Research article

3D modeling of acoustofluidics in a liquid-filled cavity including streaming, viscous boundary layers, surrounding solids, and a piezoelectric transducer

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Abstract: We present a full 3D numerical simulation of the acoustic streaming observed in full-image micro-particle velocimetry by Hagsäter et al., Lab Chip 7, 1336 (2007) in a 2 mm by 2 mm by 0.2 mm microcavity embedded in a 49 mm by 15 mm by 2 mm chip excited by 2-MHz ultrasound. The model takes into account the piezo-electric transducer, the silicon base with the water-filled cavity, the viscous boundary layers in the water, and the Pyrex lid. The model predicts well the experimental results.

Keywords: Microscale acoustofluidics, acoustic streaming, numerical simulation, 3D modeling

1. Introduction and definition of the model system

For the past 15 years, ultrasound-based microscale acoustofluidic devices have successfully and in increasing numbers been used in the fields of biology, environmental and forensic sciences, and clinical diagnostics [1, 2, 3, 4, 5]. However, it remains a challenge to model and optimize a given device including all relevant acoustofluidic aspects. Examples of recent advances in modeling include Lei et al. [6], who modeled the three-dimensional (3D) fluid domain without taking the solid domain into account; Muller and Bruus [7, 8], who made detailed models in 2D of the thermoviscous and transient effects in the fluid domain; Gralinski et al. [9], who modeled circular capillaries in 3D with fluid and glass domains without taking absorption and outgoing waves into account, effects later taken into account by Ley and Bruus [10]; and Hahn and Dual [11], who studied a 3D model for a transducer-silicon-glass device including dissipation but not the actual fields in the boundary layers.

In this paper, we present a 3D model and its implementation in the commercial software COMSOL Multiphysics [12] of a prototypical acoustofluidic silicon-glass-based device that takes into account all main acoustofluidic aspects: the piezo-electric transducer driving the system, the silicon base that contains the acoustic cavity, the Pyrex lid, and a dilute microparticle suspension filling the cavity. The presented work represents the culmination and synthesis of our previous partial modeling of stream-
Figure 1. (a) Top-view photograph of the original transducer-silicon-glass device studied in 2007 by Hagsäter et al. [14]. (b) A cut-open 3D sketch of the device in the red-dashed area of panel (a) showing the Pz26 piezo-electric transducer (green), the silicon base (gray), the water-filled cavity (blue) in the top of the silicon base, and the Pyrex lid (orange).

Table 1. The length, width, and height $L \times W \times H$ (in mm) of the six rectangular elements in the acoustofluidic device model of Fig. 1(b): The piezoelectric transducer (pz), the silicon base (si), the Pyrex lid (py), the main cavity (ca), and the two inlet channels (c1) and (c2).

<table>
<thead>
<tr>
<th>Element</th>
<th>$L \times W \times H$ (in mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pz26</td>
<td>$49 \times 15 \times 1.0$</td>
</tr>
<tr>
<td>Silicon</td>
<td>$49 \times 15 \times 0.5$</td>
</tr>
<tr>
<td>Pyrex</td>
<td>$49 \times 15 \times 0.5$</td>
</tr>
<tr>
<td>Cavity</td>
<td>$2 \times 2.02 \times 0.2$</td>
</tr>
<tr>
<td>Channel 1</td>
<td>$11.3 \times 0.4 \times 0.2$</td>
</tr>
<tr>
<td>Channel 2</td>
<td>$12.4 \times 0.4 \times 0.2$</td>
</tr>
</tbody>
</table>

