It is also possible that these slight discrepancies have to do with the decision to discount the effects of the enclosure on the vibration column, even though there is significant interaction between the vibration column and the enclosure due to the radial deformation of the column. This can be an area for further optimization in future research.

3.6 Summary of Findings

Ultrasonic horns with the dimensions calculated using the first principles analysis produced longitudinal vibrations at the selected operating frequency of 28 kHz when modelled using FEA, with minimal transfer of vibrations to the membrane module enclosure in comparison to a default configuration that did not incorporate ultrasonic horns. The maximum displacement amplitude of the ultrasonic horns, which occurred close to

the submerged emitter, was approximately an order of magnitude greater than the maximum displacement amplitude produced in the default system, which occurred within the transducer itself. While simplifications made in the first principles analysis resulted in slight differences between the locations of maximum and minimum displacement amplitude predicted by the first principles analysis and those reported by the FEA simulation, the calculated dimensions still produced the performance enhancements that motivated this investigation.

When considering the effects of variations in material properties and fabrication tolerances on resonance behaviour, it was decided that attempts to improve the theoretical performance of the horn dimensions were unlikely to produce appreciable performance improvements when the horn was fabricated and installed. Therefore, the broader experimental investigation proceeded with the dimensions stated in the First Principles Results section (Section 3.5.3.1).

Chapter 4

Experimental Setup and Analysis of the Novel Ultrasonic Horn Design

4.1 Introduction

While the results of the simulation and modelling endeavours described above represent contributions to the UFM state of the art, only experimental results can prove the practical viability of this technology. To that end, an experimental setup was designed and constructed, an experimental methodology was developed, and the resulting data was analyzed to surmise the effectiveness of UFM for pilot-scale SWRO modules. Figure 4.1 shows the constructed experimental setup. The sections below detail the nature of its various subsystems, as well as the specifics of the experiments for which it was developed.

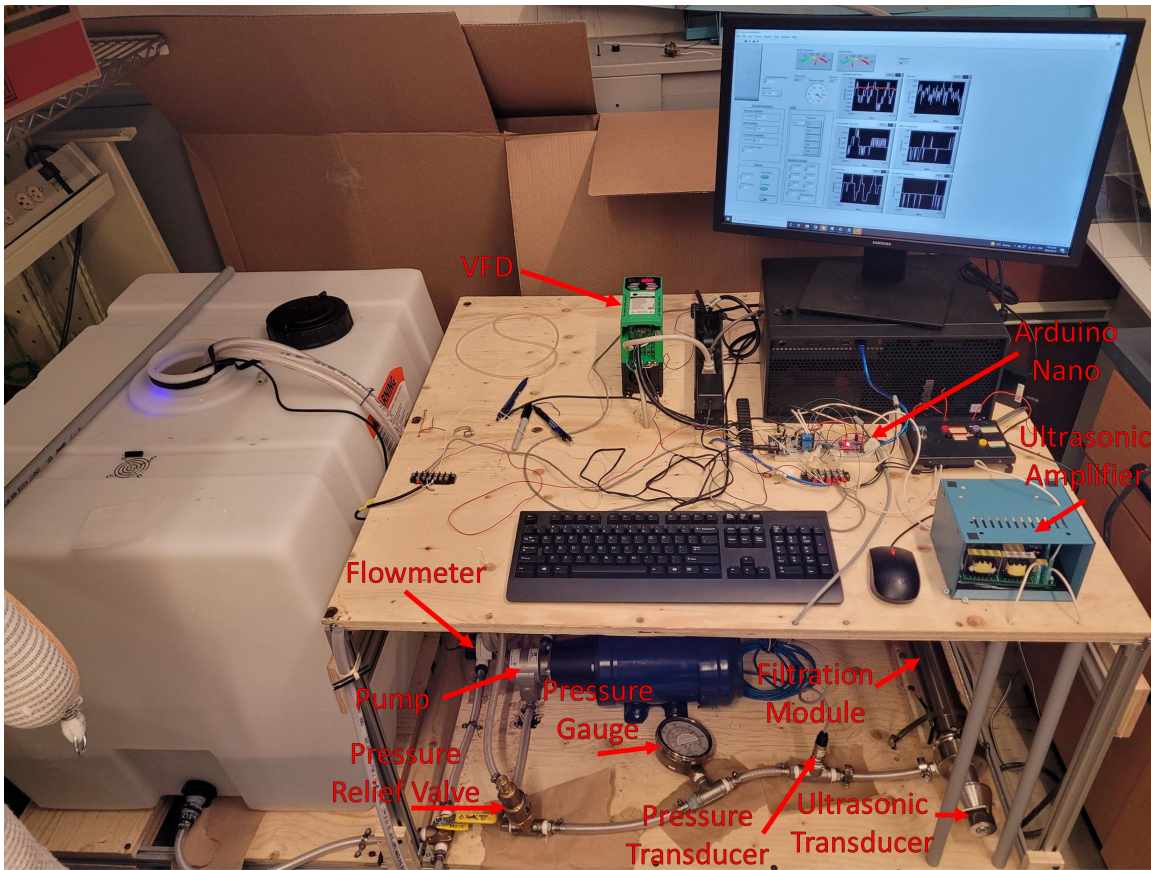


Figure 4.1: An image of the experimental setup developed and constructed for this research.

4.2 Experimental Setup

The experimental setup consists of a system of flow components controlled and monitored by an instrumentation network employing custom firmware, within which experiments are run and observed using a custom program developed on the Labview software platform. The following subsections describe in detail the operation of the different modules of the experimental setup, as well as how they interact.

