Design and Modeling of a Sonochemical Reactor
Using Geometry, Mode Shapes and Resonance

by:

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Abstract

A sonochemical reactor design which addresses deficiencies in current reactor designs is proposed. This design uses a comparatively low power electrostatic transducer because electrostatics are efficient over a wide frequency range and are not limited by their size, shape or placement in a reactor. This allows the creation of a reactor that can match the optimal frequency of a sonochemical process, maximize its sound field using mode shapes and resonance and, with the addition of a tracking system, follow system resonances that change with cavitation. The cylindrical reactor cavity and co-axial cylindrical transducer used in the design focus sound energy at the centre of the reactor, protecting the transducer from cavitation and allowing for analytic modeling of the sound field.

A model of the proposed reactor’s homogenous sound field was created in mathCAD. The model consists of a transducer model whose stiffness and damping coefficients were derived from a new thermodynamic model and a reactor model given by the reactor’s wave equation and boundary conditions. The pressure magnitude generated at the transducer scales the magnitude of the reactor sound field. This allows the transducer pressure to be expressed as a relationship between its input voltage and the reactor mode shapes.

A prototype reactor was constructed in order to verify the model experimentally. Data predicted by the model and measured experimentally were collected over a frequency range of 4 to 38 kHz. Ratios of the transducer’s calculated electrostatic pressure to the pressure at the centre of the reactor were determined for both data sets. The match between the curves of this pressure ratio versus frequency for the two data sets was very good. Differences in the widths of the curve’s frequency peaks were attributed to a smaller than expected air gap in the prototype transducer. Accounting for this produced an excellent match between the curves.

Changes to the reactor design that would allow the reactor to achieve cavitation were investigated with the model. Both decreasing the transducer gap space and replacing the air in the gap with a gas of low thermal conductivity and high dielectric strength significantly reduced the voltage required to induce cavitation in the reactor. The model also revealed that the significant effect of the stiffness of small gap space transducers on the magnitude of the reactor’s pressure field at low frequencies.
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Nomenclature

- **a**: radius of rigid electrode, m
- **A(\omega)**: phase of the transducer pressure distribution
- **A_{n,m}, B_{n,m}, C_{n,m}**: mode shape coefficients
- **\alpha**: absorption exponent, 1/m
- **b**: radius of flexible electrode, m
- **b(\omega)**: damping constant of the transducer, kg/s
- **c**: speed of sound in the reactor liquid, m/s
- **c_{H2O}**: speed of sound in water, m/s
- **C**: capacitance of the transducer, F
- **d**: gap space, m
- **d_{eq}**: equivalent air gap spacing, m
- **d_{n}**: thickness of material n, m
- **\delta_{a}**: axial displacement of the reactor’s cylindrical wall, m
- **\delta_{r}**: radial displacement of the reactor’s cylindrical wall, m
- **E**: Young’s modulus for plastic, Pa
- **\varepsilon**: permittivity of free space, F/m
- **f_{A}**: acoustic force generated by the transducer, N
- **f_{e}**: electrostatic force generated in the transducer, N
- **F_{A}, F_{A}^***: magnitudes of the conjugate exponentials of the time variant acoustic force, N
- **\phi_{function_to_electrostatic_input}**: phase difference between the function generator signal and the transducer input
- **\phi_{function^2}**: phase of the squared function generator signal
- **\phi_{hydrophone}**: phase of the hydrophone signal, equivalent to the phase of the pressure field
\( \Delta \phi \)  
phase difference

\( i(t) \)  
time dependent current, A

\( I \)  
current magnitude, A

\( \eta \)  
axial mode number

\( k_{n, \eta} \)  
wave number, 1/m

\( k_{r, \eta} \)  
radial wave number, 1/m

\( k_{z, \eta} \)  
axial wave number, 1/m

\( k(\omega) \)  
spring constant of the transducer, kg/s²

\( \kappa_n \)  
dielectric constant of material n

\( L \)  
length, m

\( L \)  
inductance of the transducer, H

\( m \)  
mass of the moving electrode, kg

\( n \)  
radial mode number

\( n \)  
ordinal

\( p(r, z, t) \)  
pressure in the reactor, Pa

\( p_b \)  
pressure at the bottom boundary of the reactor, Pa

\( p_h \)  
pressure corresponding to the hydrophone voltage, Pa

\( p_n \)  
pressure in reactor region n, Pa

\( p_t \)  
pressure at the transducer electrode, Pa

\( p_w \)  
pressure at the cylindrical wall of the reactor, Pa

\( p_{H_2O} \)  
pressure of a plane wave in water, Pa

\( P \)  
the pressure of a dielectric gas, Pa

\( P_e \)  
electrostatic pressure, Pa

\( P_t \)  
magnitude of the transducer pressure, Pa

\( P(\omega) \)  
amplitude of the transducer pressure distribution, kg/m²s²
q charge, C
q₀ constant portion of the charge input, C
Q, Q° magnitudes of the conjugate exponentials of the time variant charge input, C
r radial dimension of the reactor, m
rᵣ transducer radius, m
R resistance of the transducer, Ω
R radius of the reactor's cylindrical wall, m
R(r) radial portion of the reactor's pressure function
ρᵥ₂₀ density of water, kg/m³
S transducer surface area, m²
σₑ circumfrencial stress in the reactor’s cylindrical wall, Pa
σᵢ longitudinal stress in the reactor’s cylindrical wall, Pa
t time, s
tₘ thickness of the reactor’s cylindrical wall, m
T(t) temporal portion of the reactor’s pressure function
𝑢ᵣ velocity at the bottom boundary of the reactor, m/s
𝑢ᵣᵣ radial velocity reactor region n, m/s
𝑢ᵣᵣ velocity of the reactor’s cylindrical wall, m/s
u(t) time dependant velocity, m/s
𝑢ᵣᵣ(z, t) transducer electrode velocity, m/s
𝑢ᵣᵣ(z, t) transducer breathing velocity, m/s
𝑢ᵣᵣ(z, t) transducer displacement velocity, m/s
𝑢ᵣᵣ velocity of the plane wave in water, m/s
U magnitude of transducer velocity, m/s
v(t) time dependant voltage applied to the transducer, V
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<td>input voltage, V</td>
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<tr>
<td>$V_0$</td>
<td>constant bias voltage applied to the transducer, V</td>
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<td>V, $V^*$</td>
<td>magnitudes of the conjugate exponentials of the time variant voltage input, V</td>
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<td>$V_b$</td>
<td>breakdown voltage, V</td>
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<tr>
<td>$V_h$</td>
<td>amplitude of the hydrophone voltage signal at the reactor frequency, V</td>
</tr>
<tr>
<td>w</td>
<td>angular frequency, rad/s</td>
</tr>
<tr>
<td>$\omega_d$</td>
<td>angular frequency at which the input signals are driven, rad/s</td>
</tr>
<tr>
<td>$\omega_r$</td>
<td>angular frequency at which the reactor responds, rad/s</td>
</tr>
<tr>
<td>$\omega_n$</td>
<td>resonant frequency, rad/s</td>
</tr>
<tr>
<td>$\omega_{n,n}$</td>
<td>resonant frequency, rad/s</td>
</tr>
<tr>
<td>$\Delta \omega$</td>
<td>half-power bandwidth, rad/s</td>
</tr>
<tr>
<td>x</td>
<td>electrode displacement, m</td>
</tr>
<tr>
<td>$x_0$</td>
<td>constant portion of the displacement output, m</td>
</tr>
<tr>
<td>X, $X^*$</td>
<td>magnitudes of the conjugate exponentials of the time variant displacement output, m</td>
</tr>
<tr>
<td>z</td>
<td>axial dimension of the reactor, m</td>
</tr>
<tr>
<td>$Z(z)$</td>
<td>axial portion of the reactor pressure function</td>
</tr>
<tr>
<td>$Z_b$</td>
<td>impedance of the bottom boundary of the reactor, $kg/m^2s$</td>
</tr>
<tr>
<td>$Z_w$</td>
<td>impedance of the reactor's cylindrical wall, $kg/m^2s$</td>
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<tr>
<td>$Z_{\text{H}_2\text{O}}$</td>
<td>acoustic impedance for a plane wave in water, $kg/m^2s$</td>
</tr>
<tr>
<td>$\zeta$</td>
<td>damping ratio</td>
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Acknowledgments

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1.1 What is Sonochemistry?

Sonochemistry is the use of sound to influence chemical systems. Most sonochemical effects are caused by cavitation, or the formation and collapse of bubbles in the liquid portion of the chemical system. The phenomenon of cavitation bubbles is not limited to sonochemistry. For instance, cavitation bubbles are seen in boiling liquids and in the low pressure regions found behind turbine blades.

The low and high pressure phases of incident sound waves are responsible for acoustical cavitation. Bubbles expand in the low pressure phase of sound waves and contract in the high pressure phase. There is some disagreement as to whether gas filled micro-bubbles need to pre-exist in a fluid, either alone or attached to inclusions such as dust particles, in order for cavitation bubbles to grow in the liquid. Recent articles by Mason and colleagues assert that the rarefaction cycle of a sufficiently high intensity sound wave can overcome the intermolecular bond of the liquid medium in order to form cavitation bubbles.\(^1,2\) The pre-existence of micro-bubbles is generally accepted, however, and it has been shown that liquids with pre-existing micro-bubbles cavitate more easily.\(^3\)

Cavitation only occurs if the incident sound intensity is greater than the cavitation threshold of the system. This threshold is affected by several factors, including the amount of gas dissolved in the liquid. Liquids with high surface tension and viscosity have higher cavitation thresholds. Those with high vapour pressures and temperatures have lower cavitation thresholds. This threshold is also affected by frequency. For most liquids, the cavitation threshold is constant up to approximately 50 kHz, and then rises rapidly. The cavitation threshold for aerated water, for instance, is approximately 100 kPa (1 atm). Imploding cavitation bubbles create micro-bubbles which serve as nucleation points for more cavitation bubbles. The number of bubbles increases until a steady-state maximum has been reached. Since there are more nucleation points after cavitation has begun, less sound pressure is required to sustain cavitation than to initiate it.\(^4\)
Sonochemistry has traditionally been performed with low frequency ultrasound (20 to 100 kHz). The frequency range for sonochemistry is expanding, however, since cavitation can be made to occur within the audible range (20 Hz to 20 kHz), and at high frequencies (up to 2 MHz).

Cavitation bubbles fall into two separate classes. ‘Stable’ cavitation bubbles exist in the liquid medium for many acoustic cycles. For this to occur, the amount that these bubbles expand during the rarefaction phase of the sound wave must be equivalent to the amount that they contract during the compression phase. ‘Transient’ cavitation bubbles exist for only a few acoustic cycles. These bubbles undergo a process called rectified gas diffusion. In this process, vapour from the bulk liquid diffuses into the bubble as it expands and contracts. Since diffusion is proportional to surface area, the bubble gains more vapour during expansion than it loses during compression. It soon becomes large enough that it implodes. Whether a bubble is stable or transient depends on its initial radius, and the frequency of the incident sound wave.

1.2 What Does Sonochemistry Do?

Cavitation bubbles affect chemical systems when they pop. Imploding cavitation bubbles are thought to interact with chemical systems by different mechanisms.

The first mechanism is described in the ‘hot-spot’ theory. ‘Hot-spot’ refers to the formation of very high point-pressures, point-temperatures and point-heating/cooling rates at the location of the imploding bubbles. These values are on the order of 100,000 kPa (1000 atm), 5000 K and $10^{10}$ K/s, respectively. Extreme pressures, temperatures and heating rates have primarily chemical effects, such as catalyzing reactions, changing reaction pathways and allowing reactions that require extreme physical conditions to occur at lower pressures and temperatures. In aqueous systems, water has been found to ionize in the cavitation bubbles. The resulting hydrogen and hydroxide ions are released upon the implosion of the bubbles, creating new chemical reactions in the system.

The ‘hot-spot’ theory is not entirely uncontested. There has been some suggestion that electrical charges created on the surface of cavitation bubbles create enormous electric field gradients that can break chemical bonds on their collapse. There are some phenomena that support the electrical theory over the ‘hot-spot’ theory. There are also good arguments for discounting the electrical theory. Thus the ‘hot-spot’ theory remains the generally-accepted mechanism.
Collapsing bubbles also create shock waves, and these shock waves are the second mechanism by which cavitation interacts with chemical systems. Shock waves can break down long chain molecules and cause high-energy inter-particle collisions, which result in the agglomeration of particles and the abrasion of surfaces.

Micro-jets are the final cavitation mechanism. Most cavitation bubbles are non-spherical due to the presence of solids and pressure gradients in the chemical system. When a deformed bubble collapses, the asymmetrical implosion force results in a net motion of liquid toward the flattened side of the bubble. These jets can reach velocities of hundreds of meters per second since a portion of the implosion energy is directed into the jet. Micro-jets can remove dirt and other impurities from solid surfaces. They can also cause erosion. \(^5\)
These three cavitation mechanisms result in a wide range of physical and chemical effects. Figure 1.1 attempts to classify these sonochemical effects according to the components of the chemical system. Liquid-gas, liquid-liquid and liquid-solid chemical systems are considered. Note that sonocatalysis is common to all three classes.

It is not feasible to provide descriptions of all sonochemical processes here. Several recent papers provide excellent overviews of processes that benefit from sonochemistry. These papers include Suslick, 1997; Mason, 1998; Mason, 1999; Mason et al.; 1999; Suslick et al., 1999 and Thompson et al.

1.3 What Affects Sonochemistry?

The intensity of cavitation in a sonochemical system is influenced by several factors. It is difficult to generalize how system parameters will affect the outcome of sonochemical processes, since there are so many of them. Some generalizations about the affect of system parameters on cavitation can, however, be made.

a) Ambient Pressure

Decreasing the ambient pressure reduces the sound pressure necessary to produce pressure swings lower than the liquid vapour pressure. This lowers the cavitation threshold, which makes it easier to produce cavitation bubbles in the system. It also results in less energetic bubble implosions, so the sonochemical effect is decreased.

b) Ambient Temperature

Increasing the ambient temperature of the cavitation liquid also results in a higher equilibrium vapour pressure. High temperature liquids cavitate more easily and suffer reduced sonochemical effect.

c) Frequency

It is particularly difficult to categorize the effects of frequency on sonochemistry, since the influence of frequency is affected by the size and shape of the reaction system, the size of the cavitation bubbles and the process that is occurring. Very generally, lower frequency sound waves result in more energetic cavitation. Higher frequency sound waves create more bubbles, but less energetic cavitation. Since water ionizes in cavitation bubbles more easily at higher frequencies, some aqueous chemical processes may benefit from higher sound frequencies.
d) Other Factors

As noted, the presence of micro-bubbles in the sonochemical system reduces the cavitation threshold. Bubbling different gases into a system results in a variety of different chemical effects as well.

Cavitation occurs more easily in high vapour pressure, low viscosity and low surface tension liquids. The opposite properties encourage intense cavitation.

The effect of acoustic power on the outcomes of sonochemical processes is clouded by many issues. Certainly large power inputs into these systems are important in overcoming the cavitation threshold, but increased power once cavitation begins does not necessarily result in increased process results. This may be due in part to the frequency used, and to the formation of bubbles around the sound source. Such bubbles may impede the progress of sound waves into the system. The effect of acoustic power is also difficult to determine since there are no standard methods of determining acoustic power in sonochemical systems.

1.4 How is Sonochemistry Performed?

In industry and in the laboratory, sonochemistry is performed in a sonochemical reactor. A reactor consists of a container for the chemical system and a transducer which introduces sound waves into the liquid component of that chemical system. Improving how sonochemistry is performed is the objective of this work. A new sonochemical reactor design that improves upon existing reactor designs and that can be modeled analytically is proposed. Improvements to existing reactor designs are needed so that the many uses of sonochemistry, which are outlined above, may be more fully exploited by industry. The ability to model a design analytically makes it possible to adjust and improve the design without extensive prototyping.
2.1 Existing Reactor Designs

2.1.1 Reactor Technologies

Given the wide variety of uses for sonochemistry, one might expect to see several well-developed sonochemical reactors. In fact this is not the case. The creation of large scale reactors for industrial use is a relatively new phenomenon, and details about these reactors are few.  

Most current reactors are small-scale devices used in laboratories. Figure 2.1 groups current reactor designs into four different categories. The reactors shown in this figure are fairly broad generalizations of the reactors reported in the literature. A more thorough review of individual designs can be found in Thompson et. al.  

The first reactor type is the probe reactor. In this reactor, sound energy is introduced into the system by a sound source inserted into the liquid. Probe transducers can vibrate either axially or radially. In probe systems, the strongest sound field and the most active cavitation bubbles are centered around the probe. This results in erosion of the probe. 

The second reactor type is the axial reactor. In this design, sound is directed into the reactor from an axially vibrating transducer mounted on or near a reactor wall. Ultrasonic baths, which are ubiquitous in metals and materials laboratories for cleaning samples, fall into this category. Once again, the sound field and the cavitation are concentrated around the transducer location, which can be problematic. Both probe and axial reactor designs can have arbitrary shapes and accommodate multiple transducers.

The third reactor type is referred to as radial. Radial reactors are always tube shaped, although the tube is typically not round, since most transducers are more easily mounted on flat surfaces. Both probe transducers, and those mounted on or near the reactor walls can be used, so long as they impart radial
sound waves into the tube, and are mounted away from the tube’s central axis. One of the benefits of the tube reactor is that the circular (or almost circular) geometry focuses the sound waves and the cavitation in the centre of the reactor, rather than at the transducers.

In the examples of reactor types one through three shown in Figure 2.1, the transducers radiate sound directly into the reactor. However, all of these reactors can be designed with the transducers coupled to the reactor liquid through some other material.

The last reactor type included here is the sonotube. In the sonotube design, the transducer is mounted away from the reactor at the end of an arm. Axial sound vibrations are transmitted through the arm into the reactor. All four reactor types can be used to process single batches of chemicals, or they can have inlet and outlet tubes which deliver the chemicals to the reactor for continuous processing.
2.1.2 Transducer Technologies

Piezoelectric and magnetostrictive transducers are the most common methods of introducing sound energy into sonochemical reactors.

Piezoelectric transducers are constructed from ceramics containing materials that expand and contract in alternating electric fields. They are the favoured transducer type because they are high-power and very efficient when they are operated at their resonant frequency. Though each individual transducer is only efficient at one frequency, the range of frequencies for which piezoelectric transducers can be designed is large.

Magnetostrictive transducers are constructed from materials that expand and contract in alternating magnetic fields. They have fairly low efficiencies, and can only be made to operate up to about 70 to 100 kHz, depending on the material used. They are gaining popularity since they are well-suited for heavy-duty continuous use, and since new designs are more powerful, more compact and lighter than piezoelectrics. Like piezoelectrics, magnetostrictive transducers are most efficient when operated at resonance. The maximum power which can be delivered by both piezoelectric and magnetostrictive transducers is limited by the displacement of the transducer.

Electrostatic transducers are not common in sonochemistry. Though the concept behind these transducers is nearly a century old, high-power electrostatic transducers didn’t emerge until the 1980’s. The operation of electrostatic transducers will be described in greater detail in Chapter 3. Electrostatic transducers are not as powerful as piezoelectrics and magnetostrictives but, unlike these transducers, individual electrostatic transducers can operate efficiently over a wide frequency range. Electrostatic transducers are also lightweight, compact and easy to shape. The maximum power which can be delivered by an electrostatic transducer is limited by the pressure which can be generated by the transducer.

Other methods of cavitating the liquids in chemical systems include liquid whistle and vibrating bar technologies. These technologies have specialized applications and do not use sound waves to generate cavitation bubbles. More information on these methods can be found in the references.
2.2 Problems with Existing Reactors

As noted by Crum, "most sonochemistry reaction vessels are designed by chemists, with an emphasis on facilitating chemistry rather than simplifying the acoustics. Consequently, these systems are mechanically complex and difficult to model from an acoustics perspective." 9

Furthermore, Mason suggests that "it must also be recognized that a large number of chemists will have very little knowledge (or interest) in the mathematics and physics of cavitation. Within these disciplines lies the key to a better understanding of the ways in which acoustic cavitation could be optimized for use in chemical systems." 8

Sonochemistry is largely the domain of chemists, physicists and chemical engineers. Most of the developments in sonochemistry in the last 20 years have involved investigating the physical and chemical effects of sonochemistry, and to a smaller degree, using these effects. 3, 10

Understanding cavitation and understanding the acoustics responsible for sonochemical effects has taken a back seat. Issues of reactor design have also been largely ignored. By considering sonochemical reactors from an acoustics and design standpoint, three main deficiencies stand out.

a) Current Reactors are Constrained by Conventional Transducers

Conventional piezoelectric and magnetostrictive transducers are limited by their size, shape and placement in the reactor. They are relatively large and difficult to construct in unusual shapes. This makes it difficult to couple them to certain reaction vessels and limits their placement. As a result, reaction vessels are often designed to suit the transducer, rather than the other way around.

More importantly, conventional transducers are also limited by their operating frequencies. As noted earlier, piezoelectric and magnetostrictive transducers only operate efficiently at their resonant frequencies. Most sonochemical research has been done with resonating piezoelectric transducers, without regard to whether the transducer's operating frequency is appropriate for the sonochemical reactor system as a whole. Most low-frequency ultrasound work has been done at 20 kHz. 3, 5

The sound field in a sonochemical reactor will be strongest at the reactor's resonance frequency. The sound frequency in the reactor also affects the success of the reaction mechanism. Certainly sonochemical reactors could be designed so that the reactor and the transducer both resonate at the
frequency that best suits the process at hand. However, this would limit the reactor to certain processes, and does not account for the fact that the resonant frequencies of a cavitating liquid system are not constant. Cavitation in the reactor liquid reduces the liquid's density and decreases its bulk modulus. This increases its apparent damping and lowers its resonant frequency. Ideally, the system's transducer should provide the optimal frequency for all stages of the sonochemical process. Piezoelectric and magnetostrictive transducers do not.

b) Current Reactors do not Exploit Mode Shape and Resonance

A reactor operating at resonance will have a higher maximum sound pressure than a reactor operating off resonance with the same input power. The position of the maximum sound pressure depends on the standing waves (mode shapes) generated in the reactor. The mode shapes excited in a reactor with a constant configuration depend only on its (and, therefore, its transducer's) operating frequency. In order to operate at its peak efficiency, a sonochemical reactor must use resonance.

