Modeling Acoustic Microfluidic Phenomena in Unconventional Geometries

Andrew Ledbetter

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ABSTRACT

Modeling Acoustic Microfluidic Phenomena in Unconventional Geometries

by

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In this work, the performance of a piezoelectrically-actuated ultrasonic droplet generator is analyzed by modeling the harmonic response of a two-dimensional representation of the device cross-section. Observed vibrational and acoustic resonances provide insight into optimal design conditions to achieve efficient, robust droplet ejection. Numerical simulations highlight the importance of the coupled electrical and mechanical behavior of the resonator assembly and show that elastic modes can effectively amplify or dampen acoustic modes within the fluid chamber. Experimentally-validated modeling results guide development of an optimization strategy to further improve device performance. In addition, the standing acoustic field that is the focus of the harmonic response model is incorporated into a custom simulation of the acoustophoretic migration of microparticles. Particles achieve terminal distributions at pressure nodes in the quiescent fluid, exhibiting remarkable agreement with experimental observations. The migratory speed of microparticles in a simple rectangular fluid chamber geometry has been shown to be inversely proportional to the square of the particle radius. Here, this relationship is confirmed for particle migration in more complex acoustic microfluidic geometries.
Chapter 1

Introduction

Acoustic microfluidics is a sub-field of microfluidics focused on the application of ultrasonic waves to enhance the capabilities and overcome limitations of microfluidic devices. Finely-tuned acoustic waves can be used for fluid pumping and mixing, droplet generation or spraying, and can provide a non-contact method of manipulating small particles suspended in a fluid. Recent advances in microfabrication have led to significant growth in research and development of acoustic microfluidic devices, with applications in several high-impact areas including medicine, biotechnology, mass spectrometry, additive manufacturing, and energy [1]. This work is focused on modeling an ultrasonic droplet generator that utilizes a piezoelectric transducer to generate resonating ultrasonic waves to drive fluid ejection from an array of nozzles. The resonant acoustic field that drives fluid ejection also allows for the manipulation of microparticles. The strongly coupled physics of this novel device provide exciting opportunities for numerical analysis.

Ultrasonic waves provide a method of inducing forces in a fluid, manipulating its behavior and generating circulation or bulk flow. Furthermore, acoustic energy focused at the free surface of a fluid can result in the ejection of droplets or continuous jets, which has diverse applications including inkjet printing [2], fuel processing [3], battery material synthesis via spray pyrolysis [4], mass spectrometry [5], and medicine [6]. Piezoelectric transducers are commonly used microfluidic devices to generate high-frequency vibrational energy that is transmitted into the fluid. Several variations of successful droplet generators exist that rely on the flexural bending of a piezo to provide a pulse that pushes or squeezes fluid from one or more orifices [7]–[9], however the design of these devices inherently reduces their scalability and throughput while maintaining low power consumption [9]. A potential alternative to address these shortcomings is an acoustic atomizer. When sufficient acoustic energy is focused near a free surface of the fluid (i.e. liquid-air interface), either by surface acoustic waves (SAW) along a thin film of fluid or bulk acoustic waves (BAW) focused near the interface, intense oscillations in pressure and fluid particle acceleration perpendicular to the fluid surface overcome inertia and surface tension and can result in atomization, or fluid ejection in the form of droplets or jets with diameters on the order of micrometers (μm). For example, Tsai et al. [10], [11] reported high-throughput of 1-10 μm diameter droplet generation in the 1-3 MHz frequency range from a device that utilized resonant vibrational frequencies of a Fourier-horn structure to generate high-intensity Faraday waves that breakup into droplets at a high velocity.
Beyond atomization, ultrasonic waves can manipulate fluids in remarkable ways. Fluid mixing has been achieved by acoustic streaming [12], [13], a complicated phenomenon characterized by steady vortices induced along the boundary of a vibrating surface [14]. Acoustically-driven mixing is possible in non-conductive fluids where other established methods, which rely on electric fields, fall short [13]. Acoustic streaming has also been used to pump fluids for various applications including liquid chromatography and medical pumping devices [1]. Ultrasonic waves can also be tuned to achieve acoustic cavitation, the process of rapid bubble generation and collapse by pressure-associated phase change [15], which provides the basis for sonochemistry and sonoporation [16], [17]. While acoustic streaming and cavitation are outside the scope of this work, they are mentioned to provide a sense of the broadness of ultrasonic microfluidic capabilities. For a thorough review of ultrasonic manipulation of fluids, the reader is referred to ref. [1].

Standing, ultrasonic waves can also provide an effective method of isolating, filtering, or separating specific particles, a process called acoustophoresis. The presence of particles in a standing acoustic field causes acoustic waves to scatter, resulting in momentum transfer between the oscillating fluid and the particles. The force exerted on a small, incompressible particle due to scattering, termed the acoustic radiation force (ARF), was first studied in 1934 by L. V. King [18], and numerous investigators have since expanded on his work to include effects such as compressibility, heat transfer, viscosity, and inter-particle scattering [19]–[22]. The magnitude and direction of ARFs depend on the particle’s size and relative properties of the particle and fluid medium, driving particles to either the nodes (pressure amplitude minima) or anti-nodes (maxima) of the standing acoustic field. A remarkable application of acoustophoretic particle motion has been handling biological cells while maintaining their viability. For example, ultrasound waves have been used to separate red blood cells from plasma [23] as well as transport cells into microporous scaffolds for tissue engineering purposes [24]. Additionally, the resulting pattern of migrated particles allows for observation of an otherwise invisible pressure field, and the speed at which they become “focused” provides a means to measure of the amplitude of the pressure field [25], [26].

Ultimately, the goal of microfluidic devices is to convert input electrical power into acoustic energy within the fluid as efficiently as possible. Numerical simulations enable one to predict performance and improve design without the fabrication costs or time necessary for experimental investigation. Hahn et al. [27] reduced a generic layered resonator device for acoustophoresis to a 1-dimensional (1D) idealization and used a genetic algorithm to search a design space for the optimal geometric parameters that would result in a maximum ARF magnitude to focus microparticles. Other researchers have implemented a 2D finite element analysis (FEA) model and analyzed resonant modes of each entity of the device separately in order to predict design parameters that would produce efficient acoustic coupling and therefore optimal operation of the complete device [28]. Most recently, Garofalo et al. [29] presented an elegant approach for
identifying ideal operating conditions of acoustophoretic microfluidic devices by representing the harmonic fields with Hamiltonian and Lagrangian densities derived from the constitutive equations typically used to describe the fields. While each of these approaches proved effective for improving the design of acoustic microfluidic devices, they are limited to devices specifically for focusing particles to the centerline of a rectangular channel. Modeling efforts must continually be adapted according to the functionality of the device.

The goal of this thesis is to identify important parameters that influence operation of a novel, ultrasonic droplet generator so that a numerical model can be translated into a framework for performance optimization over a continuously varying parameter space. It has been observed that the characteristics of a generated spray are frequency-dependent [9]. To access operation of a specific reservoir at multiple spraying modes, a single transducer assembly must drive fluid atomization across a wide envelope of operating frequency. Further, in many applications (e.g. spraying of biological suspensions or corrosive liquids) the transducer must be isolated from the fluid sample necessitating implementation of a multi-layered resonator. Cell retention has also been experimentally observed during device operation with a biological suspension as the working fluid; the standing pressure field that drives fluid ejection might also trap microparticles [30], [31]. A secondary goal of this thesis is to establish a simplistic model to predict particle trajectories in a standing acoustic field such as the one generating droplet ejection, allowing this thesis to encompass both aspects of the device functionality.

This work was motivated by the ultrasonic atomizer shown in Fig. 1.1, which was designed, fabricated, and characterized by Meacham [9]. The device is driven by a multi-layered resonator consisting of a lead zirconate titanate PZT-8 piezoelectric transducer [32] and an aluminum coupling layer (A). The resonator is clamped to an injection-molded polycarbonate cartridge which encases a water-filled reservoir feeding a rectangular channel that runs between the aluminum layer and a silicon chip (C, D). A microarray of pyramidal nozzles has been chemically etched into the silicon chip (E, F). Actuation of the resonator generates elastic waves that are transmitted via the aluminum layer into the fluid as acoustic waves. At resonant frequencies of the fluid chamber, standing waves are pinned between the aluminum and silicon chip. Fluid ejection is ultimately driven by a high pressure gradient near the nozzle tips (B).
The processes of droplet formation and breakup have been studied extensively to understand the underlying physics and to harness these phenomena for various purposes. Friend and Yeo [1] have provided a thorough review of the theoretical and experimental analysis of acoustically-driven droplet ejection, including scaling laws that have been developed to relate the ejected droplet diameter to the fluid density, surface tension, and the acoustic frequency. It is well understood that periodic pressure fluctuations perturb the interface between two fluids of varying density. In the case of a water-air interface, these perturbations are characterized by capillary wave formation at the free surface of the fluid. When the perturbations are small, the fluid displaced outward by a capillary wave front returns to the free surface as the wave travels past. When the perturbations are sufficiently large, the wave fronts break away from the bulk of the fluid due to the action of surface tension, ejecting droplets. The strength of these perturbations is determined by the local acoustic pressure gradient; therefore, the occurrence of fluid ejection is determined by the gradient of the acoustic pressure amplitude at the free surface.

In the present case, the nozzle tip pressure gradients are directly influenced by the magnitude and spatial distribution of pressure throughout the fluid reservoir. Complicated fluid ejection effects can be ignored entirely by simulating the harmonic response of the device and assessing its performance by pressure gradient at the nozzle tips alone. Because the fluid chamber within the 3D device is inaccessible for observation, 2D visualization chips (Fig. 1.2) representing the device cross-section were fabricated to experimentally observe particle migration, ultimately revealing the mode shapes of the resonant acoustic fields.
Figure 1.2 Experimental characterization of the prototype ultrasonic droplet generator and a 2D representation of the 3D prototype geometry.

All harmonic simulations in this work utilize a modeling domain representative of the 2D visualization chip. Each simulation involves a harmonic response analysis that incorporates each component of the device, which is loaded by a sinusoidal voltage differential applied to the transducer. The harmonic elastic solution (displacement amplitude) and acoustic solution (pressure amplitude) are obtained simultaneously, utilizing a fluid-structure interaction (FSI) boundary condition to represent the load transfer and impedance mismatch between the fluid and the walls of the fluid chamber. The metric for evaluating fluid ejection is pressure amplitude at the nozzle tips, as the nozzles of the 2D chips are closed. Finally, the acoustic solution is used to compute the magnitude and direction of the ARF on a microparticle at any location in the fluid chamber. Therefore, the ARF-induced motion and trajectories of particles are simulated as a separate step following the harmonic analysis.

Throughout this thesis, the method of implementing the numerical model is described and the results are discussed. First, a thorough understanding of the physics underlying acoustic microfluidics is required for implementation of the model. Chapter 2 serves to provide both a general understanding of elastic waves and acoustic waves. The basic theory and general equations of elasticity, piezoelectricity, and acoustic wave propagation are introduced, followed by an analytical development of acoustic radiation force and how it affects particle motion. The idea of acoustic resonance is discussed with emphasis on rectangular geometries for which analytical expressions have been developed.

Chapter 3 covers the implementation and results of the harmonic response model, which was created using the commercial FEA software, ANSYS Mechanical APDL [33]. An overview of the finite element method (FEM) is provided, followed by discretization of the governing equations into their finite element representation. The modeling assumptions, boundary conditions, material handling and solution method
used in ANSYS are described in detail. The model is validated by experimental images, and modeling results are reported for 48 cases with varying geometric dimensions. The device performance is measured and trends discussed, as well as modeling difficulties and limitations.

In Chapter 4, flow effects are ignored to simulate ARF-induced particle motion in a quiescent fluid to observe particle trajectories over time and ensure the model is working as expected. The process of implementing the program in MATLAB is described, and the results obtained are presented and compared with experimental results as well as predictions by analytical equations. The apparent limitations of the particle trajectory simulations are discussed within the results.

The thesis concludes with a summary of the results in Chapter 5. The accuracy, efficiency, capabilities, and limitations of the numerical model are evaluated to determine where the model excels and where it needs improvement. Finally, future modeling work is suggested, including methods to further optimize the atomizer’s design parameters, new cases/geometries to which the model can be applied, and how to include the effect of fluid flow when simulating particle motion throughout the acoustic field.
Chapter 2

Background Theory

Acoustic microfluidics encompasses numerous disciplines, and a thorough understanding of the governing theory is necessary to develop a numerical model that accurately simulates and predicts the behavior of an ultrasonic microfluidic device. This first main purpose of this chapter is to provide a general introduction to the fundamental theories underlying the field—namely vibrations and acoustics. The governing physics then allow for a discussion of more advanced topics, e.g., how microparticles behave in a standing acoustic field.

2.1 Planar Resonators for Acoustic Microfluidic Devices

While the primary function of the droplet generator is to atomize liquids, its design resembles a planar resonator. As such, a brief discussion of planar resonator design characteristics provides context for the physical theory introduced herein.

Planar resonators that provide robust, resonant acoustic fields with pressure nodes oriented parallel to the direction of flow in microfluidic channels are ideal for separating or isolating particles suspended in the fluid. The symmetry of these devices allows the acoustic field to be represented using one-dimensional (1D) analytical expressions. From bottom to top, a typical device generally consists of a piezoelectric transducer, coupling layer, fluid channel or reservoir, and reflector layer as illustrated by the 2D cross-section in Fig. 2.1. The piezoelectric transducer provides vibrational energy to the system. The coupling layer thickness can be tailored to enhance the acoustic resonance within the fluid channel and may also serve as an isolation layer to protect the transducer from corrosive liquids [34]. The reflector layer serves to reflect acoustic waves back into the fluid to generate a resonant pressure field. The physical behavior of each layer is discussed in subsequent sections.
The behavior of planar resonant devices can be understood by considering each component separately, beginning with the transducer. A voltage difference applied to the transducer as a sinusoidal signal causes the transducer to vibrate at a fixed frequency corresponding to the input signal. These vibrations travel through the carrier layer, and its vibrating surface excites acoustic waves in the fluid reservoir. The initial acoustic waves are reflected back into the fluid by the reflector layer (often metal or glass), and interference between the excitation waves and reflected waves results in standing waves pinned between the carrier and reflector layer, as illustrated by the 1D schematic of a half-wavelength in Fig. 2.2. In fluid channels with a rectangular cross-section, resonance occurs at frequencies corresponding to an integer half-wavelength that coincides with the channel height. This is a useful design rule for acoustic microfluidic devices. Based on the equation shown in the figure below, a water-filled fluid channel with a height of 1 mm has resonant frequencies at integer multiples of ~750 kHz.