We summarize the coupled equations of motion for a system driven by a time-harmonic electric potential, $\tilde{\varphi} = \varphi_0 e^{-i\omega t}$ applied to selected boundaries of a piezo-electric Pz26 ceramic. Here, tilde denotes a field with harmonic time dependency, $\omega$ is the angular frequency in the low MHz range, and “$i$” is the imaginary unit. This harmonic boundary condition excites the time-harmonic fields: the electric potential $\tilde{\varphi}(r, t)$ in the Pz26 ceramic, the displacement $\tilde{u}(r, t)$ in the solids, and the acoustic pressure $\tilde{p}_1(r, t)$ in the water,

$$\tilde{\varphi}(r, t) = \varphi(r) e^{-i\omega t}, \quad \tilde{u}(r, t) = u(r) e^{-i\omega t}, \quad \tilde{p}_1(r, t) = p_1(r) e^{-i\omega t}. \quad (2.1)$$
In our simulation, we first solve the linear equations of the amplitude fields \( \varphi(r) \), \( u(r) \), and \( p_1(r) \). Then, based on time-averaged products (over one oscillation period) of these fields, we compute the nonlinear acoustic radiation force \( F_{\text{rad}} \) and the steady-state acoustic streaming velocity \( v_2(r) \).

2.1. Linear acoustics in the fluid

In the fluid (water) of density \( \rho_{\text{fl}} \), sound speed \( c_{\text{fl}} \), dynamic viscosity \( \eta_{\text{fl}} \), and bulk viscosity \( \eta_{\text{bfl}} \), we model the acoustic pressure \( p_1 \) as in Ref. [10],

\[
\nabla^2 p_1 = -\frac{\omega^2}{c_{\text{fl}}^2} (1 + i \Gamma_{\text{fl}}) p_1, \quad v_1 = -i \frac{1 - i \Gamma_{\text{fl}}}{\omega \rho_{\text{fl}}} \nabla p_1, \quad \Gamma_{\text{fl}} = \left( \frac{4}{3} \eta_{\text{fl}} + \eta_{\text{bfl}} \right) \omega \kappa_{\text{fl}}.
\]

(2.2)

Here, \( v_1 \) is the acoustic velocity which is proportional to the pressure gradient \( \nabla p_1 \), while \( \Gamma_{\text{fl}} \ll 1 \) is a weak absorption coefficient, and \( \kappa_{\text{fl}} = (\rho_{\text{fl}} c_{\text{fl}}^2)^{-1} \) is the isentropic compressibility of the fluid, see Table 2 for parameter values. The time-averaged acoustic energy density \( E_{\text{ac}}^{\text{fl}} \) in the fluid domain is the sum of the time-averaged (over one oscillation period) kinetic and compressional energy densities,

\[
E_{\text{ac}}^{\text{fl}} = \frac{1}{4} \rho_{\text{fl}} |v_1|^2 + \frac{1}{4} \kappa_{\text{fl}} |p_1|^2.
\]

(2.3)

2.2. Linear elastic motion of the solids

In the solid materials, each with a given density \( \rho_{\text{sl}} \), we model the displacement field \( u \) using the equation of motion given by [10]

\[
-\rho_{\text{sl}} \omega^2 (1 + i \Gamma_{\text{sl}}) u = \nabla \cdot \sigma,
\]

(2.4)

where \( \Gamma_{\text{sl}} \ll 1 \) is a weak damping coefficient. Here, \( \sigma \) is the stress tensor, which is coupled to \( u \) through a stress-strain relation depending on the material-dependent elastic moduli. The time-averaged acoustic energy density in the solids is given by the sum of kinetic and elastic contributions,

\[
E_{\text{ac}}^{\text{sl}} = \frac{1}{4} \rho_{\text{sl}} \omega^2 |u|^2 + \frac{1}{4} \text{Re} \left[ (\nabla u) : \sigma^* \right].
\]

(2.5)

where “Re” denotes the real value and “\(^*\)” the complex conjugate of a complex number, respectively.