4.2.1 Mechanical System

Figure 4.2 shows a diagram of the system. The operating principle is simple: feed water is stored in the reservoir, from which it is pumped into the filtration module at a rate measured using a flow meter (Omega FPR132) and a pressure determined using a pressure transducer (Honeywell PX2EN1XX250PSAAX) and limited by a relief valve. There, it is separated by the SWRO module contained therein into permeate and concentrate. The rates of permeate and concentrate production are measured independently with flow meters (McMaster-Carr 4126K74 and Omega BV1000TRN025B, respectively), allowing the control software to check the system for leaks based on mass conservation principles. The conductivities of the feed water and permeate are both measured using conductivity meters (EC/pH Transmitters A1003V8), which allows the approximate concentration of ionic constituents in the feed and permeate waters to be measured and compared. The pressure and flow rate at the inlet of the filtration module are controlled by the pump and the motorized ball valve (Valworx 565256C). The motorized ball valve was connected to the concentrate outlet of the filtration module, raising the pressure within the filtration module by resisting the flow at its outlet.

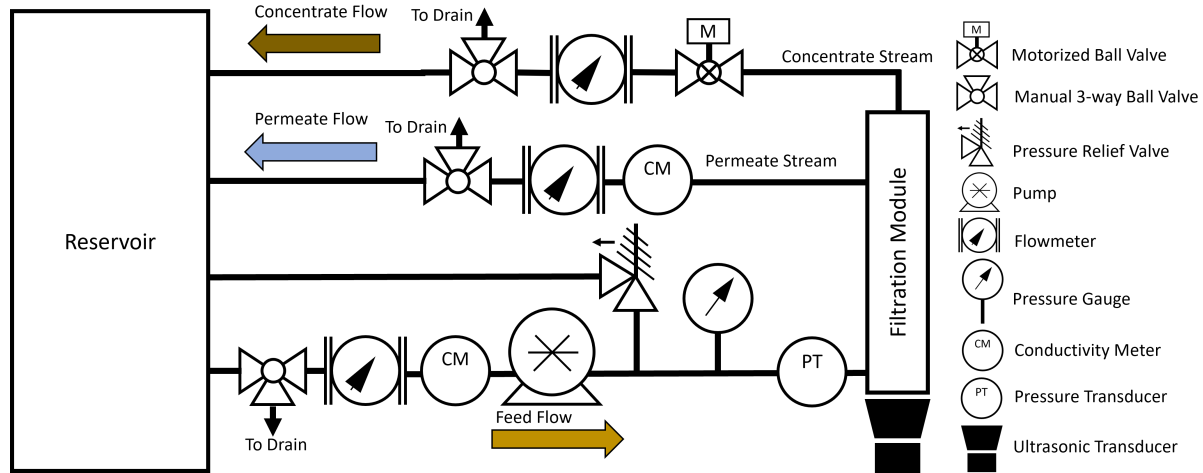


Figure 4.2: Experimental setup flow diagram.

4.2.2 Instrumentation and Firmware

Figure 4.3 shows the wiring of all instrumentation components within the experimental setup. An Arduino Nano hosting custom firmware was used to communicate with the various peripherals within the system. The peripherals used are described below:

- **Variable Frequency Drive (VFD):** This was used to drive the pump at varying frequencies based on the experimental conditions required. The VFD (Sterlitech Commander C200 series) used in this experimental setup required two digital inputs to be energized with 20 V in order to operate. The output frequency of the VFD was calculated proportionally from an analog voltage input, where the absolute maximum and minimum allowable drive frequencies were internally mapped to inputs of 10 V and 0 V, respectively. The VFD provided a 0 V to 10 V analog output corresponding to the actual frequency of the drive.
- **Motorized Ball Valve:** The valve was opened and closed to varying degrees in order to produce suitable back pressure within the filtration module. The valve required a 4 – 20 mA control signal, which was proportionally related to the rotational position of the valve such that a 4 mA signal closed the valve and a 20 mA signal fully opened the valve. The valve also provided a 4 – 20 mA corresponding to the position of the valve.
- **Ultrasonic Amplifier:** The ultrasonic amplifier converted electricity from a standard North American outlet to a signal at the voltage and frequency required by the ultrasonic transducer. The transducer is activated by a digital signal sent to a relay installed between the amplifier and its power source.
- **Flow Meters:** These devices output electrical pulses at a rate proportional to the volumetric rate of fluid flowing through them. These pulses were passed through resistor networks to bring their voltages down to an acceptable level for the digital inputs on the Arduino, and counting functionality was implemented within the Arduino firmware to track these pulses by detecting changes in the state of digital inputs from low voltage to high voltage.
- **Conductivity Meters:** These devices provide an analog voltage output between 0 and 5 V that is calibrated based on the expected conductivity range of the fluid passing through the conductivity meter.
- **Pressure Transducer:** This device provides a voltage output between 0 and 5 V, corresponding proportionally to pressures in a range of 0 to 250 psi.

Since the pins on the Arduino Nano are only rated up to 5 V, some circuitry was required to control higher voltages. In particular, simple transistor circuits were used to provide digital signals beyond 5 V, and operational amplifier circuits were constructed to produce analog voltages outside of the 0 – 5 V range. A voltage-controlled current source was constructed using an operational amplifier to drive the motorized ball valve. Since the Arduino Nano does not have the capability to produce truly analog voltage outputs, its Pulse Width Modulation (PWM) pins were used to approximate analog voltages between 0 and 5 V. Inputs to the Arduino were scaled to the appropriate voltage range using resistor networks.