**Figure 2.1** 2D schematic of planar resonator layers.

**Figure 2.2** Schematic of a “pinned” acoustic wave.
2.1.1 Vibrations in Elastic Materials

Acoustic energy travels through solid continua in the form of elastic vibrational waves. As a propagating elastic wave passes through an infinitesimal volume of a solid material, the volume contracts and expands under compressive and tensile stresses. When considering acoustic behavior, the amplitudes of these deformations are quite small, and the relationship between stress and strain can be expressed by a linear expression known as Hooke’s law,

\[ T = c S \]  

(2.1)

where \( c \) is the stiffness matrix for an isotropic material. The elastic modulus \( E \) and Poisson’s ratio \( \nu \) are necessary to define the stiffness matrix, which commonly appears as its inverse, the compliance matrix:

\[
\begin{align*}
    s_E &= c^{-1} = \\
    &= \begin{bmatrix}
        \frac{1}{E} & -\frac{\nu}{E} & -\frac{\nu}{E} & 0 & 0 & 0 \\
        -\frac{\nu}{E} & \frac{1}{E} & -\frac{\nu}{E} & 0 & 0 & 0 \\
        -\frac{\nu}{E} & -\frac{\nu}{E} & \frac{1}{E} & 0 & 0 & 0 \\
        0 & 0 & 0 & \frac{(1+\nu)}{E} & 0 & 0 \\
        0 & 0 & 0 & 0 & \frac{(1+\nu)}{E} & 0 \\
        0 & 0 & 0 & 0 & 0 & \frac{(1+\nu)}{E}
    \end{bmatrix}
\end{align*}
\]  

(2.2)

2.1.2 Piezoelectric Theory

The stresses \( T \) and strains \( S \) within a piezoelectric material are closely coupled with an internal electric field \( E \), and the material can be deformed by applying an electric potential difference. As a result, piezoelectric materials are ideal for generating vibrations when driven by an AC signal. The constitutive equations governing the coupled behavior of a piezoelectric material can be expressed in the form,

\[
\begin{align*}
    S &= s_E T + d^\top E \\
    D &= d T + \varepsilon_T E
\end{align*}
\]  

(2.3a)\hspace{1cm}(2.3b)

where \( D \) is the current displacement, \( s_E \) is the piezoelectric compliance matrix under a constant electric field, \( d \) is the piezoelectric coupling matrix, and \( \varepsilon_T \) is the electric permittivity under uniform stress. A polarized piezoelectric material exhibits transverse isotropic properties, where the elastic moduli and Poisson’s ratios in the polarized direction \( (E_p, \nu_p) \) and the unpolarized plane \( (E, \nu) \) differ. In the literature on piezoelectric materials, the poling direction is commonly denoted by the z-axis [35], and the compliance matrix is made up of 6 unique entries:
The coupling matrix, which relates the material’s strain and electric field, is made up of 3 unique entries:

\[
S_E = \begin{bmatrix}
\frac{1}{E} & -\frac{\nu}{E} & -\frac{\nu_p}{E_p} & 0 & 0 & 0 \\
-\frac{\nu}{E} & \frac{1}{E} & -\frac{\nu_p}{E_p} & 0 & 0 & 0 \\
-\frac{\nu_p}{E_p} & -\frac{\nu_p}{E_p} & \frac{1}{E_p} & 0 & 0 & 0 \\
0 & 0 & 0 & (1+\nu_p) & 0 & 0 \\
0 & 0 & 0 & 0 & (1+\nu_p) & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{(1+\nu)}{E}
\end{bmatrix}
\]  

(2.4a)

The coupling matrix, which relates the material’s strain and electric field, is made up of 3 unique entries:

\[
d = \begin{bmatrix}
0 & 0 & d_{13} \\
0 & 0 & d_{13} \\
0 & 0 & d_{33} \\
0 & d_{42} & 0 \\
d_{42} & 0 & 0 \\
0 & 0 & 0
\end{bmatrix}
\]  

(2.4b)

Finally, the electric permittivity matrix, which relates the electric displacement and electric field, is made up of 2 unique entries:

\[
\varepsilon_T = \begin{bmatrix}
\varepsilon_{11} & 0 & 0 \\
0 & \varepsilon_{11} & 0 \\
0 & 0 & \varepsilon_{33}
\end{bmatrix}
\]  

(2.4c)

2.1.3 Acoustics

For small perturbations, the behavior of acoustic wave propagation through a barotropic fluid is governed by the wave equation, which is also known as the Helmholtz equation. Formulation of the wave equation requires the constitutive equations that describe the fluid’s behavior. The continuity equation, or conservation of mass, offers one mathematical description of the fluid by considering the amount of fluid in a given space. Consider a control surface (CS) bounding an arbitrary control volume (CV), fixed in space, with finite volume and surface area. The continuity equation for a compressible fluid can be expressed by equilibrating the rate of change of mass within the control volume and the net rate of mass flow through the control surface.

\[
\frac{\partial}{\partial t} \int_{CV} \rho \, dV = -\int_{CS} \rho \, \mathbf{v} \cdot \mathbf{n} \, dA
\]  

(2.5a)

In the expression above, \(\rho\) is the density of the fluid and \(\mathbf{v} \cdot \mathbf{n}\) is the component of fluid velocity, normal to the control surface, exiting the control volume. The conservation of mass for a compressible fluid can also be expressed in differential form:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{\rho \mathbf{v}} = 0
\]  

(2.5b)
The Navier-Stokes (NS) equations, representing the conservation of momentum, govern the interactions between momentum and stresses within a fluid. Together under the continuity equation and conservation of energy, the NS equations provide a complete mathematical description of a fluid flow [36]. Neglecting body forces (gravity), the nonlinear NS equation for a viscous fluid at a given temperature may be expressed as

$$\rho \left[ \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} \right] = -\nabla p + \frac{5}{3} \mu \nabla (\nabla \cdot \mathbf{v}) + \mu \nabla^2 \mathbf{v}, \quad (2.6)$$

where $\mu$ is the dynamic shear viscosity of the fluid and we have used a value of $\frac{1}{3}$ for the ratio of dynamic to bulk viscosity to account for dilatation losses [37]. The third basic equation governing acoustic wave propagation is the equation of state, which relates the fluid’s pressure and density. Although acoustic processes are nearly isentropic [38], acoustic wave propagation is characterized by tiny fluctuations in the fluid density due to changes in pressure. The adiabat for a non-ideal gas may be expressed using Taylor’s expansion:

$$p = p_0 + \left( \frac{\partial p}{\partial \rho} \right)_{\rho_0} (\rho - \rho_0) + \frac{1}{2} \left( \frac{\partial^2 p}{\partial \rho^2} \right)_{\rho_0} (\rho - \rho_0)^2 + \cdots, \quad (2.7)$$

where the terms with a subscript ‘0’ denote equilibrium values. It turns out that $\left( \frac{\partial p}{\partial \rho} \right)_{\rho_0}$ is equal to the square of the speed of sound. Equations (2.5b – 2.7) provide all the information necessary to describe acoustic wave propagation. However, the equations are nonlinear and must be linearized before they can be combined into a single equation. Traditionally, this is done by employing perturbation theory to expand density, pressure, and velocity to the 1st order.

$$\rho = \rho_0 + \rho_1 \quad (2.8a)$$
$$p = p_0 + p_1 = p_0 + c^2 \rho_1 \quad (2.8b)$$
$$\mathbf{v} = \mathbf{v}_1 \quad (2.8c)$$

The terms of order 0, denoted by the subscript ‘0’, represent equilibrium values. The 1st-order terms in Eqns. (2.8a – 2.8c) represent the small fluctuations from equilibrium values. Note that we have assumed zero bulk flow, i.e. $\mathbf{v}_0 = 0$. Linearization is achieved by substituting the expanded terms into Eqns. (2.5b – 2.7), collecting first-order terms and neglecting products of first-order terms. After some manipulation, the lossy wave equation is obtained, which is expressed as

$$\frac{1}{c^2} \frac{\partial^2 p_1}{\partial t^2} = \left( 1 + \tau_s \frac{\partial}{\partial t} \right) \nabla^2 p_1, \quad \text{where} \quad (2.9a)$$

$$\tau_s = \frac{(2 + \beta) \mu}{\rho_0 c^2}. \quad (2.9b)$$

Here, $c$ is the speed of sound in the propagation medium, $p_1$ is the first-order pressure, and $\tau_s$ is the relaxation time for viscous processes to approach equilibrium during expansion or compression [38].
Finally, the first-order density, pressure, and velocity are given harmonic time dependence with angular velocity denoted by $\omega$.

\begin{align*}
\rho_1 &= \rho_1(x, y, z)e^{-i\omega t} \quad (2.10a) \\
p_1 &= p_1(x, y, z)e^{-i\omega t} \quad (2.10b) \\
v_1 &= v_1(x, y, z)e^{-i\omega t} \quad (2.10c)
\end{align*}

Insertion of Eqns. (2.10a–2.10c) into (2.9a) and taking the proper derivatives produces a more recognizable form of the wave equation below.

\begin{align*}
\nabla^2 p_1 &= -k^2 p_1 \quad (2.11a) \\
k &= (1 + i\gamma)\frac{\omega}{c} \quad (2.11b) \\
\gamma &= \frac{(2+\beta)\mu\omega}{2\rho_0 c^2} \quad (2.11c)
\end{align*}

Here, $k$ is termed the damped wavenumber and $\gamma$ is the coefficient of attenuation. It turns out that Eqns. (2.9) and (2.11) are approximately accurate for small bulk velocities, e.g., $v_0 \leq 0.1 \text{ m/s}$ [39]. Additionally, the viscous loss coefficient is on the order of $\sim 10^{-6}$ for ultrasonic frequencies in fluids considered in this work, and the inviscid wave equation can approximate Eqn. (2.9a) over small length scales for which attenuation is negligible:

\begin{equation}
\nabla^2 p_1 = -\left(\frac{\omega}{c}\right)^2 p_1 \quad (2.12)
\end{equation}

Together, Equations (2.1), (2.3), and (2.12) govern the elastic and acoustic behavior in a microfluidic device resembling that shown in Fig. 2.1. These equations associated with the theory of elasticity, piezoelectricity, and acoustics can be found in introductory textbooks.

### 2.2 Acoustic Radiation Force on Microparticles

The interactions between a small particle and high frequency acoustic waves are complex and require more advanced treatment than that of the previous section. While the equation describing the forces experienced by a particle in a standing acoustic field is well established, some discussion of its derivation will provide insights that will become useful when these forces are considered in the numerical model discussed in Chapter 4.

#### 2.2.1 Primary Acoustic Radiation Force

A spherical, microscale particle suspended in an acoustic field acts as a weak point-scatterer of acoustic waves, and the resulting scattered waves induce a force on the particle termed the primary acoustic radiation force ($F_{\text{rad}}$). The acoustic radiation force exerted on incompressible particles was first analyzed by King in 1934 [18], and Yosioka & Kawasima [19] considered $F_{\text{rad}}$ on compressible particles in 1955. Gorkov [20]
made further contributions in 1962. More recently, Doinikov [22] and Karlsen & Bruus [40] developed expressions considering thermal and viscous processes within the fluid, although these effects are often ignored. Bruus [41] has provided a thorough, step-by-step derivation of the acoustic radiation force on a spherical, compressible, microscale particle suspended in an inviscid fluid. His approach provides the basis for the following discussion.

Acoustophoretic particle motion occurs on a larger time scale than the μs-scale of an ultrasound wave. The forces exerted on a particle are a time-averaged effect of the oscillating acoustic field, and as such, it is useful to quantify the oscillating field terms \( X(t) \) as time-averaged quantities \( \langle X \rangle \) by taking the integral over a full period.

\[
\langle X \rangle \equiv \frac{1}{\tau} \int_{0}^{\tau} X(t) dt
\]  

(2.13)

In deriving the wave equation in the previous section, perturbation theory was employed to approximate the fluctuations of the field terms in Eqns. (2.8a – 2.8c). The first-order expansion of the NS equations was sufficient for deriving the wave equation. However, the primary acoustic radiation force requires a more accurate description, which is achieved by expanding the fields to the second-order:

\[
p = p_0 + p_1 + p_2
\]  

(2.14a)

\[
\rho = \rho_0 + \rho_1 + \rho_2
\]  

(2.14b)

\[
\nu = \nu_1 + \nu_2
\]  

(2.14c)

Inserting Eqns. (2.14a) – (2.14c) into the Eqn. (2.6) and collecting all terms of the second-order leads to the second-order expansion of the NS equations:

\[
\rho_0 \frac{\partial \nu_2}{\partial t} = -\nabla p_2 - \rho_0 (\nu_1 \cdot \nabla) \nu_1 + \eta \nabla^2 \nu_2 + \beta \eta \nabla (\nabla \cdot \nu_2) - \rho_1 \frac{\partial \nu_1}{\partial t}
\]  

(2.15)

The second-order velocity (\( \nu_2 \)) in Eqn. (2.15) represents acoustic streaming due to the fluid’s absorption of momentum from the acoustic wave. The second-order pressure (\( p_2 \)) represents the acoustic wave scattering due to the presence of the particle, which leads to \( \mathbf{F}_{rad} \). In Chapter 4, there is a discussion regarding the circumstances under which \( \mathbf{F}_{rad} \) dominates over streaming effects. For the purpose of this derivation, it is assumed that \( \nu_2 \) can be neglected. Taking the time-average of terms in Eqn. (2.15), neglecting viscosity, and manipulating terms, the second-order NS equations yield an expression for the second-order pressure:

\[
\langle p_2 \rangle = \frac{1}{2} \kappa_0 \langle p_1^2 \rangle - \frac{1}{2} \rho_0 \langle \nu_1^2 \rangle
\]  

(2.16)

where \( \kappa_0 = 1/\rho_0 c^2 \) is the compressibility of the fluid. Equation (2.16) is important because it expresses the second-order pressure, the driver of \( \mathbf{F}_{rad} \), as a function of the first-order pressure and velocity, which are much easier to solve for numerically.
Assuming there are no other particles in the vicinity, the acoustic radiation force exerted on a particle whose radius \((a)\) is much smaller than the wavelength of the standing acoustic field it resides within is obtained by computing the surface integral of the sum of the time-averaged, second-order pressure and the momentum flux tensor at a surface \(dS\) encompassing the particle.

\[
F_{rad} = -\int_{dS} \left\{ \frac{1}{2} \kappa_0 \langle p_1^2 \rangle - \frac{1}{2} \rho_0 \langle \mathbf{v}_1^2 \rangle \right\} \mathbf{n} + \rho_0 \langle \mathbf{n} \cdot \mathbf{v}_1 \rangle \right\} \, dr
\]  

(2.17)

In Eqn. (2.17), \(\mathbf{n}\) is a unit normal vector pointing outward from the surface \(dS\).

The interactions between the particle and the acoustic field are treated by scattering theory, and the acoustic field is represented by a superposition of the incoming acoustic waves and the scattered waves. Here, the definition of the velocity potential \((\phi)\) becomes useful,

\[
\mathbf{v}_1 = \nabla \phi_1 = \nabla \phi_{in} + \nabla \phi_{sc}
\]

(2.18)

where in Eqn. (2.18), the subscripts \(\text{in}\) and \(\text{sc}\) correspond to the incoming and scattered terms. We have assumed there are no other particles in the vicinity, so the only scattered acoustic waves are a result of the particle being studied. If we neglect body forces on the particle, such as gravity, the integral in Eqn. (2.17) will be the same regardless of the radius of a surface encompassing the particle. At a large integration radius as compared with the acoustic wavelength, the scattered waves can be approximated by a time-retarded multipole expansion where the monopole and dipole terms dominate [41] and have the form of Eqn. (2.19).

\[
\phi_{sc}(\mathbf{r}, t) = \phi_{mp} + \phi_{dp} = -f_1 \left[ \frac{a^3}{3 \rho_0} \frac{\partial \phi_{in}(t-r/c_0)}{\partial t} \right] - f_2 \left[ \frac{a^3}{2} \nabla \cdot \left\{ \frac{\mathbf{v}_{in}(t-r/c_0)}{r} \right\} \right] 
\]

(2.19)

Here, \(f_1\) and \(f_2\) are called the monopole and dipole coefficients, respectively.

The expression in Eqn. (2.19) for the multipole expansion of the scattered acoustic waves proves to be useful in the manipulation of Eqn. (2.17), which is outside the scope of this work but can be found in ref. [41]. The resulting expression for \(F_{rad}\) in terms of the first-order pressure and velocity is:

\[
F_{rad} = -\frac{4 \pi}{3} a^3 \nabla \left[ \frac{1}{2} Re[f_1 \kappa_0 (p_1^2) - \frac{3}{4} Re[f_2 \rho_0 \langle \mathbf{v}_1^2 \rangle] \right] 
\]

(2.20)

In the presence of a particle, the monopole scattering potential arises from scattered fluid mass. The monopole coefficient \(f_1\) is found by relating the rate of scattered mass to the rate of change in density from the incoming wave. The dipole scattering potential arises from the particle’s translational motion, and \(f_2\) is computed by balancing two expressions: one relating the particle velocity to the incoming and dipole potentials, and the second using Newton’s 2nd law to relate the particle velocity with the incoming and dipole pressure acting on the particle surface.

\[
f_1 = 1 - \frac{\kappa_p}{\kappa_0} \]

(2.21a)

\[
f_2 = \frac{2(\rho_p - \rho_0)}{2 \rho_p - \rho_0} \]

(2.21b)
In Eqns. (2.21a) and (2.21b), the equilibrium material properties $\rho_0$ and $\kappa_0$ are the fluid density and compressibility, and $\rho_p$ and $\kappa_p$ are the particle density and compressibility. Examining Eqns. (2.20), (2.21a) and (2.21b), the acoustic radiation force on a small, spherical particle in an inviscid fluid has been conveniently expressed as a function of the particle volume, the relative density and compressibility of the particle and surrounding fluid, and the first-order acoustic pressure and velocity field. For a detailed derivation of $\mathbf{F}_{\text{rad}}$, the reader can refer to refs. [18]–[20], [22], [40], [41].