Table 2. Material parameters at 25 °C for isotropic Pyrex borosilicate glass [15], cubic-symmetric silicon [16], and water [7]. Note that \( c_{12} = c_{11} - 2c_{44} \) for isotropic solids.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Pyrex</th>
<th>Si</th>
<th>Unit</th>
<th>Parameter</th>
<th>Water</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass density ( \rho_{\text{sl}} )</td>
<td>2230</td>
<td>2329</td>
<td>kg m(^{-3})</td>
<td>Mass density ( \rho_{\text{fl}} )</td>
<td>997.05</td>
<td>kg m(^{-3})</td>
</tr>
<tr>
<td>Elastic modulus ( c_{11} )</td>
<td>69.72</td>
<td>165.7</td>
<td>GPa</td>
<td>Sound speed ( c_{\text{fl}} )</td>
<td>1496.7</td>
<td>m s(^{-1})</td>
</tr>
<tr>
<td>Elastic modulus ( c_{44} )</td>
<td>26.15</td>
<td>79.6</td>
<td>GPa</td>
<td>Dyn. viscosity ( \eta_{\text{fl}} )</td>
<td>2.485</td>
<td>mPa s</td>
</tr>
<tr>
<td>Elastic modulus ( c_{12} )</td>
<td>17.43</td>
<td>63.9</td>
<td>GPa</td>
<td>Bulk viscosity ( \eta_{\text{bfl}} )</td>
<td>0.890</td>
<td>mPa s</td>
</tr>
<tr>
<td>Damping coeff. ( \Gamma_{\text{sl}} )</td>
<td>0.0004</td>
<td>0.0000</td>
<td>1</td>
<td>Damping coeff. ( \Gamma_{\text{fl}} )</td>
<td>0.00002</td>
<td>1</td>
</tr>
<tr>
<td>–</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>Compressibility ( \kappa_{\text{fl}} )</td>
<td>452</td>
<td>TPa(^{-1})</td>
</tr>
</tbody>
</table>
2.3. Stress-strain coupling in elastic solids

For a crystal with either cubic or isotropic symmetry, the relation between the stress tensor $\sigma_{ij}$ and strain components $\frac{1}{2}(\partial_x u_j + \partial_j u_i)$ is given in the compact Voigt representation as [17]

$$
\begin{bmatrix}
\sigma_{xx} \\
\sigma_{yy} \\
\sigma_{zz} \\
\sigma_{yz} \\
\sigma_{xz} \\
\sigma_{xy}
\end{bmatrix}
= \begin{bmatrix}
c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\
c_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\
c_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\
0 & 0 & 0 & c_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & c_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & c_{44}
\end{bmatrix}
\begin{bmatrix}
\partial_x u_x \\
\partial_y u_y \\
\partial_z u_z \\
\partial_y u_x + \partial_x u_y \\
\partial_z u_x + \partial_x u_z \\
\partial_z u_y + \partial_y u_x
\end{bmatrix},
$$

for Pyrex and silicon. (2.6)

Here, $c_{ij}$ are the elastic moduli which are listed for Pyrex and silicon in Table 2.

2.4. Stress-strain coupling in piezoelectric ceramics

Lead-zirconate-titanate (PZT) ceramics are piezoelectric below their Curie temperature, which typically is $200 - 400 \, ^\circ C$. Using Cartesian coordinates and the Voigt notation for a PZT ceramic, the mechanical stress tensor $\sigma_{ij}$ and electric displacement field $D_i$ are coupled to the mechanical strain components $\frac{1}{2}(\partial_x u_j + \partial_j u_i)$ and the electrical potential $\varphi$ through the relation [17]

$$
\begin{bmatrix}
\sigma_{xx} \\
\sigma_{yy} \\
\sigma_{zz} \\
\sigma_{yz} \\
\sigma_{xz} \\
\sigma_{xy}
\end{bmatrix}
= \begin{bmatrix}
c_{11} & c_{12} & c_{13} & 0 & 0 & -e_{31} \\
c_{12} & c_{11} & c_{13} & 0 & 0 & -e_{31} \\
c_{13} & c_{13} & c_{33} & 0 & 0 & -e_{31} \\
0 & 0 & 0 & c_{44} & 0 & -e_{15} \\
0 & 0 & 0 & 0 & c_{44} & -e_{15} \\
0 & 0 & 0 & 0 & 0 & c_{66}
\end{bmatrix}
\begin{bmatrix}
\partial_x u_x \\
\partial_y u_y \\
\partial_z u_z \\
\partial_y u_x + \partial_x u_y \\
\partial_z u_x + \partial_x u_z \\
\partial_z u_y + \partial_y u_x
\end{bmatrix},
$$

for Pz26. (2.7)