The geometry of a reactor, and the placement and shape of its transducers, dictate its resonant frequencies and mode shapes. It was noted above that most sonochemical research has been done with a small set of frequencies despite the fact that the reactors involved have varied greatly. In fact, most sonochemical research has ignored the presence of mode shapes and resonance, or purposely avoided resonance effects by operating away from the resonant frequency, or by using high frequency, short wave length signals.

Achieving a high intensity sound field for a relatively small input power is not the only benefit of making use of resonance and mode shapes. Some geometries, such as the cylinder, can strongly focus sound waves, resulting in very high maximum sound pressure to input sound pressure ratios. Knowledge of mode shapes also allows the transducer to be placed in the system so that the high pressure sound regions do not occur at the transducer. This protects the transducer from the erosion effects of the cavitation bubbles that form in the high pressure region.

c) Current Reactors Have Complex, Difficult to Model Sound Fields

Determining the sound field in a sonochemical reactor is an inhomogeneous boundary value problem. When reactors are built around transducers and ignore mode shapes and resonance, reactors with complex sound fields often result. Complex sound fields are usually impossible to model analytically. Numerical models are always possible, but can be difficult to implement and slow. Even if a complicated
sound field can be modeled, it is difficult to anticipate how it will be affected by changes to the reactor or its inputs. If a reactor that uses resonance and mode shapes to increase its sound field is to be designed, it must have a sound field that is easy to model and study.

d) Current Reactors Cannot Follow Frequency Shifts

As noted earlier, the frequency response of an acoustic cavity changes as cavitation is initiated. Piezoelectric and magnetostrictive transducers cannot effectively handle this phenomenon. The speed of sound decreases at the onset of cavitation because of the apparent reduction in the bulk modulus of the liquid. The driving frequency of the transducer should be reduced under these circumstances so that the wavelength of the sound within the acoustic cavity is maintained constant. A constant wavelength ensures that the transducer placement is correct with respect to the standing waves in the cavity. However, piezoelectric and magnetostrictive transducers must be operated at a fixed frequency, their resonant frequency.

Some research has been done to try to observe sound fields in existing reactors. Examples in the literature include Gonze et. al., 1998; Laborde et. al., 1998 and Faid et. al., 1998. Gonze and colleagues used sound sensitive thermocouples, light emitting reactions and piezoelectric transducers to visualize and measure reactor sound fields. Laborde’s group used high speed photography to take pictures of cavitation bubbles and, thus, their standing wave field, in an axial type transducer. Faid et. al. used mass transfer rates to measure and then visualize sound fields in a variety of reactors. The pressure fields in sonochemical reactors can also be observed when sonoluminescence - the emission of light from cavitation bubbles - occurs.

2.3 Existing Models

Most attempts at modeling sonochemical reactors have dealt with anticipating the results of sonochemical reactions. Little work has been done to mathematically model the sound fields in sonochemical reactors. None of the reported research uses reactor sound field modeling to aid in the design of new sonochemical reactors. Recent work in mathematical modeling is detailed below.

Laborde et. al. computed the pressure field in an axial type reactor with a bottom mounted transducer and cylindrical walls. They did this with two different computer packages. One computed a 2-D pressure field using the reactor’s linearized differential equations. The second used computational fluid dynamics
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Previous Work

to solve the non-linearized pressure field. Both calculations were applied to the homogenous, or non-cavitating case. Results were compared with experimental data at 28 and 500 kHz. At low frequencies, the pressure field at the reactor's centre, shown by cavitation marks on a thin foil, matched the non-linear calculation fairly well. At high frequencies, the calculated sound field was well matched by observations taken from a light emitting cavitation reaction. Differences between the experiments and models were attributed to the lack of cavitation bubbles in the computer models, and to the increased importance of non-linear effects in the low frequency, nearly resonant sound field. 16

Most of the work in modeling sonochemical pressure fields has been done by Keil and Dähnke. Their first papers, in 1997 outline a numerical method of solving the linearized pressure field in a homogenous reactor of arbitrary shape. 17,18 This is done by assuming the reactor to be made up of point spherical sound sources whose combined effect yields the overall sound field. Results were obtained for a selection of reactor types. Computation times were on the order of several hours. In 1998 Dähnke and Keil refined their model to include cavitation bubbles. 19,20 They did this by adjusting the parameters in the differential wave equation to attempt to account for the volume fraction of the vapour bubbles. The sound field is calculated in incremental shells moving away from the transducer. Initial bubble volume fractions and the distribution of bubbles were assumed. Again, results were obtained for a selection of reactor types. In 1999, Dähnke, Keil and Swamy used this model to calculate the pressure field in two different experimental reactors, and compared the modeled results to sound field measurements reported for these reactors. 21,22 They declared the matches 'quite good', though there were definite discrepancies which were attributed to difficulties in obtaining accurate measurements of the sound field.

2.4 From Previous to Proposed

The above discussion highlights the need for improvement in sonochemical reactor design. Most existing reactors have been assembled by chemists and not designed by engineers. Most do not exploit the sound-field in the reactor, and all use transducers ill-suited to the needs of sonochemistry. The proposed reactor design addresses these deficiencies by considering the design of a sonochemical reactor from an engineering standpoint. The above discussion also highlights the areas of sonochemical reactor modeling that have received little attention - namely analytical modeling and the use of reactor models as a design tool. In this work, an analytic model of the proposed reactor design is created, verified and used to suggest improvements to the design.
3.1 Design Impetus

"...research and development for sonochemical reactors are mostly based on empirical reaction data." - Keil and Dähnke

Currently, sonochemical reactors are not designed using engineering principles. Instead, they are developed by putting combinations of reaction vessels and transducers together and seeing what happens. The previous section outlined some of the results of this method. They are:

- reactors that are ineffective because they do not use mode shapes and resonance
- awkward transducers that can’t track the resonant frequency of a cavitating reactor
- sound fields that are difficult to model and analyze.

The proposed sonochemical reactor design breaks this pattern by approaching sonochemical reactor development from an engineering design standpoint, using the following criteria:

- The reactor must have a transducer that isn’t limited by its size, shape, or placement
- The transducer used in the reactor must be efficient over a wide range of frequencies
- The reactor must operate at resonance for maximum efficiency
- The geometry and mode shapes of the reactor must maximize the magnitude of the sound field
- Mode shapes and transducer placement must be used to reduce cavitation against the transducer
- The sound field must be easily modeled so that modeling can be used to refine the design.

The following sections of this chapter reveal how the proposed sonochemical reactor design meets these criteria.
3.2 Electrostatic Transducers

It is clear from the discussion in Chapter 2 that the only transducer technology that is not constrained by its shape, size, or placement in the reactor is the electrostatic transducer. These transducers can be made to conform to a variety of shapes, they are thin enough to fit a variety of spaces and their flexibility of construction allows them to be placed anywhere in a reactor. Electrostatic transducers are also the only transducer technology that is efficient over a wide frequency range. Consequently, they can be used to ensure a reactor system always operates at its resonant frequency, despite the shifts in the resonant frequency which occur during cavitation. The greatest limitation of electrostatic transducers is the limited pressure which they can generate.

3.2.1 General Principles

Figure 3.1 depicts a basic electrostatic transducer and its parameters. It consists of two electrode plates that are electrically isolated from each other by a small space which is usually filled with air.

One or both of the electrode plates are allowed to move, either because the plate or plates are flexible, or because the spacers between the two plates are compliant. Figure 3.1 shows a transducer with one moving plate. An alternating voltage applied across the plates creates an alternating electrostatic pressure between them. The attractive force between the plates from the applied voltage causes the plates to oscillate and generate sound.

![Figure 3.1 Basic Electrostatic Transducer](image)

- **V** = input voltage, V
- **d** = gap spacing, m
- **p_e** = electrostatic pressure, Pa
- **p_t** = pressure at the electrode, Pa
- **u** = electrode velocity, m/s
- **x** = electrode displacement, m
- **k** = transducer stiffness, kg/s
- **b** = transducer damping, kg/s²
The electrostatic pressure developed between the plates is given by the following relation:

\[ P_e = \frac{\varepsilon V^2}{2d^2} \] \hspace{1cm} 3.1

Where

\[ \varepsilon = \text{the permittivity of free space, F/m} \]

and \( P_e, V, \) and \( d \) are as described in Figure 3.1. The displacement of the plates is normally small compared to their separation. If the gap between the electrodes contains several materials, or a material other than air, then the following equation can be used to find the equivalent air filled gap spacing:

\[ d_{eq} = \sum_n \left[ \frac{d_1}{\kappa_1} + \frac{d_2}{\kappa_2} + \ldots + \frac{d_n}{\kappa_n} \right] \] \hspace{1cm} 3.2

Where

\[ d_n = \text{thickness of material n, m} \]
\[ \kappa_n = \text{the dielectric constant of material n} \]
\[ d_{eq} = \text{the equivalent air gap spacing, m} \]

Because the electrostatic pressure is proportional to the square of the applied voltage, the frequency of the electrostatic pressure may differ from that of the applied voltage. Figure 3.2 illustrates the case of a sinusoidal input voltage. The frequency of the electrostatic pressure is twice that of the input voltage, and the average pressure is above zero, which results in a slight elevation of the fluid’s gauge pressure.

Applying a DC bias voltage that is large compared with the sinusoidal input voltage will result in a pressure response that has the same frequency as the applied voltage.

The increase in the transducer’s electrostatic pressure with increasing input voltage has its limitations. If the voltage applied across the electrode gap is too great, the gas in the gap will ionize. The presence of charged ions in the gap will allow electrical flow. This loss of the electrical isolation between the electrode plates is called breakdown.
Paschen's law describes the voltage at which breakdown will occur, $V_b$, as a function of the product of the pressure of the dielectric gas, $P$, and the dielectric gap space, $d$: \[ V_b = f(Pd) \]
This product is called the Paschen product. This functional relationship between the Paschen product and the breakdown voltage must be determined experimentally for individual gases, but most relationships, or Paschen curves, are similar to that for air, shown in Figure 3.3. The value of the Paschen product at which the breakdown voltage is lowest is referred to as the Paschen Minimum.

Once the Paschen curve has been determined for a gas, the maximum electric field strength, $V_b/d$, can be determined for any combination of gas pressure and electrode spacing. Figure 3.4 shows the electric field strength versus gap space for air at atmospheric pressure. This reveals the gas’ dielectric strength, or resistance to electrical breakdown. Changing the gas, its pressure or the gap spacing in an electrostatic transducer, changes the breakdown voltage of the transducer.

Unfortunately, a transducer’s electrical isolation can be compromised at voltages lower than breakdown. At very small values of the Paschen product the dielectric strength does not become infinite, as Figure 3.4 might suggest.

![Paschen Curve for Air at 101 kPa](image.png)
Ionization does not occur at very low values of Pd, because the mean free path between individual gas molecules is so small. Instead, electrons are actually pulled away from the negative electrode (cathode) and accelerated towards the positive one (anode). When these free electrons strike the anode, positive ions are discharged and accelerated towards the cathode. This process, called electron field emission, continues until there are so many charged particles in the gap that breakdown does occur.

Theory predicts that electron field emission will occur at electric field strengths on the order of $5 \times 10^9$ V/m. In practice, field emission occurs at nominal electric fields as low as $2 \times 10^7$ V/m. Irregularities in the electrode surface create concentrations in the electric field, resulting in a local electric field gradient that is higher than the nominal one. The mechanism is analogous to stress concentration. Solid dielectric coatings, such as mylar, on the electrodes can reduce field emission by reducing the concentration of the electric field before it reaches the electrode. Conditioning the transducer by exposing it to gradually increasing voltages erodes field emitting sites and also helps to eliminate field emission. Well prepared electrodes can operate in electric fields with strengths on the order of $5 \times 10^8$ V/m.
For an electrostatic transducer to operate properly, the spacers holding the electrode plates apart must also insulate the electrodes from one another electrically. The bulk dielectric strength of solids is used to determine whether the spacers will accommodate similar voltages to the dielectric gas. Like gases, the dielectric strength of solids increases with reducing thickness. Some solids can also breakdown prior to their breakdown voltage. Gases ionize at solid surfaces first. The ions from this corona bombard the surface causing heating, erosion and, ultimately, premature breakdown. Some materials, such as mylar, will breakdown in electric fields one order of magnitude smaller than their nominal breakdown voltage due to corona damage. Others, such as silicone and mica, will not breakdown prematurely.

### 3.2.2 Electrostatic Transducer Design

The design concept for the electrostatic transducer used in this project is illustrated in Figure 3.5. Engineering drawings of the transducer, with dimensions, are included in Appendix A.
This transducer has one stationary aluminum plate and one flexible plate made of aluminized mylar. The aluminized side of the mylar faces away from the stationary plate to ensure complete electrical separation. The flexible plate is wrapped around the stationary one and separated from it with foam tape, allowing it to radiate in two directions.

The seams along the edge of the transducer are sealed with a waterproof silicone material, and the whole device is wrapped in clear vinyl to insulate it from the liquid in the sonochemical reactor. An alternating voltage is applied to the transducer through wires that are applied to the electrodes - one to the stationary electrode and one to the flexible one.

This style of transducer can be constructed in a variety of shapes and sizes by changing the shape and size of the stationary electrode, and by applying spacers so that they maintain the desired gap space. If the spacers are arranged so that gap space is divided into closed sections that are isolated from one another, then only the area of the moving membrane over each individual section should be used to calculate the electrostatic pressure generated by that section of the transducer.

3.3 Cylindrical Geometry

A cylindrical geometry was chosen for the proposed reactor design. As noted in Chapter Two, a cylindrical reactor strongly focuses sound waves towards its centre axis, thereby maximizing the sound field there. The sound field of a cylindrical reactor can also be modeled analytically. Modeling the reactor’s sound field allows its mode shapes and resonant frequencies to be used in the design process, and simplifies the process of refining the design.

The focusing effect of this reactor geometry can be seen by considering the standing waves in an unforced cylindrical reactor. Figure 3.6 shows the mode shapes of an unforced cylinder with pressure relief boundaries. (For a reactor to have pressure relief boundaries, the impedance of the boundary material to must be low compared to that of the reactor liquid.) The axial mode shapes are sine waves and the radial mode shapes are J-type Bessel functions. The Bessel functions show the expected concentration of the sound field at the centre of the reactor. Thus, this reactor shape fits the design criteria for a geometry that magnifies the sound field.
Figure 3.6 Mode Shapes of a Cylindrical Reactor
3.4 Mode Shapes and Transducer Placement

Once the shape of the reactor has been chosen, “The ultrasonic pressure intensity profile in the reactor depends entirely on the design and location of the transducer.”- Dähnke, Swamy, Keil

Placing a transducer in a reactor changes the system from an unforced to a forced system. It also changes the boundary conditions of the reactor, which influences the mode shapes. The mode shapes of the unforced system can, however, be used to guide the placement of the transducer. Indeed, the design criteria for the proposed sonochemical reactor design require that it use mode shapes to govern the transducer’s placement in the reactor. The three primary reasons for this requirement are detailed below:

a) Avoiding cavitation against the transducer
As noted in Chapter 2, energetic cavitation bubbles can corrode solid materials, such as those used to construct the transducers used in sonochemical systems. High energy cavitation occurs at high sound pressures. In order to reduce cavitation against the transducer in a reactor system, the transducer should be placed away from pressure maxima, where the most energetic bubble implosions occur. The mode shapes of the unforced reaction vessel indicate where those pressure maxima are.

b) Maximizing the sound field in the reactor
Though the cylindrical reactor geometry focuses the reactor’s sound field, the shape and placement of the transducer in the reactor governs how much the sound field is increased. First, because the reactor focuses sound radially, the input sound waves should also be radial. The most efficient and uniform way to introduce radial waves into a cylindrical reactor is to use a cylindrical transducer centered on the reactor’s axis. In this configuration, the mode shapes inside the transducer (between it and the centre of the reactor) will be J-type Bessel functions, just as they are in the unforced reactor.

Next, it must be noted that the sound pressure at the centre of such a cylindrical reactor system depends on both the transducer’s pressure and its radius. This is demonstrated in Figure 3.7, which shows the second radial mode shape of a cylindrical reactor. First, assume that the cylindrical transducer element has a radius of zero, such that it is coincident with the axis of the reactor, and assume that the transducer introduces a pressure, P, into the reactor. The maximum pressure in the reactor, by virtue of its Bessel function radial mode shapes, is also located on the axis of the reactor, and must be equal to the pressure.
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that the transducer introduces there. This pressure is $P$. Thus, if the transducer is placed on the reactor’s axis, no focusing, and no increase in the magnitude of the introduced sound pressure, are achieved.

Next, imagine that the transducer’s radius places it where the reactor pressure is half that at the centre of the reactor. It is still introducing pressure $P$ into the reactor, but now $P$ will be half the centre pressure, and the centre pressure will be proportional to $(1/0.5)P$ or $2P$. Finally, assume that the transducer’s radius is such that it is placed at the radius where the reactor pressure is normally zero - a pressure node - and it continues to introduce pressure $P$. Now the centre pressure will be proportional to $(1/0)P$ - an infinite increase. This won’t happen in practice, but this thought exercise does demonstrate that placing a transducer on, or very near, a pressure node of one of the unforced mode shapes will result in the greatest possible magnification of the transducer input. Thus, placing the transducer near a pressure node reduces the pressure it must generate to produce cavitation in the centre of the reactor. This is especially important in the proposed reactor design because, as noted in Chapter 2, electrostatic transducers are less powerful than the piezoelectrics and magnetostrictives commonly used in sonochemical reactors.

![Figure 3.7 Sound Pressure as a Function of Transducer Position](image-url)
c) Tracking the resonance frequency

The design criteria for the proposed reactor require it to operate at its resonant frequency for maximum efficiency. Since a cavitating system's resonant frequency is transient, some method of tracking that resonant frequency must be employed in the final design. The proposed reactor does not include a resonance tracking mechanism, but it has been designed to accommodate the addition of one.

It has already been noted that an electrostatic transducer was chosen partly because it can operate efficiently over a wide frequency range. This will allow future designs to operate at varying resonances without penalty. In this section, the use of mode shapes to isolate a distinct and, therefore, easily tracked resonant frequency is described.

The resonant frequencies of an unforced cylindrical reactor are given by the following equation:

\[ \omega_{n,\eta} = ck_{n,\eta} = c\sqrt{k_{r_n}^2 + k_{z_\eta}^2} \]  

3.4

Where

- \( \omega_{n,\eta} \) = angular resonant frequency, rad/s
- \( k_{r_n} \) = radial wave number, 1/m
- \( k_{z_\eta} \) = axial wave number, 1/m
- \( k_{n,\eta} \) = wave number, 1/m
- \( c \) = speed of sound, m/s
- \( n \) = radial mode number
- \( \eta \) = axial mode number

Each resonant frequency is a function of one radial and one axial wave number. Some combinations of wave numbers may result in resonant frequencies that are very close to one another, while others may yield resonant frequencies that are far apart. This phenomenon can be observed by looking at a wave number contour plot, such as the one shown in Figure 3.8. Because wave numbers are proportional to resonant frequencies, a wave number contour plot is equivalent to a resonant frequency contour plot.
In Figure 3.8, the x-axis grid lines represent the radial wave numbers for the radial modes of a cylindrical reactor of radius R and length L. The y-axis grid lines represent the axial wave numbers for the axial modes of same reactor. The intersection of the radial and axial wave number lines denotes the value of the wave number that corresponds to the reactor mode of the same radial and axial numbers. The curves through those intersections are the wave number contours, which are proportional to the resonant frequency contours. For the reactor shown in the figure, the first radial, first axial mode has a very distinct resonance - there are no contours near it. The first radial, second axial and the second radial, zero axial modes have fairly close contours - indicating that the resonant frequencies for these modes are close in value.
In a cavitating reactor, these resonant frequencies would decrease, but at different rates, since the size, density and placement of cavitation bubbles in the reactor would have a different effect on each frequency. As they decrease, the resonant frequencies that are already close might become closer, coincide, or even switch places. If this were to happen, it would be difficult to track a particular resonance, since the tracking equipment could easily mistake a nearby resonant frequency for the one it was initially following. In order for resonant frequency tracking to take place, the proposed reactor design must favour a mode with a single, distinct resonant frequency.

Like in the radial case, the axial configuration of the transducer dictates which axial modes will be strongly supported by the reactor, and which will not be supported at all. The simplest axial configuration for the transducer is one where the transducer extends along the whole length of the reactor. This results in an input pressure at the transducer radius that is constant along the reactor’s length, but zero at the upper and lower axial boundaries. Thus, the pressure input from the transducer takes the form of a square wave. The reactor pressure at the transducer equals the transducer pressure, so the axial modes excited by the transducer also form a square wave. For this to occur, the reactor’s axial response must be a sum of odd axial modes only. Even axial modes have a pressure node at the center of the reactor’s axis so no sum of even axial modes produces a square wave. This principle is illustrated in Figure 3.9. It can also be seen in this figure that the reactor’s first axial mode, which consists of one sine wave peak, most closely approximates a square wave, and will be strongly excited as a result.

Knowledge of how the transducer’s configuration in the reactor excites specific radial and axial mode shapes allows the proposed reactor design to be configured such that it will strongly excite a mode with a distinct, trackable resonant frequency.