2.2.2 Acoustophoretic Particle Manipulation

The ARF-induced acceleration of a particle is resisted by drag forces due to fluid flowing over its surface. The Stokes’ drag on a spherical object with radius $a$ is a well-known expression,

$$ F_{\text{drag}} = 6\pi \mu a v $$

(2.22)

where $v$ is the ambient velocity of the fluid. Considering a particle moving with a velocity $v_p$ relative to a static observer, we can substitute $v$ in Eqn. (2.22) with the quantity $(v_f - v_p)$, the particle velocity relative to the fluid. Newton’s 2nd law governs the motion of bodies subjected to external forces, and the particle motion can be determined by the expression,

$$ m_p \frac{dv_p}{dt} = F_{\text{rad}} + F_{\text{drag}} $$

(2.23)

where $m_p$ is the particle mass, and gravity and buoyancy are negligible. The time scale of a microparticle’s inertial acceleration is negligible compared to the time scale of its acoustophoretic motion, and it is accurate to consider the acceleration as instantaneous for numerical simulation purposes [42]. After inserting Eqn. (2.22) into (2.23) and neglecting the particle inertia, we obtain the particle velocity.

$$ v_p = \frac{F_{\text{rad}}}{6\pi \mu a} - v_f $$

(2.24)

Equations (2.20), (2.21), and (2.24) govern the acoustophoretic motion of spherical particles and provide the basis for the particle-tracking aspect of our proposed numerical model. Particles of varying size, density, and compressibility will behave differently within a given acoustic field. Larger particles will move with higher velocities than smaller particles, as $F_{\text{rad}} \propto a^3$ and $F_{\text{drag}} \propto a$. The direction of $F_{\text{rad}}$ exerted on a particle is parallel to the local pressure gradient and is determined by the acoustic contrast factor ($\Phi_{ac}$), which may be expressed as the following [26], [41], [43]:

$$ \Phi_{ac} = \frac{1}{3} f_1 + \frac{1}{2} f_2 $$

(2.25)

When $\Phi_{ac} < 0$, the particle moves in the direction of increasing pressure amplitude, i.e., toward the antinode where the time-averaged pressure amplitude is a maximum. When $\Phi_{ac} > 0$, the particle moves in the opposite direction, i.e., towards the pressure node where $P_1 = 0$. Recalling the definition of $f_1$ and $f_2$
in Eqns. (2.21a – 2.21b), it is notable that the direction of the ARF is independent of the standing acoustic field properties.

2.2.3 Acoustic Streaming

The time averaged 2\textsuperscript{nd}-order velocity \( \langle \nu_2 \rangle \) corresponds to a secondary acoustic radiation force termed acoustic streaming, steady bulk fluid motion driven by absorbed acoustic energy along the fluid boundary walls [39], [44]. Streaming results from the inability of a fluid to sustain shear stresses. When vibrational shear waves propagating through a solid layer reach a fluid layer, the energy is absorbed by the fluid at the interface [38]. The no-slip condition of a viscous fluid at a vibrating wall results in rotational motion of the fluid within a thin layer at the wall, termed the Stokes’ layer or viscous boundary layer. These vortices transfer momentum to adjacent fluid outside the Stokes’ layer via viscous processes. Sufficient momentum transfer results in slow, steady motion (streaming) within the bulk fluid. The width of the Stokes’ layer is given by,

\[
\delta = \sqrt{\frac{2\nu}{\omega}} \tag{2.26}
\]

where \( \nu \) is the kinematic viscosity of the fluid, given by \( \nu = \mu / \rho \). A general equation to determine the streaming velocity field has not been developed due to the complexity of the 2\textsuperscript{nd}-order continuity and NS equations (which must be simultaneously satisfied by \( \langle \nu_2 \rangle \)), but the reader is encouraged to see Ref. [44] for a more in-depth discussion of the topic.
Chapter 3

Harmonic Response Model

This chapter encompasses the investigation of the harmonic response of a 2D microfluidic chip and actuator assembly representing the cross-section of the droplet generator device. The key acoustic, electronic, and vibrational indicators that signify ideal conditions for fluid ejection are identified using numerical simulations. By characterizing the effects of geometric design parameters on device performance, this study lays the groundwork for setting up an optimization routine to enhance droplet generator design for efficient ejection.

3.1 Modeling Domain

While the 3D acoustic field in the actual atomizer device cannot be wholly represented by a 2D model, the behavior of acoustic wave focusing in a planar domain representing the fluid chamber cross-section is representative of that in the 3D chamber, as verified by 3D modeling of an infinite array of nozzles [9]. The 2D visualization chip shown in Fig. 3.1 serves as the basis for all simulations discussed herein. The fluid reservoir, triangular horns, and curved inlet arms were etched in a silicon substrate to a depth of 200 µm. A glass layer was bonded to the silicon chip to seal the fluid reservoir and enable observation of the fluid chamber during operation. The circular inlet/outlets were etched through to allow filling and emptying of the chamber. The curved inlet arms were designed to minimize reflected, lateral acoustic waves (across the length of the channel) to best preserve the longitudinal resonant modes expected in the 3D device. The resonator assembly shown at the top of Fig. 3.1 consists of a lead zirconate titanate PZT-8 piezoelectric transducer and aluminum coupling layer, which are clamped to the base of the silicon chip during operation. The thin layer of silicon between the aluminum and fluid chamber is not characteristic of the 3D device, but it is necessary in the visualization chip to prevent leakage and should be considered as part of the resonator assembly. For a complete description of the chip’s fabrication methods, the reader is referred to [30].
The nozzle tips terminate in the silicon chip, precluding fluid ejection and rendering the nozzles effectively “closed” in the visualization chip. As a result, there is no bulk fluid flow within the chamber during operation. Near resonant frequencies, acoustic wave crests are “pinned” at the nozzle tips, resulting in high pressure amplitudes rather than pressure gradients. Hence, the average pressure amplitude across the nozzle tips is the main indicator of ejection for a given resonator mode. The height-to-depth ratio of the fluid chamber, where height is measured from base to nozzle tip and depth measured between the silicon substrate and glass cover, is around 5:1 for a 1.0 mm chamber height. In the frequency range of interest (0.5 – 2.5 MHz), the standing acoustic field generated within the fluid chamber varies minimally across the depth of the channel, and the acoustic phenomena can be well-represented with a 2D model, neglecting the glass cover and silicon substrate beneath the fluid. Taking advantage of horizontal symmetry, the chip is modeled using the planar domain illustrated in Fig. 3.2, labeled with the dimensions of each component. The geometric design variables being considered are the thicknesses of the piezoelectric transducer ($t_{pZT}$), aluminum coupling layer ($t_{Al}$), and silicon isolation layer ($t_{Si}$), as well as the height of the fluid chamber ($h_{c}$). The fluid chamber height is measured from the silicon isolation layer to the base of a nozzle; this distance does not include the 0.5 mm height of the pyramidal nozzles. The nozzle width is fixed at 40 µm for all simulations. The in-plane dimensions of the silicon chip itself remain fixed for all simulations, however the location of the fluid chamber within the substrate is shifted vertically to enable varying of $t_{Si}$. 

**Figure 3.1** 2D visualization chip (scale bar is 5 mm).
It should be noted that the acoustic field predicted by the closed-nozzle model of the 2D visualization chip is not expected to identically represent the acoustic field within the 3D device. Rather, these simulations are focused on observing trends that are indicative of the 3D device with respect to resonant behavior and ejection performance as functions of the design parameters mentioned above.

### 3.2 Numerical Methods

Most practical engineering problems are far too complicated for an exact solution to exist or be derived using analytical methods. A common approach to solving these problems is the finite element method (FEM), a powerful mathematical tool that can be used to approximate solutions to partial differential equations that cannot be solved directly. The mathematics underlying the finite element method (FEM) were first formulated in the 1950s and 1960s [45], [46], with significant theoretical development in the 1970s and early 1980s [47], [48]. The technology was quickly commercialized in the form of MSC Nastran [49]. Today, there are many finite element analysis (FEA) software packages available for a variety of engineering problems including those involving static elasticity, fluid dynamics, heat transfer, transient and harmonic motion, among others. The term finite element analysis (FEA) refers to application of the FEM to analyze a specific problem.
In general, the finite element involves discretizing, or dividing, a solution domain into a mesh, or grid, of finite elements by using a weighted residual method to define a set of basis functions specifically designed to be nonzero at individual elements or their boundaries and zero elsewhere [50]–[52]. The basis functions can be generated by polynomials defined on simple element shapes (generally rectangles or triangles in 2D, and hexahedrons, pentahedrons, or tetrahedrons in 3D) that satisfy solution continuity requirements across element boundaries. Elements of the solution domain are then mapped onto “real” elements by mapping functions so that the resulting mesh accurately represents the true physical domain of the problem being analyzed. Once the constitutive equations that govern the physical system have been discretized, the mapped basis functions are arranged in a large system of equations that can be solved to approximate the behavior throughout a body or system under specific loading conditions and constraints. FEA is used extensively for structural analysis in the civil, aerospace, and automotive industries as well as for academic research such as the harmonic response modeling described in this work.

The elastic and acoustic response of the ultrasonic atomizer are simulated using ANSYS Mechanical APDL, a commercial finite element analysis (FEA) code that offers numerous types of structural analyses including static (linear elasticity and geometric or material nonlinear analyses), transient, mode-frequency, harmonic, and several others [33]. An acoustic analysis package is also available in ANSYS with a capability to couple structural dynamics and acoustics for problems involving fluid-structure interactions. The program can be controlled entirely through ANSYS Parametric Design Language (APDL), and complicated models can be generated, modified, solved, and post-processed with the use of APDL scripts.

The ultrasonic atomizer consists of four materials: aluminum, silicon, water, and a piezoelectric ceramic. ANSYS contains an element library of over 200 element types, each with unique properties and modeling capabilities [53]. Three 2D element types were used in all harmonic response simulations, and their shape functions, governing equations, and other characteristics are discussed in the following sections.

### 3.2.1 Modeling the Linear Elastic Solids

In solid mechanics, the principle of virtual work provides a technique for discretizing deformable, elastic bodies using finite elements based on the equations of equilibrium, the strain-displacement relations, and the constitutive stress-strain relations [50]. The principle of virtual work mathematically states that the work done by internal stresses due to a small perturbation (virtual displacement) must be equal to the virtual work done by external loads imposing the perturbation. Application of the FEM and the principle of virtual work, when considering the structural dynamics of a solid continuum body or system of bodies, leads to the discretized equation of motion:

$$\begin{align*}
\begin{bmatrix} M_s \end{bmatrix} \{ \ddot{u}_s \} + \begin{bmatrix} C_s \end{bmatrix} \{ \dot{u}_s \} + \begin{bmatrix} K_s \end{bmatrix} \{ u_s \} &= \{ F_s \}
\end{align*}$$

(3.1)
where \([M_s]\), \([C_s]\), and \([K_s]\) are the structural mass, damping, and stiffness matrices, which are based on the geometry, material properties, and finite element shape functions; \({\ddot{u}}_s\), \({\dot{u}}_s\), and \({u}_s\) are the generalized, nodal acceleration, velocity, and displacement vectors; and \({F}_s\) is the applied structural load vector. The quantity of interest, i.e., the solution to Eqn. (3.1), is the vector of nodal displacements that minimize the potential energy of the system.

In ANSYS, Eqn. (3.1) is used to model the harmonic response of the aluminum and silicon materials in the 2D chip, where the displacement and strain are related by Hooke’s law for isotropic, linear elastic materials (recall Eqn. 2.1). These materials are modeled under plane stress assumptions with the PLANE183 element type: a 2D, 8-node quadrilateral with displacement degrees-of-freedom (DOF). Vibrations are assumed to be steady-state; all loads and displacements oscillate sinusoidally at the same frequency (but not necessarily in phase). Deformations remain elastic, and the relative stiffness, damping, and mass effects are constant. Friction and thermal effects are neglected. The relevant material properties of aluminum and silicon are given in Table 3.1.

<table>
<thead>
<tr>
<th>Property</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density, water</td>
<td>(\rho_w)</td>
<td>1000 kg/m(^3)</td>
</tr>
<tr>
<td>Dynamic viscosity, water</td>
<td>(\mu_w)</td>
<td>0.001 kg/m-s</td>
</tr>
<tr>
<td>Speed of sound, water</td>
<td>(c_w)</td>
<td>1500 m/s</td>
</tr>
<tr>
<td>Elastic modulus, aluminum</td>
<td>(E_{Al})</td>
<td>70 GPa</td>
</tr>
<tr>
<td>Poisson's ratio, aluminum</td>
<td>(\nu_{Al})</td>
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</tr>
<tr>
<td>Density, aluminum</td>
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</tr>
<tr>
<td>Elastic modulus, silicon</td>
<td>(E_{Si})</td>
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</tr>
<tr>
<td>Poisson's ratio, silicon</td>
<td>(\nu_{Si})</td>
<td>0.21</td>
</tr>
<tr>
<td>Density, silicon</td>
<td>(\rho_{Si})</td>
<td>2330 kg/m(^3)</td>
</tr>
<tr>
<td>Structural damping coefficient</td>
<td>(\gamma_{Al}), (\gamma_{Si})</td>
<td>(6x10^{-9})</td>
</tr>
</tbody>
</table>

### 3.2.2 Modeling the Piezoelectric Transducer

The stress, strain, and electric field of the piezoelectric material are governed by the coupled field equations (recall Eqns. 2.3a and 2.3b). In ANSYS, these equations have the form,

\[
\begin{bmatrix}
\{S\} \\
\{D\}
\end{bmatrix} =
\begin{bmatrix}
[s_E] & [d] \\
[d]^T & [\epsilon_T]
\end{bmatrix}
\begin{bmatrix}
\{T\} \\
\{E\}
\end{bmatrix}
\]  (3.2)
where the piezoelectric coupling matrix \([d]\) used in ANSYS is the transpose of the form in which it was presented in Chapter 2 (both forms are used in the literature). The discretized form of Eqn. (3.2) used in ANSYS to simultaneously solve for displacement \([u]\) and voltage \([V]\) is expressed as,

\[
\begin{bmatrix}
[M] & [0] \\
[0] & [0]
\end{bmatrix}\{\ddot{u}\} + \begin{bmatrix}
[L] & [0] \\
[0] & [-C^{rh}]^T
\end{bmatrix}\{\ddot{V}\} + \begin{bmatrix}
[K] & [K^Z] \\
[K^Z]^T & -[K^d]
\end{bmatrix}\{u\} = \{F\}
\]

(3.3)

where \([-C^{rh}\)] is the element dielectric damping matrix, \([K^Z]\) is the piezoelectric coupling matrix, \([K^d]\) is the dielectric permittivity coefficient matrix, and \([F]\) and \([L]\) are applied structural and electrical (charge) load vectors. The finite element matrices are formulated internally in ANSYS [54].