The values of the material parameters for the PZT ceramic Pz26 are listed in Table 3. Due to the high electric permittivity of Pz26, we only model the electric potential $\varphi$ in the transducer, and since we assume no free charges here and only low-MHz frequencies, $\varphi$ must satisfy the quasi-static equation,

$$\nabla \cdot D = 0, \quad \text{for Pz26.}$$

(2.8)

### Table 3. Material parameters of Ferroperm Ceramic Pz26 from Meggitt A/S [18]. Isotropy in the $x$-$y$ plane implies $e_{66} = \frac{1}{2}(e_{11} - e_{12})$. The damping coefficient is $\Gamma_{sl} = 0.02$ [11].

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Parameter</th>
<th>Value</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho_{sl}$</td>
<td>7700 kg/m$^3$</td>
<td>$\epsilon_{11}$</td>
<td>828 $\epsilon_0$</td>
<td>$\epsilon_{33}$</td>
<td>700 $\epsilon_0$</td>
</tr>
<tr>
<td>$c_{11}$</td>
<td>168 GPa</td>
<td>$c_{33}$</td>
<td>123 GPa</td>
<td>$\epsilon_{31}$</td>
<td>$-2.8$ C/m$^2$</td>
</tr>
<tr>
<td>$c_{12}$</td>
<td>110 GPa</td>
<td>$\epsilon_{44}$</td>
<td>30.1 GPa</td>
<td>$\epsilon_{33}$</td>
<td>14.7 C/m$^2$</td>
</tr>
<tr>
<td>$c_{13}$</td>
<td>99.9 GPa</td>
<td>$c_{66}$</td>
<td>29.0 GPa</td>
<td>$\epsilon_{15}$</td>
<td>9.86 C/m$^2$</td>
</tr>
</tbody>
</table>
2.5. Boundary conditions and boundary layers in the fluid at the fluid-solid interfaces

The applied boundary conditions are the usual ones, namely that (1) the stress and the velocity fields are continuous across all fluid-solid and solid-solid interfaces, (2) the stress is zero on all outer boundaries facing the air, (3) the piezoelectric ceramic is driven by a given electric potential at specified surfaces that represent the presence of infinitely thin, massless electrodes, and (4) there are no free charges on the surface of the ceramic. The influence \((A \leftarrow B)\) on domain A from domain B with the surface normal \(n\) pointing into A, is given by

\[
\begin{align*}
Pz26 \text{ domain } \leftarrow \text{phase electrode:} & \quad \varphi = \varphi_0, \quad \text{(2.9a)} \\
Pz26 \text{ domain } \leftarrow \text{ground electrode:} & \quad \varphi = 0, \quad \text{(2.9b)} \\
Pz26 \text{ and solid domain } \leftarrow \text{air:} & \quad \sigma \cdot n = 0 \quad \text{and} \quad n \cdot D = 0, \quad \text{(2.9c)} \\
\text{Solid domain } \leftarrow \text{fluid:} & \quad \sigma \cdot n = -p_1 n - i k_s \eta_0 (v_{sl} - v_1), \quad \text{(2.9d)} \\
\text{Fluid domain } \leftarrow \text{solid:} & \quad v_1 \cdot n = v_{sl} \cdot n - \frac{1}{k_s} \nabla \parallel \cdot (v_{sl} - v_1)\parallel. \quad \text{(2.9e)}
\end{align*}
\]