There is one final point to make regarding mode shapes and transducer placement. Recall that the reactor’s radial mode shapes were determined by assuming the radial wall is pressure release. This makes the wall radius a pressure node for all radial mode shapes. It was also determined that the cylindrical transducer should be placed so that it coincided with a radial node. Let it now be assumed that the transducer is placed at a node inside the reactor - not on the reactor wall. This creates two separate regions in the reactor - one between the centre of the reactor and the transducer, and one between the transducer and the reactor wall. These regions are both influenced by the transducer since it applies the same pressure to each region, but are isolated otherwise.
Figure 3.9 Axial Modes Which Approximate a Square Wave

The centre region is where the reactor's largest pressure maximum is developed. It is where the sound field from the transducer is focused and cavitation is induced. In the outer region, one or more pressure maxima are developed between the transducer and the wall, but these are low-amplitude maxima that don't do anything useful. Generating them is unnecessary and inefficient. Placing all of the reactor
vessel at the radius of the next anti-node of the radial pressure profile will suppress the generation of a pressure field in the outer region. The maximum pressure in the outer region will equal the transducer pressure, while the maximum pressure in the inner region is much greater than the transducer pressure because of the mode shapes.

3.5 Resonance

Much has already been said about resonance in the above discussions of frequency tracking and excitation of distinct mode shapes. It bears mentioning, however, that the reason the proposed reactor design must always operate efficiently at one of its resonant frequencies, is that the response of the reactor is always largest, and the reactor itself is always most efficient, at a resonant frequency. If for some reason the transducer, or some other reactor component, does not operate efficiently at the reactor's resonance, the maximum pressure amplitude in the reactor will not be achieved.

It also bears mentioning that, although the proposed reactor design can be tuned to strongly favour one particular mode and its corresponding resonant frequency, the reactor will also have other modes with other resonant frequencies. In some cases, the maximum pressure at another one of these resonances may be higher that the maximum pressure at the intended resonant frequency.

For the proposed reactor design to function as is intended, it must operate at one of its resonant frequencies.

3.6 Final Reactor Design

Complete drawings of the reactor and the transducer, with dimensions, are shown in Appendix A. A plastic bucket, filled with water, is used as the reaction vessel. The plastic sides and bottom of the bucket are pressure release boundaries, as is the free water surface at the top of the reactor.

For bucket's plastic walls to be considered pressure relief boundaries, their impedances must be significantly less than the impedance of the water inside the reactor. From a mechanical standpoint, this means that they must either be much less massive or much less 'acoustically stiff' than the water, or both.

The mass impedance of water is on the same order of magnitude of that of plastic, because the two have similar densities. The acoustic impedance of water is given by: $^{25}$
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\[
Z_{H_2O} = \frac{p_{H_2O}}{u_{H_2O}} = \rho_{H_2O}c_{H_2O} = 1.5 \times 10^6 \frac{kg}{m^2s}
\]

Where

- \(Z_{H_2O}\) is the acoustic impedance for a plane wave in water, kg/m²s
- \(p_{H_2O}\) is the pressure of the plane wave in water, Pa
- \(u_{H_2O}\) is the velocity of the plane wave in water, m/s
- \(\rho_{H_2O}\) is the density of water, kg/m³
- \(c_{H_2O}\) is the speed of sound in water, m/s

The acoustic impedance of the cylindrical plastic wall is also given by its pressure divided by its velocity. The pressure experienced by the cylindrical wall is related to its circumferential or hoop stress, which is given by:

\[
P_w = \frac{\sigma_c t_w}{R} = \frac{E_p \delta_r t_w}{R^2}
\]

Where

- \(p_w\) is the pressure at the cylindrical wall, Pa
- \(\sigma_c\) is the circumferential stress in the cylindrical wall, Pa
- \(t_w\) is the thickness of the cylindrical wall, m
- \(R\) is the radius of the cylindrical wall, m
- \(E_p\) is Young's modulus for plastic, Pa
- \(\delta_r\) is the radial displacement of the cylindrical wall, m

The velocity, \(u_w\), of the bucket’s cylindrical wall is given by the product of its displacement and the frequency at which the sound waves in the water force it to move:

\[
u_w = \delta_r \omega
\]

Thus, the impedance of the cylindrical plastic wall is given by:
The traditional frequency range for sonochemistry was given in Chapter 2 as 20 to 100 kHz. For the version of the proposed reactor design that was built for this research, these frequencies correspond to wall impedances of approximately 7500 to 1500 kg/m$^2$s. In Chapter 5, it will be shown that the lowest frequency used in this research is 4 kHz. This corresponds to cylindrical wall impedance of 39,000 kg/m$^2$s. These impedances are significantly lower than the impedance of water, which confirms that it is appropriate to assume that the cylindrical reactor wall is a pressure relief boundary.

The impedance at the bottom of the bucket can be approximated in a similar manner to that of the cylindrical wall, except that the pressure must be calculated using the longitudinal stress experienced by the cylinder, instead of the circumferential stress. Deflection of the bucket’s plastic bottom will also play a role in the impedance of the bottom boundary, but its effect is neglected in this approximation. Thus, the impedance of the bottom boundary is given by:

$$Z_B = \frac{p_b}{u_b} = \frac{2t_w \sigma_l \frac{1}{R}}{\delta_a \omega} = \frac{2t_w E \delta_b}{LR \frac{1}{\delta_a \omega}} = \frac{2Et_w}{LR \frac{1}{\omega}} = \frac{1200 \times 10^6}{\omega} \frac{kg}{m^2s^2}$$

Where

- $p_b$ = pressure at the bottom boundary, Pa
- $u_b$ = velocity at the bottom boundary, Pa
- $\sigma_l$ = longitudinal stress in the cylindrical wall, Pa
- $L$ = length of the cylindrical wall, m
- $\delta_a$ = axial displacement of the cylindrical wall, m

At 4 kHz, this corresponds to an impedance of 300,000 kg/m$^2$s for the test reactor. This value is one order of magnitude less than the impedance of water. Deflections of the bucket’s bottom will make this impedance even smaller, so it is also appropriate to assume the bottom of the bucket is a pressure release boundary.
The transducer used in the final reactor design was constructed as described earlier in the Chapter 3. It is mounted in the reactor so that its centre axis coincides with the bucket’s centre axis. It extends from the bottom of the bucket to the top of the water. The transducer is attached to the bucket with a silicone based adhesive. The silicone creates a water proof seal that prevents water from flowing between the interior and exterior regions of the reactor.

The transducer and wall radii for the final reactor design were chosen so that they would coincide with the first node and second maximum of a cylinder’s second radial mode. This is shown in Figure 3.10. As discussed earlier in the chapter, this configuration forces the interior region of the reactor to respond strongly at the resonant frequency that corresponds to this mode and nearly eliminates the sound field in the outer region.

It can be seen from the figure, however, that the radius of the bucket does vary slightly from the bottom to the top. In the actual test reactor, the outer radius is about 10% greater at the waterline than it is at the middle of the bucket. Similarly, the radius at the bottom of the bucket is about 10% smaller than the centre radius. The transducer was also built and mounted by hand, so it is not perfectly cylindrical or centered. The error in the radius of the transducer is ± 5% at the most. This may seem to be contrary to the design process, which demonstrated that the placement of the reactor elements determined the effectiveness of the reactor, but these deviations do not threaten the success of the reactor. Instead, they demonstrate the flexibility of the proposed reactor design.

Deviations in the transducer’s radius cause the resonant frequency of the reactor to shift slightly. It was noted above that the reactor’s strongest response (resonance) is produced when the transducer is at the node of an the unforced radial mode. If the transducer is slightly inside or outside its intended location, then that position will be the new nodal position. This node will be slightly closer to, or further away from, the centre of the reactor than was originally presumed. This causes the radial wave length of the mode to be a little shorter or a little longer. As a result, the reactor’s resonant frequency for that mode will be a little larger or smaller than was originally thought. Since the proposed reactor design uses an electrostatic transducer, these slight variations in the expected resonant frequency are easily accommodated. Therefore, a tight tolerance on the transducer’s radius is only necessary when a very specific pre-cavitation resonant frequency is required. Deviations in the radius of outer wall only affect how quickly the sound field in the outer region goes to zero.
Though the proposed reactor design is a batch reactor (it applies sound energy to discrete quantities of liquid), it could easily be made into a flow-through reactor for continuous operation. In a continuous reactor, the bottom of the reaction vessel would be removed and the cylindrical walls would act like a pipe. This change in the reactor's top and bottom boundaries, and the motion of the liquid through the cylinder, would alter the reactor's axial boundary conditions. These changes would not, however, negate the design principles behind the reactor. The radial mode shapes would be unchanged and the axial ones would be modified slightly. This would once again result in a slight change in the reactor's resonant frequencies, which would be simple to accommodate.

Figure 3.10 Final Reactor Design
Chapter Four  

Mathematical Modeling

Mathematical modeling of the homogenous pressure fields in a sonochemical reactor is "... a first step of the design of sonochemical reactors..." (Keil & Dähnke, 1996) Furthermore, "The characterization of sonoreactors is essential when one is aiming to optimize the reaction conditions." (Keil, Dähnke & Swamy, 1999)

As discussed in Chapter 2, previous reactor modeling has focused on creating models of existing reactors so that they can be compared and modified, without considering the merits of the original design. What distinguishes the modeling done in this research is that it is used as a design tool. The proposed sonochemical reactor design, discussed in Chapter 3, proceeded from good design principles, but this in of itself does not guarantee that the design will be successful. Its performance is unproven, particularly in regards to its electrostatic transducer which, despite its many advantages, generates comparatively low power output. Once it is shown to be accurate, the mathematical model of the reactor design detailed in this chapter can be used to determine whether this design is feasible and, if so, how it should be refined.

In constructing a model of the whole reactor system, models of the transducer and the reaction container were created. These models were combined to create the complete model of the sonochemical reactor.

4.1 Transducer Model

A basic mathematical model for an electrostatic transducer had to be adapted for use in this research. Specifically, the model needed to accommodate a sinusoidal input frequency, the curved geometry of the transducer and the transducer's stiffness and damping characteristics.

4.1.1 Basic Transducer Model

A mathematical model of a transducer relates its input parameters to its output parameters by a transfer function. In the case of an electrostatic transducer, the input parameters are the current and voltage supplied to the transducer; the output parameters are the pressure and velocity of the moving
diaphragm. The electrostatic pressure generated in the transducer is not equivalent to the pressure of the moving diaphragm. Instead, the stiffness and damping forces within the transducer modify the electrostatic pressure, resulting in the pressure acting on the moving diaphragm. This force creates the acoustic pressure in the reactor liquid.

The transfer function of an electrostatic transducer can be derived as shown below. This derivation assumes that the input signal to the transducer consists of both a constant bias voltage and a sinusoidal voltage signal.

The derivation starts with a mechanical force balance for the transducer:

\[ f_A = m\ddot{x} + b(\omega)\dot{x} + k(\omega)x + f_e \]  \hspace{1cm} (4.1)

Where

- \( f_A \) = the acoustic force generated by the transducer, N
- \( f_e \) = the electrostatic force generated in the transducer, N
- \( x \) = the displacement of the moving diaphragm, m
- \( b(\omega) \) = the damping constant of the transducer, kg/s
- \( k(\omega) \) = the spring constant of the transducer, kg/s²
- \( \omega \) = the angular frequency at which the transducer is driven, rad/s

The electrostatic force can be replaced by the expression given in equation 3.1. In order to do this, the electrostatic pressure given in equation 3.1 is converted to a force, and the voltage is replaced by a charge, as follows:

\[ f_e = P_e S \quad V = \frac{qd}{\varepsilon S} \quad P_e = \frac{\varepsilon V^2}{2d^2} \Rightarrow f_e = \frac{q^2}{2\varepsilon S} \]  \hspace{1cm} (4.2)

Where

- \( q \) = the charge on a transducer plate, C
Thus, the mechanical force balance for the transducer becomes:

\[ f_A = m\ddot{x} + b(\omega)\dot{x} + k(\omega)x + \frac{q^2}{2\varepsilon S} \]  \hspace{1cm} \text{(4.3)}

The next step is to consider an electrical description of the electrostatic transducer. Assuming that the transducer has some resistance and inductance as well as its considerable capacitance, the electrical description will take the following form:

\[ V_0 + v(t) = L\ddot{q} + R\dot{q} + \frac{q}{C} \]  \hspace{1cm} \text{(4.4)}

Where

\[ V_0 = \text{the constant bias voltage applied to the transducer}, \ V \]
\[ v(t) = \text{the time-dependent voltage applied to the transducer}, \ V \]
\[ L = \text{the inductance of the transducer}, \ H \]
\[ R = \text{the resistance of the transducer}, \ \Omega \]
\[ C = \text{the capacitance of the transducer}, \ F \]
\[ t = \text{time}, \ s \]

This equation is modified by replacing the capacitance with an equivalent expression. Recall that \( d \) is the nominal gap space and \( x \) is the displacement of the flexible electrode from its neutral position.

\[ C = \frac{\varepsilon S}{d + x} \]

\[ V_0 + v(t) = L\ddot{q} + R\dot{q} + \frac{d + x}{\varepsilon S} \]  \hspace{1cm} \text{(4.5)}

Together, equations 4.3 and 4.5 form the basis for computing the transfer function of an electrostatic transducer. All the required elements are present - the input voltage, \( V \), the input current, which is represented by the charge, \( q \), the output force, \( f_A \), and the membrane velocity, which is found from the displacement, \( x \).
To develop the final transfer function, appropriate expressions for the input and output variables are assumed and inserted into these equations. The most general time-variant input or output signals can be constructed by expanding each signal into a Fourier series. Only the constant and first harmonic terms of each series are used in this derivation. This is equivalent to assuming that the system is linear about the dc bias voltage. The first harmonic is most easily represented as a sum of complex exponentials. The charge and displacement will also have bias values, since a constant voltage imparts a constant charge and, therefore, a constant attraction to the plates. The input and output signals are as follows:

\[ v(t) = \frac{1}{2}V e^{j\omega t} + \frac{1}{2}V^* e^{-j\omega t} \]  \hspace{1cm} (4.6)

\[ q = q_0 + \frac{1}{2}Q e^{j\omega t} + \frac{1}{2}Q^* e^{-j\omega t} \]  \hspace{1cm} (4.7)

\[ f_A = \frac{1}{2}F_A e^{j\omega t} + \frac{1}{2}F_A^* e^{-j\omega t} \]  \hspace{1cm} (4.8)

\[ x = x_0 + \frac{1}{2}X e^{j\omega t} + \frac{1}{2}X^* e^{-j\omega t} \]  \hspace{1cm} (4.9)

Where

- \( V, V^* \) = magnitudes of the conjugate exponentials of the time-variant voltage input, \( V \)
- \( q \) = total charge input, \( C \)
- \( q_0 \) = constant portion of the charge input, \( C \)
- \( Q, Q^* \) = magnitudes of the conjugate exponentials of the time-variant charge input, \( C \)
- \( f_A \) = total force output, \( N \)
- \( F_A, F_A^* \) = magnitudes of the conjugate exponentials of the time-variant force output, \( N \)
- \( x \) = total displacement output, \( m \)
- \( x_0 \) = constant portion of the displacement output, \( m \)
- \( X, X^* \) = magnitudes of the conjugate exponentials of the time-variant displacement output, \( m \)
Equations 4.3 and 4.5 include the first and second time derivatives of the displacement and charge expressions, so these must be calculated as well:

\[
\dot{x} = \frac{j\omega}{2} X e^{j\omega t} - \frac{j\omega}{2} X^* e^{-j\omega t} \quad 4.10
\]

\[
\ddot{x} = -\frac{\omega^2}{2} X e^{j\omega t} - \frac{\omega^2}{2} X^* e^{-j\omega t} \quad 4.11
\]

\[
\dot{q} = \frac{j\omega}{2} Q e^{j\omega t} - \frac{j\omega}{2} Q^* e^{-j\omega t} \quad 4.12
\]

\[
\ddot{q} = -\frac{\omega^2}{2} Q e^{j\omega t} - \frac{\omega^2}{2} Q^* e^{-j\omega t} \quad 4.13
\]

Inserting equations 4.6 through 4.13 into equations 4.3 and 4.5 results in two equations which have the following form:

\[
A_n e^0 + B_n (e^{j\omega t} \pm e^{-j\omega t}) + C_n (e^{j2\omega t} \pm e^{-j2\omega t}) = 0 \quad 4.14
\]

The two equations can be separated into several workable equations by equating terms with similar powers of \( e \). The equations for the positive powers of \( e \) are given below:

Powers of 0:

\[
0 = 2k(\omega)x_0 + \frac{q_0}{\xi S} \quad 4.15
\]

\[
V_0 = \frac{1}{\xi S}(2dq_0 + 2x_0g_0 + XQ^* + X^*Q) \quad 4.16
\]

Powers of \( j\omega t \):

\[
F_A = X(-m\omega^2 + jb(\omega)\omega + k(\omega)) + \frac{Qq_0}{\xi S} \quad 4.17
\]
\[ V \approx Q \left( -L\omega^2 + jR\omega + \frac{d + x_0}{\varepsilon S} \right) + \frac{Xq_0}{\varepsilon S} \]  

4.18

Powers of \( j2\omega t \):

\[ 0 \approx \frac{Q^2}{4\varepsilon S} \]  

4.19

\[ 0 \approx \frac{1}{2} XQ \]  

4.20

Of these new equations, only 4.17 and 4.18 reveal anything useful about the relationship between the transducer's input and output signals. To generate the final transfer function, the charge and displacement in these equations are replaced with the current, \( i(t) \), and transducer velocity, \( u_0(t) \). This is possible because current and velocity are the time derivatives of charge and displacement, respectively.

\[ i(t) = Ie^{j\omega t} = \frac{\partial}{\partial t} Qe^{j\omega t} = j\omega Qe^{j\omega t} \quad u_0(t) = U_0 e^{j\omega t} = \frac{\partial}{\partial t} Xe^{j\omega t} = j\omega Xe^{j\omega t} \]  

4.21

Putting these new values into equations 4.17 and 4.18 gives:

\[ f_A(t) = -\frac{q_0}{j\omega \varepsilon S} i(t) + \frac{(-m\omega^2 + jb(\omega)\omega + k(\omega))}{j\omega} u_0(t) \]  

4.22

\[ v(t) = \frac{(-k(\omega)\omega^2 + j\omega R + d + x_0)}{j\omega \varepsilon S} i(t) + \frac{q_0}{j\omega \varepsilon S} u_0(t) \]  

4.23
These equations constitute the transfer function for the transducer. Equation 4.24 casts equations 4.22 and 4.23 into matrix form:

\[
\begin{bmatrix} F_A \\ V \end{bmatrix} e^{j\omega t} = \begin{bmatrix} \frac{q_0}{j\omega \varepsilon} & j \left( m \omega - \frac{k}{\omega} \right) + b \\ j \left( L \omega - \frac{d + x_0}{\omega \varepsilon} \right) + R & \frac{q_0}{j\omega \varepsilon} \end{bmatrix} \begin{bmatrix} I \\ U_r \end{bmatrix} e^{j\omega t} \tag{4.24}
\]

It can be seen from equation 4.24 that, when a sinusoidal and bias voltage are applied to an electrostatic transducer, the resulting acoustic force has the same frequency as the time-variant input voltage. This agrees with the discussion in Chapter 3.

### 4.1.2 Pure Sinusoidal Input

In this research, the input voltage to the transducer was sinusoidal. In Chapter 2, it was noted that the frequency of an electrostatic transducer’s output signals is twice that of its input signals, when no constant bias voltage is applied. As a result, the first-harmonic term of the Fourier series for both output signals is proportional to $e^{j\omega t}$ and not $e^{j\alpha t}$, as was used in the derivation of the transfer function shown above. To address this issue, the above derivation can be modified to create a transfer function appropriate for a purely sinusoidal input. For this situation, the assumed input and output signals are:

\[
v(t) \equiv \frac{1}{2} V e^{j\omega t} + \frac{1}{2} V^* e^{-j\omega t} \tag{4.25}
\]

\[
q \equiv \frac{1}{2} Q e^{j\omega t} + \frac{1}{2} Q^* e^{-j\omega t} \tag{4.26}
\]

\[
f_A \equiv \frac{1}{2} F_A e^{j2\omega t} + \frac{1}{2} F_A^* e^{-j2\omega t} \tag{4.27}
\]

\[
x \equiv x_0 + \frac{1}{2} x e^{j2\omega t} + \frac{1}{2} x^* e^{-j2\omega t} \tag{4.28}
\]
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Where

\[ \omega_d = \text{angular frequency at which the input signals are driven, rad/s} \]

What distinguishes equations 4.25 through 4.28 from equations 4.6 through 4.9 is that the doubling of the force and displacement frequencies is included in the Fourier transforms descriptions, and some constant values are left out, since there is no constant bias voltage and, thus, no constant charge response. Also, for reasons that will become clear later, the angular frequency of the input signals is referred to as \( \omega_d \) or the driving frequency.