The 2D ANSYS model is drawn in the x-y plane, with the piezoelectric polarized parallel to the y-axis. This requires a rotation of the transversely isotropic compliance matrix from Ch. 2. Furthermore, the Cartesian directional components of a tensor are re-ordered in ANSYS in a manner that differs from the IEEE standards (ANSI/IEEE Standard 176-1987). The 4th, 5th, and 6th rows and/or columns of a 6-by-6 tensor in ANSYS correspond to the xy, yz, and xz components, respectively. As a result, the compliance matrix is converted to the form of Eqn. (3.4).

\[
s_E = \begin{bmatrix}
1/E & -v_p/E_p & -v/E & 0 & 0 & 0 \\
-v_p/E_p & 1/E & -v_p/E_p & 0 & 0 & 0 \\
-v/E & -v_p/E_p & 1/E & 0 & 0 & 0 \\
0 & 0 & 0 & 2(1 + v_p)/E_p & 0 & 0 \\
0 & 0 & 0 & 0 & 2(1 + v_p)/E_p & 0 \\
0 & 0 & 0 & 0 & 0 & 2(1 + v)/E
\end{bmatrix}
\]

(3.4)

Note the three, lower-right diagonal entries of the compliance matrix were multiplied by a factor of 2 to remain consistent with ANSYS [54]. Similarly, the transposed piezoelectric strain matrix is re-ordered as shown in Eqn. (3.5).

\[
d = \begin{bmatrix}
0 & 0 & 0 & d_{42} & 0 & 0 \\
d_{13} & d_{33} & d_{13} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & d_{42} & 0
\end{bmatrix}
\]

(3.5)

The lead zirconate titanate (PZT-8) material of the piezoelectric ceramic is modeled using the PLANE223 element: a 2D, 8-node coupled-field quadrilateral, with voltage and displacement DOF. An electric potential difference can be simulated by applying voltage boundary conditions to the nodes along the top and bottom edges of the transducer, where the voltage difference between the top and bottom represents the peak-to-peak voltage \((V_{pp})\) of the signal applied to the transducer. The coupled field Eqn. (3.3) is solved in ANSYS for the nodal displacement and voltage throughout the piezoelectric material elements. The
displacement current per unit depth ($i_{disp}$) can be extracted from the finite element solution at each node along the transducer’s top edge to compute its electrical input impedance,

$$Z = \frac{V_{pp}}{j\omega (i_{disp})d}$$  

(3.6)

where $j = \sqrt{-1}$, $\omega$ is the angular frequency of vibration, and $d$ is the depth of the 3D transducer represented by the 2D model in ANSYS.

Nominal PZT-8 material properties were provided by the vendor, APC International, Ltd. [32]. These parameters have tolerances as large as ±20% [55]. To accurately represent the piezoelectric element, it was modeled in ANSYS in free vibration (isolated from the 2D chip) to compare its natural impedance response with that measured experimentally. For reference, the electrical response of three bare transducers of the same material were obtained experimentally by applying a sinusoidal electrical signal at constant $V_{pp}$ swept over a wide frequency range (0.5 – 2.5 MHz) and measuring the impedance. The cross section of each transducer was modeled in ANSYS with voltage amplitudes of $V_{pp} = 0$ and $V_{pp} = 10$ V applied to the top and bottom surface nodes, respectively, over the experimental frequency range in increments of 5 kHz. The input material properties were modified such that the modeled impedance response most accurately reflected the measured response. The optimal material properties are reported below in Table 3.2. All values were within ±1.5% of the vendor’s material properties with the exception of $d_{33}$ (10.9% difference) and $d_{13}$ (22.7% difference).

**Table 3.2 Properties of Lead Zirconate Titanate (PZT-8) Material**

<table>
<thead>
<tr>
<th>Property</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td>$\rho$</td>
<td>7600 kg/m$^3$</td>
</tr>
<tr>
<td>Elastic modulus in unpolarized direction</td>
<td>$E$</td>
<td>79.403 GPa</td>
</tr>
<tr>
<td>Elastic modulus in polarized direction</td>
<td>$E_p$</td>
<td>54.697 GPa</td>
</tr>
<tr>
<td>Poisson’s ratio (unpolarized/unpolarized)</td>
<td>$\nu$</td>
<td>0.2932</td>
</tr>
<tr>
<td>Poisson’s ratio (polarized/unpolarized)</td>
<td>$\nu_p$</td>
<td>0.3615</td>
</tr>
<tr>
<td>Coupling matrix entries</td>
<td>$d_{13}$</td>
<td>$-1.400 \times 10^{-10}$ m/V</td>
</tr>
<tr>
<td></td>
<td>$d_{33}$</td>
<td>$3.050 \times 10^{-10}$ m/V</td>
</tr>
<tr>
<td></td>
<td>$d_{42}$</td>
<td>$3.999 \times 10^{-10}$ m/V</td>
</tr>
<tr>
<td>Permittivity matrix entries</td>
<td>$\varepsilon_{11}$</td>
<td>735</td>
</tr>
<tr>
<td></td>
<td>$\varepsilon_{33}$</td>
<td>510</td>
</tr>
<tr>
<td>Structural damping coefficient</td>
<td>$\gamma$</td>
<td>$2 \times 10^9$</td>
</tr>
</tbody>
</table>

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Figure 3.3 Electrical impedance of the bare piezoelectric transducer over the frequency band of interest; Numerical model (M) vs experiment (E).

Figure 3.3 shows the comparison between the experimental measurements and the modeling results obtained using the tabulated material properties. In general, the model predicts the overall behavior of the piezoelectric element quite well, with the resonance (minimum impedance) and anti-resonance (maximum impedance) pair falling nearly on top of the measured response for both the 1.5 mm and 2.5 mm transducers. While the peaks are translated slightly (by ~50 kHz) for the 2.0 mm transducer, the width of the gap between the resonance and anti-resonance is well represented. The secondary resonances in the experimental impedance response, indicated by sharp peaks/troughs, were not observed in the ANSYS model. This could be attributed to the damping coefficient being too large, however the effect on the overall microfluidic chip is expected to be negligible, and the parameters in Table 3.2 were used for all subsequent simulations.

3.2.3 Modeling the Fluid

The behavior of the fluid domain is governed by the acoustic wave equation. The finite element representation of Eqn. (2.12) is formulated in ANSYS using the Ritz-Galerkin weighted residual method [56]. The complete derivation can be found in [54], and in the absence of mass source terms, the resulting expression is,

\[
[M_f] \dddot{p} + [C_f] \ddot{p} + [K_f] p + \rho_0 [R]^T \dddot{u}_f = 0 \tag{3.7}
\]

where \( \dddot{p} \) and \( \ddot{p} \) are the 1st and 2nd time derivatives of the pressure \( p \), respectively; \( \rho_0 \) is the fluid’s equilibrium density; \( \dddot{u}_f \) is the acceleration of the fluid; \([M_f]\), \([C_f]\), and \([K_f]\) are the fluid mass, damping, and stiffness matrices, and \([R]\) is called the acoustic fluid boundary matrix. The matrices are represented by the following integral expressions.

\[
[M_f] = \rho_0 \iiint_{\Omega_f} \frac{1}{\rho_0 c^2} \{N_p^f\} \{N_p^f\}^T dV \tag{3.8a}
\]
\[ [C_f] = \rho_0 \iiint_{\Omega_f} \frac{4\mu}{3\rho_0 c^2} [\nabla N_p^f]^T [\nabla N_p^f] \, dV \]  
(3.8b)

\[ [K_f] = \rho_0 \iiint_{\Omega_f} \frac{1}{\rho_0} [\nabla N_f^f]^T [\nabla N_f^f] \, dV \]  
(3.8c)

\[ [R]^T = \oint_{\Gamma_f} \{N_p^f\} \{N_u^f\}^T \hat{n} \, dS \]  
(3.8d)

In Eqns. (3.8a) – (3.8d), \(dV\) is a differential volume element of the acoustic fluid domain \((\Omega_f)\), \(dS\) is a differential surface element of the acoustic fluid boundary \((\Gamma_f)\), \(\hat{n}\) is a unit normal vector pointing outward from the boundary, and \(\{N_p^f\}\) and \(\{N_u^f\}\) are the fluid element shape functions for pressure and displacement.

In an acoustic analysis in ANSYS, it is assumed there is no bulk flow (recall from Ch. 2 the assumption that \(v_0 = 0\)).

The fluid medium (water) is represented in ANSYS by the FLUID29 element type, which has displacement and pressure DOF in the bulk fluid. The fluid elements along the fluid-structure boundary have pressure DOF only. The density, viscosity, and speed of sound of water at room temperature, listed in Table 3.1, are assigned to the FLUID29 elements. In this analysis, ANSYS solves the inviscid wave equation in which viscous dissipation, or attenuation, is neglected. There is no bulk motion in the fluid, which is assumed to be compressible and irrotational. It is also assumed there are no body forces and pressure disturbances are small. Thermal effects are neglected; hence temperature-dependent material properties remain constant throughout the fluid.

### 3.2.4 Boundary Conditions

In simulating the complete resonator-chip combination, the boundary conditions shown in Fig. 3.4 are applied. An electrical signal to the piezoelectric transducer provides the input load to the system, indicated by green and yellow arrows at the nodes along the top and bottom of the piezoelectric (A). The amplitude of the signal is specified by voltage boundary conditions applied to the piezoelectric transducer using the same method as described for the bare transducer. The signal frequency is also specified, and this value governs the frequency of all oscillating fields in this harmonic analysis. The electric potential difference generates elastic displacements according to the coupled piezoelectric equations, and these vibrations propagate through the domain.

Symmetry boundary condition are applied to all nodes along the left edge of the domain, indicated by red arrows in Fig. 3.4 (B). This inhibits the displacement degrees-of-freedom normal to the edge, effectively simulating a full chip. Furthermore, this prevents rigid body translation in the x-direction as well as rotation. While rigid body motion in the y-direction is not explicitly restricted by any boundary conditions, rigid
body motion is disallowed by ANSYS automatically. The top and right edges of the 2D chip are allowed to vibrate freely.

A perfect couple is assumed between the piezoelectric, aluminum, and silicon materials. In reality, some vibrational energy is lost due to gaps between the materials in contact, however this cannot be predicted or simulated with a great deal of accuracy. These losses are expected to be small in reality and are neglected from the simulations.

To most accurately simulate the impedance mismatch between water and silicon, the model implements a two-way, fluid-structure interaction (FSI) condition along the acoustic fluid boundary by prescribing the following coupling conditions along the fluid-structure boundary (C). By doing so, the elastic waves in the silicon are transmitted into the fluid as acoustic waves. Furthermore, the damping effect of the acoustic waves interacting with the vibrating walls, is captured. This enables a more accurate representation of the impedance response of the transducer.

\[
\bar{\sigma}(u_s) \hat{n} + p_f \hat{n} = 0 \quad (3.9a)
\]

\[
u_s \cdot \hat{n} - u_f \cdot \hat{n} = 0 \quad (3.9b)
\]

The two-way FSI conditions are defined mathematically by Eqns. (3.9a) and (3.9b), where \(\bar{\sigma}\) is the solid material stress tensor, a function of the local displacement \((u_s)\). Equation (3.9a) satisfies force equilibrium at the fluid boundary by equilibrating the fluid pressure at the boundary with the normal stress at the wall along \(\Gamma_{FS}\), allowing the fluid and structure to impose forces and/or momentum on one another. The fluid pressure at a particular location along the boundary oscillates between a positive and negative amplitude, which corresponds to a normal stress in the solid wall (at the same location) that fluctuates between a compressive and tensile amplitude, respectively. Similarly, Eqn. (3.9b) satisfies continuity along \(\Gamma_{FS}\) by equilibrating normal displacements between the fluid and solid, which additionally equilibrates velocity and acceleration. The FSI conditions allow the harmonic model to consider the structural and acoustic FE equations simultaneously. The coupled equations may be expressed in the following form:

\[
\begin{bmatrix}
[M_s] & 0 \\
\rho_0[R]^T & [M_f]
\end{bmatrix}
\begin{bmatrix}
\{\ddot{u}\} \\
\{\ddot{p}\}
\end{bmatrix}
+ \begin{bmatrix}
[C_s] & 0 \\
0 & [C_f]
\end{bmatrix}
\begin{bmatrix}
\{\dot{u}\} \\
\{\dot{p}\}
\end{bmatrix}
+ \begin{bmatrix}
[K_s] & -[R] \\
0 & [K_f]
\end{bmatrix}
\begin{bmatrix}
\{u\} \\
\{p\}
\end{bmatrix}
= \begin{bmatrix}
F_s \\
F_f
\end{bmatrix}
\quad (3.10)
\]

Expressions for the structural mass, damping, and stiffness matrices are found in ref. [54].
3.2.5 Solution Methodology

The field quantities (displacement and pressure) oscillate harmonically at a constant frequency ($\Omega$). This is conveniently represented using complex notation.

\[
\{u\} = \{U e^{i\phi}\} e^{i\omega t} \quad (3.11a)
\]
\[
\{p\} = \{P e^{i\phi}\} e^{i\omega t} \quad (3.11b)
\]

In Eqns. (3.11a) and (3.11b), \(\{U\}\) and \(\{P\}\) represent the amplitude of oscillation, \(\phi\) is the spatial phase shift in units of radians, and \(\omega\) is in radians per second and is related to the frequency by \(\omega = 2\pi f\). Separating the spatial term of (3.11a) into real and imaginary components, the displacement is expressed as,

\[
\{u\} = (\{u_1\} + i\{u_2\}) e^{i\omega t} \quad (3.12a)
\]

where \(\{u_1\} = \{U\cos\phi\}\) and \(\{u_2\} = \{U\sin\phi\}\), by Euler’s identity. Then, after taking the first and second derivatives of Eqn. (3.12a), the velocity and acceleration vectors are obtained as shown in Eqns. (3.12b) and (3.12c).

\[
\{\dot{u}\} = i\omega (\{u_1\} + i\{u_2\}) e^{i\omega t} \quad (3.12b)
\]
\[
\{\ddot{u}\} = -\omega^2 (\{u_1\} + i\{u_2\}) e^{i\omega t} \quad (3.12c)
\]
The same development can be done for pressure. By expressing the amplitude of each field term with a complex representation, the effects of damping are accounted for; the physical displacement, velocity, and acceleration are described by the real components of Eqns. (3.12a) – (3.12c). Finally, insertion of the complex representation of terms into the governing Eqn. (3.10) yields the following equation.

\[
-\omega^2 \begin{bmatrix}
[M_s] & 0 \\
0 & -[M_f]/\rho_0 - [M_s]/\rho
\end{bmatrix}
\begin{bmatrix}
\{u\} \\
\{p\}
\end{bmatrix}
+ i\omega \begin{bmatrix}
[C_s] & -[R] \\
-[R]^T & [-\kappa]/\rho_0
\end{bmatrix}
\begin{bmatrix}
\{u\} \\
\{p\}
\end{bmatrix}
+ \begin{bmatrix}
[K_s] & 0 \\
0 & -[\kappa_f]/\rho_0
\end{bmatrix}
\begin{bmatrix}
\{u\} \\
\{p\}
\end{bmatrix}
= \begin{bmatrix}
F_s \\
iF_f/\omega\rho_0
\end{bmatrix}
\] (3.13)

ANSYS solves the system of equations in (3.13) during a harmonic analysis involving fluid-structure interactions. Notice the temporal component \(e^{i\omega t}\) has been cancelled out from all terms. As a result, the temporal phase shifts are invisible to the FEA model, solving for the real and imaginary components of displacement or pressure amplitude at discrete points, but leaving no way to ascertain the relative amplitude between separate regions of the domain at a specific point in time during the oscillation period.

The same methods are used to express Eqns. (3.1), (3.3), and (3.7) for the linear elastic materials, the piezoelectric, and bulk fluid, respectively. Together, these equations are transformed into the following linear system of equations to be solved simultaneously,

\[
[K]\{u\} = \{F\} \tag{3.14}
\]

where [\(K\)] is called the global stiffness matrix, \(\{u\}\) is the global vector of nodal field terms, and \(\{F\}\) is the global applied load vector. There are numerous methods to solve a large system of simultaneous linear equations. The Cholesky factorization of a matrix provides an efficient method for solving large systems of linear equations, avoiding the complicated task of directly inverting a large matrix. ANSYS offers a sparse direct solver and a large number of iterative solver options to solve the system of linear equations [57]. The sparse solver takes a primarily Gaussian elimination approach by first computing the LDL decomposition (a variant of Cholesky decomposition) of the matrix [\(K\)], substituting the result into Eqn. (3.14), and then implementing a forward pass operation followed by back substitution to solve for \(\{u\}\), the global vector of nodal unknowns. These steps are expressed mathematically in the series of Eqns. (3.15a) – (3.15e) shown below.

\[
[K] = [L][D][L]^T \tag{3.15a}
\]
\[
[L][D][L]^T\{u\} = \{F\} \tag{3.15b}
\]
\[
\{w\} = [D][L]^T\{u\} \tag{3.15c}
\]
\[
[L]\{w\} = \{F\} \tag{3.15d}
\]
\[
[D][L]^T\{u\} = \{w\} \tag{3.15e}
\]
The forward pass follows from the LDL decomposition of $[K]$ shown in Eqn. (3.15a), when the product of the 2nd and 3rd factorized matrices with $\{u\}$ are conveniently substituted with a single vector $\{w\}$ that is found trivially by solving Eqn. (3.15d). Back substitution refers to Eqn. (3.15e), in which the solution vector $\{u\}$ is obtained using the original definition of $\{w\}$. The global stiffness $[K]$ in Eqn. (3.14) is a symmetric matrix that is sparsely populated by non-zero entries clustered around the main diagonal, with zero entries elsewhere. The sparse solver is designed to take advantage of this by treating non-zero entries only. Its efficiency is further optimized by an algorithm that reorders the equations in $[K]$ in a manner that minimizes the production of additional non-zero entries during the LDL matrix factorization [58]. The sparse direct solver uses complex arithmetic to solve Eqn. (3.14) for the harmonic analysis conducted in this work.