While the overall structure of these boundary conditions is the usual continuity in stress and velocity, the details of Eqs. (2.9d) and (2.9e) are not conventional. They are the boundary conditions for the surface stress \(\sigma \cdot n\) of Eq. (2.4) and the acoustic velocity \(v_1\) of Eq. (2.2) (proportional to the gradient of the acoustic pressure \(p_1\)) derived by Bach and Bruus using their recent effective pressure-acoustics theory [13]. In this theory, the viscous boundary layer of thickness \(\delta = \sqrt{2 \eta_0 / (\rho_0 \omega)} \approx 0.35 \mu m\) at 2.3 MHz has been taken into account analytically. As a result, terms appear in Eqs. (2.9d) and (2.9e) that involve the shear-wave number \(k_s = (1 + i) \delta^{-1}\) as well as the tangential divergence of the tangential component of the difference between the solid-wall velocity \(v_{sl} = -i \omega u\) and the acoustic velocity \(v_1\) at the fluid-solid interface. This boundary condition also takes into account the large dissipation in the boundary layers, which leads to an effective damping coefficient \(\Gamma_{\text{eff}} \approx \frac{\delta}{H} \approx 0.002\), the ratio of the boundary layer width \(\delta\) to the device height \(H\) [7, 11, 13]. Remarkably, this boundary-layer dissipation dominates dissipation in the fluid domain, because \(\Gamma_{\text{eff}} \ll 1\).

2.6. The acoustic streaming

The acoustic streaming is the time-averaged (over one oscillation period), steady fluid velocity \(v_2\) that is induced by the acoustic fields. In our recent analysis [13], we have shown that the governing equation of \(v_2\) corresponds to a steady-state, incompressible Stokes flow with a body force in the bulk due to the time-averaged acoustic dissipation proportional to \(\Gamma_{\text{eff}}\). Further, at fluid-solid interfaces, the slip velocity \(v_{2bc}\) takes into account both the motion of the surrounding elastic solid and the Reynolds stress induced in viscous boundary layer in the fluid,

\[
\begin{align*}
\nabla \cdot v_2 &= 0, \quad \eta_0 \nabla^2 v_2 = \nabla p_2 - \frac{\Gamma_{\text{eff}} \omega}{2 c_s^2} \text{Re} \left[ p_1^i v_1 \right], \quad v_2 = v_{2bc}, \quad \text{at fluid-solid interfaces,} \quad \text{(2.10a)} \\
\n\cdot v_{2bc} &= 0, \quad (1 - nn) \cdot v_{2bc} = -\frac{1}{8 \omega} \nabla \parallel v_{1\parallel}^2 - \text{Re} \left[ \left( 2 - \frac{i}{4 \omega} \nabla \parallel v_{1\parallel}^* + \frac{i}{2 \omega} \partial_{\perp} v_{1\perp}^\perp \right) v_{1\parallel} \right]. \quad \text{(2.10b)}
\end{align*}
\]

Here, we have used a special case of the slip velocity \(v_{2bc}\), which is only valid near acoustic resonance, where the magnitude \(|v_1|\) of the acoustic velocity in the bulk is much larger than \(\omega |u_{sl}|\) of the walls.
2.7. The acoustic radiation force and streaming drag force on suspended microparticles

The response of primary interest in acoustofluidic applications, is the acoustic radiation force \( F_{\text{rad}} \) and the Stokes drag from the acoustic streaming \( v_2 \) acting on suspended microparticles. In this work, we consider 1- and 5-\( \mu \)m-diameter spherical polystyrene "Styron 666" (ps) particles with density \( \rho_{\text{ps}} \) and compressibility \( \kappa_{\text{ps}} \). For such large microparticle suspended in water of density \( \rho_{\text{fl}} \) and compressibility \( \kappa_{\text{fl}} \), thermoviscous boundary layers can be neglected, and the monopole and dipole acoustic scattering coefficients \( f_0 \) and \( f_1 \) are real numbers given by [19],

\[
\begin{align*}
\frac{f_0}{f_1} &= 1 - \frac{\kappa_{\text{ps}}}{\kappa_{\text{fl}}} = 0.468, \\
\frac{f_1}{f_0} &= \frac{2(\rho_{\text{ps}} - \rho_{\text{fl}})}{2\rho_{\text{ps}} + \rho_{\text{fl}}} = 0.034. 
\end{align*}
\]  

(2.11a)