To develop the new transfer function, equations 4.25 through 4.28, and the new charge and displacement derivatives, which are shown below, are substituted into the mechanical and electrical descriptions of the transducer. The new charge and displacement derivatives are:

\[ \dot{x} \approx j \omega_d X e^{j2\omega_d t} - j \omega_d X^* e^{-j2\omega_d t} \]

\[ \ddot{x} \approx -2 \omega_d^2 X e^{j2\omega_d t} - 2 \omega_d^2 X^* e^{-j2\omega_d t} \]

\[ \dot{q} \approx \frac{j \omega_d}{2} Q e^{j\omega_d t} - \frac{j \omega_d}{2} Q^* e^{-j\omega_d t} \]

\[ \ddot{q} \approx \frac{-\omega_d^2}{2} Q e^{j\omega_d t} - \frac{\omega_d^2}{2} Q^* e^{-j\omega_d t} \]

Once again, inserting equations 4.25 through 4.32 into equations 4.3 and 4.5 results in large equations that can be simplified by equating common powers of \( e \). In the sinusoidal case the equations for positive powers of \( e \) are:

Powers of 0:

\[ 0 \approx \frac{1}{2} QQ^* + 2kx_0 \]
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Powers of $j\omega t$:

\[ V \approx \frac{1}{\varepsilon S} \left( (d + x_0)q + \frac{1}{2} x_0 Q^* \right) \quad 4.34 \]

Powers of $j2\omega t$:

\[ F_A \approx X(-4\omega_d^2 m + j2\omega_d b(\omega) + k(\omega)) + \frac{Q^2}{4\varepsilon S} \quad 4.35 \]

Powers of $j3\omega t$:

\[ 0 \approx \frac{XQ}{2\varepsilon S} \quad 4.36 \]

For this derivation, only equations 4.34 and 4.35 are useful for constructing the transfer function. Once again, the charge and displacements in these equations are replaced by currents and velocities using:

\[ i(t) = Ie^{j\omega_d t} = \frac{\partial}{\partial t} Qe^{j\omega_d t} = j\omega_d Qe^{j\omega_d t} \quad 4.37 \]

This results in the following equations:

\[ f_A(t) = -\frac{1}{4\omega_d^2\varepsilon S} i(t)^2 + \left( b(\omega) + j \left( 2\omega_d m - k(\omega_d) \right) \right) u_i(t) \quad 4.38 \]

\[ v(t) = \frac{d}{j\omega_d\varepsilon S} i(t) \quad 4.39 \]

Note that in converting equation 4.35 to equation 4.39, the $xq^*$ term has been dropped. This is valid for two reasons. First, the gap spacing, $d$, in the transducer is much bigger than the membrane displacement, $x$, so the $xq^*$ term is not significant. Second, the resulting equation for $V$ matches the known impedance expression for a capacitor as shown below:

\[ v(t) = \frac{d + x}{j\omega_d\varepsilon S} i(t) = \frac{1}{j\omega_d C} i(t) \quad 4.40 \]
One could construct a matrix transform from equations 4.38 and 4.39. However, since 4.39 now gives a direct relationship between the voltage and current signals, a single transform equation can be constructed. Using equation 4.39 to eliminate \( i \) from equation 4.38 yields:

\[
f_A(t) = -\frac{\varepsilon S}{4d^2} v(t)^2 + \left( b + j \left( 2\omega_d m - \frac{k}{2\omega_d} \right) \right) u_i(t)
\]

To use this equation in the reactor system, it is useful to cast it into a few different forms. The first form uses the acoustic pressure at the transducer instead of the acoustic force. This pressure will be referred to as \( p_t \) or the transducer pressure, to distinguish it clearly from pressures in the reactor. It is given as:

\[
p_t(t) = -\frac{\varepsilon}{4d^2} v(t)^2 + \left( b + j \left( 2\omega_d m - \frac{k}{2\omega_d} \right) \right) \frac{u_i(t)}{S} = \frac{f_A(t)}{S^2}
\]

The second uses the frequency of the pressure signal imparted to the reactor, given by \( \omega_r \) where \( r \) refers to the reactor frequency, rather than the driving frequency, \( \omega_d \). Recall that \( \omega_r = 2\omega_d \). The exponential time dependence is also shown explicitly in this equation:

\[
P e^{j\omega_r t} = -\frac{\varepsilon}{4d^2} V^2 e^{j\omega_d t} + \left( b + j \left( \omega_r m - \frac{k}{\omega_d} \right) \right) \frac{U_i e^{j\omega_d t}}{S}
\]

### 4.1.3 Curved Transducer

The derivation above assumes that the transducer electrodes are parallel plates. The transducer used in this research is a cylindrical surface divided into square transducer elements. Each transducer element consists of a pair of arc-shaped plates separated by a constant distance. A transducer element is illustrated in Figure 4.1. In order to use the transfer function derived above, it must be shown that the equations for the curved transducer elements are sufficiently similar to those of a flat one.
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If the displacement, \( x \), is assumed to act in a direction normal to the curved transducer, then the only difference between the curved and flat transducer elements is the expression for the capacitance which is given below:

\[
C = \frac{2\Theta \varepsilon L}{\ln \left(1 + \frac{d}{a}\right)} = \frac{2\Theta \varepsilon L}{\ln \left(\frac{a + d}{a}\right)}...
\]

\( a, d \) and \( L \) are as given in Figure 4.1. The logarithmic term in this equation can be replaced with a series representation. For this natural logarithmic form, the Maclaurin Series is given by:

\[
\ln \left(1 + \frac{d}{a}\right) = \frac{d}{a} - \frac{\left(\frac{d}{a}\right)^2}{2} + \frac{\left(\frac{d}{a}\right)^3}{3} - \frac{\left(\frac{d}{a}\right)^4}{4} + \ldots \quad (-1 < \frac{d}{a(x)} < 1)
\]

The condition that the absolute value of the variable term must be less than one is easily met in this case, since the transducer radius, \( a \), is much larger than the electrode spacing, \( d \). In fact, it is reasonable to neglect the higher-order terms of the equation, since the powers of \( d \) get smaller and smaller, while the powers of \( a \) get larger and larger.

\[
\begin{align*}
a & = \text{radius of rigid electrode, m} \\
b & = \text{radius of flexible electrode, m} \\
d & = \text{gap space, m} \\
x & = \text{flexible electrode displacement, m} \\
L & = \text{length of transducer element, m (into page)}
\end{align*}
\]

Figure 4.1 Illustration of an Arc Shaped Transducer Element
Neglecting the higher-order terms in equation 4.45, and recalling that the area, $S$, of a portion of a cylinder of length $L$ and radius $a$ is given by $2\Theta aL$, yields the following:

$$C \approx \frac{2\Theta \varepsilon L a}{d} \approx \frac{\varepsilon S}{d} \quad \text{4.46}$$

The only thing needed to make the capacitance of the cylindrical reactor elements match that of the planar transducer elements is to add the membrane displacement, as shown below:

$$C \approx \frac{\varepsilon S}{d + x} \quad \text{4.47}$$

### 4.1.4 Transducer Stiffness and Damping

Expressions for the transducer’s stiffness and damping are all that is needed to complete the transfer function. The expressions used in this research are based on a thermodynamic model of the transducer system developed by Dunwoody. 29

The plates of an electrostatic transducer are pulled together by the electrostatic force. The air, or other gas, between the plates compresses, creating a pressure rise that acts like a spring and resists the motion. This seemingly simple process is complicated by the fact that the pressure rise in the gas increases its temperature. As the temperature rises, heat flows from the gas to the transducer plates. Half a cycle later the plates move apart, the pressure in the gap decreases and heat flows from the transducer plates to the gas. Since the flow of heat from the gas to the plates and back again is not instantaneous, a phase difference results between the pressure and temperature, and ultimately between the pressure fluctuations and the displacement of the plates. This phase difference results in a dissipation of energy in the system, and creates a damping effect.

The model developed by Dunwoody makes a few assumptions about the transducer. The horizontal extent of the transducer element is assumed to be much greater than the gap spacing so that all heat flow is unidirectional. This is a valid assumption for the transducer used in this research. The gas in the
transducer is assumed to follow the polytropic gas law, which is reasonable for normal operating temperatures and pressures. The heat transfer within the gas is assumed to take place entirely by conduction because the gaps in most transducers, including the one used in this research, are so small that convective cells cannot be formed. Finally, the transducer plates are assumed to be ideal heat sinks. This assumption is reasonable because the aluminum plates used in the research transducer have much higher thermal capacities and conductivities than the air in the gaps.

The thermal model for the transducer's stiffness and damping uses the polytropic gas law, the conservation of energy within a control mass and the conductive heat transfer of air to find the transducer's temperature and pressure distributions. The magnitude and phase of these quantities are used to generate the spring and damping coefficients for the transducer, given below:

\[
\begin{align*}
    k(\omega) &= SP(\omega) \cos(A(\omega)) \\
    b(\omega) &= \frac{S}{\omega} P(\omega) \sin(A(\omega))
\end{align*}
\]

Where

\[
    P(\omega) = \text{the amplitude of the pressure distribution, kg/m}^2\text{s}^2
\]

\[
    A(\omega) = \text{the phase of the pressure distribution}
\]

4.2 Reactor Model

The next step in producing a mathematical model of the whole reactor system is to determine the pressure distribution in the reaction vessel. This first part of section 4.2 outlines the development of the pressure field in a reactor without considering damping in the reactor liquid. Damping is incorporated in the second part.

4.2.1 Undamped Pressure Distribution

Recall from Chapter 3 that the reactor designed for this research, and illustrated in Figure 4.2 below, has a pressure distribution that can be determined analytically.
The solution starts with the wave equation for sound. Solving the homogenous, or unforced, form of this equation will yield the reactor's eigenfunctions. These eigenfunctions are used to find the reactor's response to the input pressure from the transducer. This homogenous wave equation is given by:

\[
\frac{\partial^2 p(r,z,t)}{\partial^2} - c^2 \nabla^2 p(r,z,t) = 0
\]

or, in cylindrical co-ordinates:

\[
\frac{\partial^2 p(r,z,t)}{\partial^2} - c^2 \left( \frac{\partial^2 p(r,z,t)}{\partial^2 r} + \frac{1}{r} \frac{\partial p(r,z,t)}{\partial r} + \frac{\partial^2 p(r,z,t)}{\partial z^2} \right) = 0
\]

Where

\[
p(r, z, t) = \text{pressure in the reactor, Pa}
\]
\[
r = \text{radial dimension of the reactor, m}
\]
\[
z = \text{axial dimension of the reactor, m}
\]
\[
t = \text{time, s}
\]
\[
c = \text{speed of sound in the reactor liquid, m/s}
\]

Note that, by virtue of symmetry, the reactor pressure is not dependent on the angular position in the reactor. The partial differential equation given above can be simplified using separation of variables. For this technique, \(p(r, z, t)\) is assumed to take the following form:

\[
p(r, z, t) = R(r)Z(z)T(t)
\]

Where

\[
R(r) = \text{radial portion of the pressure function}
\]
\[
Z(z) = \text{axial portion of the pressure function}
\]
\[
T(t) = \text{temporal portion of the pressure function}
\]
Substituting this form of the pressure function into the wave equation, and assuming that the time variance of the pressure function will have eigenvalues, $-\omega_{n,\eta}^2$, yields the following relations:

$$c^2 \left( \frac{R''(r)}{R(r)} + \frac{1}{r} \frac{R'(r)}{R(r)} + \frac{Z''(z)}{Z(z)} \right) = \frac{T''(t)}{T(t)} = -\omega_{n,\eta}^2$$ \hspace{1cm} (4.53)

$$\frac{R''(r)}{R(r)} + \frac{1}{r} \frac{R'(r)}{R(r)} + \frac{Z''(z)}{Z(z)} = -k_{r,\eta}^2 = -(k_{r,\eta}^2 + k_{z,\eta}^2)$$ \hspace{1cm} (4.54)

Where

- $k_{r,\eta} = \text{radial wave number, 1/m}$
- $k_{z,\eta} = \eta \pi / L = \text{axial wave number, 1/m}$
- $k_{n,\eta} = \text{reactor wave number, 1/m}$
Equations 4.53 and 4.54 yield three ordinary differential equations that can be solved easily. These are:

\[ T''(t) + \omega_{n,\eta}^2 T(t) = 0 \quad 4.55 \]
\[ Z''(z) + k_{\eta}^2 Z(z) = 0 \quad 4.56 \]
\[ r^2 R''(r) + r R'(r) + r^2 k_{\eta}^2 R(r) = 0 \quad 4.57 \]

To solve these equations, the boundary conditions for the reactor must be applied. In Figure 4.2, the reactor is divided into two separate regions - region one, which is inside the transducer and region two, which is outside of it. In region 1, which extends from the centre of the reactor at \( r = 0 \) m, to the transducer at \( r = r_n \), the radial boundary conditions are as follows:

\[ u_{r1}(0, z, t) = 0 \quad 4.58 \]
\[ p_1(r, z, t) = p_1(t) \quad 4.59 \]

Where

\[ u_{r1}(r, z, t) = \text{radial velocity of the sound wave in region one, m/s} \]

Note that the radial velocity of the sound wave in the reactor can be determined from the pressure by the following relation:

\[ \frac{\partial u_r(t)}{\partial t} + \frac{1}{\rho} \frac{\partial p(t)}{\partial r} = 0 \quad 4.60 \]
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In region 2, which extends from the transducer at \( r = r_n \) to the wall of the reactor at \( r = R \), the radial boundary conditions are as follows:

\[
p_2(r, z, t) = p_2(t) \tag{4.61}
\]

\[
p_2(R, z, t) = 0 \tag{4.62}
\]

Recall that pressure at \( R \) is zero because the plastic outer wall of the reactor is assumed to act as a pressure release boundary.

Finally, the axial boundary conditions, which extend from the bottom of the reactor at \( z = 0 \) m, to the top of the reactor at \( z = L \), are given by:

\[
p_{1,2}(r, 0, t) = 0 \tag{4.63}
\]

\[
p_{1,2}(r, L, t) = 0 \tag{4.64}
\]

Again, the pressures at both the top and bottom of the reactor are zero because both the plastic bottom surface and the free water surface at the top of the reactor are assumed to act as pressure release boundaries.

Applying these boundary conditions to the separated ordinary differential equations that describe the reactor system gives the following eigenfunctions for the reactor:

Radial eigenfunction in region one:

\( J_0(k_{r_n} r) \) \tag{4.65}

Radial eigenfunctions in region two:

\( J_0(k_{r_n} r) \)

\( Y_0(k_{r_n} r) \)

Axial eigenfunctions:

\( \sqrt{2} \sin(k_{z_n} z) \) \tag{4.67}

The factor of \( 2^{1/2} \) in the axial eigenfunction normalizes the function. The response of the unforced reactor also has a time variation given by:
The eigenfunctions given in equations 4.65 through 4.67 describe the mode shapes of the reactor system, and can be used to find the forced response. This is because the response of a linear system which is subjected to a time varying forcing function consists of a sum of its mode shapes vibrating at the input frequency. For the reactor used in this research, the forced response is described by the following equations:

Region one:

\[ p_1(r, z, t) = \sum_{n, \eta} \sqrt{2} A_{n, \eta} J_0(k_n r) \sin(k_z z) e^{\omega t} \]  \hspace{2cm} 4.69

Region two:

\[ p_2(r, z, t) = \sum_{n, \eta} \sqrt{2} (B_{n, \eta} J_0(k_n r) + C_{n, \eta} Y_0(k_n r)) \sin(k_z z) e^{\omega t} \]  \hspace{2cm} 4.70

Where

\[ A_{n, \eta}, B_{n, \eta}, C_{n, \eta} = \text{mode shape coefficients} \]

The coefficients of each individual mode shape indicate how much of the forced response is due to each individual mode. These coefficients can be determined by equating the forcing function, which is the pressure at the transducer, to the reactor pressure distribution at the transducer. The pressure at the transducer is a constant value that extends from \( z = 0 \) m to \( z = L \) at the transducer radius. Equating the transducer and reactor pressures at the transducer location gives:

Region one:

\[ p_1 e^{\omega t} = \sum_{n, \eta} \sqrt{2} A_{n, \eta} J_0(k_n r_t) \sin(k_z z) e^{\omega t} \]  \hspace{2cm} 4.71

Region two:

\[ p_2 e^{\omega t} = \sum_{n, \eta} \sqrt{2} (B_{n, \eta} J_0(k_n r_t) + C_{n, \eta} Y_0(k_n r_t)) \sin(k_z z) e^{\omega t} \]  \hspace{2cm} 4.72

To isolate the mode coefficients, both sides of equations 4.71 and 4.72 are multiplied by an axial mode shape and then integrated over the axial dimension, \( z \). Mode shapes that have different mode numbers are orthogonal, so the integral of their product is zero. If the chosen mode shape has the same mode number as the mode that it multiplies, then the integral is not equal to zero. The integrals that aren't equal to zero are solved for the mode coefficients. This process yields the following equations for the coefficients:
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\[ A_{n,\eta} = \frac{p_1 \int_0^L \sin(k_z z) \, dz}{L J_0(k_{\eta, r})} \]  \hspace{1cm} (4.73)

\[ B_{n,\eta} = \frac{-p_1 \int_0^L \sin(k_z z) \, dz}{L(J_0(k_{\eta, r} R) Y_0(k_{\eta, r}) - Y_0(k_{\eta, R}) J_0(k_{\eta, r})))} \]  \hspace{1cm} (4.74)

\[ C_{n,\eta} = \frac{p_1 \int_0^L \sin(k_z z) \, dz}{L(J_0(k_{\eta, R} R) Y_0(k_{\eta, r}) - Y_0(k_{\eta, R}) J_0(k_{\eta, r})))} \]  \hspace{1cm} (4.75)

With these equations, the coefficients can be calculated for each radial wave number. This is implemented in the research model by using the following relation for the frequency that the reactor is driven at:

\[ \omega_r^2 = c[k_{\eta} + k_{z, \eta}] \]  \hspace{1cm} (4.76)

This equation yields a value for the radial wave number for each actual value of the axial wave number that is used. Some of these values of \( k_z \) are complex. The value of \( k_r \) and the axial wave number are substituted into equations 4.73 to 4.75 to find values for the coefficients. Note that the Bessel functions that describe the radial mode shapes can have complex arguments. If the axial wave number is for a mode that is not supported by the reactor at the given frequency, the coefficients approach zero. If the value of \( k_r \) that is used does not match a radial wave number for the region of the reactor being considered, or if it matches a radial mode number that is not supported by that region of the reactor at the given frequency, then the coefficients also approach zero. Thus, when all of the pressure equations for all of the input values of \( k_z \) are added up, only those that represent the mode shapes that are present in the response contribute to the summation. The new forms of the summations that yield the pressure distribution are:
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Region one:
\[ p_1(r,z) = \sum_{\eta} \sqrt{2} A_\eta J_0(k_r(\eta)r) \sin(k_z z) \]  

Region two:
\[ p_2(r,z) = \sum_{\eta} \sqrt{2} (B_\eta J_0(k_r(\eta)r) + C_\eta Y_0(k_r(\eta)r)) \sin(k_z z) \]

Note that the time dependence, which is the same on both sides of the equation, is not shown.

4.2.2 Damped Pressure Distribution

The above equations for the sound pressure distribution in the reactor do not account for sound attenuation in the reactor. As sound travels through media it loses small amounts of acoustic energy to heat. Some energy is dissipated at the system's boundaries and some is lost in the transmitting medium.

Sound energy dissipation at the boundaries of an acoustic system is primarily due to energy absorption by the walls. Since the research reactor has been designed to minimize the sound energy between the transducer and the reactor walls, the energy absorbed by the walls of the reactor is negligible. Thus, boundary dissipation is not considered in this analysis.

Sound energy losses in the transmitting medium are considered, but they are small, due to the small volume of water used in the reactor. There are three primary mechanisms to which heat losses in liquids are attributed. These are viscous losses, heat conduction losses and losses due to molecular energy exchanges. Viscous losses are caused by the relative motion of the fluid as it undergoes compression and expansion. Heat conduction losses occur during the adiabatic expansion and contraction of the fluid due to sound waves. The changes in pressure result in temperature changes within different regions of the fluid. These temperature disparities tend to equalize, reducing the pressure amplitude and creating heat. Losses due to molecular exchanges are caused by delays in changing the energy of compression to molecular vibration energy and molecular vibration energy to the energy of expansion. These delays tend to promote pressure equalization and, therefore, reduced sound amplitude.

The effect of these fluid losses is commonly expressed in terms of absorption exponents, which modify the amplitude of the pressure wave as it gets farther away from its sound source. For plane waves, the absorption exponent is applied to the pressure equation as follows:

\[ P_{\text{plane}}(x,t) = A e^{i \omega t} e^{-j k x} e^{-\alpha x} \]
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Where

\[ \alpha = \text{absorption exponent, } 1/m \]

The transducer in the reactor is a curved. It radiates sound into the reactor radially, so it is arguably similar to a planar transducer, which radiates in a linear direction. Sound pressure in the reactor is, however, dependent on both the radial and the axial dimension. Nevertheless, applying the absorption coefficient to the radial part of the pressure equation yields:

\[
p_i(r,z,t) = \sum_{n,q} \sqrt{2} A_{n,q} J_0(k_{n,q} r) \sin(k_{n,q} z) e^{\alpha(r-r)} e^{i\omega t} \tag{4.80}
\]

Region two:

\[
p_2(r,z,t) = \sum_{n,q} \sqrt{2} (B_{n,q} J_0(k_{n,q} r) + C_{n,q} Y_0(k_{n,q} r)) \sin(k_{n,q} z) e^{\alpha(r-r)} e^{i\omega t} \tag{4.81}
\]

Since this research concentrates on the radial concentration of the pressure field, it is appropriate to concentrate on radial dissipation and neglect axial dissipation. Furthermore, the model calculations prove that the effect of including fluid damping in the reactor description is negligible.

Another way to apply the absorption coefficient to a multi-variable pressure description is to make the damping exponent modify the time variable, rather than a spatial variable: 30

\[ e^{-\alpha x} = e^{-\alpha t} \tag{4.82} \]

If the reactor were large enough that fluid damping had a significant effect on the reactor pressure, this form of the damping coefficient would be more appropriate than the pseudo-planar model.

The final step in incorporating damping into the model is to determine what the absorption exponent is for the reactor fluid, which in this case is water. Damping due to viscous effects and heat transfer can be calculated using classical equations although, for water, the effects of heat transfer are negligible since pressure fluctuations don’t affect the temperature of water to a great extent. Molecular effects are thought to account for the differences between calculated absorption exponent values and observed values. Calculated and observed absorption exponents for water are shown in Table 4.1. Note that these values are proportional to the cyclic frequency, \( f \), which is equivalent to \( \omega/2\pi \). The research model uses the observed value of the absorption exponent.