3.3 Solution Verification and Validation

The aforementioned assumptions and material properties were considered to simulate the harmonic response of the 2D closed-nozzle model in Fig. 3.2 using ANSYS. All combinations of the geometric parameters shown in Fig. 3.2 were considered, resulting in a total of 48 simulations. In each case, an input voltage of 10 Volts was applied to the piezoelectric transducer, and Eqn. (3.14) was solved over a frequency range from 0.5 – 2.5 MHz in increments of 5 kHz, resulting in a total of 400 frequency steps.

<table>
<thead>
<tr>
<th>Table 3.3 Modeling Parameters Considered</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parameter</td>
</tr>
<tr>
<td>Silicon layer thickness</td>
</tr>
<tr>
<td>Reservoir height</td>
</tr>
<tr>
<td>Aluminum layer thickness</td>
</tr>
<tr>
<td>Transducer thickness</td>
</tr>
<tr>
<td>Frequency</td>
</tr>
</tbody>
</table>

3.3.1 Solution Convergence

When conducting any study using FEA, it is important to show that approximation errors associated with the numerical solution are small. In the ANSYS harmonic response simulation, elements used to represent the solution domain are limited by their linear and quadratic shape functions. In other words, the solution across any one element can only be represented by 1st or 2nd-order polynomials. The complexity of the 2D chip geometry coupled with ultrasonic resonances results in complicated vibrational and acoustic mode shapes with rapid gradients in displacement and pressure amplitude, and significant mesh refinement is required to capture the harmonic response in high resolution. A consequence of refining the finite element mesh is an increase in the number equations involved in Eqn. (3.14), resulting in a longer computational
A balance between accuracy and efficiency is key, and this can be achieved by refining the mesh in areas of interest as well as locations where the solution behavior is more complicated, while maintaining a coarser mesh in other regions.

![Finite element mesh](image)

**Figure 3.5** Finite element mesh for the case of $t_{si} = 2.0\text{ mm}$, $h_c = 0.9\text{ mm}$, $t_{Al} = 3.0\text{ mm}$, and $t_{PZT} = 1.5\text{ mm}$.

The finite element mesh shown in Fig. 3.5 is representative of all 48 cases modeled. In this particular case, a total of approximately 53,000 quadrilateral elements were used. Due to geometric mesh refinement, cases with larger design parameters (e.g. a thicker aluminum layer) generally contain more elements, and those with smaller parameters contain less. The height of the fluid chamber ($h_c$) has the most significant effect on number of elements, because the mesh is very fine in the fluid domain to accurately approximate the
acoustic behavior. The nozzles are characterized by the most refinement, where the pressure amplitude is of upmost interest. The average element edge length across the nozzle tip is \( \sim 8 \mu m \). The fluid-structure interface consists of a single layer of FLUID29 elements with a thickness of 50 \( \mu m \) along the base of the chamber that tapers to \( \sim 5 \mu m \) at either side of the nozzle tips. The mesh is coarsened as one moves away from the fluid chamber; the average element edge length is \( \sim 120 \mu m \) within the transducer material.

To show mesh independence, the quantities of interest extracted from the finite element solution are compared at various levels of mesh refinement. Theoretically, for a well-posed problem, the finite element solution approaches the exact solution as the number of DOF approaches infinity \([50]\). Hence, the error is reduced as the number of degrees-of-freedom (DOF) are increased as a result of refining the mesh. The quantities of interest that characterize the spraying performance of the device are the electrical impedance of the piezoelectric transducer and the sum of the pressure amplitude at each nozzle tip. These data will be used to quantify the error.

In the following mesh independence study, the mesh shown in Fig. 3.5 (denoted “Current Mesh”) was refined, uniformly across the domain, two consecutive times (“Refinement 1” and “Refinement 2”). The total number of DOFs of the three meshes were 236,103, 913,295, and 2,057,854, respectively. With identical loads and boundary conditions, each mesh was solved from \( f = 0.5 – 2.5 \) MHz in 5 kHz increments. After extracting the quantities of interest at each frequency step, the approximation error of the finite element solution associated with mesh \( j \) was computed as the normalized, absolute difference between the solution quantity from the mesh being studied \( (S_j) \) and a reference mesh \( (S_{ref}) \). The most refined mesh, Refinement 2, was used as the reference mesh.

\[
(error)_j = \left| \frac{S_j - S_{ref}}{S_{ref}} \right|
\]  

(3.16)

In Figure 3.6, the amplitude of the electrical impedance and nozzle tip pressure are plotted as a function of frequency for all 3 meshes for comparison. Both responses are normalized with respect to the overall maximum value across all 48 cases investigated. Below the impedance or tip pressure response curves, the associated error is plotted as a function of frequency for the Current Mesh and Refinement 1.

In Fig. 3.6a, the impedance response curves appear to fall on top of one another, indicating that the solution is not changing as more DOF are added; the impedance response, computed from the FE solution, is mesh independent. The error for the Current Mesh is mostly flat with a few jumps between 0.95 and 1.70 MHz. The average and maximum error were 0.08\% and 1.21\%, respectively. For the Refinement 1 mesh, the average and maximum error were 0.01\% and 0.15\%. A maximum error of 1.21\% is more than acceptable for the impedance response, therefore the Current Mesh is sufficient for capturing the electromechanical response of the device.
In Fig. 3.6b, the normalized tip pressure response curves for the 3 meshes fall practically on top of one another, with some slight differences visible around 2.20 MHz. The average and maximum error for the Current Mesh were 1.59% and 19.91%, respectively, while the same values were reduced to 0.23% and 3.10% for the more refined mesh. The Current Mesh error spikes are located at frequencies where the corresponding tip pressure amplitude is low. Furthermore, the general pattern or shape of the tip pressure response vs frequency is not affected by the refinement. Since the goal of the simulations is to observe trends in the behavior of the device as the design parameters are varied, the Current Mesh was deemed acceptable.
The plots in Fig. 3.6 clearly show the approximation error decreasing in an asymptotic manner as the number of DOF were increased, indicating convergent behavior. This verifies the use of the Refinement 2 mesh as the reference for this mesh independence study, and also rules out the chance of any singularities in the domain (i.e., reentrant corners at the base of the nozzles and the edge of the chip where the transducer and aluminum meet) affecting the solution quantities of interest.
The error values reported for this case are representative of all of the geometric combinations considered in this work. A more converged result would not better represent the acoustic phenomena we are trying to study. Therefore, the refinement levels in the Current Mesh were used to generate all modeling results presented in the following sections.

3.3.2 Model Validation

In order to validate the model, experimental observations were made using the 2D visualization chips to be compared with modeling results. This is necessary to ensure that the model accurately predicts resonances where we would predict droplet ejection or jetting and portrays accurate predictions of mode shapes. It is well known that the terminal particle distribution for suspensions of micrometer-sized particles (with positive acoustic contrast factor) are known to represent nodal pressure locations in a standing pressure field [25], [26].

A visualization chip fabricated to specifications $t_{Si} = 2\text{mm}$, $h_c = 0.9\text{ mm}$, $t_{Al} = 3.0\text{ mm}$, and $t_{PZT} = 1.5\text{ mm}$ is shown in Fig. 3.7. The chip was loaded with water containing 10 $\mu$m diameter polystyrene (PS) beads at a density of $2 \times 10^6$ beads/mL. The piezoelectric transducer was driven using a 500 mV AC signal amplified between 30 – 180 V_{pp}. When rapid particle migration was observed, this indicated that the device was operating at or near a resonant frequency of the fluid chamber. At each resonance, a microscope was used to image the terminal particle distribution.

![Figure 3.7](image.png)

**Figure 3.7** Harmonically-varying pressure field computed in ANSYS (right) compared with terminal distribution of 20-$\mu$m polystyrene (PS) beads, imaged during experiment (left), at resonant frequencies within the fluid reservoir.
The first three integer half-wave resonant frequencies of the geometry were identified at 0.610 MHz, 1.10 MHz, and 1.665 MHz. Images of the terminal particle distribution at each frequency are shown on the left-hand side of Fig. 3.7. On the right, contour plots of the amplitude of the standing pressure field are shown at each corresponding frequency as simulated in ANSYS, where the red and blue colors correspond to regions of maximum and minimum pressure amplitude, respectively. Due to the positive acoustic contrast factor of the PS beads, they were focused at the nodes of the standing pressure field. Qualitatively, the mode shapes predicted by the FEA model are strikingly similar to that revealed by the terminal particle distributions observed experimentally. These results indicate the planar model accurately predicts mode shape characteristics of the actual 2D visualization chip at resonant frequencies of the fluid chamber.

3.4 Identification of Ejection Modes

The ultimate goal of this work is to find trends in design parameters that lead to improved and/or optimal performance of the ultrasonic atomizer. In order to do this, the conditions that signify “good” ejection must be easily recognized from the model. Here, we describe those indicators.

In a previous study that involved modeling a variant of the 3D atomizer that consisted of just the transducer, fluid chamber, and silicon chip, the piezoelectric was in direct contact with the working fluid [59]. In the absence of the aluminum coupling layer, ejection modes for a particular geometry were clearly identifiable from the electrical impedance response. Local minima/maxima (resonance/anti-resonance) pairs in the impedance magnitude corresponded to fluid chamber resonances. In the 2D chips analyzed in this work, inclusion of aluminum and silicon layers, sandwiched between the piezoelectric and fluid chamber, significantly affect the electrical behavior of the piezoelectric transducer. As a result, resonant frequencies of the fluid chamber become impossible to identify directly from the impedance response alone. Instead, ejection modes are identified as local maxima in the pressure amplitude summed across the nozzle tips.

Nonetheless, the impedance response provides insight into the kinetic behavior of the device by highlighting frequencies characterized by efficient transfer of electrical energy into mechanical energy. When the transducer is coupled with the aluminum coupling layer and microfluidic chip, it is effectively loaded by the aluminum and silicon chip/fluid chamber combination. The resulting impedance response provides indications of constructive and destructive vibrational coupling between the piezo and the other components of the device. Together, the total nozzle tip pressure and electrical impedance responses tell a great deal about the phenomena occurring within the 2D device.

In Fig. 3.8, the electrical input impedance is plotted as a function of frequency for all 48 combinations of aluminum coupling layer thickness (2.5, 3.0, and 3.5 mm), silicon carrier layer thickness (0.2, 0.5, 1.0, and 2.0 mm), and chamber height (0.5 and 0.9 mm) for 1.5 mm and 2.0 mm thick piezoelectric transducers. The
actual values of the impedance were normalized to best represent all cases on a single plot. The solid green curves correspond to cases in which a 1.5 mm transducer thickness was considered, and the black dashed curves represent the use of a 2.0 mm transducer. The overall disorder of the plots indicate the sensitivity of the device to the design parameters; however, some trends can be extracted from these plots. In the absence of the aluminum coupling layer, the piezoelectric element’s natural longitudinal resonance was easily identifiable, but when the coupling layer and silicon are included, this is no longer possible for any individual case. Here, the addition of the aluminum, silicon, and fluid layers introduces additional local minima/maxima pairs corresponding to device resonances. These additional resonances are viewed as potential operating frequencies, but further analysis of the tip pressure response is required to conclude whether or not ejection is likely. Nonetheless, the input impedance response provides useful information regarding the behavior of the device by locating resonances within the resonator, the fluid chamber, or both.

![Figure 3.8](image)

Figure 3.8 Impedance response due to various resonator geometry combinations, with (a) 900-µm height reservoir and (b) 500-µm reservoir.

Figure 3.9 shows the total tip pressure, or the sum of the pressure amplitude at each nozzle tip, as a function of frequency for all 48 geometric combinations. These values were normalized by the overall maximum value among the 48 simulations (2.302 MPa between 3 nozzles).

An infinite array of 2D nozzles was simulated with constant-amplitude displacement conditions applied to the base of the fluid chamber and a sound-hard boundary condition applied to the walls of the nozzle. This eliminated the vibrational effects of the resonator to effectively isolate the acoustic resonances of the fluid chamber alone. The first four half-wavelength resonant modes corresponding to pressure wave focusing (indicated by the vertical red lines in Fig. 3.9) are observed as clearly identifiable maxima in tip pressure at approximately 0.63, 1.13, 1.63, and 2.17 MHz for the 0.9 mm fluid chamber height. Similarly, the first three half-wave modes are observed at approximately 0.88, 1.54, and 2.23 MHz for the 0.5 mm chamber. The location of the integer half wave resonances \( \left( \frac{n}{2} \lambda \right) \) in the fluid chamber can be roughly approximated by the analytical equation for a 1D standing wave pinned between two parallel plates \( f_n = \frac{n c}{2 W} \), where
in this case is the distance between the reservoir base and the tip of a nozzle, i.e., \( h_c + 500 \mu m \). While the clearly identifiable resonances from an infinite array of nozzles become obscured when the additional components of the real device are included, they provide a general location near which resonant should frequencies exist for a given chamber height. The conglomeration of local maxima in tip pressure amplitude for the 48 cases tend to exist near these fundamental chamber resonances.

It is important to clarify nomenclature. Used throughout the remainder of the thesis, \textit{chamber resonance} refers to the integer half-wave, acoustic resonant frequencies of a particular fluid chamber. The corresponding mode shape, or the pattern of the pressure amplitude, has characteristics similar to those shown in the contour plots at the top of Fig. 3.9. When the resonator is included in the simulation, the resulting acoustic mode shape varies from case to case. This can make identifying a chamber resonance at a single frequency challenging, and thus a chamber resonance is often defined over a narrow range of frequencies. However, the fundamental mode shapes in Fig. 3.9 serve as a guide for properly identifying chamber resonances. \textit{Chamber resonances} are also referred to as \textit{ejection modes} because they correspond to operating frequencies that will most likely lead to fluid ejection.

In addition to the local maxima corresponding to chamber resonances, there exist additional peaks in normalized nozzle tip pressure, particularly at lower frequencies. As it turns out, there are many factors that can lead to spikes in pressure amplitude at the nozzle tips, and thus a system was employed for selecting ejection modes. For a given potential resonant frequency:

1. Find the largest tip pressure maxima in the vicinity of the fundamental resonant frequency.
2. Observe the pressure amplitude contour; does it resemble a fundamental mode shape?
   a. If yes, this is an ejection mode.
   b. If no, find next largest tip pressure maxima close to fundamental resonant frequency and repeat.

In choosing operating frequencies, there is a key balance between the chamber acoustic resonance in the sense of the fundamental mode shapes shown in Fig. 3.9 and the amplitude of the normalized tip pressure, since the latter is what ultimately drives ejection. The next two sections will provide examples of the identification process for ideal and non-ideal cases.
Figure 3.9 Acoustic response of the fluid reservoir due to various resonator geometry combinations. Pressure mode shapes are shown for an infinite array of nozzles in the (a) 900 µm height reservoir and (c) 500 µm reservoir. Additionally, the nozzle tip pressure response is shown due to various resonator geometry combinations for the (b) 900-µm height reservoir and (d) 500 µm reservoir.