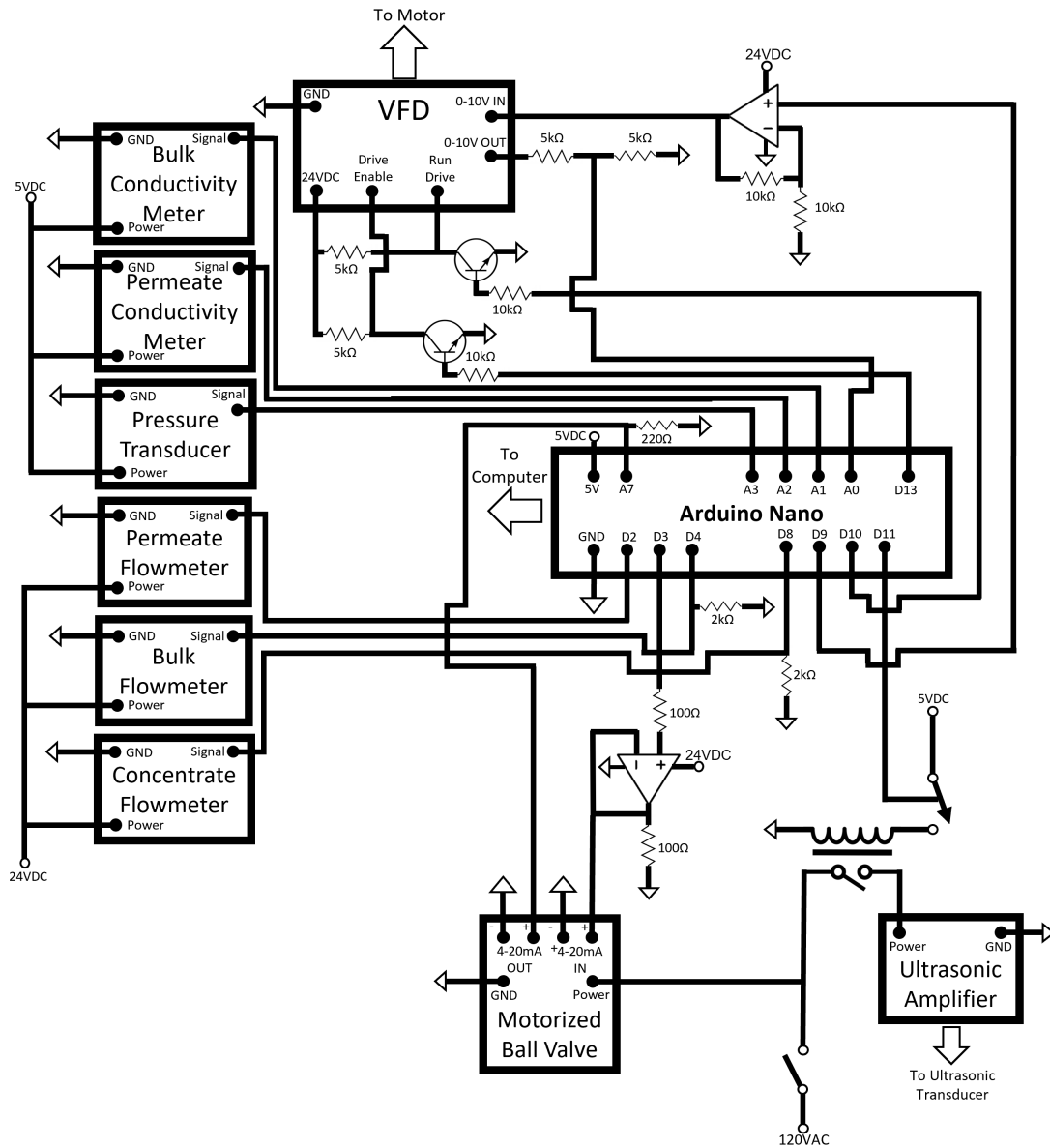


Figure 4.3: Diagram of the instrumentation used for the experimental setup.

4.2.3 Software

The system was developed using the Labview software package. The primary purpose of the software was to compile and unpack the 8 byte integer arrays used to communicate with the custom firmware running on the Arduino to which the experimental setup is wired. The software also converted the outputs of the Arduino into appropriate units for their measurements based on calibration constants that can be supplied by the user via the user interface. Figures 4.4 and 4.5 show the user interface and logic used to control the experimental setup.

It was discovered in the development of the experimental setup that the execution frequency of the Labview loop deteriorates rapidly as the complexity of the code increases. This introduced problems with flow rate measurements, as the pulse frequencies of the flow meters were beyond the attainable operating frequency of the Labview loop at flow rates well within the operational envelope of the setup. To combat this, the firmware installed on the Arduino was designed to return a count of pulses over a 100 ms interval, and the Labview program was designed to operate at 10 Hz.

Control of the system was rudimentary: user-supplied integers between 0 and 255 in the “Valve Control” and “Motor Control” inputs were sent directly to the Arduino as duty cycle values for the PWM pins corresponding to the ball valve position and VFD frequency. Theoretically, feedback control principles could be used to calculate the control values for the VFD frequency and ball valve position from user-provided pressure and flow rate setpoints; however, manual control was considered sufficient for initial investigations.