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Table 4.1 Absorption Coefficients in Water

<table>
<thead>
<tr>
<th>Viscous Absorption Exponent</th>
<th>Heat Conduction Absorption Exponent</th>
<th>Observed Absorption Exponent</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(8.1 \times 10^{-15})^2$</td>
<td>-</td>
<td>$(24 \times 10^{-15})^2$</td>
</tr>
</tbody>
</table>

4.3 Complete Model

To complete the model, the transducer and reactor models must be integrated. The transducer model describes the pressure at the transducer in terms of the input voltage and the velocity of transducer's moving electrode. The transducer velocity is unknown, but is related to the liquid's radial velocity at the transducer location. The liquid's radial velocity can be determined from the reactor's pressure distribution at the transducer. The reactor model gives the pressure distribution in the reactor, but the calculation assumes that the transducer pressure is known, which it is not, because the reactor pressure is not yet known. This is the problem that must be addressed before the transducer and reactor models can be used to create a complete description of the system.

The first step is to determine the relationship between the liquid velocity at the transducer, and the velocity of the moving electrode. This is complicated by the complex motion of the transducer. First, the flexible electrodes on either side of the transducer oscillate due to the changing input voltage. Since the voltage change is the same on both sides of the transducer, the displacements of both electrodes are also the same, but in different directions. The velocities of the moving electrodes, which are the velocities that are required for the transducer model, are determined by taking the derivative of their displacements over time. Second, the transducer itself expands and contracts slightly in response to differences in the radial velocities of the liquid on either side of the reactor. This velocity is referred to as the breathing velocity. These velocities are related as follows:

$$u_b(z,t) = \frac{u_{zr}(r_z,z,t) + u_{ir}(r_z,z,t)}{2}$$  \hspace{1cm} 4.83

$$u_d(z,t) = u_i(z,t) = u_b(r_z,z,t) - u_{ir}(r_z,z,t)$$  \hspace{1cm} 4.84
Where

\[ u_b(z, t) = \text{breathing velocity, m/s} \]
\[ u_d(z, t) = \text{displacement velocity, m/s} \]

Recall that equation 4.60, which relates the time derivative of the radial velocity to the radial derivative of the pressure, can be used to calculate \( u_r(r, z, t) \) and \( u_{r2}(r, z, t) \), which are used to calculate the breathing and displacement velocities. The expression for the displacement velocity is long and complex, and is not shown here. However, the new expression for the transducer pressure, which incorporates the equivalence of the transducer and displacement velocities, is:

\[
p_t(z, t) = -\frac{\varepsilon}{4d^2} V^2(z, t) + \left( b + j \left( \omega, m - \frac{k}{\omega r} \right) \right) u_d(z, t)
\]

In this equation, the transducer’s output pressure and input voltage are shown as functions of the axial dimension, even though the voltage applied to the transducer, and the resulting pressure, are constant. This is because the reactor pressure equations, from which the electrode velocity is calculated, have axial dependancies. To match the transducer and reactor equations, the axial variable is included.

Now that the relationship between the transducer and reactor radial velocity equations has been derived, a method to attack the dependent relationship between the reactor pressure and the transducer pressure can be developed. Iteration is a common method for solving dependent relations such as these. In this case, however, there is a more straight-forward method. Recall equation 4.77 which is used in the model to describe the reactor pressure in region one:

\[
p_1(r, z) = \sum_{\eta} \sqrt{2} A_{\eta} J_0(k_{r}(\eta)r) \sin(k_{z\eta}z)
\]

The coefficients, \( A_{\eta} \), are solved for using the following relation:

\[
A_{\eta} = \frac{p_t \int_0^L \sin(k_{z\eta}z)dz}{LJ_0(k_{r}(\eta)r_1)}
\]
The transducer pressure, $p_t$, is a constant and acts as a scaling factor for each individual mode coefficient and, therefore, each individual mode that makes up the reactor pressure in region one. The same is true for the pressure distribution in region two. Because of this, the shape of the pressure distribution can be found for the reactor by solving the pressure equations with a unit transducer pressure. The actual pressure distribution can be found by multiplying the unit result by an appropriate factor.

The transducer velocity is developed by performing differentiation and integration on each pressure equation and then adding and subtracting the results. Since none of these operations removes the multiplying effect of the transducer pressure, $p$, also acts as a scaling factor for the transducer velocity expression. This means that the relationship between the transducer pressure, displacement velocity, and input voltage can represented in an equation that relates the transducer pressure to the input voltage through the transducer stiffness and damping and the eigenfunctions of the pressure distribution. This relationship is given below:

$$\frac{\varepsilon V^2}{4d^2 \left( p_{\text{unit}}(r,z) - \left( b(\omega) + j \left( m\omega - \frac{k(\omega)}{\omega} \right) \right) u_{d\text{-unit}}(z) \right)}$$

Equation 4.87 allows a complete reactor description to be constructed using the following procedure:

1. Compute the shape of the reactor's pressure distribution by assuming that the transducer pressure is 1 Pa.
2. Use the unit pressure equations, determined in step one, to compute the corresponding displacement velocity for the transducer.
3. Substitute the unit pressure and corresponding displacement velocity into equation 4.85, along with the actual input voltage, and calculate the actual transducer pressure. Since the pressure and velocity values are constant along the transducer's axis, the simplest way to do this calculation is to set $z$ equal to $L/2$. In the computer model, the computed transducer pressure has a negligibly small imaginary component, which is an artifact of summing the reactor mode shapes to express a pressure that is constant along the reactor's axis. As a result, the magnitude of the complex calculated transducer pressure is used in the next step.
4. Scale the reactor’s pressure function using the actual transducer pressure, which was determined in step four.

This complete reactor model has been implemented using mathCAD, which is a program that represents and computes mathematical processes in a workbook-like layout. An example of the mathCAD sheet ‘force’, which implements the model, is included in Appendix B. This sheet finds the pressure distribution for any reactor with the same general geometry, boundary conditions and sinusoidal input as the test reactor. The transducer radius, wall radius, reactor/transducer length, input frequency, input voltage and most of the other system parameters can be varied. Given appropriate inputs, the model calculates the pressure distribution for the modeled reactor. It also exports input values such as the input voltage and frequency, useful parameters such as the hydrophone position, and output values such as the pressure magnitude at the hydrophone, to other mathCAD sheets that compare the values predicted by ‘force’ with those that have been experimentally determined.

4.4 Validating the Model

Several different methods were used to ensure the accuracy of the mathematical model of the reactor that was developed in this chapter. The simplest was to use the graphics capabilities in mathCAD to visualize the results of intermediate calculations in the model. Some of these graphs are included in Appendix B.

Contour plots of the final pressure distributions calculated by the program were also plotted. These contour plots were checked for accuracy over a wide frequency range. The purpose of this check was to ensure that the calculated pressure distributions revealed the expected mode shapes. Recall from Chapter 3 that only the odd axial modes are supported by the proposed reactor design, because the transducer generates a step input pressure - zero pressure at the top and bottom of the reactor and transducer pressure along the length of the transducer/reactor. Also recall from Chapter 3 that radial modes whose nodes fall near the transducer radius are strongly supported by the proposed reactor. Finally, recall that the pressure distribution in the reactor is equivalent to the sum of the pressure distributions due to each of the reactor’s supported mode shapes, regardless of the frequency at which it is forced. Thus, contour plots of the pressure distribution in the reactor, at any frequency, should contain visual evidence of the supported mode shapes.
Figure 4.3 illustrates two different pressure distributions in the reactor. These distributions were calculated using the same dimensions and parameters as those of the reactor that was built for the experiments described in Chapter 5. Details of this reactor are given in Appendix A. Each distribution represents the response of the reactor at the resonant frequency of one of the reactor modes. The radial and axial modes that correspond to the resonant frequencies used in the figure are clearly visible. As expected from the discussion in Chapter 3, the axial modes in these plots are odd, and the radial modes have nodes near the transducer.

The pressure distribution in Figure 4.3 (a) is at the frequency (11,076 Hz) for which the experimental reactor was optimized. At this frequency, the first axial mode shape is excited because it most closely resembles the transducer's square-wave pressure input. The radial mode shape can be described as the first radial mode of the reactor's inner region, since its first node is at the transducer. Finally, the outer wall of the reactor is positioned such that it coincides with a pressure maximum of the inner region's radial mode shape. This causes the sound field to be attenuated in the outer region of the reactor.

The pressure distribution in Figure 4.3 (b) is for another of the reactor's resonant frequencies (27,117 Hz). Here, the third axial mode shape and the second radial mode shape of the reactor's inner region are excited. The outer wall does not coincide with a pressure maximum of this radial mode, so the magnitude of the pressure field in the outer region is larger.

Figure 4.4 shows the predicted pressure distribution for the experimental reactor at a non-resonant frequency (16,000 Hz). This response is smaller in magnitude than the resonant pressure responses and consists of a combination of the reactor's resonant mode shapes instead of a single resonant mode. The axial response consists primarily of the first and third axial modes. These are the axial modes that were excited in the two resonant frequency responses in Figure 4.3. Similarly, the radial response in Figure 4.4 consists primarily of the first and second radial modes of the inner region, which were the radial modes that were excited in the Figure 4.3 resonant responses. This is to be expected, since the frequency of the non-resonant response shown in Figure 4.4 (16,000 Hz) lies between the frequencies of the two resonant responses.

The first axial and first radial modes clearly dominate in Figure 4.4. Thus, the outer wall is once again near a pressure maximum of the radial mode that dominates in the inner region. The outer region sound is effectively eliminated as a result.
Figure 4.3 Predicted Resonant Pressure Distributions and their Mode Shapes* (a) 11076 Hz
*mode shape magnitudes not to scale
Figure 4.3 Predicted Resonant Pressure Distributions and their Mode Shapes* (b) 27117 Hz
*mode shape magnitudes not to scale
Figure 4.4 Predicted Non-Resonant Pressure Distribution with Mode Shapes* (16000 Hz)
*mode shape magnitudes not to scale
The reactor pressure distributions shown in Figures 4.3 and 4.4 show excellent agreement with the pressure fields that the proposed reactor was designed to produce. As such, these pressure field contours, and the pressure field contours produced by the model over a wide range of frequencies, provide compelling evidence that the mathematical model created for the reactor design is accurate.

The fact that the radial mode shapes of the interior region of the reactor all have nodes near the transducer suggests a final method of confirming the validity of the model. If the transducer were a pressure release boundary, the radial mode shapes of the interior region would all have nodes that coincided exactly with the transducer radius. Thus, the resonant frequencies of an unforced reactor of the same length as the test reactor with a pressure release wall at the transducer position, $r_p$, can be compared to the resonant frequencies of the test reactor. If they match, the forced reactor model is accurate. Note that the resonant frequencies of an unforced cylindrical reactor can be easily calculated using the $J_0$-type Bessel equation.

These results of this comparison are shown in Table 4.2. Note that the radial wave number used in this table refers to both the radial wave number of the radial modes of a reactor of radius $r$, and the radial wave numbers in the interior region of a reactor with a transducer at $r_p$.

The match between the resonant frequencies for the two reactor designs are excellent. Discrepancies between the two values for each individual mode are very small, and can be accounted for by the fact that the pressure at the transducer of the forced reactor isn’t actually zero. In fact, it is slightly above or below zero, resulting in a slight shift in the position of the actual node, and a slight change in the resonant frequency. This final method of checking the mathematical model of the reactor also provides compelling evidence of its accuracy.

<table>
<thead>
<tr>
<th>Axial Wave Number</th>
<th>Radial Wave Number</th>
<th>Resonant Frequencies (Hz) of the Unforced Reactor</th>
<th>Predicted Resonant Frequencies (Hz) of the Forced Test Reactor</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>11,074</td>
<td>11,076</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>17,650</td>
<td>17,658</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>23,353</td>
<td>23,354</td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>26,254</td>
<td>26,267</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>27,097</td>
<td>27,117</td>
</tr>
<tr>
<td>1</td>
<td>3</td>
<td>36,141</td>
<td>36,151</td>
</tr>
</tbody>
</table>
Chapter Five

Verifying the Model Experimentally

The reactor model developed in Chapter 4 performs as expected from a theoretical standpoint, but the true test of this model comes in comparing it to experimental data. Validating the model experimentally will make it possible to use the model as a replacement for prototype reactors during the design process.

5.1 Apparatus

The sonochemical reactor model determines the pressure distribution in a reactor from the known input voltage. In order to validate the model experimentally, the pressure response of a physical reactor to a known input voltage must be compared with the values predicted by the model. A schematic and photograph of the experimental apparatus used to obtain these data are shown in Figure 5.1.

The sonochemical reactor is described in detail in Appendix A. The reactor was constructed from a plastic bucket with a rim near the top. The reactor bucket was hung in a cylindrical mount that supported it at the rim. This support mechanism, which is shown in Figure 5.2, ensured that the bottom of the bucket remained a pressure release boundary. A cylindrical transducer was constructed as described in Chapter 3, and mounted inside the bucket, coincident with its centre axis. The transducer was attached to the bottom of bucket using a silicon adhesive. The seal prevents the reactor liquid from flowing between the inner and outer regions of the reactor. A Plexiglass bucket cover, which prevents electrical components from falling into the reactor, was also constructed. It has holes for the electrical leads and a hydrophone. The reactor is filled to the top of the transducer with ordinary, room-temperature tap water.

The sinusoidal input signal was created by a function generator and then amplified and transformed to increase it’s voltage amplitude. This signal was then sent to the electrostatic transducer. The lead that connects to the interior, plate-type electrode is fused for safety. The signal generated by the function generator, and the signal input to the electrostatic transducer, were both fed into an oscilloscope for analysis, and to ensure that the input signal remained sinusoidal through the amplifier and transformer. The amplitude of the signal to the transducer was measured with both the oscilloscope and a voltmeter.
Figure 5.1 Experimental Apparatus
The sinusoidal signal input to the electrostatic transducer caused it to oscillate and to generate a pressure field in the reactor. This field was measured using a hydrophone - an underwater microphone. The hydrophone sent a voltage signal to the oscilloscope which was proportional to the instantaneous magnitude of the pressure field that it was detecting.

The hydrophone was lowered into the reactor through a hole in the Plexiglass cover. The hydrophone was placed so that its centre of pressure (the point on the hydrophone where the pressure signal is measured most accurately) was located at both the radial and axial centers of the reactor. Data were taken from the centre of the reactor where the pressure field is highest. Since this is where the pressure field is the highest, hydrophone measurements were taken from this location only. The maximum pressure in the reactor is due to the pressure field in the reactor as a whole. Therefore, if the pressures predicted by the model match with the experimentally determined pressure values at this maximum pressure location, it is not necessary to compare pressure values over the whole reactor volume. The
relative magnitude of the pressure field at various locations in the reactor was visually checked on the oscilloscope before any measurements were taken. This was done to confirm that the pressure field had the expected shape.

The axial position of the hydrophone was determined by measuring the distance by which it was lowered into the reactor. The radial position was achieved by centering the hydrophone inlet hole on the axis of the reactor. In the initial tests, a guide constructed of stainless-steel mesh was used to ensure that the hydrophone stayed along the axis of the reactor, but the mesh was found to interfere electrically with the experimental system.

The hydrophone used in this research was a Bruel and Kjær 8100. It is described by the company as “a wide-range underwater transducer for absolute sound measurement over the frequency range 0.1 Hz to 200 kHz”. The calibration curve for this hydrophone is shown in Figure 5.3. It shows that the frequency response of this hydrophone is flat only to approximately 40 kHz.

![Figure 5.3 Calibration Curve for the Hydrophone](image)

Figure 5.3 Calibration Curve for the Hydrophone 31
The oscilloscope used to collect the data was a Tektronix Digitizing Oscilloscope. This oscilloscope has several functions useful for data collection and analysis, including high frequency filtering, high-resolution acquisition and the ability to save waveform data to disk in mathCAD compatible data files.

### 5.2 Data Collection and Analysis

#### 5.2.1 Data Collection

Input and output data were acquired from the experiment over a wide frequency range. Input and output signals, and specific information regarding these signals, were recorded for driving frequencies ranging from 2 to 19 kHz. This is equivalent to an acoustic frequency range of 4 to 38 kHz. These frequencies fell within the flat response frequency range of the hydrophone. Over most of the frequency range, measurements were taken using 100 Hz increments of the driving frequency, which corresponded to 200 Hz increments of the reactor frequency. The sonochemical reactor designed, built and modeled for this research was, however, expected to have a resonance peak near 11 kHz reactor frequency, so measurements were taken in 50 Hz increments of the driving frequency (100 Hz reactor) between driving frequencies of 5.0 and 5.8 kHz (10 and 16.0 kHz reactor). The response of the reactor between driving frequencies of 14.5 and 17.0 kHz was essentially constant, so few measurements were taken over this range. Measurements were taken at driving frequencies of 14.5, 15.0, 16.0 and 17.0 kHz (29, 30, 32 and 34 kHz reactor).

It was not possible to use driving frequency increments of less than 50 Hz because the uncertainty of the frequency of the input signal to the transducer was on the order of ± 3 Hz. (It became as much as ± 5 Hz at high frequencies where larger increments were used.) The percentage uncertainty of the input frequency would have been too large for smaller input frequency increments to be valid.

The simplest way to analyze the difference between the input signal to the electrostatic transducer and the output signal from the hydrophone would have been to record both signals using the oscilloscope. This was not possible, however, because the amplitude of the input voltage over most the frequency range was too great. Instead, the signal generated by the function generator was recorded, and the oscilloscope was used to measure the phase shift between this signal and the transducer input. The phase difference measurements had an uncertainty of ± 3°. The amplitude of input voltage was measured using the voltmeter. It had an uncertainty of ± 0.5 V.
The data for the project were acquired as follows:

- The hydrophone was inserted into the reactor and the oscilloscope was turned on to warm up. After 20 minutes, the oscilloscope's signal path compensation function was run to ensure that the measurements would not be affected by changes in the system's ambient temperature or aging of the components. This was done before any electrical signals were applied to the oscilloscope.

- The oscilloscope's upper frequency limit was set to 20 MHz. It was reasonable to eliminate frequencies over 20 MHz, because the highest reactor frequency to be measured during the experiment was 38 kHz. The oscilloscope was also set to its high-resolution acquisition mode. In this display mode, the oscilloscope takes several measurements during each time interval and averages them to produce a result for that time interval. The main benefit of this mode over the other acquisition modes ('sample mode', where the first data point in each time interval is chosen, and 'peak detect mode' which uses high and low values in two intervals) was that it reduced random noise in the signal. The record length, or the number of data points recorded by the oscilloscope, was set to 5000.

- The transducer was connected to the transformer to receive its input signal. The function generator was set to a sinusoidal signal, and the amplitude and frequency dials were turned to zero. The function generator and amplifier were then turned on to begin the tests.

- The input signal was adjusted to the first test frequency, and the amplitude of the function generator's output signal was adjusted so that the transducer input voltage had a low enough amplitude to be measured by the oscilloscope. The phase difference between the function generator signal and the transducer input signal was recorded.

- The function generator's output voltage was increased until the transducer input voltage reached an appropriately high value. How high the voltage could be set was dependent on frequency. Voltages used in the experiment ranged from 5 to 140 V. As the test frequency increased, the maximum voltage that could be generated by the transformer decreased, regardless of the function generator voltage. If too much voltage was introduced to the transformer by the function generator, distortion was induced in the transducer response, so care was taken to avoid voltages that were too high for the test system at the given frequency. The input voltage to the transducer was recorded.
Using the run/stop function on the oscilloscope, the function generator signal and the hydrophone signal were captured. The oscilloscope's triggering mechanism was used to ensure that simultaneous signals were captured so that the phases of the signals could be compared.

The function generator and hydrophone signals were saved to disk, using the mathCAD compatible file format provided by the oscilloscope.

The oscilloscope was reset so that it displayed the real time signal, and adjusted to the next frequency so that the measurements could be repeated.

5.2.2 Data Analysis

The experimental data was imported into several mathCAD programs for analysis. First, the function-generator signal and the hydrophone signal for each frequency data point were imported into a mathCAD sheet called 'view'. A sample of this sheet is included in Appendix C. The sheet served two main purposes. The first was to ensure that the input and output signals recorded by the oscilloscope were consistent with established principles - namely that the frequency of the output signal was twice that of the input signal and that both signals were dominated by their first harmonic. The sheet calculated the expected period of the hydrophone output signal. The squared input signal and the output signal were then graphed and checked visually to ensure that they had the expected period. A Fourier transform was also performed on the squared input signal and the output signal. The transforms were graphed and compared visually with the expected reactor frequency to ensure that they were strongly centered about this frequency.

Figure 5.4 shows a sample of the graphs from the sheet that were used to examine frequency doubling in the output signal. Analyzing the input and output signals in this way revealed several interesting points. By and large the input and output signals had the expected form - the hydrophone output response frequency was twice that of the input signal frequency (and the same as that of the squared input signal). For frequencies at which the amplitude of the hydrophone signal was very low, however, the doubled reactor frequency was not as strong. Indeed the amplitude of the response at the reactor frequency was of the same order of magnitude as the response at the driving frequency.
The Fourier transforms show this effect most clearly. Figure 5.5 shows the Fourier Transforms of the hydrophone signal at 11,000 Hz, which is near resonance and is representative of a high amplitude response, and at 16,000 Hz, which is not. Interestingly, the Fourier transforms of the function generator signals show small peaks at half the driving frequency (which shows up as driving frequency response on the plot of the squared signal). This effect was likely an artifact of the fact that the transducer tended to have a small response at the driving frequency, which would show up on the input side of the transducer as an input of half that frequency. Two of these responses are shown in Figure 5.6.

These characteristics of the Fourier transforms of the two signals is indicative of two things. One is that, although the transducer response is treated as a linearized system that contains only a response at the reactor frequency, it is actually a sum of harmonics including that of the driving frequency. Second, as
was made clear in the description of the model in Chapter 4, the electrical input to the sonochemical reactor and its pressure response are not independent, but are coupled. What happens on one side of the transducer affects what happens on the other and vice versa.