Figure 3.9 also illustrates the effect that fluid chamber height and its interplay with piezoelectric thickness have on predicted operating frequency for 24 cases at each of the two chamber heights (0.5 and 0.9 mm). The fundamental resonance of the 1.5 mm thick piezoelectric occurs at 1.35 MHz, making it a good choice for the 2nd and 3rd characteristic ejection frequencies of the 900 µm chamber and the 3rd ejection frequency for the 500 µm chamber. As the first ejection frequency for each of the fluid reservoirs occurs well below the fundamental resonance of the 1.5 mm thick piezoelectric, it may not be the better choice for driving ejection from devices at lower frequencies. Conversely, the 2.0 mm thick piezoelectric is better matched to ejection frequencies in the 0.8 to 1.2 MHz range, making it ideal for driving ejection from smaller chamber heights. These results are significant as they suggest that reservoir height and piezoelectric thickness are most important in dictating the frequencies at which a particular device will best perform. The geometry of the other device components plays an important role in whether or not ejection will occur; however, it does not significantly alter the specific frequencies at which ejection is most likely to occur for a given reservoir height.

3.5 Influence of Resonator Geometry (Case 1)

The impedance and tip pressure responses are essential to identifying the ejection modes. However, they do not provide sufficient information for understanding why the device behaves the way it does. For this
reason, 2 cases have been chosen for further analysis in which we compare the impedance and tip pressure responses as well as the pressure and displacement field contours throughout the domain.

In Fig. 3.10, the input impedance and total nozzle tip pressure amplitude are plotted as a function of frequency for Case 1 \((t_{PZT} = 1.5 \text{ mm}, t_{Al} = 3.0 \text{ mm}, h_c = 0.9 \text{ mm}, \text{ and } t_{Si} = 0.2 \text{ mm})\). The first four half-wave chamber resonances are clearly identifiable from the tip pressure response, and each peak in tip pressure corresponds to a local minimum in impedance. This makes sense; a resonance in the fluid chamber should result in a reduced vibrational resistance as seen by the resonator, and hence a reduced electrical impedance of the piezoelectric transducer. Clearly defined local maxima in nozzle tip pressure are observed within the prescribed range of frequencies identifying each chamber resonance, making the selection of ejection modes straightforward.

The total pressure amplitude of the three nozzles is indicated by the solid blue curve, while the black/gray curves represent the tip pressure amplitudes of the individual nozzles. It is notable that nozzle 3, which corresponds to the outermost nozzle of the array, displays a significantly reduced tip pressure amplitude compared to nozzles 1 and 2 at the first and second ejection modes. At lower-order, half-wave resonances, the pressure mode shape tends to be more focused towards the center of the chamber, as shown in Fig. 3.11. The field amplitude decreases away from the symmetry line, particularly near the 3rd nozzle. At higher ejection modes, the pressure mode shape generally becomes more uniform across the length of the chamber, resulting in a more equal contribution among the nozzles to the total tip pressure. This result suggests that it is more likely for fewer nozzles to eject fluid at lower operating frequencies. This behavior has been observed in experiments with the droplet generator device.
Figure 3.10 Harmonic behavior of Case 1 resonator/chip geometry as a function of frequency. It is evident that the (a) impedance and (b) fluid chamber resonance modes occur at relatively similar frequencies, indicating a good match of geometric parameters.

Figure 3.11 shows contours of the displacement and pressure amplitude in the piezoelectric/aluminum/silicon and fluid, respectively, at each of the resonator and fluid chamber resonances. The displacement resonances ($f_{SI/Al/PZT}$) were found based on maxima in the resonator displacement amplitude by extracting the nodal $y$-displacement amplitude along the base of the reservoir. At these frequencies, planar patterns are clearly identifiable from the displacement mode shape throughout the resonator. The first half-wave displacement resonance was not observed in the frequency range of interest. While it is possible it occurred below 500 kHz, the first transverse mode shape may be difficult to develop in the resonator whose thickness is dominated by the aluminum coupling layer. Based on the three observed resonances, it appears the resonator vibrates most efficiently when a standing half-wave (or nearly a half-wave) exists in the piezoelectric material. This makes sense, as it is a piezoelectric chip vibrating in the thickness-mode that generates transverse waves. The speed of sound is only slightly higher in the aluminum than the piezoelectric material, hence a single half-wave displacement mode through the entire resonator may be less than ideal.
For broadband operation, Case 1 is close to ideal in that the resonator frequencies occur quite close to the chamber resonant modes; within 25 kHz for the 2nd and 4th modes, and within 150 kHz for the 3rd. The nozzle tip pressure amplitude at the 2nd and 3rd ejection modes were near 80% of the overall maximum among all 48 cases studied. A quick glance at Fig. 3.9 shows the 4th ejection mode was in the upper echelon of tip pressure amplitude for this chamber height. Based on these results, it is evident that the alignment of the PZT/Al/Si resonances with the chamber’s resonant frequencies leads to strong coupling between the resonator and fluid channel. The efficient transfer of acoustic energy into the fluid was evidenced by the strong acoustic focusing at the nozzle tips. This result agrees with observations made by Bora and Shusteff [28], who simulated a piezoelectric transducer bonded to a glass chip containing a rectangular fluid channel and found that coupling the vibration mode of the piezoelectric with the elastic modes of the chip resulted in an increased pressure amplitude in the fluid channel. In summary, Case 1 is a satisfactory combination of design parameters that lead to efficient energy transfer from the piezoelectric into the fluid due to strong coupling throughout the multi-layered resonator when operating near the fluid chamber resonant frequencies.
3.6 Influence of Reservoir (Case 2)

Case 2 ($t_{PZT} = 1.5 \text{ mm}, t_{Al} = 3.0 \text{ mm}, h_c = 0.5 \text{ mm}, \text{ and } t_{Si} = 0.5 \text{ mm}$) is an example of a non-ideal case that portrays the effects of poor acoustic coupling between the fluid chamber and resonator. Notice that the geometry of the resonator is almost identical to Case 1; only the silicon layer has been slightly increased. However, the shorter fluid chamber is considered to highlight the effects the fluid reservoir can have on the behavior of the device when the resonator is left relatively unchanged.

In Fig. 3.12, the electrical impedance and the nozzle tip pressure amplitude are plotted as a function of frequency, as indicated by the red lines. The immediate effect of the reduced chamber height is that ejection modes have been shifted to higher frequencies and become more spread apart. In fact, the 4th half-wave chamber resonance does not exist within the frequency range considered. The first ejection mode was determined to be located at 880 kHz, about 175 kHz below the second vibrational resonance of the resonator. As a result, the pressure amplitude at this ejection mode is quite low. The 2nd elastic mode of the resonator occurs at 1.055 kHz, and the overall amplitude of the acoustic field in the fluid has been significantly augmented leading to a locally large normalized tip pressure, despite the acoustic mode shape in Fig. 3.13 showing no resemblance to a “typical” chamber resonance. This suggests the possibility of ejection when operating at frequencies where the components of the resonator assembly are coupled well, and the vibrational resonance can overcome a less-than-ideal acoustic mode shape in the fluid reservoir in order to generate sufficient acoustic energy to drive ejection. Thus, the device could be operated at either the chamber resonance or the PZT-Al resonance. This behavior has been observed experimentally in the 3D droplet generator.
Figure 3.12 Harmonic behavior of Case 2 resonator/chip geometry as a function of frequency. The (a) impedance and (b) fluid chamber resonance modes are offset by significant frequency gaps, indicating bad resonant coupling between the resonator and fluid reservoir.

Similarly, the 3\textsuperscript{rd} and 2\textsuperscript{nd} resonances of the resonator and fluid chamber, respectively, are separated by a 135 kHz gap. A strong total tip pressure is seen at the chamber resonance, and a secondary peak is observed at the frequency corresponding to the resonator resonance. While the acoustic mode shape at 1.435 MHz represents a chamber resonance slightly better than that at 1.570 MHz, the latter was chosen as the ejection mode due to its more dominant nozzle tip pressure amplitude. However, the similarity between the two acoustic mode shapes is quite striking; they are nearly identical. This strongly suggests that we may be able to design the atomizer such that it is relatively insensitive to a specific design frequency of operation. This would have multiple benefits. The various components of the device would not need to be machined to within such a tight tolerance. Similarly, the material properties of the device, particularly the highly-varying piezoelectric properties, would not need to be perfectly known for the numerical model in order to achieve a desired performance.
Together, Cases 1 and 2 provide invaluable information regarding the behavior of the device and how design parameters affect its performance. The relative frequencies of the elastic modes of the resonator and acoustic modes of the fluid chamber can either augment or suppress chamber resonance behavior.

3.7 Resonance Alignment Study (Case 3)

In Case 3, the 0.9 mm fluid chamber height is considered with a 1.5 mm piezoelectric thickness, a 3.0 mm aluminum coupling layer, and a 1.0 mm silicon layer. This case immediately drew attention due to the fact that its 3rd ejection mode resulted in the largest total nozzle tip pressure (2.302 MPa) out of all ejection modes across the 48 cases analyzed. What caused the large tip pressure?

Figure 3.14 shows the electrical impedance and nozzle tip pressure as a function of frequency. The 3rd ejection mode occurs at 1.645 MHz, which happens to be within 200 kHz of the 3rd vibrational mode of the resonator. The large resonance/anti-resonance pair near this frequency in the impedance response suggests
remarkably strong coupling between the piezoelectric, aluminum, and silicon layers of the resonator. At this particular frequency, the resonator transmits an enormous amount of acoustic energy into the fluid.

**Figure 3.14** Harmonic behavior of Case 3 resonator/chip geometry as a function of frequency.

Based on the observations from Case 1, it is worthwhile to try and further optimize the geometry. To increase the energy transfer from the resonator into the fluid chamber, the resonance frequency of the transducer stack can be shifted so that it coincides with the fluid chamber resonance for improved energy efficiency. By reducing the thickness of the piezoelectric transducer, its natural longitudinal resonance can be shifted to a higher frequency. The aluminum thickness must be adjusted accordingly in order to maintain optimal coupling within the resonator assembly.

Figure 3.15 shows the impedance and nozzle tip pressure amplitude as a function of frequency for five variations of the Case 3 geometry. The piezoelectric thickness was reduced to 1.2 mm, and numerous aluminum thicknesses between 2.2 mm and 3.0 mm were investigated. Each of the five cases outperformed the Case 3 geometry in terms of maximum tip pressure.
Figure 3.15 Harmonic responses of Case 3 variations with $t_{SI} = 1.0 \, \text{mm}$, $h_c = 0.9 \, \text{mm}$, $t_{PZT} = 1.2 \, \text{mm}$, and aluminum thicknesses varying between 2.2 mm and 3.0 mm.

The impedance response for the 3.0 mm aluminum thickness case shows the global impedance minimum at 1.535 MHz, where the 3$^{rd}$ half-wave resonance of the transducer stack occurs, verified at the top of Fig. 3.16. There is a secondary local impedance minimum at 1.6575 MHz, characterized by the global maximum in nozzle tip pressure amplitude, indicating the fluid chamber’s 3$^{rd}$ half-wave resonance, shown at the bottom of Fig. 3.16. The transducer stack resonance and chamber resonance are separated by roughly 123 kHz. Decreasing the aluminum thickness is expected to increase the resonant frequency of the transducer stack to better coincide with the chamber resonance.
Figure 3.16 Contours of the y-component of displacement amplitude and pressure amplitude at (top) the 3\textsuperscript{rd} half-wave transducer resonance at 1.535 MHz and (bottom) the 3\textsuperscript{rd} half-wave fluid chamber resonance at 1.6575 MHz for the 3.0 mm aluminum thickness case.

The impedance response for the 2.8 mm aluminum thickness case shows the 3\textsuperscript{rd} half-wave resonance of the transducer stack has moved to 1.58 MHz, as shown at the top of Fig. 3.17. The tip pressure response shows two peaks. The first peak, at 1.6075 MHz, happens to be the fluid chamber’s 3\textsuperscript{rd} half-wave resonance (bottom of Fig. 3.17) and is characterized by large pressure amplitudes at each of the nozzle tips. A secondary maximum in tip pressure occurs at 1.67 MHz, and although it is a slightly higher amplitude than at 1.6075 MHz, the pressure mode shape shows the pressure wave is focused at the 2\textsuperscript{nd} and 3\textsuperscript{rd} nozzle tips, however the pressure amplitude has decreased significantly in the 1\textsuperscript{st} (symmetry) nozzle.
Figure 3.17 Contours of the $y$-component of displacement amplitude and pressure amplitude at (top) the 3rd half-wave transducer resonance at 1.58 MHz and (bottom) the 3rd half-wave fluid chamber resonance at 1.6075 MHz for the 2.8 mm aluminum thickness case.

The impedance response for the 2.6 mm aluminum thickness case is similar to the 2.8 mm case, with the impedance minima shifted to slightly higher frequencies. An interesting difference, however, is that the displacement resonance in the transducer stack has shifted to the higher frequency impedance minima.
Figure 3.18 Contours of the y-component of displacement amplitude and pressure amplitude at (top) the 3rd half-wave fluid chamber resonance at 1.6225 MHz and (bottom) the 3rd half-wave transducer resonance at 1.6975 MHz for the 2.6 mm aluminum thickness case.

Ultimately, the transducer stack’s displacement resonance never quite coincides with the acoustic resonance of the fluid chamber. There are two discrete frequencies corresponding to each resonance, and they are generally characterized as a primary and secondary dip (peak) in impedance (summed tip pressure). As the aluminum thickness was decreased from 2.8 mm to 2.6 mm, the displacement resonance of the transducer stack passed the acoustic resonance of the fluid chamber, and neither case represented a significantly amplified nozzle tip pressure.

Surprisingly, further reducing the aluminum layer thickness to 2.2 mm resulted in the maximum total tip pressure with a normalized value of 2.54 at 1.6375 MHz, despite the transducer stack’s displacement resonance occurring at 1.7775 MHz. At the chamber’s resonant frequency, the displacement pattern in the transducer stack appears close to a one and one-quarter-wave resonance (2.5 half-wave), with a displacement node occurring just below where the silicon meets the fluid chamber, as shown at the top of Fig. 3.19. This is a remarkable result that indicates the behavior of the transducer stack near the base of the
reservoir may play a significant role in the amplification of the acoustic field and summed tip pressure, based on the fluid-structure interaction.

When identifying y-displacement resonances of the transducer stack, there is an integer half-wave through the piezo, aluminum, and silicon, resulting in a local maximum displacement near the reservoir base (in other words, a phase angle of 90 degrees if it is considered like a sine wave). In the harmonically oscillating solid material, the y-component of normal stress is at a minimum amplitude when the y-component of displacement is at a maximum amplitude. While operating at a transducer n<sup>th</sup> half-wave is optimal from an efficiency standpoint (low input voltage to achieve maximum vibrational energy), it does not constitute the ideal boundary condition for acoustic excitation in the fluid chamber due to the vertical component of normal stress in the solid material being close to minimal near the base of the reservoir. This translates to a reduced acoustic pressure amplitude at the base of the fluid chamber.

Instead, the optimal case with the maximum total tip pressure amplitude results when the transducer stack operates at its 2.5 half-wave, transverse resonance, resulting in a displacement amplitude node near the base of the fluid chamber. This condition translates to a high acoustic pressure amplitude at the base of the fluid chamber, setting up a robust acoustic resonance characterized by an amplified pressure amplitude at the nozzle tips. Although it does not coincide with the 3<sup>rd</sup>, half-wave resonance of the transducer stack, the chamber resonance is evidenced by a local minimum in the impedance response of the piezoelectric. This result suggests that operating near the global impedance minimum of the transducer stack can increase the power efficiency of the device. However, modeling attempts to design the transducer stack so its vibrational resonance coincides with the acoustic resonance of the fluid chamber illustrate the importance of considering the acoustic boundary condition at the base of the fluid chamber for achieving optimal device performance, i.e., maximum pressure amplitude at the nozzle tips.
Figure 3.19 Contours of the y-component of displacement amplitude and pressure amplitude at (top) the 3rd half-wave fluid chamber resonance (1.6375 MHz) and (bottom) the 3rd half-wave transducer resonance (1.7775 MHz) for the 2.2 mm aluminum thickness case.