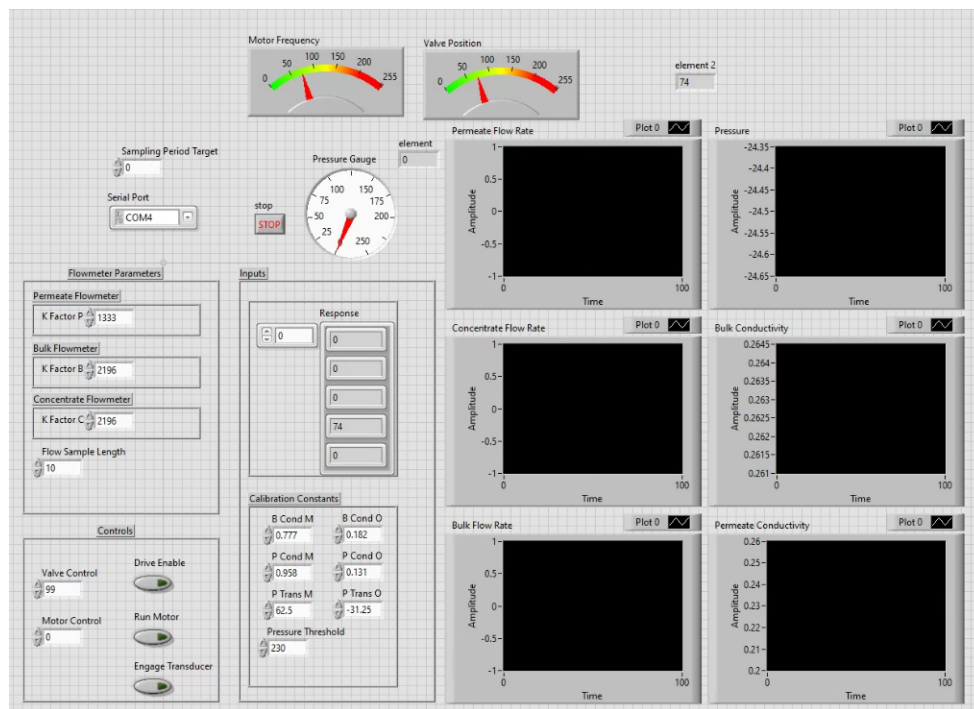


Figure 4.4: User interface of the experimental setup control program, built using Labview.

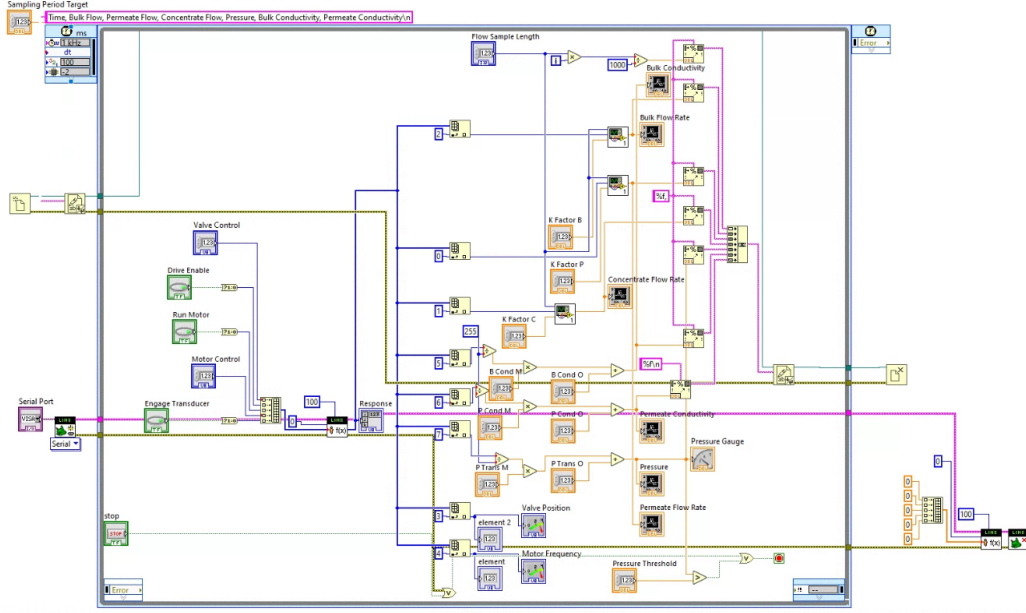


Figure 4.5: Control logic of the experimental setup control program, built using Labview.

4.3 Experiment Design

The overall goal of the research is to determine whether UFM can be effective in mitigating fouling within SWRO modules. The findings of the cavitation propagation modelling research suggested that UFM would be most effective when implemented as part of an intermittent cleaning regime due to the reduction in operating pressure required to produce cavitation onset throughout the module. Therefore, the experiment was designed with the goal of assessing the effectiveness of a UFM cleaning regime at restoring the performance of a fouled membrane.

4.3.1 Feed Water Design

The primary purpose of applying RO to brackish groundwater is the removal of dissolved inorganic constituents [4]. Concentration of inorganic solutes within fluids can be measured fairly simply by monitoring the conductivity of the solutions [78]. Inorganic fouling is a significant contributor to the fouling developed when treating brackish groundwater with RO [4]. Therefore, the decision was made to test the effectiveness of UFM for mitigating inorganic fouling within SWRO modules treating inorganic solutions.