The second purpose of the 'view' mathCAD sheet was to determine the phase difference between the input signal to the transducer and the pressure in the reactor as determined by the hydrophone. This was done by using the argument of the Fourier transform of the squared input signal and the hydrophone output signal, at the reactor frequency only, to find the phase of these signals. Phase varies with frequency, so the phase difference at unforced frequencies is not meaningful. The phase difference between the actual electrostatic signal in the transducer and the pressure signal in the reactor, was determined as follows:

![Figure 5.5 Fourier Transforms of the Hydrophone Output Signal at 11 and 16 kHz](image-url)
\[ \Delta \phi = \phi_{\text{function}^2} + 2\phi_{\text{function to electrostatic input}} - \phi_{\text{hydrophone}} \]  

Where

\[ \phi_{\text{function}^2} = \text{phase of the squared function generator signal} \]

\[ \phi_{\text{function to electrostatic input}} = \text{phase difference between the function generator signal and the input to the transducer - when the signals are squared, the phase difference doubles} \]

\[ \phi_{\text{hydrophone}} = \text{phase of the hydrophone signal, which is equivalent to the phase of the pressure field} \]
The mathCAD sheet used for data analysis is called 'profile'. A sample of 'profile' is given in Appendix D. This sheet finds the predicted and experimental ratios of the transducer’s electrostatic pressure to the pressure at the centre of the reactor. To do this, the sheet uses data exported from the mathCAD sheet 'force' that is described in Chapter 4. As a result, 'force' was run for each of the experimental frequencies and corresponding voltages. 'Force' exported the test frequency, test voltage, calculated electrostatic pressure at the transducer, modeled hydrophone position co-ordinates, and the predicted output pressure at the hydrophone, to 'profile'. The modeled hydrophone's axial position was taken to be L/2, which placed the centre of pressure at the axial centre of the reactor, as in the experiment. Its radial position was taken to be -0.0092m, which assumed that the hydrophone was centered on the axis, as in the experiment. The co-ordinate wasn’t zero because the hydrophone has a radius of 0.0092m.

'Profile' imported this information, along with the hydrophone output signal for the appropriate experiment. It used the predicted hydrophone pressure and the electrostatic pressure imported from 'force' to compute the predicted ratio. To compute the experimental ratio the pressure detected by the hydrophone had to be calculated from the voltage signal. The first step in this calculation was to obtain the appropriate value for the voltage from the hydrophone signal. As discussed in Chapter 3, the transducer is assumed to be linear, so the only portion of the output signal from the transducer that isn’t considered to be random or harmonic noise is that portion whose frequency is twice the driving frequency (also known as the reactor frequency). Thus, the only portion of the response at the centre of the reactor that was considered was the portion that oscillated at the reactor frequency. The voltage magnitude of this portion of the signal was taken from the value of the Fourier transform at the reactor frequency only. (Note that the transform will still pick up noise at the reactor frequency.)

The magnitude of the voltage response at the centre of the reactor was converted into a pressure using the hydrophone’s sensitivity, which is given in the hydrophone documentation as:  

$$p_h = \frac{V_h \times 1Pa}{30.6 \times 10^{-6} V} + 1 \times 10^{-6} Pa$$

Where

- \(V_h\) = the amplitude of the voltage signal at the reactor frequency, V
- \(p_h\) = the pressure corresponding to the hydrophone voltage signal, Pa
This expression is valid for the linear region of the response. The experimental pressure ratio was calculated using the pressure determined from this relationship and the electrostatic pressure imported from ‘profile’.

Pressure ratios were calculated for every test frequency except 3.9 kHz driving (7.8 kHz reactor), as the output signal recorded for this frequency was found to be in error. It was determined from the output observed on the oscilloscope during testing, and from the pressure ratio curve, that this frequency was not in a critical region of the pressure ratio curve. Thus, no effort was made to retest it.

5.3 Comparison of Experimental and Predicted Results

To compare the experimental pressures with those predicted by the model, their pressure ratios and phase differences over the entire frequency range and their individual values at each test frequency were assembled into vectors using mathCAD. These vectors were then exported for use in mathCAD sheets that displayed the vectors as functions of frequency.

5.3.1 Direct Comparison of Predicted and Experimental Results

Figure 5.7 shows the calculated electrostatic pressure, predicted hydrophone pressure, and experimentally measured pressures over the tested frequency range. Note that the electrostatic pressures generated in the transducer were very low. For the low frequency, higher voltage (140 V) tests, the electrostatic pressure was slightly greater than 1 Pa, but most of the electrostatic pressures were well below this value. The output pressures, both predicted and measured, peak at the frequencies that correspond to the predicted and measured resonances. For most of the resonant frequencies, the predicted pressure amplitude is actually lower than the experimental value, except at the first resonance, which is the one that the system was designed to excite.

A clearer picture of how the predicted and measured pressures compare is given in Figure 5.8, which shows the ratios of the pressures predicted by the model and of the measured pressures to the electrostatic pressure. This is a more direct comparison, because the effect of the changing electrostatic pressure is eliminated.

When comparing the predicted and measured pressure ratios, three features of the curves are considered - their resonant frequencies, their shapes and their magnitudes.
a) Frequency

If the model of the reactor design is accurate, then the resonant frequencies that it predicts will be similar to those found experimentally. The predicted and measured resonant frequencies, shown by the peaks of the curves in Figure 5.8, are very similar. The first resonance, whose mode the reactor was specifically designed to excite, matches very closely. The higher resonances, which are for modes that can physically occur in the reactor, but that it was not specifically designed to excite, show slight differences. This is likely due to slight dimensional differences between the modeled reactor and the hand-built experimental reactor.

Figure 5.7 Calculated Electrostatic and Predicted and Measured Hydrophone Pressures
Note that the predicted resonant frequencies shown in Figure 5.8 are not exactly the same as those given in Table 4.2. This is because the experimental pressures are only available in 200 Hz increments (100 Hz near the first resonance peak), while resonant frequencies found by the model were resolved to within 0.5 Hz increments. To make an appropriate comparison, only frequencies matching the experimental frequencies were used to obtain the curve for the predicted pressure ratios.

Another way to validate the experimental resonant frequencies is to look at the phase shift between the transducer’s input and output signals, which was determined as described in the last section. At resonance, the phase shift should undergo a 180° change centered at 90°. A plot of the phase difference versus frequency is shown in Figure 5.9.
A smoothing routine was applied to the phase difference curve before it was plotted. This was necessary because the uncertainty of the phase measurements was on the order of ±3°. This was problematic when phase values approached 180 or -180°. With an uncertainty of ±3°, a measured phase of -180° could in reality be 178°. If the two phase values flanking this -180° measurement were both positive, then using a positive value within the uncertainty range, such as 178°, in place of -180°, eliminated apparent phase shifts that were due only to experimental uncertainty, and produced a smoother curve.

The phase curve shows the appropriate behaviour at the resonant frequency for which the reactor was designed - 11,076 Hz (first axial, first radial mode). It also shows close to the appropriate behaviour at the second radial, first axial mode (23,354 Hz). The other resonant frequencies are not evident on the phase curve. The reason for this has not yet been determined.

![Figure 5.9 Phase Difference Between the Input and Output Signals versus Frequency](image)
b) Shape

The shape of a resonance curve, in terms of the width and height of the resonant peaks, is indicative of the damping in the system. The main source of damping in the design used in this research is the transducer damping. This damping is assumed to be viscous. In this case, the damping constant is related to the non-dimensional damping ratio as follows: \[ \zeta = \frac{b(\omega_n)}{2m \omega_n} \]  

Where

\[ \zeta = \text{damping ratio} \]
\[ \omega_n = \text{resonance frequency, rad/s} \]

The width of the resonant peak at half of the peak's amplitude, is called the half-power bandwidth. It is proportional to the damping ratio, according to the following: \[ \Delta \omega \approx 2\zeta \omega_n \]  

Where

\[ \Delta \omega = \text{half-power bandwidth, rad/s} \]

Furthermore, the area under each resonant peak, which is representative of the energy consumed by the system when it undergoes broadband excitation, is proportional to \( 1/\zeta \). It is evident from Figure 5.8 that the shapes of the predicted and experimental resonant peaks are similar, but not the same. The experimental peaks are wider, and in some cases, higher than those predicted by the model. These differences suggest that the damping coefficient calculated in the mathematical model is not quite the same as the damping coefficient of the experimental transducer.

c) Magnitude

The greatest disparity between the predicted and experimental pressure ratio curves is seen in their magnitudes. As can be seen in Figure 5.8, there are really three different kinds of magnitude disparity.
between the predicted and experimental curves. The first is due to the disparity between the widths of
the resonant peaks. This is especially noticeable at the higher frequencies. The slopes of the predicted
and experimental curves are similar at the bottoms of the two peaks; thus the peak of the curve with the
wider base is higher than the peak of the curve with the narrower base. This magnitude disparity is
related to the shape issue discussed above and can be addressed with the method discussed in that
section.

The second magnitude issue is the noticeably larger magnitude of the experimental response at high
frequencies. The high frequency experiments had to be performed at very low input voltages (~5 to 15V)
and, therefore, very low electrostatic pressures. These low electrostatic pressures yielded very low
pressures at the centre of the reactor. As a result, the voltage signal generated by the hydrophone in
response these low centre pressures was also quite low. Unfortunately, these small hydrophone voltages
were not large enough to dominate over the ever - present noise in the hydrophone signal. Thus, the
percent increase in the hydrophone signal due to noise was not negligible for the high frequency, low
input voltage tests. The large influence of the noise signal accounts for the apparent doubling and
tripling of the magnitude of the experimental pressure ratio over the pressure ratio predicted by the model
at the higher frequencies.

The third issue in considering the magnitude of the predicted and experimental curves relates to the
heights of the resonance peaks. Although the experimental resonance peaks were obtained only to a
resolution of 100 to 200 Hz, the heights of these curves are fairly accurate (neglecting the issues
discussed above), because the peaks were clearly observable during the experiments. The measured
pressure ratio at the design frequency of 11 kHz was approximately 95. Thus, at this frequency, the
pressure at the centre of the reactor was 95 times greater than the electrostatic pressure of the transducer.

The peaks predicted by the model, however, could well be much higher than those that appear in Figure
5.8. In this figure, the predicted centre pressure is approximately 110 times greater than the electrostatic
pressure but, as noted above, the resonances predicted by the model were actually resolved to within 0.5
Hz. If the predicted magnitudes at the resolved resonant frequencies are included in the pressure ratio
curves, Figure 5.10 results. In this figure the peaks predicted by the model are very high, but probably
representative of values that are not achievable in real life.
5.3.2 Comparison of Predicted and Measured Results with Adjusted Gap Spacing

It is worthwhile to revisit the issue of disparate damping coefficients between the modeled transducer and the experimental one. In the last section, the relationship between the area under each resonance peak and the damping coefficient was discussed. Thus the disparity between the shapes of the measured and predicted curves can be reduced by adjusting the damping ratio in the model to better reflect what is happening in the actual test reactor.

The method used to determine the transducer’s damping coefficient is assumed to be valid, so changes to the damping coefficient must be made by changing the values used to calculate it. The simplest and most reasonable way to alter the predicted damping coefficient is to alter the gap spacing in the transducer. The size of the gap space in the transducer was assumed to be 0.381mm, which was the thickness of the...
Tape used to maintain the spacing between the rigid plate electrode and the aluminized mylar electrode. There are a number of reasons why the gap space was likely smaller than this in practice.

**a) Stretching and Compression of the Spacing Tape**

The 3M VHB (Very High Bond) double-sided foam tape used to create the spacers in the electrostatic transducer is pliable. A small degree of stretching, which caused a reduction in the tape’s thickness, occurred as the tape was cut and applied to the rigid electrode. The tape also compressed slightly when the flexible electrode was applied to it, although great care was taken to minimize this occurrence.

**b) Sagging of the Membrane**

Great care was also taken not to allow either tension or looseness in the flexible electrode as it was mounted to the transducer. Some sagging of the transducer at the middle of the individual cells created by the separator tape was unavoidable, however, and this reduced the gap spacing.

**c) Hydrostatic Pressure**

The pressure inside the transducer’s air gaps is the ambient pressure. When the water is added to the system reactor, it exerts a hydrostatic pressure on the transducer cells that is proportional to the depth of the water. This pressure compresses the air gaps. The difference between the gap space used by the reactor model and the actual gap space in the experimental reactor is most likely due primarily to the effects of hydrostatic pressure on the experimental transducer. Unfortunately this means that the gap spacing in the transducer cells varies slightly along the axis of the reactor. This effect is neglected in the calculations below.

Once it was determined that the gap spacing was most likely responsible for the discrepancy in damping coefficients, a new gap spacing was determined for the model. This was done by using the fact that the area under the resonance peak is proportional to the inverse of the damping ratio, as discussed in the previous section. First the ratio of the area of the experimental resonance peak to the predicted resonance peak at 11 kHz was calculated. This ratio was used to determine a damping ratio, and corresponding gap space, that would make the resonance peak area ratio as close to 1:1 as possible. Using this process it was determined that the actual gap spacing in the transducer was approximately 0.228mm, instead of 0.381mm. Thus the actual gap is thought to be approximately 2/3 the thickness of the gap spacing tape. A gap space reduction of 33%, due to stretching of the spacing tape, sagging of the transducer membrane and hydrostatic pressure, is physically reasonable.
Changing the gap spacing changes the calculated electrostatic pressure. Therefore, assuming a new transducer gap space for the reactor used in this research changes both the experimental pressure ratio curve and the pressure ratio curve predicted by the model. The new curves are shown in Figure 5.11. The new predicted pressure ratio is similar to the previous one, while the new experimental curve is slightly different from its predecessor. It is clear that modifying the gap spacing results in a much better match between the curves.

Unfortunately, reducing the gap space also reduces the experimental pressure increase that the reactor achieves. It appears that the changes in the stiffness and damping coefficients caused by using a smaller, corrected gap spacing has a more pronounced effect on the system’s outcome than the change in the electrostatic pressure. If the electrostatic pressure were the only factor in the new outcome, then reducing the gap spacing should increase the electrostatic pressure and the centre pressure of the reactor.
6.1 Immediate Applications of the Model

The sonochemical reactor that was constructed, modeled and tested in this research did not create cavitation bubbles. The experimental and predicted results (0.228 mm air gap) in Figure 6.1 show that a 5.5 kHz sinusoidal input voltage with an approximate amplitude of 7000 V would be required to excite the 11 kHz reactor resonance. A 7000 V input is potentially dangerous and much greater than the 900 V estimated breakdown voltage of the test transducer. Fortunately, creating a cavitating reactor was not the research objective. As discussed in Chapter 3, it was to use sound design principles to create a sonochemical reactor that exploited geometry, resonance and mode shapes, was not limited by its transducer and had an easily modeled sound field so that modeling could be used to refine the design.

![Figure 6.1 Voltage Required for Cavitation](image-url)
As a result, the research has involved the creation of a reactor design which met the above mentioned design objectives (Chapter 3) and the creation of a mathematical model of the design (Chapter 4) that accurately represents the reactor's behaviour (Chapter 5). The next step would be to use the reactor model to investigate the design changes that are necessary to create a cavitating reactor.

Some of the design changes that could be made to create a cavitating reactor include the following:

- Replace the air in the transducer gaps with a gas having a low thermal conductivity and high dielectric strength. Low thermal conductivity prevents the transfer of heat from the gas to the electrode plates, reducing the effects of thermal damping. High dielectric strength allows higher voltages to be applied to the transducer, which generates a higher pressure. A potential candidate is R11 gas (CCl\textsubscript{3}F), which has a dielectric constant of approximately 3.5 and a thermal conductivity approximately 1/3 that of air.

- Decrease the air gap thickness, thereby increasing the electrostatic pressure in the transducer. This would presumably increase the pressure generated by the transducer, creating a corresponding increase in the pressure at the centre of the reactor.

While these changes may seem to have straightforward benefits, changes to the reactor parameters can have complex and unexpected effects. For instance, a different gap material not only has a new thermal conductivity and dielectric strength, but also a new constant volume heat capacity and density. These values also have an effect on the damping and stiffness coefficients, so the expected benefits may not result. Similarly, though a reduced gap space increases the transducer's electrostatic pressure, it also alters the transducer's stiffness and damping coefficients. Thus, once again, implementing this change might not result in an increased acoustic pressure in the reactor.

Figures 6.2 and 6.3 compare several pressure ratio curves predicted by the model. In Figure 6.2, the model is used to predict how replacing the gap material in the test reactor will affect the ratio of the reactor's centre pressure to the electrostatic pressure generated in the transducer. Curves are shown for the test reactor with the corrected gap space (0.228 mm), and for the test reactor with the corrected gap space filled with R11 instead of air.

Two plots are shown in Figure 6.2. The first shows the predicted pressure ratio curves for both reactor designs. The curves are almost identical, but, because R11 has a dielectric constant 3.5 times larger than
that of air, the apparent gap thickness in the R11 transducer is much smaller. Thus, the electrostatic pressure in the R11 transducer and the centre pressure generated by the R11 transducer are much larger than those of the air-filled transducer.

Figure 6.2 Comparison of Air and R11 Filled Transducers
This difference in the relative pressures experienced in the two reactor systems is evident in the second plot in Figure 6.2, which compares the magnitude of the voltage signal necessary to generate cavitation at the design frequency for the two reactors. It was established in Figure 6.1 that a signal amplitude of approximately 7000 V is necessary to create cavitation in the design reactor with the air-filled transducer. The model predicts that only 2200 V would be required to produce the equivalent response using an R11-filled transducer with the same gap space.

As predicted, using R11 as the transducer gas instead of air reduces the voltage needed to achieve cavitation. Furthermore, the R11 reactor design responds similarly to the original design over the tested frequency range. This indicates that the stiffness and damping coefficients of the two transducer designs have similar frequency variations.

Though achieving cavitation with a 2200 V input signal is certainly preferable to requiring a 7000 V signal, there is still room for improvement. This voltage is still large, and will likely cause breakdown. The required improvements may be achieved by the second suggested design change - reducing the transducer gap space. In Figure 6.3, the reactor model is used to predict how changes to the transducer gap spacing will affect the pressure ratios achieved at the centre of the reactor. The plot includes the curve for the test reactor with the corrected gap space of 0.228 mm, and curves that assume that the transducer in the test reactor is replaced with similarly designed transducers with gap spaces of 0.01 and 0.001 mm.

At higher frequencies, the ratio of the pressure generated at the centre of the reactor to the electrostatic pressure generated in the transducer is similar for all three gap spaces. Since the electrostatic pressure is larger for the transducer with the smallest gap space, the centre pressure will also be largest for this transducer. Thus, decreasing the gap spacing has the desired effect at higher frequencies. At low frequencies, such as the 11 kHz test reactor design frequency, the pressure ratios predicted for the transducers with reduced gap spaces are extremely low - at most, these transducers generate centre pressures 5 times larger than the electrostatic pressure. Thus, for these frequencies, reducing the gap space is highly detrimental. Investigation into the reason for this behaviour is warranted.
Insight into the behaviour of the different reactors may be gained by considering the stiffness and damping ratios of their transducers. Figure 6.4 shows the effect of the transducer’s gap space on the transducer impedance over the test frequency range. The transducer impedance is a function of frequency, stiffness and damping. The impedance of the test transducer, with a gap space of 0.228 mm, is very low near the 11 kHz design frequency, as well as the higher test frequencies. This is in contrast to the impedances of 0.01 and 0.001 mm transducers, which are high at the design frequency. The impedance of the 0.01 mm transducer is comparable to that of the 0.228 mm transducer at high frequencies. The impedance of the 0.001 mm transducer is still very high at high frequencies, but its high frequency impedance is still low relative to its low frequency impedance.
Figure 6.4 Effect of Gap Space on Transducer Impedance

Figure 6.5 shows the changes in the stiffness and damping coefficients at the design frequency as a function of gap spacing. It is apparent from this figure that transducer stiffness dominates the behaviour of the low gap space transducers. This explains the reduction in the low frequency pressure ratios for these transducers, since very stiff objects have high resonant frequencies. They are not easily excited by low input frequencies and, therefore, do not generate significant centre pressures. The damping ratio does not make a significant contribution to the difference in the transducer’s responses. It does show a small variation with gap space, but the damping coefficients of the 0.228, 0.01 and 0.001 mm transducers are of the same order of magnitude.

Although a design frequency of 11 kHz was chosen for the test reactor and for this analysis, there is no reason why this has to be the operating frequency. Higher frequencies, for which low gap space transducers operate effectively, are just as valid.
Figures 6.6 and 6.7 show the voltages at which the reactors built with the 0.01 and 0.001 mm transducers are expected to cavitate, as predicted by the model.

Figure 6.6 shows the centre pressures predicted by the model for the 0.01 mm transducer over the test frequency range at three different input voltages. The upper plot in the figure shows the centre pressure curves as lines on a frequency versus pressure plot. The cavitation threshold, which is approximately 1 atm or 100 kPa, is marked. The bottom plot shows the area under each curve. Each pressure curve area is cropped at the cavitation threshold pressure. Both the upper and lower plots show which frequencies are expected to achieve cavitation in response to the three input voltages considered. Different readers may find one or the other easier to analyze.
Figure 6.6 Reactor Centre Pressure with 0.01 mm Transducer at Assorted Input Voltages
For this reactor configuration, it is predicted that cavitation would occur at the design frequency, and most other test frequencies, with an input voltage of approximately 2000 V. Despite the reduced pressure ratio, the high electrostatic pressure makes this a considerably lower cavitation voltage than for the 0.228 mm transducer. However, it is still not low enough to prevent breakdown. The model predicts that an 800 V input will cause cavitation at most of the reactor's middle to high resonant frequencies. Finally it predicts that the reactor will cavitate with only a 400 V input signal, if it is operated at its high resonant frequencies. This would be a remarkable improvement. Still, the breakdown voltage for the 0.01 mm transducer is estimated at 300 V. It might be possible to increase this breakdown voltage by applying mylar to the transducer's stationary electrode, as well as to the flexible membrane.