Given an acoustic pressure \( p_1 \) and velocity \( v_1 \), a single suspended microparticle of radius \( a \), experience an acoustic radiation force \( F_{\text{rad}} \), which, since \( f_0 \) and \( f_1 \) are real, is given by the potential \( U_{\text{rad}} \) [20],

\[
F_{\text{rad}} = -\nabla U_{\text{rad}}, \quad \text{where} \quad U_{\text{rad}} = \frac{4\pi}{3} a^3 \left( f_0 \frac{1}{4} \kappa_{\text{fl}} |p_1|^2 - f_1 \frac{3}{8} \rho_{\text{fl}} |v_1|^2 \right). 
\]  

(2.11b)

The microparticle is also influenced by a Stokes drag force \( F_{\text{drag}} = 6\pi \eta_{\text{fl}} a (v_2 - v_{ps}) \), where \( v_2 \) and \( v_{ps} \) is the streaming velocity and the polystyrene particle velocity at the particle position \( r_{ps}(t) \), respectively. In the experiments, the streaming and particle velocities are smaller than \( v_0 = 1 \text{ mm/s} \), which for a 5-\( \mu \)m-diameter particle corresponds to a small particle-Reynolds number \( \frac{1}{\rho_{\text{fl}} \eta_{\text{fl}} v_0} = 0.6 \). Consequently, we can ignore the inertial effects and express the particle velocity for a particle at position \( r \) from the force balance \( F_{\text{rad}} + F_{\text{drag}} = 0 \), between the acoustic radiation force and streaming drag force,

\[
v_{ps}(r) = v_2(r) + \frac{1}{6\pi \eta_{fl} a} F_{\text{rad}}(r). 
\]  

(2.12)

The particle trajectory \( r_{ps}(t) \) is then determined by straightforward time integration of \( \frac{d}{dt} r_{ps} = v_{ps}(r_{ps}) \).

2.8. Numerical implementation

Following the procedure described in Ref. [10], including mesh convergence tests, the coupled field equations (2.2) and (2.4) for the fluid pressure \( p_1 \) and elastic-solid displacement \( u \) are implemented directly in the finite-element-method software Comsol Multiphysics 5.3a [12] using the weak form interface “PDE Weak Form”. We extend the model of Ref. [10] by including the transducer with the piezoelectric stress-strain coupling Eq. (2.6) and implementing the governing equation (2.8) for the electric potential \( \varphi \) in weak form. Similarly, the boundary conditions Eq. (2.9) are implemented in weak form. In a second step, we implement Eq. (2.10) for the acoustic streaming \( v_2 \) in weak form. Finally, the acoustic radiation force \( F_{\text{rad}} \) acting on the particles is calculated from Eq. (2.11) using the acoustic pressure \( p_1 \) and velocity \( v_1 \), and subsequently in a third step, following Ref. [21], we compute the particle trajectories \( r_{ps}(t) \) from the time-integration of Eq. (2.12).

We optimize the mesh to obtain higher resolution in the water-filled cavity, where we need to calculate numerical derivatives of the resulting fields to compute the streaming and radiation forces, and less in the surrounding solids and in the transducer. We ensure having at least six nodal points per wave length in all domains, which for the second-order test function we use, corresponds to maximum mesh
sizes of 0.52 mm, 0.59 mm, 0.50 mm, and 0.22 mm in the domains of Pz26, silicon, Pyrex, and water, respectively. The final implementation of the model contains 1.1 and 0.4 million degrees of freedom for the first- and second-order fields, respectively. On our workstation, a Dell Inc Precision T7500 Intel Xeon CPU X5690 at 3.47 GHz with 128 GB RAM and 2 CPU cores, the model requires 45 GB RAM and takes 18 min per frequency. When running frequency sweeps of up to 70 frequency values, we used the DTU high-performance computer cluster requiring 464 GB RAM and 11 min per frequency.