To simplify the preparation of experimental materials and the correlation of conductivity to concentration, it was decided that the feed water should have only one inorganic constituent [78]. Calcium sulphate (CaSO_4) was selected as the solute. It was chosen due to the high prevalence of both calcium and sulphate in groundwater samples taken as part of previous studies investigating RO treatment of brackish groundwater, as well as the existence of prior research investigating calcium sulphate fouling in RO contexts [4, 26, 79, 80]. A similar argument could have been made for the use of calcium carbonate (CaCO_3); however, the solubility of calcium carbonate decreases with temperature, whereas the solubility of the least soluble solid form of calcium sulphate increases with temperature in the temperature ranges considered for this experiment [4,

26, 59, 81]. Therefore, to prevent scaling from occurring within the pump due to elevated temperatures, calcium sulphate was selected.

To produce severe fouling as quickly as possible, it was decided that the solution should be saturated with calcium sulphate. This corresponds to a concentration of about 2000 mg/L, which is within the definition of “brackish” established earlier [16].

4.3.2 Experimental Conditions

When membranes are depressurized between extended operation intervals, they typically exhibit a temporary but significant performance recovery when operation is resumed [4]. This is due to the dissipation of Concentration Polarization developed during operation, as well as some fouling mitigation due to mild flow reversal as the forward osmotic pressure exceeds the driving pressure and pushes clean water back through the membrane [4, 24, 82, 83]. Because of this, an observed performance recovery after a UFM cleaning cycle would not be sufficient to demonstrate that the UFM itself was effective, as there is no way to distinguish the performance recovery attributable to the natural effects described above from performance recovery produced by UFM. To that end, a control cleaning cycle had to be established for comparison, that was identical to the UFM-enabled cleaning cycle in all attributes except the application of ultrasound.

The establishment of a control cleaning cycle only facilitates effective comparison if the cleaning cycles are conducted on membranes that are fouled to similar degrees. Therefore, the extent to which the membranes have been fouled must be monitored in order to ensure that the cleaning cycles are applied consistently. Membrane performance in the presence of inorganic fouling tends to be asymptotic, as the decreasing rate of permeate flux through the membrane reduces the rate of solute exclusion at the membrane surface, thus limiting the extent to which the elevated contaminant concentrations necessary for solute precipitation can develop [4, 25, 26]. Therefore, it was decided that cleaning would occur when membrane performance reached approximate stability, as the stable performance of the membrane should remain unchanged by cleaning cycles unless the permeability of the membrane itself were somehow altered (by damage from the high intensity ultrasound, for example). The practical quantification of stability was not decided upon at this stage, as it was expected to depend on the specific properties of the experimental setup and feed water.

4.3.3 Cleaning Cycle Design

The design of the cleaning cycle itself is extremely important to the success of the experiment. The nature of the experimental setup does not allow the modulation of ultrasonic intensity, so three parameters control the operating conditions during a UFM-enabled cleaning cycle: inlet pressure, inlet flow rate, and cleaning cycle duration. The research conducted on cavitation propagation found that maintaining a fixed flow rate while varying the inlet pressures between 335 – 355 kPa could produce inertial cavitation throughout a SWRO module assuming nominal performance characteristics for the module. However, it was noted from the literature that membrane fouling can also increase the hydrodynamic resistance of the SWRO module feed channel, resulting in the pressure drop along the length of the module being higher than the nominal parameters used in the modelling research would predict [84]. For this reason, it was decided that the cleaning cycle would begin and end at the filtration operating pressure of 1551 kPa, reaching a minimum value of 335 kPa halfway through the cleaning duration, while the flow rate would be kept at the nominal system flow rate of $8.796 \times 10^{-5} \text{ m}^3/\text{s}$ whenever possible.

Prior art was consulted to determine a reasonable duration for the cleaning process. A study involving the reversal of organic fouling of MF and UF membranes on small, flat-sheet membranes using a combination of water washing and sonification applied via an ultrasonic bath successfully employed a cleaning period of 40 minutes [42]. An article investigating the chemical cleaning of RO membranes subjected to both organic and inorganic fouling showed that cleaning durations of greater than 15 minutes were effective, with durations of 30 minutes restoring membranes to nearly 100% effectiveness [85]. Since there exist cleaning technologies that are effective in the time frame of 15 – 40 minutes, it was decided that the initial cleaning cycles would employ a nominal duration of 30 minutes.

4.3.4 Data Collection and Interpretation

Throughout the experiment, the pressure and flow rate at the inlet of the SWRO module were controlled and recorded. Permeate production rate, permeate conductivity, and feed water conductivity were recorded. The permeate production rate was used to assess membrane performance M_P , expressed at time t using equation (4.1):

$$M_P(t) = \frac{P(t)}{P_i} \quad (4.1)$$

Here, $P(t)$ is the permeate production at time t , and P_i is the permeate flux achieved when the fresh membrane was first exposed to the filtration cycle operating conditions.

The ratio of permeate conductivity σ_P to feed water conductivity σ_F can be used to assess the rejection ratio of the membrane R_R as shown in equation (4.2):

$$R_R = 1 - \frac{\sigma_P}{\sigma_F} \quad (4.2)$$

Here, a value of 1 corresponds to perfect rejection of contaminants by the membrane, with lower values corresponding to reduced rejection ratios.

Figure 4.6 illustrates the progression in the parameter values defined above in the case of a successful experiment. Successful UFM should show that the UFM cleaning cycle produces a recovery in the value of M_P that is greater than the recovery produced by the control cycle. Additionally, the minimum M_P during the UFM cleaning cycle should be higher than that of the control, as the effects of UFM should begin to take effect as the membrane is cleaned.