Figure 6.7 shows the centre pressures predicted by the model for the 0.001 mm transducer over the test frequency range at three different input voltages. The first and second plots are similar to those in Figure 6.6. For this configuration, it is predicted that cavitation is possible at the design frequency with an input voltage of approximately 1000 V - half that of the previous case. Similarly, the voltage near which the medium to high frequency resonant inputs are predicted to achieve cavitation is 400 V, and the frequency at which the high frequency resonances alone are predicted to achieve cavitation is 200 V. Depending on the condition of the electrodes and the coatings applied to them, the breakdown voltage of the 0.001 mm transducer is estimated to be between 20 and 500 volts. Thus, according to the model, the proposed reactor design, with a carefully designed and constructed 0.001 mm transducer would produce cavitation.

It is apparent that the relationships between reactor parameters are complex, and that the effects of changing these parameters are not always as expected. How the reactor parameters interact needs to be investigated in order to make intelligent and efficient design changes to the sonochemical reactor. This kind of investigation will rely on the predictions of the reactor model. By investigating proposed design changes using the model, as has been done here, numerous design concepts can be investigated relatively quickly. Also, the unexpected trends resulting from changing reactor parameters can be easily identified, thereby eliminating or reducing the amount of trial and error required in the prototyping process.

Based on the predictions of the model, a reactor of the same dimensions as the test reactor, with a carefully designed and built, air filled, 0.001 mm gap space transducer, should cavitate in response to an input signal of approximately 200 V and 36.5 kHz. This is likely not the ultimate solution, however, since a 0.001 mm gap space may be too small to be practical.
Design and Modeling of a Sonochemical Reactor

Refining the Design

Figure 6.7 Reactor Centre Pressure with 0.001 mm Transducer at Assorted Input Voltages
Design and Modeling of a Sonochemical Reactor

Refining the Design

It would be worthwhile to investigate the effects of using a transducer with 0.01 mm gap space filled with R11, since the predictions for both the 0.01 mm gap space transducer, and the transducer filled with R11, showed significant improvement over the test reactor. R11 has a higher dielectric constant and a higher strength than air, so a greater electrostatic pressure will be generated for a given voltage difference and a greater voltage can be applied across the gap without breakdown.

Note also that the radius and length of the test reactor, and the associated resonant frequencies, used in this research were basically arbitrary. The model will prove an invaluable tool in investigating cylindrical type reactors built to certain geometries, or for certain resonant frequencies.

6.2 Modeling an Inhomogeneous Sound Field

The work done in this research concentrated on the modeling and testing of a homogenous (non-cavitating) pressure field. This is valuable in constructing a sonochemical reactor which generates sufficient pressure to initiate cavitation. There is much work to be done to model a cavitating reactor properly, and to ensure that the sonochemical reactor design not only initiates cavitation efficiently, but also maintains it.

The reactor design developed in this research is already well suited for a system that both creates and maintains cavitation. Cavitation in the reactor liquid reduces the liquid’s density, decreases its bulk modulus and increases its apparent damping. It also lowers the resonant frequency of the reactor system. The input frequency of the electrostatic transducer can be adjusted to compensate for the change in resonant frequency. The pressure required to create cavitation is less than that required to initiate it, so refining the design such that it creates cavitation, will also allow the reactor to maintain cavitation.

Modeling a cavitating sound field is a difficult problem. It is necessary to determine both the properties of a bubbly fluid and the distribution of cavitation bubbles in the sound field. Once the fluid properties and bubble distributions have been determined, they must be incorporated into the model and checked against experiment. Some work has been done to address this problem, including that by Dähnke, Keil and Swamy, in 1999. This work was described briefly in Chapter 3.
Conclusions

The deficiencies of current reactors were addressed in this research by approaching a sonochemical reactor from a design standpoint, and by creating a reactor model for use specifically as a design tool. A preliminary reactor design was created to meet the design criteria detailed below:

- The transducer wasn’t limited in size, shape or placement in the reactor. Electrostatic transducers are easily constructed in a variety of shapes and sizes. For this research, a curved transducer that was slim enough to have a minimal presence in the reactor was constructed. It was also sealed so that it could be placed directly into the reactor.

- The transducer wasn’t limited in its operating frequency. Electrostatic transducers operate efficiently over a wide frequency range, unlike traditional transducer technologies. A sonochemical reactor built with an electrostatic transducer can always operate effectively at one of the resonant frequencies of the reactor, even if irregularities in the transducer location or cavitation bubbles shift the reactor resonant frequency away from the design frequency.

- The reactor used mode shapes, resonance and its own geometry to increase the magnitude of the sound field. A cylindrical reactor with Bessel function radial mode shapes and a cylindrical transducer directing sound into the centre of the reactor were chosen for their focusing affect on the sound field. The transducer was also constructed so that the sound field would contain odd axial mode shapes only. Exciting the reactor at a frequency which corresponded to an odd axial mode and a radial mode with a pressure node coincident with the transducer radius caused the whole reactor system to resonate, thereby generating the largest possible sound pressure at the focal point of the reactor.

- The mode shapes and the placement of the transducer within the sound field were used to prevent cavitation against the transducer. In this design the transducer was placed away from the reactor’s axis where sound pressure and cavitation are concentrated.

- The sonochemical reactor was designed to have easily modeled sound field. The cylindrical geometry with cylindrical forcing allowed the reactor’s pressure field to be solved as a standard boundary value problem.
A model was developed to assist in refining the sonochemical reactor design. The purpose of this model was to accurately predict the pre-cavitation, homogenous sound field in the reactor. Since less sound energy is required to sustain cavitation that to create it, it is valid to model a homogenous reactor to determine if cavitation will be initiated. To create the complete reactor model, models of the electrostatic transducer and the reaction vessel were created, and then linked together.

The transducer model was constructed by adapting an established calculation to the research reactor. This yielded an expression relating the transducer's voltage and pressure output to the velocity of the transducer membrane. The stiffness and damping coefficients in the expression were calculated using a thermodynamic model developed by Dunwoody. This model is based on the phase difference between the air compression and the heat flow in the transducer.

The reaction vessel model was developed by applying the boundary conditions of the reactor to the wave equation for sound. The reactor's boundaries were the pressure relief plastic walls of the reactor, the pressure relief free water surface at the top of the reactor and the transducer, whose pressure matched the liquid's pressure at the transducer's radius. Solving the boundary value problem yielded a relationship between the transducer pressure and the reactor's pressure field. Determining the pressure field also allowed the reactor's radial velocity and, in turn, the velocity of the transducer membrane to be determined.

Development of the complete reactor model was complicated by the fact that the transducer pressure and the reactor pressure field were not independent. To address this problem, the reactor pressure field and, therefore, the transducer pressure and velocity, were expressed as sums of mode shapes multiplied by a pressure scaling factor. This allowed the shape of the reactor's pressure field and, therefore, the relative pressure magnitude between any two points in the reactor, to be determined independent of the magnitude of the transducer pressure. The transducer pressure could then be determined from the pressure field mode shapes and the input voltage.

The reactor model was checked in several different ways to ensure its accuracy. Two checks were done on the model alone:

- The sonochemical reactor conceived and modeled in this research was specifically designed to excite the first radial mode in the region between the transducer and the centre of the reactor, and the first axial mode of the reactor, when a frequency matching the resonant frequency of those modes was
applied. At other frequencies, the reactor was expected to support combinations of odd axial modes and other radial modes with pressure nodes at or near the transducer radius. The pressure fields that were generated by the model were checked graphically to confirm that this was the case. It was.

- The resonant frequencies of the modeled reactor configuration were the same as the resonant frequencies of an unforced reactor with a pressure release radial wall at the transducer radius. The unforced resonant frequencies of this configuration were compared with the resonant frequencies calculated by the model for the forced reactor. The match was found to be excellent.

The reactor model was also compared with experimental data. In order to make this comparison, a sonochemical reactor based on the modeled reactor configuration was constructed, and the pressure magnitude at the centre of the reactor was determined for a wide range of frequencies. The expected electrostatic pressure developed in the reactor for each measurement was also calculated from the input voltage. The ratio of the reactor's experimentally determined centre pressure to the calculated electrostatic pressure was determined. This ratio was compared to the ratio of the centre pressure predicted by the model to the calculated electrostatic pressure. The match between pressure ratios predicted by the model and measured experimentally was quite good. Both the model and the reactor showed the same resonant frequencies, and similar relationships between pressure ratio and frequency.

The main difference between the experimental and predicted pressure ratio curves was the width of their resonant peaks. The width and/or area of a resonance peak is proportional to the damping of the system at the resonant frequency. In the proposed sonochemical reactor design, the damping of the whole system is governed by the transducer damping. Thus it was anticipated that the difference in the widths of the resonant peaks was due to a difference between the experimental transducer’s damping coefficient, and the damping coefficient used by the model. The source of this difference is thought to be due to a smaller than expected gap space between the plates of the electrostatic transducer used in the experiment. The gap space was adjusted so that the area of the predicted and measured resonant peaks at the main reactor resonances were similar, and the pressure ratios were recalculated. Correcting the gap space changed both pressure ratio curves, since the calculated electrostatic pressure was dependent on the gap spacing. The agreement between the modeled and experimental curves with the correct gap spacing was excellent.
The excellent agreement between the pressure ratios predicted by the model and those found experimentally confirmed the validity of the reactor model developed in this research. Confirming the validity of the reactor model was important for several reasons:

- The thermodynamic model of electrostatic transducer stiffness and damping was untested prior to this research. Since the research results suggest that the whole transducer model is valid, they also suggest that the individual parts of the model, such as the method used to calculate the stiffness and damping, are also be valid.

- Although the reactor proposed in this research was carefully designed, the specific design details of the experimental reactor, such as the length and radius of the reactor cavity, the gap space of the transducer and the resonant frequency for which the reactor was designed, were arbitrarly chosen, though interrelated. Since the model has been verified using the configuration of the experimental reactor, it can also be used to analyze different design configurations without building new reactors.

- The power output of electrostatic transducers is low compared to those of the transducer technologies traditionally used in sonochemical reactors. As a result, there is some question as to whether electrostatic transducers can be used effectively in sonochemical reactors despite their aforementioned benefits. The verified model can be used to investigate the sonochemical potential of electrostatic transducers.

In fact, the sonochemical reactor built, modeled and tested in this research did not generate sufficient pressure to cause cavitation. According to the predicted pressure ratio at the design frequency, an input signal of 7000 V would be necessary to achieve cavitation in the test reactor. At this voltage, the transducer would break down. Thus, the reactor model was used, as suggested above, to investigate changes to the reactor design. Two changes were studied. They were:

- Reducing transducer damping by reducing heat conduction from the gap space gas. This was done by modeling the reactor with the air in the transducer gap replaced with R11, a gas with low thermal conductivity and high dielectric strength. This change reduced the voltage needed for cavitation to 2200 V, which is much improved, but will still cause breakdown.

- Reducing the transducer's gap space to increase electrostatic force. This was done by decreasing the size of the transducer gap space in the model to 0.01 and 0.001 mm. For these gap spaces the model indicated that the resonance at the design frequency is significantly reduced, but that cavitation is achievable at higher frequencies with voltage inputs of 400 and 200 V, respectively.
The low cavitation initiation voltages predicted by the model for small gap space transducers confirm that it is possible to generate cavitation in sonochemical systems using carefully chosen electrostatic transducers.

Using the model to predict the behaviour of the sonochemical reactor design in different configurations and for different inputs yielded unexpected results, such as the reduction in the magnitude of the design resonance with decreased gap spacing. This finding demonstrates that the reactor variables and, specifically, the transducer parameters, are heavily interrelated, which makes predicting the results of changes to reactor parameters difficult. This is where the model developed in this research is particularly useful for sonochemical reactor design.
References


Appendix A

Sonochemical Reactor Schematics
Figure A.1 Prototype of Proposed Sonochemical Reactor
Figure A.2 Cut-Away Section of Electrostatic Transducer Prototype
Figure A.3 Cross-Section Detail of Electrostatic Transducer Prototype
Appendix B
Sonochemical Reactor Model in mathCAD
Sonochemical Reactor Model

Damping Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gap Pressure</td>
<td>$P_0 := 0.1-10^6 \text{ Pa}$</td>
</tr>
<tr>
<td>Temperature</td>
<td>$T_0 := 293 \text{ K}$</td>
</tr>
<tr>
<td>Density air</td>
<td>$\rho_{\text{air}} := 1.2 \text{ kg-m}^{-3}$</td>
</tr>
<tr>
<td>Specific Heat</td>
<td>$c_V := 716 \text{ joule-kg}^{-1}\text{K}^{-1}$</td>
</tr>
</tbody>
</table>

Thermal Conductivity $\kappa_T := 0.025 \text{ joule-sec}^{-1}\text{m}^{-1}\text{K}^{-1}$

Permittivity free space $\varepsilon := 8.85 \times 10^{-12} \text{ farad-m}^{-1}$

Maximum Pressure Amplitude $P_{\text{max}} := 10^4 \text{ Pa}$

Transducer Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Assumed Pressure</td>
<td>$P_t := 1 \text{ Pa}$</td>
</tr>
<tr>
<td>Air Gap Thickness</td>
<td>$H := 0.381 \text{ mm}$</td>
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<tr>
<td>Mylar Thickness</td>
<td>$d_m := 0.0254 \text{ mm}$</td>
</tr>
<tr>
<td>Dielectric Const</td>
<td>$\kappa_m := 3$</td>
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<tr>
<td>Apparent Air Gap Thickness</td>
<td>$d := H + d_m \kappa_m^{-1}$</td>
</tr>
<tr>
<td>Radius:</td>
<td>$r_t := 0.057 \text{ m}$</td>
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</tbody>
</table>

Test Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Driving Frequency</td>
<td>$v_d := 5538 \text{ sec}^{-1}$</td>
</tr>
<tr>
<td>Reactor Frequency</td>
<td>$v := 2 \cdot v_d$</td>
</tr>
<tr>
<td>Approximate Radial Hydrophone Position</td>
<td>$r_h := 0.375 - 0.0245 \text{ m}$</td>
</tr>
<tr>
<td>Approximate Axial Hydrophone Position</td>
<td>$r_h := 9.188 \times 10^{-2} \text{ m}$</td>
</tr>
<tr>
<td>Test Voltage</td>
<td>$V_{\text{test}} := \sqrt{2 \cdot 70 \text{ volt}}$</td>
</tr>
</tbody>
</table>

Test Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reactor Frequency</td>
<td>$v := 1.108 \times 10^4 \text{ sec}^{-1}$</td>
</tr>
<tr>
<td>Approximate Radial Hydrophone Position</td>
<td>$r_h := 0.375 - 0.0245 \text{ m}$</td>
</tr>
<tr>
<td>Approximate Axial Hydrophone Position</td>
<td>$r_h := 9.188 \times 10^{-2} \text{ m}$</td>
</tr>
<tr>
<td>Test Voltage</td>
<td>$V_{\text{test}} := \sqrt{2 \cdot 70 \text{ volt}}$</td>
</tr>
</tbody>
</table>

Reactor Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Approximate Radius</td>
<td>$R := 3.7 - 0.0254 \text{ m}$</td>
</tr>
<tr>
<td>Length</td>
<td>$L := 6 \cdot 0.0254 \text{ m}$</td>
</tr>
<tr>
<td>Density $H_2\rho$</td>
<td>$\rho_0 := 1000 \text{ kg-m}^{-3}$</td>
</tr>
<tr>
<td>Speed of Sound $H_2\rho$</td>
<td>$c_0 := 1482 \text{ m-sec}^{-1}$</td>
</tr>
<tr>
<td>Damping Coefficient $H_2\rho$</td>
<td>$\alpha := 24 \cdot 10^{-15} \cdot v^2 \cdot \text{sec}^{-2} \cdot \text{m}^{-1}$</td>
</tr>
<tr>
<td>Range of Radial Values</td>
<td>$r := 0 \text{ m, } 0.001 \text{ m}$</td>
</tr>
<tr>
<td>Range of Axial Values</td>
<td>$z := 0 \text{ m, } 0.001 \text{ m}$</td>
</tr>
<tr>
<td>Diaphragm Cell Mass</td>
<td>$m_t := \rho_d \cdot S$</td>
</tr>
<tr>
<td>Diaphragm Mass</td>
<td>$m_t := 1.4 \times 10^{-4} \text{ kg}$</td>
</tr>
</tbody>
</table>

Diaphragm Parameters
Transducer Stiffness and Damping Parameters
Stiffness and damping parameters are calculated assuming that the air inside the transducer is the primary source of stiffness and damping.

Function Definition
\[ \text{odd}(n) := \text{mod}(n, 2) = 1 \]

Temperature distribution (per unit pressure amplitude)

Phase angle (component)
\[ \phi(n, \omega) := \arctan \left[ \sqrt{\frac{n \pi}{H}} \left[ \omega \left( c \sqrt{\rho_{\text{air}} + \frac{P_0}{T_0}} \right)^{-1} \right] \right] \]

Amplitude (component)
\[ \Theta(n, \omega) := 4 \cdot \omega \cdot \text{odd}(n) \cdot \left[ \frac{n \pi}{H} \cdot \left( \omega \cdot \sqrt{\frac{n \pi}{H}} \cdot \sin(\phi(n, \omega)) + \omega \left( c \sqrt{\rho_{\text{air}} + \frac{P_0}{T_0}} \cdot \cos(\phi(n, \omega)) \right) \right]^{-1} \]

\[ T(x, t, \omega) := \left[ \sum_{n=1}^{19} \left( \sin\left( \frac{n \pi x}{H} \right) \cdot \Theta(n, \omega) \cdot \cos(\omega t + \phi(n, \omega)) \right) \right] \cdot P_{\text{max}} \]

Pressure distribution (per unit displacement amplitude)

Phase angle
\[ A(\omega) := \arctan \left[ \frac{2 \cdot H}{\pi \cdot T_0} \cdot \left( \sum_{n=1}^{19} \frac{\Theta(n, \omega) \cdot \sin(\phi(n, \omega))}{n} \right) \cdot \left( \frac{2 \cdot H}{\pi \cdot T_0} \cdot \sum_{n=1}^{19} \frac{\Theta(n, \omega) \cdot \cos(\phi(n, \omega))}{n} - \frac{H}{P_0} \right)^{-1} \right] \]

Amplitude
\[ P(\omega) := \left[ \left( \frac{2 \cdot H}{\pi \cdot T_0} \cdot \sum_{n=1}^{19} \frac{\Theta(n, \omega) \cdot \sin(\phi(n, \omega))}{n} \right)^2 + \left( \frac{2 \cdot H}{\pi \cdot T_0} \cdot \sum_{n=1}^{19} \frac{\Theta(n, \omega) \cdot \cos(\phi(n, \omega))}{n} - \frac{H}{P_0} \right)^2 \right]^{-0.5} \]

Spring coefficient
\[ k(\omega) := S \cdot P(\omega) \cdot \cos(A(\omega)) \]

Damping coefficient
\[ b(\omega) := \sum_{\omega} S \cdot P(\omega) \cdot \sin(A(\omega)) \]

Radially Forced Boundary Conditions
A cylindrical sonochemical reactor with a cylindrical (or near cylindrical) transducer radiating radially into the core of the reactor can is modeled by considering two regions and the transducer. Region 1 extends from the center of the reactor \((r=0)\) to the transducer. Region 2 extends from the transducer to the wall of the reactor.
Region 1
At the center of the reactor \((r=0)\), the radial velocity of the sound wave will be zero. The pressure at the transducer \((r=r_t)\) is the same as the transducer pressure, \(p_t(z)\). The axial boundaries are the same as in the free field case. Damping is assumed to be exponential - similar free field plane waves.

**Pressure in region 1:**
\[
p_t(r, z, t) = \text{Sum}(A_n J_0(k r_t) \sin(k z) e^{jwt} e^{\alpha (r-r_t)})
\]
**Radial velocity in region 1:**
\[
u_t(r, z, t) = \text{Sum}(A_n \omega p_0 (k r_t) J_1(k r_t) \alpha J_0(k r_t)) \sin(k z) e^{jwt} e^{\alpha (r-r_t)})
\]
Applying the boundary conditions yields the following equations:
**Outer boundary:**
\[
p_t(r_t, z, t) = \text{Sum}(A_n J_0(k r_t) \sin(k z) e^{jwt}) = p_t(z) e^{iw t}
\]
**Inner boundary:**
\[
u_t(0, z, t) = \text{Sum}(A_n \omega p_0 (kr_t) J_1(k r_t) \alpha J_0(k r_t)) \sin(k z) e^{jwt} e^{\alpha (0-r_t}) = 0
\]
For the inner boundary, \(J_1(k r_t) = 0\), so this equation is automatically met. Integrating the outer boundary equation times an axial mode shape over the length of the reactor and solving for \(A_n\) yields the following equation for the coefficient:

**Region 1 coefficient:**
\[
A_n = \int_0^L (\sin(k z) p_t(z) dz) / L J_0(k r_t)
\]

Region 2
Since the radial wall of the reactor is a pressure release boundary, the pressure at the wall \((r=R)\) will be zero. The pressure at the transducer \((r=r_t)\) is the same as the transducer pressure, \(p_t(z)\). The axial boundaries are the same as in the free field case. Damping is assumed to be exponential - similar free field plane waves.