3. Results for the transducer-glass-silicon acoustofluidic device

We apply the 3D model of Section 2 to the transducer-glass-silicon acoustofluidic device by Hagsäter et al. [14], shown in Fig. 1 and using the parameter values listed in Tables 1, 2, and 3. In Fig. 2 we compare the experimental results from Ref. [14] with our model simulations. In Fig. 2(a1) we show the measured micro-particle image velocimetry (micro-PIV) results obtained

![Figure 2](image_url)

**Figure 2.** (a1) Micro-PIV measurements adapted from Ref. [14] of the particle velocity $v_{ps}$ after 1 ms (gray arrows, maximum 200 µm/s) superimposed on a micrograph of the final positions (black curved bands) of 5-µm-diameter polystyrene particles in water with a standing ultrasound wave at 2.17 MHz. (a2) Same as panel (a1), but for 1-µm-diameter polystyrene particles moving in a 6-by-6 flow roll pattern without specific final positions. (b1) Numerical 3D COMSOL modeling with actuation voltage $\varphi_0 = 10$ V of the acoustic potential $U^{rad}$ from $-1.2$ fJ (black) to 3.5 fJ (orange) and the velocity (gray arrows, maximum 500 µm/s) after 1 ms of 5-µm-diameter polystyrene particles in the horizontal center plane of the water-filled cavity at the resonance $f = 2.292$ MHz. (b2) Numerical modeling at the same conditions as in panel (b1), but at the slightly higher frequency 2.297 MHz, of the particle velocity $v_{ps}$ (magenta vectors) and its magnitude $v_{ps}$ from 0 (black) to 400 µm/s (white) of 1-µm-diameter polystyrene particles.
on a large number of 5-µm-diameter tracer particles at an excitation frequency of 2.17 MHz. The yellow arrows indicate the velocity of the tracer particles 1 ms after the ultrasound has been turned on, and the black bands are the tracer particles focused at the minimum of the acoustic potential $U_{rad}$ after a couple of seconds of ultrasound actuation. A clear pattern of 3 wavelengths in each direction is observed. Similarly, in Fig. 2(a2) is shown the micro-PIV results for the smaller 1-µm-diameter tracer particles. It is seen that these particles, in contrast to the larger particles, are not focused but keep moving in a 6-by-6 flow roll pattern. This result is remarkable, as the conventional Rayleigh streaming pattern [7, 8, 21] has four streaming rolls per wavelength oriented in the vertical plane, but here is only seen two rolls per wavelength, and they are oriented in the horizontal plane.

In Fig. 2(b1) and (b2) we see that our model predicts the observed acoustofluidics response qualitatively for both the larger and the smaller tracer particles. Even the uneven local amplitudes of the particle velocity $v_{ps}$ in the 6-by-6 flow roll pattern, which shifts around as the frequency is changed 5 kHz, is in accordance with the observations. In Ref. [14] it is mentioned that “If the frequency is shifted slightly in the vicinity of 2.17 MHz, the same vortex pattern will still be visible, but the strength distribution between the vortices will be altered.”. We chose the 5-kHz higher frequency in Fig. 2(b2) to obtain a pattern similar to the observed one.

Quantitatively, we find the following. The acoustic resonance is located at 2.29 MHz, approximately 6 % higher than the experimental value of 2.17 MHz. This disagreement may be due to the fact that we had to assume a certain length and width of the Pz26 transducer, because its actual size was not reported in Ref. [14]. Another source of error is that we have not modeled the coupling gel used in the experiment between the Pz26 transducer and the silicon base. Moreover, because the actual actuation voltage in the experiment has not been reported, we use $\phi_0 = 10$ V corresponding to the 20 V peak-to-peak function generator mentioned in Ref. [14]. With these assumption we compute the velocity $v_{ps} \approx 550$ µm/s for the large 5-µm-diameter, only a factor of 2.5 higher than the 200 µm/s reported in the experiment.