As mentioned earlier in this thesis, UFM can potentially cause damage to filtration membranes [14]. This damage is characterized by a sudden increase in permeate flux through the membrane, which would correspond to an increase in M_P as it is characterized within this work [14]. Therefore, M_P cannot be used on its own to distinguish between performance enhancements due to UFM and the effects of UFM-induced membrane damage as it was defined within this work. Distinguishing between these two circumstances requires the examination of R_R , which declines when membranes are damaged [14]. Figure 4.7 shows what parameter behaviours would be expected if UFM produced membrane damage.

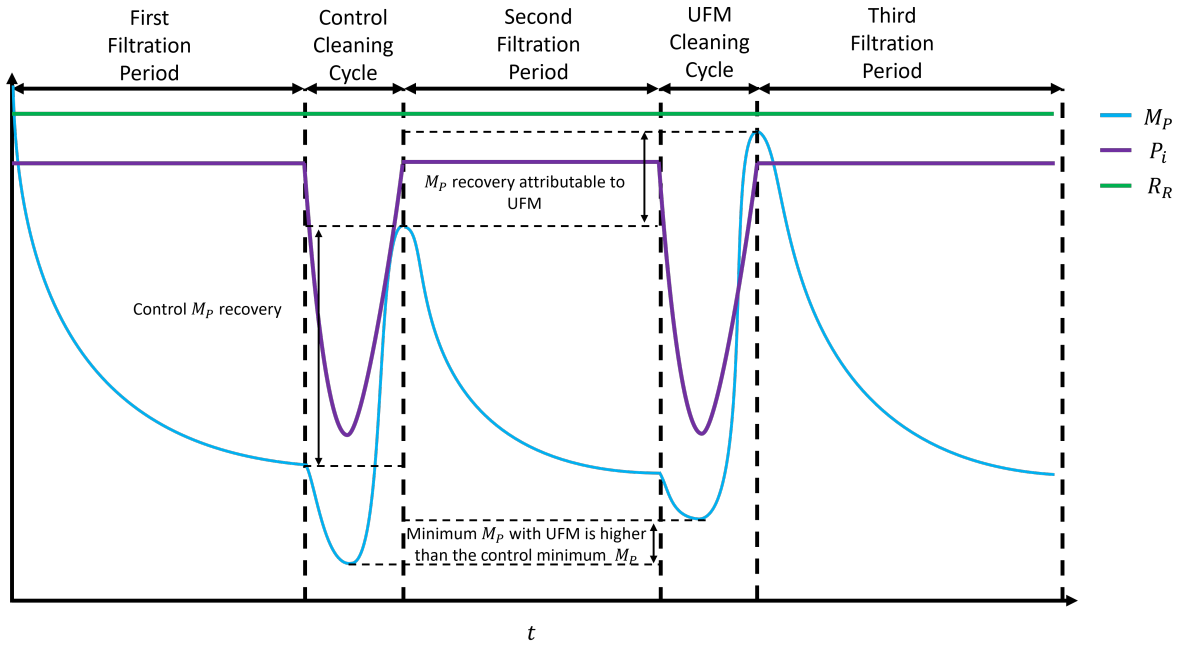


Figure 4.6: Illustration of the expected behaviour of the system if UFM is successful. Key indicators of UFM success are the increases in membrane performance both during and after the UFM cleaning cycle relative to the control, while the constant rejection ratio indicates that the membrane has maintained its integrity.

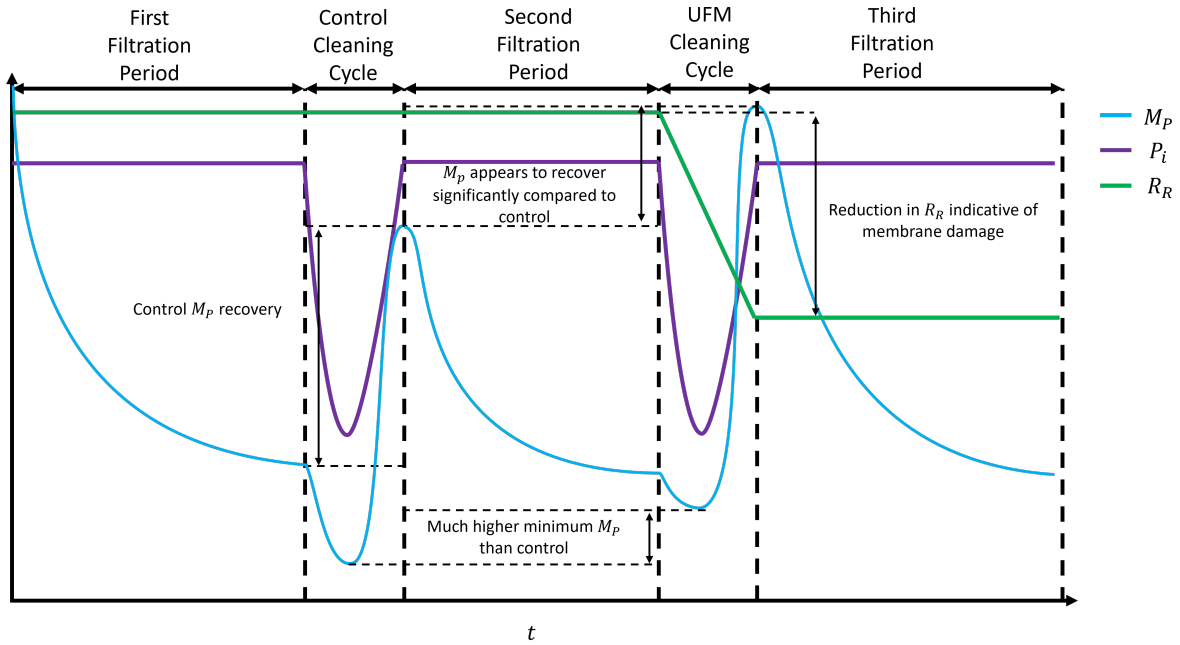


Figure 4.7: Illustration of the expected behaviour of the system if UFM damages the membrane. Membrane damage can only be distinguished from the successful use of UFM by a decrease in the rejection ratio of the membrane.