**Pressure in region 2:**
\[
p_2(r, z, t) = \text{Sum}(B_n J_0(k r) e^{jwt} + C_n Y_0(k r) \cos(k z) e^{jwt} e^{\alpha (r-R)})
\]
**Radial velocity in region 2:**
\[
u_2(r, z, t) = \text{Sum}(i \omega r_0 [B_n J_1(k r) + \alpha J_0(k r)] + C_n [k r Y_1(k r) \alpha Y_0(k r)]) \cos(k z) e^{jwt} e^{\alpha (r-R)})
\]
Applying the boundary conditions yields the following equations:
**Outer boundary:**
\[
p_2(R, z, t) = \text{Sum}(B_n J_0(k r) e^{jwt} + C_n Y_0(k r) \cos(k z) e^{jwt} e^{\alpha (R-R)}) = 0
\]
**Inner boundary:**
\[
u_2(r_t, z, t) = \text{Sum}(B_n J_0(k r_t) e^{jwt} + C_n Y_0(k r_t) \cos(k z) e^{jwt}) = p_t(z) e^{iw t}
\]
Integrating both boundary equations times an axial mode shape over the length of the reactor and solving for \(B_n\) and \(C_n\) yields the following equations for the coefficients:

**Region 2 coefficient, \(B_n\):**
\[
B_n = -Y_0(k r) \text{Integral}_0^L (\sin(k z) p_t(z) dz) / L [J_0(k r_t) Y_0(k r) - Y_0(k r_t) J_0(k r)]
\]
**Region 2 coefficient, \(C_n\):**
\[
C_n = J_0(k r) \text{Integral}_0^L (\sin(k z) p_t(z) dz) / L [J_0(k r_t) Y_0(k r) - Y_0(k r_t) J_0(k r)]
\]
Response to unit pressure at the transducer

The response of the reactor to a radial input frequency is given by the region 1 and 2 pressure equations found above. The input frequency and unit pressure are generated by the radial transducer in response to an unknown input voltage and the specified frequency.

Transducer input frequency (rads/sec) \( \omega := 2 \pi \nu \) \( \omega = 6.959 \times 10^4 \ \text{sec}^{-1} \)

Range of axial wave numbers used in calculations
\( n := 0 \ldots 50 \)
\( k_z := n \frac{\pi}{L} \)

Range of radial wave numbers generated from axial numbers
\( k_r(n) := \sqrt{\left( \frac{\omega}{c_0} \right)^2 - \left( k_z \right)^2} \)

Axial pressure mode shapes
\( Z(z,n) := \sqrt{2} \cdot \sin \left( k_z \cdot z \right) \)

Radial pressure mode shapes

'J0' type Bessel Response
\( R_{J0}(r,n) := \begin{cases} J_0(k_r(n) \cdot r) & \text{if} \ (k_r(n))^2 \geq 0.1 \cdot m^2 \\ 0 & \text{otherwise} \end{cases} \)

'Y0' type Bessel Response
\( Y_{0}(r,n) := \begin{cases} Y_0(k_r(n) \cdot r) & \text{if} \ (k_r(n))^2 \geq 0.1 \cdot m^2 \\ K_0(k_r(n) \cdot r) & \text{otherwise} \end{cases} \)

Radial pressure mode shapes

'J1' type Bessel Response
\( R_{J1}(r,n) := \begin{cases} J_1(k_r(n) \cdot r) & \text{if} \ (k_r(n))^2 \geq 0.1 \cdot m^2 \\ 0 & \text{otherwise} \end{cases} \)

'Y1' type Bessel Response
\( Y_{1}(r,n) := \begin{cases} Y_1(k_r(n) \cdot r) & \text{if} \ (k_r(n))^2 \geq 0.1 \cdot m^2 \\ K_1(k_r(n) \cdot r) & \text{otherwise} \end{cases} \)

Axial variation of transducer pressure
\( p_z(z) := 1 \)

Plot of the shape of the axial forcing function and the axial mode shape
Pressure Coefficients

The response coefficients for each mode are found using the defined input pressure and frequency at the transducer and the equations given in the discussion above.

Region 1 pressure and radial velocity

Coefficient multiplier

\[
M_1 := \int_0^L p(z) \cdot Z(z, n) \, dz
\]

Coefficient \( A_n \)

\[
A_n := \frac{p \cdot t \cdot M_1}{L \cdot R \cdot J_0(r, n)}
\]

Region one pressure equation

\[
p_1(r, z) := \sum_n A_n \cdot R \cdot J_0(r, n) \cdot Z(z, n) \cdot e^{\alpha(r-t)}
\]

Region one radial velocity equation

\[
u_{1r}(r, z) := \sum_n \frac{j \cdot A_n}{\omega \cdot \rho} \left( k \cdot J_1(r, n) - \alpha \cdot R \cdot J_0(r, n) \right) \cdot Z(z, n) \cdot e^{\alpha(r-t)}
\]

Region 2 pressure and radial velocity

Coefficient multiplier

\[
M_2 := \int_0^L p(z) \cdot Z(z, n) \, dz
\]

Coefficient \( B_n \)

\[
B_n := -\frac{1}{L \cdot R \cdot J_0(r, n) \cdot R \cdot Y_0(r, n) \cdot R \cdot J_0(r, n)}
\]

Coefficient \( C_n \)

\[
C_n := \frac{p \cdot t \cdot R \cdot J_0(r, n) \cdot M_2}{L \cdot R \cdot J_0(r, n) \cdot R \cdot Y_0(r, n) \cdot R \cdot J_0(r, n)}
\]

Pressure equation

\[
p_2(r, z) := \sum_n \left( B_n \cdot R \cdot J_0(r, n) + C_n \cdot R \cdot Y_0(r, n) \right) \cdot Z(z, n) \cdot e^{\alpha(r-t)}
\]

Radial velocity equation

\[
u_{2r}(r, z) := \sum_n \frac{j}{\omega \cdot \rho} \left( B_n \cdot (k \cdot J_1(r, n) - \alpha \cdot R \cdot J_0(r, n)) \right) \cdot Z(z, n) \cdot e^{\alpha(r-t)}
\] 

\[
+ \sum_n \frac{j}{\omega \cdot \rho} \left( C_n \cdot (k \cdot Y_1(r, n) + \alpha \cdot R \cdot Y_0(r, n)) \right) \cdot Z(z, n) \cdot e^{\alpha(r-t)}
\]

Pressure and Radial Velocity Distributions Along the Radius of the Reactor

Using the calculated coefficients and the pressure and velocity equations for each region, a pressure distribution for the whole reactor is constructed. The assumed transducer pressure is 1 atm.
Pressure distribution
\[
\text{Pressure}(r,z) := \begin{cases} 
\rho_1(r,z) & \text{if } r \leq r_t \\
\rho_2(r,z) & \text{otherwise}
\end{cases}
\]

Radial velocity distribution
\[
\text{Velocity}_r(r,z) := \begin{cases} 
\mathbf{u}_1(r,z) & \text{if } r \leq r_t \\
\mathbf{u}_2(r,z) & \text{otherwise}
\end{cases}
\]

Pressure and radial velocity profiles at center cross section

Location of profile on z axis
\[
Z_{\text{mid}} := \frac{L}{2}
\]

Check for unit transducer pressure
\[
\text{Pressure}(r_t, Z_{\text{mid}}) = 1.013 \text{ kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-2}
\]

Pressure distribution

Radial velocity distribution
Transducer Velocity Profile
The fluid velocity on each side of the transducer is related to the "breathing velocity" of the whole transducer due to its motion back and forth, as well as the displacement velocity of the transducer membrane. The magnitude of the membrane displacement velocity is equal on both sides of the transducer, but the direction of the velocity on each side is different. This calculation is approximate since the transducer membranes are not continuous, but divided into square sections.

Breathing velocity

\[ u_b(z) := \frac{u_2(r, z) + u_1(r, z)}{2} \]

Displacement velocity

\[ u_d(z) := u_b(z) - u_1(r, z) \]

Comparison of breathing velocity, displacement velocity and the total velocities of each transducer membrane

Transducer Displacement Profile
The "breathing displacement" of the transducer is due to its total motion back and forth. Both membranes have equal displacements relative to the transducer structure, but their total displacements differ due to the "breathing" of the transducer. This calculation is approximate since the transducer membranes are not continuous, but divided into square sections.

Region one displacement

\[ \Delta_1(z) := \frac{u_1(r, z)}{\omega} \]

Region two displacement

\[ \Delta_2(z) := \frac{u_2(r, z)}{\omega} \]

Breathing displacement

\[ \Delta_b(z) := \frac{u_b(z)}{\omega} \]

Membrane displacement

\[ \Delta(z) := \frac{u_d(z)}{\omega} \]

Comparison of breathing displacement, membrane displacement and the total displacement of each transducer membrane
Voltage Required for Unit Acoustic Pressure at Transducer
Transducer pressure and displacement velocity equations have been developed using an assumed transducer pressure of 1 Pa. The voltage required for unit transducer pressure can be determined using the voltage transfer function, which includes the transducer's pressure and displacement velocity, plus the mass, springiness and damping of its elements.

Voltage transfer function
\[ V(z) = \frac{2d}{\varepsilon^0.5}\left[p_1(z) - (b(\omega) + j(m_1 - k(\omega)/\omega)u_d(z))\right]^{0.5} \]

Voltage function
\[ V(z) := \frac{d \cdot 2}{\sqrt{\varepsilon}}\left[p_1(t, z) - \left[b(\omega) + j\left(m_1 - k(\omega)/\omega\right)\right] u_d(z)\right]^{0.5} \]

Voltage required for unit transducer pressure
\[ V_{\text{input}} := \int_{0 \cdot m}^{L} V(z) \, dz \left(\int_{0 \cdot m}^{L} 1 \, dz\right)^{-1} \]
\[ V_{\text{input}} = 1.179 \cdot 10^3 \text{ volt} \]

Electrostatic pressure required for unit transducer pressure
\[ P_{\text{elec input}} := \frac{\varepsilon \cdot V_{\text{input}}^2}{2 \cdot d^2} \]
\[ P_{\text{elec input}} = 40.564 \text{ Pa} \]

Pressure as a Function of Input Voltage
The pressure and velocity profiles in the reactor are related linearly to the magnitude of the pressure generated at the transducer. The transducer pressure is a function of input voltage and transducer velocity. In order to determine the pressure and velocity responses to an actual test voltage, a scaling factor for the responses to unit input pressure must be determined.
Transducer impedance

\[ z_t := \left[ b(\omega) + j \left( m_1 \omega - \frac{k(\omega)}{\omega} \right) \right] \frac{1}{S} \]

Unit pressure

\[ p_{\text{unit}}(z) := \sum_n M_1 n \cdot R J_0(r_t, n) \cdot Z(z, n) \]

Unit displacement velocity

\[ u_{\text{unit}}(z) := \sum_n \frac{j}{2\omega \rho_0} \cdot M_2 n \left[ -R Y_0(r_t, n) \cdot (k(n) \cdot Ru J_1(r_t, n) + \alpha \cdot R J_0(r_t, n)) \right] Z(z, n) \]

Electrostatic pressure due to test voltage

\[ P_{\text{e_test}} := \frac{e \cdot V_{\text{test}}^2}{2 \cdot d^2} \quad P_{\text{e_test}} = 0.286 \cdot \text{Pa} \]

Transducer pressure due to test voltage

\[ P_{\text{t_test}} := \frac{P_{\text{e_test}}}{2 \cdot p_{\text{unit}}(L/2) - z_t u_{\text{unit}}(L/2)} \quad |P_{\text{t_test}}| = 4.214 \cdot 10^{-3} \cdot \text{Pa} \]

Unit pressure to test pressure scaling factor

\[ P_{\text{scale}} := \frac{P_{\text{t_test}}}{P_t} \quad |P_{\text{scale}}| = 4.214 \cdot 10^{-3} \]

Scaled Pressure and Radial Velocity Profiles
Using the scale factor, the pressure and radial velocity profiles for the test frequency and input voltage can be calculated and displayed.

Test Pressure

\[ \text{Pressure}_{\text{test}}(r, z) := P_{\text{scale}} \cdot \text{Pressure}(r, z) \]

Test Radial Velocity

\[ \text{Velocity}_{\text{test}}(r, z) := P_{\text{scale}} \cdot \text{Velocity}_r(r, z) \]

Pressure and Radial Velocity Matrices

Reactor matrix size

\[ \sigma := 50 \quad i := 1..\sigma \quad t := 1..\sigma \]

Unit pressure matrix

\[ P_{\text{matrix}}_{\text{unit}} := \text{Pressure} \left( i \cdot \frac{R}{\sigma}, t \cdot \frac{L}{\sigma} \right) \]

Test pressure matrix

\[ P_{\text{matrix}} := P_{\text{scale}} \cdot P_{\text{matrix}}_{\text{unit}} \]

Unit radial velocity matrix

\[ U_{\text{matrix}}_{\text{unit}} := \text{Velocity}_r \left( i \cdot \frac{R}{\sigma}, t \cdot \frac{L}{\sigma} \right) \]

Test radial velocity matrix

\[ U_{\text{matrix}}_{\text{unit}} := P_{\text{scale}} \cdot U_{\text{matrix}}_{\text{unit}} \]
Maximum reactor pressure
\[ \text{max}(P_{\text{matrix}}) = 1.081 \text{ Pa} \]

Minimum reactor pressure
\[ \text{min}(P_{\text{matrix}}) = 88.258 \text{ Pa} \]

Ratio of maximum pressure to electrostatic pressure
\[ \frac{\text{max}(P_{\text{matrix}})}{P_{e_{\text{test}}}} = 3.781 \]
Reactor pressure at hydrophone

\[ p_{h\_tst} := \text{Re} \left( P_{\text{scale}} \cdot P_{\text{pressure}}(r_h, z_h) \right) \]

\[ p_{h\_tst} = 85.081 \text{ Pa} \]

Ratio of hydrophone pressure to electrostatic pressure

\[ \frac{p_{h\_tst}}{p_{e\_test}} = 297.599 \]

Reactor Radial Velocity Contours

Radial Velocity Contours: 11,076 Hz

Maximum reactor radial velocity

\[ \max(\text{Urmatrix}) = 2.75 \cdot 10^{-9} \text{ m-sec}^{-1} \]

Minimum reactor radial velocity

\[ \min(\text{Urmatrix}) = 3.118 \cdot 10^{-5} \text{ m-sec}^{-1} \]

Model Verification

The output from this model must be compared with test data. The following commands export data that is used to analyze and compare test data.

Unit pressure at hydrophone position

\[ \text{Pressure}_{\text{unith}} := \text{Pressure}(r_h, z_h) \]
Pressure at hydrophone

\[ p_{h_{\text{test}}} = | \text{Re} \left( P_{\text{scale}} \cdot \text{Pressure} \left( r_{h}, z_{h} \right) \right) | \]

\[ p_{h_{\text{test}}} = 85.081 \text{ Pa} \]

Data for Export

Data for comparison
(Driving frequency, pressure ratio / driving frequency, hydrophone pressure)

\[ \text{WRITEPRN} \left( "\text{pressure.txt}" \right) := v \cdot \text{sec} \left[ \frac{p_{h_{\text{test}}}}{p_{e_{\text{test}}}} \right] \]

\[ \text{WRITEPRN} \left( "\text{abs.txt}" \right) := v \cdot \text{sec} \left[ \frac{p_{h_{\text{test}}}}{p_{a}} \right] \]
Appendix C
mathCAD Sheet 'View'
View the measured input and output

Phase difference between Input Signal and Transformer Signal
deg := 159
rad := \frac{deg \cdot \pi}{180}

Test Frequency
i := 0..6
data_i := READ("data.txt")
data := READ("data.txt")

Driving Frequency
v_d := \frac{data_i}{sec} = 5.5 \cdot 10^3 \text{ sec}^{-1}
v_d := 5.5 \cdot 10^3 \text{ sec}^{-1}

Reactor Frequency
v_r := 2 \cdot v_d = 1.1 \cdot 10^4 \text{ sec}^{-1}

Test Period
T_r := \frac{1}{v_r} = 9.091 \cdot 10^{-5} \text{ sec}

Input Signal
n := 5003
i := 0..n
INIT := READ("Indata.txt")
INIT_i := READ("Indata.txt")

Reactor Signal
The frequency of the reactor signal is twice that of the input signal. The reactor signal calculated here represents the frequency of the reactor signal BUT NOT THE MAGNITUDE.

Fourier Transform of Reactor Signal
INPUT := CFFT(input)

Output Signal
Measured from the hydrophone
OUT_i := READ("Outdata.txt")
output_i := OUT_{i+4}

Fourier Transform of Output Signal
OUTPUT := CFFT(output)

Timescale of Signal
T := INIT_i \cdot sec
T = 2 \cdot 10^{-6} \text{ sec}

Frequency Range
\nu := \frac{\eta}{N \cdot T}

Graph of Reactor Signal

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{reactor_signal_graph.png}
\caption{Graph of Reactor Signal}
\end{figure}
Fourier Transform of Reactor Signal

Graph of Output Signal

Fourier Transform of Output Signal
Determining Phase Difference Between Reactor Signal and Output

Algorithm for determining the increment of test frequency

\[
\phi_{\text{num}}(\text{freq}, \text{freqd}) :=
\]
\[
\begin{align*}
\text{num} &\leftarrow 0 \\
\text{for } n &\in 0..\text{rows(freq)} - 1 \\
\text{freq}_{\text{num}} &\leftarrow n \text{ if } \frac{\text{freq}_{\text{num}}}{\text{freqd}} = 1 \\
\text{num} &\leftarrow 0
\end{align*}
\]

Increment of test frequency

\[
\text{num} := \phi_{\text{num}}(v, v_r)
\]

Phase of test frequency

\[
\arg\left(\text{INPUT}_{\text{num}}\right) = 0.942
\]

Algorithm for finding the reactor/output phase difference between -180 and 180 degrees

\[
\text{phasediff}(\text{INPUT}, \text{OUTPUT}, \text{shft}, \text{num}) :=
\]
\[
\begin{align*}
\text{del}\phi &\leftarrow (\arg(\text{INPUT}_{\text{num}}) + 2\cdot\text{shft} - \arg(\text{OUTPUT}_{\text{num}})) \frac{180}{\pi} \\
\text{del}\phi &\leftarrow \text{del}\phi - 360 \text{ if } \text{del}\phi > 180 \\
\text{del}\phi &\leftarrow 360 + \text{del}\phi \text{ if } \text{del}\phi < -180 \\
\text{del}\phi &\leftarrow \text{del}\phi \text{ otherwise}
\end{align*}
\]

Phase difference

\[
\Delta\phi := \text{phasediff}(\text{INPUT}, \text{OUTPUT}, \text{rad}, \text{num})
\]

\[
\Delta\phi = -77.716
\]

Phase difference data file

\[
\text{WRITEPRN}("p.txt") := [v \cdot \text{sec}] \\
\Delta\phi
\]

Output transform data file

\[
\text{WRITEPRN}("\text{fourier.txt}"") := \text{OUTPUT}
\]
Appendix D

mathCAD Sheet 'Profile'
Input Output Profile

Test Parameters \( i := 0..5 \)

Driving Frequency \( v_d := \text{Input}_i \cdot \text{sec}^{-1} \)

Reactor Frequency \( v_r := 2 \cdot v_d \)

Test Voltage \( \text{Vin}_{\text{test}} := \text{Input}_i \cdot \text{volt} \)

Hydropone Position \( \text{hydro}_{rz} := [\text{Input}_2, \text{Input}_3] \cdot \text{m} \)

Electrostatic Pressure \( p_e := \text{Input}_4 \cdot \text{Pa} \)

Modeled Output Pressure \( p_{\text{mod}_{out}} := \text{Input}_4 \cdot \text{Pa} \)

Modeled Hydrophone Output Voltage \( V_{\text{mod}_{out}} := 30.6 \cdot 10^{-6} \frac{\text{volt}}{\text{Pa}} \cdot (p_{\text{mod}_{out}} - 1 \cdot 10^{-6} \cdot \text{Pa}) \)

Measured Output Voltage

\( n := 5003 \quad i := 0..n \)

Output Time Interval \( T := \text{OUT}_i \cdot \text{sec} \)

Output Voltage Curve \( \eta := 0..4999 \quad N := 5000 \)

Fourier Transform

\( \text{OUTPUT} := \text{CFFT}(\text{out}) \)

Fourier Frequencies \( \nu_{\eta} := \frac{\eta}{N \cdot T} \)

Magnitude of Measured Output Voltage at Reactor Frequency

Reactor Frequency \( \text{round}(x) := \text{if}(x - \text{floor}(x) < 0.5, \text{floor}(x), \text{ceil}(x)) \)

Increment Value \( \eta_r := \text{round} \left( v_r \cdot N \cdot T \right) \)

\( \eta_r = 110 \)

Magnitude of Output Voltage (reactor frequency)

\( V_{\text{test}_{out}} := |\text{OUTPUT}_{\eta_r}| \cdot \text{volt} \)

\( V_{\text{test}_{out}} = 6.223 \cdot 10^{-4} \cdot \text{volt} \)

Magnitude of Measured Output Pressure at Reactor Frequency

\( \text{P}_{\text{test}_{out}} := \frac{V_{\text{test}_{out}} \cdot \text{Pa}}{30.6 \cdot 10^{-6} \cdot \text{volt}} + 1 \cdot 10^{-6} \cdot \text{Pa} \)

\( \text{P}_{\text{test}_{out}} = 20.336 \cdot \text{Pa} \)
Pressure Increase Ratio - Reactor Pressure/Electrostatic Pressure

Model to Calculated Electrostatic

\[ P_{\text{inc}_m} := \frac{P_{\text{mod\_out}}}{P_e} \]

\[ P_{\text{inc}_m} = 69.5 \]

Experiment to Calculated Electrostatic

\[ P_{\text{inc}_t} := \frac{P_{\text{test\_out}}}{P_e} \]

\[ P_{\text{inc}_t} = 71.129 \]

Data Output

Data Matrix

\[ \text{data := } [v, \text{sec}, P_{\text{inc}_m}, P_{\text{inc}_t}] \]

Data Output Command

\[ \text{WRITEPRN("pressure.txt") := data} \]

Measured Output Voltage

![Measured Output Voltage Graph]

Measured Output Voltage (zoom)

![Measured Output Voltage (zoom) Graph]