In terms of optimization, the first 48 cases studied were effectively an exhaustive search over a very limited design space based on discrete allowable parameter values. Case 3 was chosen as the optimal geometric combination found, and it was further optimized over a local search space by allowing the piezoelectric and aluminum thicknesses to vary. This methodology shows that, for a given frequency range of interest, an optimization routine could be designed to search over a continuous design space for the optimal parameters for ejection, i.e., an increase in the nozzle tip pressure. Based on the inconsistencies regarding the selection of ejection modes as highlighted in the discussion of Case 2, a more objective method for identifying operating frequencies is necessary. Perhaps, narrowing the search to a more limited range of frequencies could alleviate the issue. Furthermore, operating at the piezoelectric natural longitudinal resonance is typically avoided, as it generally results in significant heating and frictional losses. These losses are unaccounted for in ANSYS and could potentially alter the feasibility of specific operating frequencies.
3.8 Summary

By characterizing methods to successfully identify ejection frequencies and highlighting important trends in device performance, this study has provided valuable information for designing an efficient droplet generator. Comparison to experiment has shown that the harmonic response model can predict ejection frequencies with reasonable accuracy. The above results have confirmed that the fluid chamber height and piezoelectric thickness are the most important parameters in dictating the frequencies of ejection. The thicknesses of the aluminum and silicon strongly influence the likelihood of ejection, however. Finally, elastic modes of the resonator assembly can (and should) be utilized to amplify the acoustic response.
Chapter 4

Acoustophoresis Simulation in Static Fluid

It is well known that small particles in a standing acoustic field experience acoustic radiation forces due to the scattering of acoustic waves. In a quiescent fluid, particles with a positive acoustic contrast factor migrate to the pressure nodes of the acoustic field. This behavior has been observed when polystyrene beads (5 – 20 µm in diameter) were suspended in water within the 2D visualization chips during operation at the characteristic resonant frequencies of the fluid chamber. In this chapter, the migratory acoustophoretic motion of polystyrene beads in 2D visualization chips is simulated using MATLAB and the acoustic pressure obtained from the harmonic response simulations presented in the previous chapter. Successfully modeling particle trajectories in a quiescent fluid is a first step in predicting the particle trapping and retention abilities of the 3D ultrasonic atomizer.

4.1 Assumptions

Experimental operation of the 2D visualization chip was subject to several indeterminate variables (device heating, different clamping conditions, variable drive voltage, etc.); therefore, the model serves as a numerical proof-of-concept rather than an exact representation of what occurs in the actual device. In this context, simplifying assumptions that allow prediction of acoustophoretic particle motion are justified.

The time-averaged effect of the primary acoustic radiation force \( F_{\text{rad}} \) exerted on a small particle can be determined using the first-order acoustic field provided by ANSYS. While acoustic streaming effects have been analyzed using numerical simulations [60]–[62], the phenomena is not included in this work. \( F_{\text{rad}} \) is proportional to the cube of the particle radius, indicating that larger particles will experience exponentially stronger forces than smaller particles. For a given particle in a standing acoustic field, there exists a critical radius \( a_c \) that determines whether a particle’s motion will be dominated by streaming or by primary radiation forces.

\[
\begin{align*}
\text{If } a &< a_c, \text{ streaming dominates.} \\
\text{If } a &> a_c, \ F_{\text{rad}} \text{ dominates.}
\end{align*}
\]

Bruus [43] used scaling law arguments to approximate the critical particle radius order of magnitude to be \(~1 \mu m\) in the case of a 1 MHz standing wave parallel to a planar wall in water at room temperature. This seems to agree with the results from a numerical study by Muller et al. [61], in which the motion of 5 µm
diameter polystyrene (PS) beads in a rectangular, water-filled channel (377 x 157 µm cross-section) subject to acoustic excitation at 1.94 MHz were dominated by the radiation force, whereas 0.5 µm diameter beads were dominated by streaming effects. The cases analyzed in this work are limited to PS particles (a_{min} \geq 2.5 \mu m) suspended in water, subjected to ultrasonic frequencies within 0.5 MHz \leq f \leq 2.5 MHz, which falls within the range for streaming effects to be negligible. During all experiments with the 2D visualization chips, no evidence of acoustic streaming effects was observed. For these reasons, acoustic streaming effects were neglected from the MATLAB model.

In microfluidic applications, the particle concentration is low and does not have a noticeable effect on the fluid properties, such as density, speed of sound, and viscosity. It is common practice to simulate an acoustic microfluidic device without particle suspensions present in the working fluid and then use the resulting acoustic field to simulate particle motion. In other words, the presence of particles is assumed to have no effect on the standing acoustic field. It is also assumed that, initially, the particles are uniformly dispersed and the acoustic waves scattering from each particle have a negligible local effect on the acoustic field. As a result, particle-particle effects on F_{rad} become irrelevant. Thus, particle motion can be simulated based on the results of a single ANSYS harmonic response simulation on a particle-free fluid.

Additionally, the model neglects particle inertia and assumes instantaneous acceleration due to the balance of acoustic radiation and drag forces. The instantaneous, ARF-induced velocity in a quiescent fluid, Eqn. (2.24) reduces to the following expression:

\[ v_p = \frac{F_{rad}}{6\pi \mu a} \]  
(4.1)

The radiation force equation from Chapter 2 neglected viscous and thermal effects within the acoustic field, which can cause the magnitude of F_{rad} to vary considerably in certain situations [22]. For simplicity, these effects are ignored in the model presented herein. Heating of the fluid, particle-wall collisions, and other particle-particle interactions are also ignored. The limitations associated with some of these assumptions are explored later in this chapter. Nonetheless, it will be shown that reasonable results can be generated with a simplified model.

4.2 MATLAB Implementation

Forces exerted on a particle depend on the local acoustic pressure amplitude and gradient as the particle migrates within a standing acoustic field. In order to predict its trajectory through a fluid reservoir, these forces and the resulting particle velocity must be computed continuously throughout the transient process. Simulating the motion of numerous particles simultaneously requires hundreds of thousands of intermediate calculations and organized data storage. MATLAB [63] was used to handle acoustic field results from
ANSYS and simulate particle motion, and a few of the MATLAB functions essential to the particle tracking model are mentioned in this section.

4.2.1 Pressure Field Representation

The standing acoustic field results from ANSYS, in the form of nodal pressure amplitude data, were imported into MATLAB and mapped onto a 2D triangulation using the Delaunay function. As shown in Fig. 4.1, the triangulation method draws triangles between nearest neighbors in a 2D point cloud.

![Figure 4.1 Example triangulation from arbitrary 2D points.](image)

The usefulness of the triangulation stems from its representation of a scalar field defined by arbitrarily-spaced points, a situation where rectangular grids cannot be applied. In this case, the scalar field is pressure amplitude, and the triangulation vertices are defined by the x- and y-locations of the nodes in the ANSYS finite element mesh. A typical triangulation applied to the closed-nozzle reservoir geometry is shown in Fig. 4.2.

![Figure 4.2 Triangulation of 2D reservoir.](image)
In MATLAB, the Delaunay function takes a vector \( \{V\} \) of point coordinates and creates an organized \( < n \times 3 > \) array that represents a triangulation of \( n \) triangles, each defined by 3 vertices which are indexed by the corresponding points in \( \{V\} \). The mapped triangulation is useful for approximating the gradient of some scalar field value that is not readily available from the ANSYS post-processor, such as the square of the pressure amplitude. The gradient of a specific scalar quantity was approximated at each triangle vertex using the function \texttt{trigradient\_Hanselman} [64] in MATLAB, which first computes the face gradient of all triangles sharing the corresponding vertex and then interpolates the face gradient to the vertex location where each face gradient value is weighted by an inverse-distance method.

The triangulation object in MATLAB is also useful for determining when a particle has left the fluid domain. The function \texttt{pointLocation} takes the coordinates of an arbitrary point \( P(x,y) \) and returns the index of the triangle containing it. The same function returns \texttt{NaN} (Not-A-Number) if the input coordinates correspond to a location outside the triangulation.

### 4.2.2 Particle Injection

Acoustic radiation forces drive particles with a positive acoustic contrast factor towards the pressure field nodes. In a quiescent fluid, the trajectory of a particle through an arbitrary, standing acoustic field depends on its starting location. The acoustic mode shapes generated in the fluid chamber of the 2D chips are dependent on the frequency of operation and the chip geometry, therefore it is useful to simulate a large number of randomly distributed particles to capture the migration to their terminal distribution. This also allows for comparison between the behaviors of different particles. Furthermore, particle suspensions are initially uniformly distributed throughout the fluid chamber during an experiment. During the injection step of the model, parameters are used to define the particle density, compressibility, speed of sound, as well as the total number to be simulated. A corresponding number of particles are then injected at random starting locations (rather than along a uniform grid) throughout the fluid chamber to represent a true particle suspension. The MATLAB Random Number Generator is employed to produce initial particle locations, and the \texttt{shuffle} function is used to seed the random number generator based on the current time. This guarantees randomized initial particle locations for each simulation, for consistency. In most cases presented below, between 500 and 2500 total particles are considered at a time. For all cases, spherical PS beads are simulated in water at room temperature using the material properties shown in Table 4.1.
Table 4.1 Material Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density, water</td>
<td>$\rho_w$</td>
<td>1000 kg/m$^3$</td>
</tr>
<tr>
<td>Speed of sound, water</td>
<td>$c_w$</td>
<td>1500 m/s</td>
</tr>
<tr>
<td>Compressibility, water</td>
<td>$\kappa_w$</td>
<td>4.444x10$^{-10}$ 1/Pa</td>
</tr>
<tr>
<td>Density, polystyrene</td>
<td>$\rho_p$</td>
<td>1050 kg/m$^3$</td>
</tr>
<tr>
<td>Speed of sound, polystyrene</td>
<td>$c_p$</td>
<td>2350 m/s</td>
</tr>
<tr>
<td>Compressibility, polystyrene</td>
<td>$\kappa_p$</td>
<td>1.725x10$^{-10}$ 1/Pa</td>
</tr>
</tbody>
</table>

4.2.3 Computing $\mathbf{F}_{\text{rad}}$

Recalling its definition in Eqn. (2.20), $\mathbf{F}_{\text{rad}}$ depends on the field terms $\langle p_1^2 \rangle$ and $\langle v_1^2 \rangle$. However, only the extraction of nodal pressure amplitude is necessary from the harmonic response solution, as it is straightforward to compute the fluid particle velocity in MATLAB. The first-order fluid velocity is related to the gradient of pressure by the equation,

$$\mathbf{v}_1 = \frac{1}{i \rho_0 \omega} \nabla p_1$$  \hspace{1cm} (4.2)

and the time-average of the squared, first-order velocity field can be computed by

$$\langle v_1^2 \rangle = -\frac{1}{\rho_0 \omega^2} \langle (\nabla p_1)^2 \rangle$$  \hspace{1cm} (4.3)

where we note that squaring a vector is analogous to taking the dot product with itself. Inserting Eqn. (4.3) into Eqn. (2.20) allows for $\mathbf{F}_{\text{rad}}$ to be expressed in terms of first-order pressure only.

$$\mathbf{F}_{\text{rad}} = -\frac{4\pi}{3} a^3 \left[ \frac{1}{2} f_1 \kappa_0 \nabla \langle p_1^2 \rangle + \frac{3}{4} f_2 \frac{1}{\rho_0 \omega^2} \nabla \langle (\nabla p_1)^2 \rangle \right]$$  \hspace{1cm} (4.4)

The first-order pressure oscillates harmonically at a given frequency with an amplitude of $P_a$, which is computed by ANSYS. The time-dependent, first-order pressure at an arbitrary point in the acoustic field can be expressed mathematically by the equation,

$$p_1(t) = P_a \cos(\omega t)$$  \hspace{1cm} (4.5)

where $\omega$ is the angular frequency in units of radians per second. The period of oscillation is now conveniently $2\pi$ radians. Squaring both sides of Eqn. (4.5) and inserting into the time average integral of Eqn. (2.13) leads to the following equation:

$$\langle p_1^2 \rangle = \frac{1}{2\pi} \int_0^{2\pi} [P_a \cos(\omega t)]^2 dt = \frac{1}{2\pi} \left[ \frac{\sin^2(4\pi \omega)}{4\omega} + \pi \right] P_a^2$$  \hspace{1cm} (4.6)

Considering frequencies in the MHz range, the first bracketed term becomes negligible, and the expression reduces to the following expression:

$$\langle p_1^2 \rangle = \frac{1}{2} P_a^2$$  \hspace{1cm} (4.7a)
Due to its periodic nature, the time average of $p_1(t)$ in Eqn. (4.5) will always yield the result given by Eqn. (4.7a). Since all points in the acoustic field are oscillating at a single frequency, the gradient operator on $p_1$ will have no effect on the time average integral, and the second time-averaged term in Eqn. (4.4) becomes:

$$\langle (\nabla p_1)^2 \rangle = \frac{1}{2} (\nabla p_a)^2$$

(4.7b)

Therefore, the magnitude and direction of the acoustic radiation force on a PS bead of a given radius ($a$) can be approximated at any point in the acoustic field based on the local pressure amplitude ($P_a$) with the following expression:

$$F_{rad} = -\frac{4\pi}{3} a^3 \left[ \frac{1}{4} f_1 \kappa_0 \nabla (P_a^2) + \frac{3}{8} f_2 \frac{1}{\rho_0 \omega^2} \nabla \nabla (P_a)^2 \right]$$

(4.8)

The scalar quantities of Eqns. (4.7a) and (4.7b) are used to compute $F_{rad}$ at the nodal locations of the ANSYS finite element mesh. The MATLAB function scatteredInterpolant is then used to approximate the components of $F_{rad}$ at a given particle location.

### 4.2.4 Particle Tracking Algorithm

Particle motion is simulated over a sequence of discrete time steps using the iterative solution algorithm described below. Let the superscript $i$ denote the current time step and subscript $j$ denote the current particle of the set of $N$ total particles. At $i = 0$, the particles are located at their initial positions with no initial velocity.

1) Use `pointLocation` to find the triangle containing particle $j$ located at ($x_j^i$, $y_j^i$).

2) Compute $F_{rad}$ on particle $j$ using the `scatteredInterpolant` function.

3) Use Eqn. (4.1) to compute the resulting velocity of the particle at the current location, i.e., $V(x_j^i, y_j^i)$.

4) Compute the particle’s new position after a small time step $\Delta t$ by the equations

   $$x_j^{i+1} = x_j^i + V_x(x_j^i, y_j^i) \Delta t,$$
   $$y_j^{i+1} = y_j^i + V_y(x_j^i, y_j^i) \Delta t.$$  

(4.9a)

(4.9b)

5) Loop over $N$ particles.

6) Repeat steps 1 – 5 until stopping criterion is satisfied.

Note that an explicit numerical method was employed to compute the particle’s new location based on the forces exerted on it at its current location. The stopping criterion can be defined by a number of things, including a fixed number of time steps, a maximum computation duration, or a subroutine used to sense when particle focusing has been achieved to some degree of completion (or tolerance). The simulation duration, or the length of time over which particles are tracked, is determined by the length and total number
of time steps. Particles are translated at constant velocity in step 4, which is accurate as long as the resulting displacement is sufficiently small such that changes in $F_{\text{rad}}$ exerted on the particle between subsequent steps is also small. A smaller value of $\Delta t$ will minimize this approximation error, but it will increase the required number of steps, hence computation time, required to simulate particle motion over a given duration. The time step must be chosen carefully to balance accuracy and speed.

4.3 Results

4.3.1 Mesh Independence

In the previous chapter, the quantity of interest was a single value: the total pressure amplitude at the nozzle tips. For simulating the motion of particles throughout the fluid domain, the solution throughout entire acoustic field must be reliable. In order to verify the finite element solution to the wave equation, we can treat the pressure amplitude throughout the acoustic field as a 3D surface whose x- and y-dimension span the fluid chamber domain and the z-dimension represents pressure amplitude. In this manner, the approximation error can be computed by comparing subsequently refined solutions in a least squares sense. The $\ell_2$ norm difference between the current finite element solution to the wave equation, $P_1$, and a reference solution, $P_{\text{ref}}$, is computed as follows:

$$ error = \sqrt{\frac{\int (P_1 - P_{\text{ref}})^2 dA}{\int (P_{\text{ref}})^2 dA}} $$

(4.10)

where $P_{\text{ref}}$ is a good approximation of the exact numerical solution.