4.4 Summary of Findings and Conclusion

Initial tests of the experimental setup have been conducted. Both RO filtration and membrane fouling have been achieved using a saturated Calcium Sulphate feed water solution. Initial UFM tests have been conducted; however, the data collected is not yet sufficient to draw meaningful conclusions about UFM performance. Future work will include rigorous experimental investigations of UFM.

Chapter 5

Conclusion

5.1 Introduction

The research completed as a part of this thesis resulted in four principal contributions to the state of the art of UFM. The research also opened several avenues for future exploration in the field of fouling mitigation technologies. The sections below summarize the state of the art of UFM prior to the commencement of the work, review the main research contributions of this thesis, and outline potential research questions that researchers interested in this field could choose to investigate in the future.

5.2 Summary of the State of the Art

Membrane filtration technologies such as RO can be combined with renewable energy sources to provide clean water to remote rural communities, but are limited by the progressive obstruction of their membrane surfaces known as fouling [2, 13, 26]. Ultrasonic fouling mitigation uses a phenomenon known as inertial cavitation to scour contaminants from the surfaces of filtration membranes, and has been shown to be effective at a lab scale on RO, MF, and UF membranes [14, 15, 86]. Prior to the commencement of the research compiled in this thesis, the scalability of the technology was limited by its energy inefficiency, as well as challenges adapting UFM technology to work with the more complicated membrane geometries used for practical implementations [14, 42]. The use of ultrasonic transducers equipped with specially-designed attachments known as ultrasonic horns to enhance the transfer of ultrasound to fluids had been investigated for a range of applications [62–64]. The dynamics of bubbles subject to acoustic cavitation, as well as the attenuation of ultrasonic waves within fluid media undergoing cavitation, had also been investigated extensively [32, 41, 49, 53].

5.3 Summary of Contributions and Findings

The research contained within this thesis consisted of four primary contributions:

1. Temperature distribution modelling within SWRO modules subject to axial sonification;
2. Cavitation onset modelling within axially sonified SWRO modules with respect to a range of operating parameters;
3. Design of a novel ultrasonic horn to enhance the transfer of ultrasound across membrane module boundaries;
4. Development and construction of an experimental setup and an associated experimental regimen to investigate UFM in the context of SWRO modules.

The nature of these contributions are outlined below.

5.3.1 Temperature Distribution Modelling

Temperature distributions within SWRO modules subjected to UFM were investigated to gauge the effects of UFM on filtration performance and establish a means to use these temperature distributions to

analyse ultrasonic absorption efficiency. A mathematical characterization of the heat and mass transfer occurring within a SWRO module was developed by expanding existing models within the literature. A de-coupled model neglecting the effects of temperature on mass transfer was developed and compared to a model that fully accounted for these effects by solving both numerically using system properties representative of a typical SWRO module and sonification intensity. The results showed excellent agreement between the two models, indicating that the de-coupled model could be effectively used for modelling temperature distributions within SWRO modules. The temperature distributions predicted were expected to have negligible effects on filtration performance within SWRO modules.

5.3.2 Cavitation Onset Modelling

The onset position of inertial cavitation along the length of an axially-sonified SWRO undergoing different combinations of inlet pressure and flow rate was investigated using a numerical model to compute ultrasonic intensity and bulk flow properties incrementally along the length of the module. A set of operating flow rates and pressures conducive to effective UFM throughout a typical SWRO module was compiled to form a UFM cleaning regime. The power consumption associated with this regime was estimated, and found to be similar to the power consumption of the SWRO system under standard operating conditions.

5.3.3 Ultrasonic Horn Design

An ultrasonic horn with an enhanced capacity for vibration transfer across membrane module boundaries was designed. An analytical approach was used to calculate theoretically optimal dimensions for key elements of the horn based on a simplified model of the horn. The efficacy of these dimensions was then verified against an FEA model comparing a horn employing the analytically-calculated dimensions to a default approach. The FEA analysis showed that the calculated dimensions outperformed the default approach, and the vibration behaviour of the system was similar to the behaviour predicted by the analytical approach.

5.3.4 Experimental Setup Development

An experimental setup was developed to incorporate the SWRO sonification apparatus into a fully functional pilot-scale SWRO filtration system, with instrumentation to continuously control operating parameters while monitoring filtration performance. Experiments using the experimental setup were developed, involving inorganic foulants and a prescribed UFM cleaning cycle.