![Figure 3](image-url)
In Fig. 3 we show another result that is in agreement with the experimental observations, namely the particle trajectories $r_{ps}(t)$ for suspensions of tracer particles of different size. The larger 5-µm-diameter particles are focused along the bottom of the troughs in the acoustic potential $U_{rad}$, shown in Fig. 2(b1), after a short time $\frac{1}{12}(2 \text{ mm})/(550 \mu\text{m}/\text{s}) \approx 0.3$ s, forming the red wavy bands in Fig. 3(a) very similar to the observed black bands in Fig. 2(a1). In contrast, the smaller 1-µm-diameter particles are caught by the 6-by-6 streaming vortex pattern and swirl around without being focused, at least within the first 1.5 s as shown in Fig. 3(b), in full agreement with the experimental observation shown in Fig. 2(a2).

4. Discussion

Our full 3D numerical model, which takes into account the piezo-electric transducer, the silicon base with the water-filled cavity, the viscous boundary layers in the water, and the Pyrex lid, has been validated both qualitatively and quantitatively by comparing the results for the acoustic radiation force, for the streaming velocity, and for the trajectories of tracer particles of two different sizes with the decade-old experimental results presented by Hagsäter et al. [14]. However, we did find that although the determination of the first-order pressure $p_1$ and the acoustic potential $U_{rad}$ is fairly robust, the computation of the streaming velocity $\nu_2$ from the Stokes equation (2.10a) is sensitive to the exact value of the frequency and of the detailed shape of the fluid solid interface. To lower this sensitivity, we artificially increased the damping $\Gamma_{fl}$ by a factor of 4 in the second term of (2.10a), the so-called Eckart bulk force due to dissipation in the bulk away from the viscous boundary layers. This increase has been introduced in the computation of Figs. 2(b2) and 3(b). Remarkably, as predicted by Bach & Bruus (2018), this Eckart term is responsible for the characteristic 6-by-6 flow pattern for the small 1-µm-diameter particles. While Fig. 3(b) shows the flow rolls appearing with a 4-fold increased Eckart term, Fig. 3(c) reveals that the flow rolls disappear completely, when the Eckart term is suppressed. In this case, the particle motion in the horizontal plane have clear divergent behavior, similar to that of the large particles due to the radiation force. This conclusion runs contrary to the conventional wisdom that the Eckart bulk force is only important in systems of a size, which greatly exceeds the acoustic wave length. Here, in a system of the size of three acoustic wavelengths, we find that the existence of in-plane flow rolls are controlled by the Eckart bulk force. This phenomenon deserves a much closer study in future work.

While our model takes many of the central aspects of acoustofluidics into account, it can still be improved. One possible improvement would be to include the influence of heating on the material parameters as in Ref. [7]. One big challenge in this respect is to determine the material parameters of the solids, which may be temperature and frequency dependent. Another difficult task is to model the coupling between the transducer and the chip, which in experiments typically are coupled using coupling gels or other ill-characterized adhesives. The last point we would like to raise is use of the simple Stokes drag law on the suspended particles in the cavity. Clearly, this model may be improved by including particle-wall effects and particle-particle interactions. However, as direct simulations of both of these effects are very memory consuming their implementation would require effective models.
5. Conclusion

We have described the implementation of a full 3D modeling of an acoustofluidic device where we have taken into account the viscous boundary layers and acoustic streaming in the fluid, the vibrations of the solid material, and the piezoelectricity in the transducer. As such, our simulation is in many ways close to a realistic device, which is also reflected in the agreement between the simulation and the experiment shown in Figs. 2 and 3. Our model has correctly predicted the unusual streaming pattern observed in the device: a 6-by-6 flow roll pattern in the horizontal plane, much different form the 12-by-2 Rayleigh streaming pattern expected in the horizontal plan. Moreover, our model has revealed the surprising importance of the Eckart bulk force in a device with a size comparable to the acoustic wavelength. In future work, we must analyze the sensitivity of the streaming velocity, and how to avoid the artificial four-fold increase of the Eckart bulk force.

By introducing the model, we have demonstrated that simulations can be used to obtain detailed information about the performance of an acoustofluidic device in 3D. Such simulations are likely to be useful for studies of the basic physics of acoustofluidics as well as for engineering purposes, such as improving existing microscale acoustofluidic devices.

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Conflict of interest

All authors declare no conflicts of interest in this paper.

References


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