The $\ell_2$ norm measure of error was computed for the Case 1 and Case 2 chip geometries at the frequencies of interest, namely the resonant frequencies of the fluid chamber. While particle migration could theoretically be simulated at any frequency, we are most interested in acoustophoretic behavior at the frequencies that characterize ejection in a 3D atomizer. The harmonic analyses conducted in the previous chapter were repeated at the chamber resonant frequencies with incremental mesh refinement performed. The h-discretization, or mesh refinement, was applied uniformly throughout the domain, as the acoustic harmonic solution (i.e., pressure field) is sensitive to the solution quality of the elastic harmonic solution outside the fluid domain. In the figures below, it was observed that a converged pressure field solution required a more refined mesh than a converged nozzle tip pressure amplitude.
Figure 4.3 Pressure error in the $\ell_2$ norm sense as a function of DOF for the pressure field computed in ANSYS at 2.150 MHz for the Case 1 chip geometry.

Figure 4.3 shows how the $\ell_2$ norm measure of error decreased for the Case 1 chip geometry at the 4th chamber resonance as the DOF were increased due to mesh refinement. The reference mesh contained over 3.6 million DOF. A summary of the error, as measured by the $\ell_2$ norm method, is given in Table 4.2 for all frequencies of interest. Of the chamber resonances, the largest error occurs at the highest resonant mode due to the increased number of wavelengths in the standing acoustic field; approximating a pressure field at a higher mode requires more DOF than at a lower mode.

A side-by-side comparison of the pressure field computed at each mesh is shown in Fig. 4.4 shows that the pressure field computed with 2,057,854 DOF (2.34% error) is practically identical to the reference mesh.
Figure 4.4 Fringe contour plots of the pressure amplitude for the Case 1 chip geometry at 2.150 MHz at each mesh refinement level: a) 236,103 DOF, b) 913,295 DOF, c) 2,057,854 DOF, and d) 3,637,078 DOF (reference).

By observation, the acoustic mode shapes computed using the 3 meshes of highest DOF are of equal resolution. To quantify the difference in another manner, Fig. 4.5 shows the convergence of the maximum pressure amplitude as the DOF are increased.
Figure 4.5 Convergence of the maximum pressure amplitude for the Case 1 chip geometry at 2.150 MHz.

The asymptotic behavior of the maximum pressure indicates strong convergence. The maximum pressure amplitude, which occurs at the tip of the 1st nozzle (closest to symmetry line), is computed to within 1.46% of the reference mesh value of 160.5 kPa at 913,295 DOF and within 0.33% at 2,057,854 DOF.

This is well within reasonable accuracy for the purposes of simulating particle migration behavior. In the previous chapter, differences were seen between the ANSYS acoustic solution and experimentally observed acoustic mode shapes. Those experimental uncertainties are greater than the numerical error shown in the figures above. Therefore, this level of mesh refinement (913,295 DOF for the Case 1 chip geometry) was used for simulating acoustophoretic particle trajectories in the subsequent sections of this chapter.

Table 4.2 Summary of Pressure Error at Each Mesh Refinement Level

<table>
<thead>
<tr>
<th>f (MHz)</th>
<th>236,103 DOF</th>
<th>913,295 DOF</th>
<th>2,057,854 DOF</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.620</td>
<td>0.137</td>
<td>0.057</td>
<td>0.028</td>
</tr>
<tr>
<td>1.110</td>
<td>0.678</td>
<td>0.089</td>
<td>0.029</td>
</tr>
<tr>
<td>1.665</td>
<td>2.495</td>
<td>0.431</td>
<td>0.106</td>
</tr>
<tr>
<td>2.150</td>
<td>11.885</td>
<td>2.338</td>
<td>0.524</td>
</tr>
</tbody>
</table>

4.3.2 Terminal Particle Distributions

For a given particle, the primary acoustic radiation force magnitude depends on the pressure amplitude and pressure gradient at the particle location. During actuation, particles in regions of high pressure amplitude and strong pressure gradients will quickly migrate away to regions of lower potential, i.e., to the pressure
nodes for a positive acoustic contrast factor particle. As shown in the previous chapter, the acoustic mode shapes within the 2D chip can have unusual shapes, with regions of high pressure gradient and regions of low pressure gradient in the same mode shape. Particles may focus to the pressure node quickly in some areas, while they may never quite reach the pressure node in other areas. Thus, a terminal distribution can be assumed when the overall particle population becomes stagnant (i.e., average particle velocity drops below a threshold value). By computing the average velocity magnitude of all particles ($V_{avg}$) at each time step, we can define an assumed terminal distribution as the state of the particles when $V_{avg}$ reaches 5% of its initial value. In the following particle simulation results, the stopping criterion for the iterative solution algorithm was satisfaction of the terminal condition.

$$V_{avg}^i = 0.05 \times V_{avg}^{i=0} \quad (4.11)$$

Figure 4.6 shows a typical time history plot of the average particle velocity normalized to the initial average velocity. The average velocity declines sharply soon after initialization as the particles migrate to the nodes and decelerate asymptotically to zero velocity. Theoretically, the velocity will never quite reach 0 because the pressure node computed from the harmonic simulation has an infinitesimal width, and because the time step $dt$ is finite. Once a particle reaches the pressure node, it oscillates back and forth due to the sign change of the local pressure gradient. Furthermore, the neglect of particle-particle interactions prevents the agglomeration of particles along pressure nodal lines as observed during experiments. Instead, particles are allowed to pass through one another or overlap at any location within the fluid chamber.

![Time History of Particle Motion](image)

**Figure 4.6** Time history plot of normalized, average particle velocity. Case 1 chip geometry at 1.110 MHz, 40 V$_{pp}$.
While the particles exhibit acoustophoretic motion throughout the entire fluid chamber, including within the curved inlet arms, the region of interest for observing particle migration and trapping is within the rectangular section of the chamber, and near the nozzles in particular. In Figs. 4.7 and 4.8, 1000 PS beads of 10 µm diameter were injected at random locations in the rectangular portion of the fluid chamber, including the nozzles, and their acoustophoretic motion was simulated in the Case 1 and Case 2 chip geometries at the ejection frequencies of each chip. It is evident that in regions exhibiting strong pressure gradients, the particles have migrated to a tight formation along the pressure nodes. Conversely, in regions where the pressure gradient is weaker, the particles have clearly migrated towards the pressure node; however, they have not yet achieved a narrow distribution along the pressure node. This behavior suggests that terminal particle distributions observed experimentally in the 2D visualization chips could potentially portray aspects of the standing acoustic field such as differences between regions of high pressure gradient and weaker pressure gradient.

**Figure 4.7** Initial and final particle distributions for Case 1 chip geometry, 10 µm-dia. PS beads.
Interestingly, the particles are most tightly focused at the 3\textsuperscript{rd} half-wave resonance (1.665 MHz) in the Case 1 geometry where the pressure mode shape is the most planar. Conversely, the mode shape resulting from the 2\textsuperscript{nd} half-wave resonance (1.110 MHz) shows a merger of the pressure node in the 3\textsuperscript{rd} nozzle with the pressure node that runs along the base of the fluid reservoir, which has led to a large region of low pressure gradient that exhibits high particle dispersion at steady-state. This result suggests that resonant frequencies with more planar mode shapes could potentially have higher particle trapping abilities in a 3D ultrasonic atomizer.

![Figure 4.8 Initial and final particle distributions for Case 2 chip geometry, 10 \textmu m-dia. PS beads.](image)

### 4.3.3 Transient Behavior of Particle Motion

Viewing the terminal particle distribution verifies that particle trajectories predicted using the described implementation in MATLAB are qualitatively correct; the PS particles, with a positive acoustophoretic contrast factor in water, migrate to the pressure nodes as expected. A more interesting observation is the transient motion of particles. In particular, observing the contrast in migration behavior of larger and smaller particles is noteworthy.

The acoustophoretic motion of 5 \textmu m and 20 \textmu m diameter PS beads suspended in water was observed simultaneously in the Case 3 chip geometry presented in the previous chapter at a frequency of 0.983 MHz, where strong particle motion was observed [31]. 20 \textmu m beads became more or less focused after approximately 12 seconds of actuation, while the 5 \textmu m beads remained significantly dispersed.
In Fig. 4.9 below, the experimental results (shown in black and white) are compared with particle trajectories predicted using the MATLAB particle motion simulation (shown in color), based on an ANSYS simulation of the Case 3 chip geometry at a frequency of 1.020 MHz and a driving voltage of 8.5 Vpp. The frequency of 1.020 MHz was chosen due to it coinciding with the local maxima in nozzle tip pressure amplitude and its similarity to the experimentally-observed acoustic mode shape revealed by the terminal particle distribution. The contrast in focusing speed between the smaller and larger particles was captured remarkably by the numerical simulation.

![Figure 4.9](image)

**Figure 4.9** Transient behavior of 5 and 20 µm diameter PS beads in the Case 3 chip geometry at a chamber resonance of 0.983 MHz (experiment; 1.020 MHz numerical model). Each image pair corresponds to the particle suspension after a) 0, b) 4, c) 8, and d) 12 seconds of actuation.

The drive voltage was adjusted so that the simulated transient behavior of the particles closely resembled the experimental images after 4, 8, and 12 seconds of actuation. In theory, the pressure amplitude of the acoustic field within the 2D chip could be measured based on the focusing speed of the particles, and this has been done in rectangular microchannels [26]. However, for complicated reservoir geometries such as the horned microarray represented by the 2D chips, this would require significant control over experimental variabilities and a very robust numerical model. Thus, it is outside the scope of the current work.

4.3.4 Particle Focusing Time

In the idealized case of a 1D standing half-wave pinned between two parallel plates, it has been shown with a scaling law argument that a particle’s focusing time \( \tau_{foc} \), defined as the time it takes for a particle to travel from one plate to the pressure node, is inversely proportional to the square of the particle radius [43].

\[
\tau_{foc} \propto \frac{1}{a^2}
\]

(4.11)

This is an interesting characteristic with regard to this work, as its applicability to a more complicated geometry can easily be tested. In the idealized case, all possible particle trajectories are known; a particle with a positive acoustic contrast factor will always travel in a direction perpendicular to the parallel plates until it reaches the pressure node. The pressure mode shapes characteristic of the rectangular channel with pyramidal horns are significantly more complex, and an infinite number of acoustophoretic particle trajectories are possible. However, the average path length can be approximated from the trajectories of several hundred particles injected at randomized starting points. Previously, we defined the assumed
terminal distribution as the state of the particles when the average velocity of the particles reached 5% of their initial average velocity. The time it takes to reach the terminal distribution, denoted \( \tau_t \), is analogous to focusing time and thus expected to have the same dependence on particle size.

In Fig. 4.10 below, the time required for a particle suspension to achieve its assumed terminal distribution was plotted as a function of PS particle radius at each acoustic resonant frequency of the Case 1 chip geometry. In each case, 2000 particles were injected at random locations of the fluid chamber in the vicinity of the nozzles. Particle migration behavior in the inlet arms was not considered. The data was fitted using MATLAB’s Curve Fitting Tool [65]. When plotting the linear regression of \( \tau_t \) vs \( 1/\alpha^2 \), the data fit the curve with an R-squared value greater than 0.998 at each resonant frequency. This result strongly suggests that \( \tau_t \) is analogous to focusing time in complex geometries when a large number of randomly dispersed particles are considered.

![Figure 4.10 Relationship between \( \tau_t \) and PS particle radius at chamber frequencies, Case 1 chip geometry, 40 Vpp.](image)

Parameters such as the time step, total number of particles, etc. are fixed during the transient computation, and cautionary steps were taken to ensure the results were reasonable. Since the particles are initialized at randomized locations, a large number of particles must be simulated to ensure the computed \( \tau_t \) is reliable. In order to assess this, each simulation was repeated with an increasing number of particles until the resulting \( \tau_t \) changed by no more than 2%. It was found that simulating 2000 particles adequately represented all possible particle trajectories in the fluid chamber.
The assumption of instantaneous acceleration combined with a finite time step allows for the simulation to displace particles at a constant velocity at each time step based on the local magnitude and direction of \( \mathbf{F}_{\text{rad}} \). A particle’s trajectory can be reasonably approximated with a sufficiently small time step. The maximum particle displacement at each time step was monitored so that large “jumps” could be avoided. When a large displacement (greater than 10 µm) occurred, the simulation was stopped so that the time step could be reduced.

Reducing the time step parameter has the consequence of significantly increasing the computational time, as for-loops in MATLAB are not efficient, yet this was unavoidable for this simulation. However, a second issue with having too large a time step parameter directly affected computation of \( \tau_t \). When the particles reach the pressure node, the finite time step can have the effect of causing the particles to oscillate about the pressure node. If the value of the time step is too large, the particles will oscillate with a velocity magnitude large enough to prevent the average particle velocity from decreasing as expected. To visualize this effect, 2000 PS particles of 6 µm diameter were simulated in the Case 1 chip geometry at 1.110 MHz at various time step values. The time history plot in Fig. 4.11 shows that too large a time step can result in an inaccurate computation of \( \tau_t \). In extreme cases, the particles may never reach the assumed terminal distribution at all, as evidenced by oscillations in the time history plot of normalized, average particle velocity. As the time step value is reduced, the simulation converges to a final value of \( \tau_t \). A similar sensitivity analysis was done for each case shown in Fig. 4.10, and the time step parameter was reduced until the computed \( \tau_t \) deviated by less than 2%. 
Some issues that arose during the development of this model include particles leaving the fluid domain, as well as hyper-focusing of the particles, where they would migrate to the nodes and become superimposed on one another. Both of these phenomena are due to neglect of particle-particle and particle-wall interactions in the model. Nonetheless, the results found with the simplistic model have highlighted some interesting behaviors. While the magnitude of the acoustic pressure amplitude directly affects the strength of $\mathbf{F}_{\text{rad}}$, the terminal particle distributions shown in Figs. 4.7 and 4.8 suggest that the energy density as displayed by the acoustic mode shape also may play a role in the particle retention capabilities of the 3D ultrasonic atomizer.

### 4.4 Summary

In summary, the model developed herein has successfully demonstrated accurate predictions of acoustophoretic particle motion in a quiescent fluid. The transient migratory behavior of 5 and 20 µm diameter PS beads agrees remarkably well with experiment. Additionally, it has been shown in a complicated geometry that the time it takes for a particle suspension to reach its assumed terminal distribution in a quiescent fluid is inversely proportional to the square of the particle radius.
Chapter 5

Conclusion

The goals of this thesis were to identify important variables that impact the operational performance of an ultrasonic droplet generator and to construct a model capable of predicting acoustophoretic particle trajectories in standing acoustic fields characteristic of the device.

A series of 48 harmonic response simulations were conducted in 2D geometries representing the device cross-section, supported by previously conducted experimental work, to investigate the effects of varying specific design parameters that significantly alter the resonant behavior of the device. Methods for predicting and identifying vibrational and acoustic resonances were established. The simulations provided insight into the coupled electrical and acoustic behavior of the device, which led to further improvement of the optimal case studied.

A simplistic MATLAB model was established to predict the migratory behavior of microparticles within standing acoustic fields generated from the harmonic response simulations, showing remarkable agreement with experimentally observed transient particle motion. In addition, the modeling results support an inverse-square relationship between particle focusing time and particle radius in complex geometries.

Having established models that accurately portray experimentally-observed acoustic microfluidic behavior, the following topics are suggested for future research:

- Develop an automated routine to search over a continuous space for the optimal design parameters for fluid ejection.
- Incorporate particle image velocimetry (PIV) measurements in experimental work to better quantify how accurately the acoustophoretic particle migration model predicts transient particle motion.
- Incorporate particle-particle and particle-wall collisions into the particle migration model.
- Design and fabricate 2D visualization chips that allow for fluid ejection, and incorporate the effects of bulk fluid flow in the acoustophoretic particle migration model. Other follow-up topics can be explored, including:
  - Establish a model that accurately predicts particle retention behavior due to particles becoming trapped in the standing acoustic field.
- Study the influence of design and other input parameters on particle retention behavior. This information would be useful for designing a device that separates a particle mixture by trapping specific particles and ejecting others, i.e. a filtering device.
- Assess the influence on particle retention of a limited number of nozzles ejecting vs all nozzles ejecting simultaneously.
References