5.4 Areas for Future Investigation

The next logical step in this research is the experimental procedure outlined within this thesis. This was meant to be a part of the work outlined above, but was not completed due to time constraints and campus access limitations brought about by the COVID 19 pandemic. The dimensions of the ultrasonic horn could be further optimized for vibration transfer purposes. Different cross-sectional geometries could be examined, as has been done in the literature for other applications of ultrasonic horns [62]. The analytical model used could be further refined to account for the resistance to the lateral expansion and contraction of the vibration column produced by the membrane enclosure. The scope of the analytical model could also be expanded to include the transducer. The models developed could be made more accurate by investigating variations

in SWRO flow parameters within the plane perpendicular to the direction of flow. Boundary layers, in particular, have the potential to store significant thermal energy in the relatively stagnant fluid contained therein, and could be worth modelling to produce a more accurate picture of the effects of ultrasound on RO membrane performance.

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Appendices

5.5 Appendix A: Derivation of Rayleigh-Plesset Equation

Assume first that viscous effects within the body of the fluid (though not necessarily at its boundaries) are negligible, liquids within the fluid medium are incompressible, and body forces are negligible [46]. These assumptions allow for the use of the following mass conservation and Euler equations in spherical coordinates:

$$\frac{\partial \rho}{\partial t} + \frac{1}{r^2} \frac{\partial r^2 \rho u}{\partial r} = 0 \quad (5.1)$$

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial r} + \frac{1}{\rho} \frac{\partial \rho}{\partial r} = 0 \quad (5.2)$$

The radius of the bubble can be described as $R(t)$, with a time derivative $\dot{R}(t)$. Since the motion in the bubble is expected to be oscillatory, a linearized wave equation can be used to describe the velocity potential Φ within the bubble in terms of time t and the speed of sound c within the media. While the dynamics of the system are expected to be non-linear, this assumption is justified by the fact that the non-linearity introduced by the bubble being modelled is far greater than the non-linearity that would exist within the system if the bubble did not exist (which is true in general for idealized single-bubble dynamics) [46]. The equation for the wave is:

$$\nabla^2 \Phi - \frac{1}{c^2} \frac{\partial^2 \Phi}{\partial t^2} = 0 \quad (5.3)$$

Where:

$$u = \nabla \Phi \quad (5.4)$$

In spherical coordinates, the wave equation becomes:

$$\Phi = \frac{\psi(t - r/c)}{r} \quad (5.5)$$

With ϕ being an amplitude function. Assuming that the wavelength of the oscillatory motion of the bubble is far greater than the radius of the bubble itself, the assumption that $\nabla^2 \phi = 0$ holds true. It follows that:

$$\Phi = \frac{\psi(t)}{r} \quad (5.6)$$

At the instantaneous radius of the bubble R , $\frac{\partial \Phi}{\partial r} = \dot{R}$, leading to the following expressions of the amplitude function and velocity potential:

$$\psi = -R^2 \dot{R} \quad (5.7)$$

$$\Phi = \frac{-R^2 \dot{R}}{r} \quad (5.8)$$

Equation (5.2) becomes:

$$\frac{\partial^2 \Phi}{\partial t \partial r} + \frac{1}{2} \frac{\partial}{\partial r} \left(\frac{\partial \Phi}{\partial r} \right)^2 + \frac{1}{\rho} \frac{\partial \rho}{\partial r} = 0 \quad (5.9)$$

At some radius r_1 that is simultaneously much larger than the bubble radius and much smaller than the pressure wave wavelength, the pressure within the fluid medium is primarily a function of the hydrostatic pressure p_0 and the forcing pressure $p(t)$ as opposed to those related to the presence of the bubble. Because of this, equation (5.10) can be integrated from a variable radius r to an r_1 satisfying the conditions above to produce the following:

$$\frac{\partial \Phi(r, t)}{\partial t} + \frac{1}{2} \left(\frac{\partial \Phi(r, t)}{\partial r} \right)^2 = \frac{p(r, t) - p_0 - p(t)}{\rho} \quad (5.10)$$

This can be evaluated at bubble radius R . The derivatives of Φ with respect to r and t at $r = R$ become:

$$\frac{\partial \Phi(r, t)}{\partial t} = -R\ddot{R} - 2R^2 \quad (5.11)$$

$$\frac{\partial \Phi(r, t)}{\partial r} = \dot{R} \quad (5.12)$$

The result is the Rayleigh-Plesset equation expressed in terms of bubble radius:

$$R\ddot{R} + \frac{3\dot{R}^2}{2} = \frac{p_L(t) - p_0 - p(t)}{\rho} \quad (5.13)$$

5.6 Appendix B: Derivation of Dynamic Pressure Equilibrium

Recalling equation (5.8) and the definition in equation (5.4) allows for the derivation of $\frac{\partial u_r}{\partial r}$ as follows:

$$\begin{aligned} \frac{\partial u_r}{\partial r} &= \frac{\partial \nabla \Phi}{\partial r} \\ &= \frac{\partial}{\partial r} \nabla \frac{-R^2 \dot{R}}{r} \\ &= \frac{\partial}{\partial r} \frac{R^2 \dot{R}}{r^2} \\ &= -2 \frac{R^2 \dot{R}}{r^3} \end{aligned} \quad (5.14)$$

At $r = R$, equation (5.14) reduces to:

$$\frac{\partial u_r}{\partial r} = -2 \frac{\dot{R}}{R} \quad (5.15)$$

Substituting into equation (2.39) gives:

$$\sigma_{rr} = -4\mu \frac{\dot{R}}{R} \quad (5.16)$$

The outcome is the dynamic form of equation (2.33) [32, 45]:

$$p_I = p_L + \frac{4\mu \dot{R}}{R} + \frac{2\sigma}{R} \quad (5.17)$$