Simulation of SAW-Driven Microparticle Acoustophoresis Using COMSOL Multiphysics®

Nitesh Nama¹, R. Barnkob², C. J. Kähler², F. Costanzo¹, and T. J. Huang¹

¹ Department of Engineering Science and Mechanics
The Pennsylvania State University, State College, PA, USA

² Institute of Fluid Mechanics and Aerodynamics
Bundeswehr University Munich, Neubiberg, Germany
Outline

- Introduction
- Numerical scheme
- Model validation
- COMSOL Modeling and convergence
- Results
- Conclusion and Outlook
Acoustofluidics
Integration of acoustics with microfluidics

Acoustic Streaming

- Oscillating boundaries
- Time-averaged motion of the fluid

Useful for fluid and particle manipulation

Acoustic Radiation Force

- Scattering of incident acoustic waves from the particles
- ARF acting towards pressure node or antinode

Tatsuno et al, Album Fluid Motion, 1982.


\[ F^{\text{rad}} = -\pi a^3 \left[ \frac{2k_0}{3} \text{Re} [f_1^* p_{in}^* \nabla p_{in}] - \rho_0 \text{Re} [f_2^* v_{in}^* \cdot \nabla v_{in}] \right] \]
Surface Acoustic Wave (SAW) systems have gained prominence for various lab-on-a-chip applications.

Questions:
- Type of acoustic fields setup inside the channel?
- Effect of PDMS walls as opposed to harder materials (e.g. silicon)
- Critical transition size for particle motion inside the microchannel?
Governing equations

Balance of mass

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

Balance of linear momentum

\[ \rho \frac{\partial \mathbf{v}}{\partial t} + \rho (\mathbf{v} \cdot \nabla) \mathbf{v} = -\nabla p + \mu \nabla^2 \mathbf{v} + \left( \mu_b + \frac{1}{3} \mu \right) \nabla (\nabla \cdot \mathbf{v}) \]

Constitutive relation

\[ p = c_0^2 \rho \]

Numerical Challenges:

- Widely separated time scales – Characteristic oscillation period \((10^{-7} \text{ s})\) vs. characteristic times dictated by streaming speeds \((10^{-1} \text{ s})\)
The nonlinear problem is divided into two sets to linear equations which can be solved successively.

**Numerical Scheme**: COMSOL Multiphysics 5.1 with P2-P1 elements for velocity and pressure.
Model System and Boundary conditions

Impedance condition on the channel walls (PDMS)

\[ n \cdot \nabla p_1 = i \frac{\omega \rho_0}{\rho_m c_m} p_1 \]

Standing SAW displacement on the bottom wall

\[ u_y(t, y) = 0.6u_0 e^{-C_{ay}} \left[ \sin \left( \frac{-2\pi(y - w/2)}{\lambda} + \omega t - \Delta \phi \right) 
+ \sin \left( \frac{-2\pi(w/2 - y)}{\lambda} + \omega t \right) \right], \]

\[ u_z(t, y) = -u_0 e^{-C_{ay}} \left[ \cos \left( \frac{-2\pi(y - w/2)}{\lambda} + \omega t - \Delta \phi \right) 
+ \cos \left( \frac{-2\pi(w/2 - y)}{\lambda} + \omega t \right) \right], \]

The displacement on the bottom wall was adopted from the results of numerical simulations by Gantner.

Step 1: Assume a solution for both pressure and velocity.

Step 2: Plug into PDEs to get the forcing and boundary conditions.

\[
\begin{align*}
\frac{\partial v}{\partial t} & - \nu_1 \Delta v - \nu_2 \nabla (\nabla \cdot v) + \nabla p = f_v \\
\frac{\partial p}{\partial t} + \nabla \cdot v & = f_p \\
v & = g
\end{align*}
\]
in \( \Omega \), \( t > 0 \)
on \( \partial \Omega \), \( t > 0 \)

Step 3: Use the computed forcing and boundary conditions in the numerical model to obtain a solution.

Step 4: Compare the obtained solution with the assumed solution.
COMSOL Modeling and convergence

- Weak PDE interface
- Parametric sweep over mesh size.
- Finer mesh near the boundaries to resolve the boundary layers.

\[ C(g) = \sqrt{\frac{\int (g - g_{\text{ref}})^2 \, dy \, dz}{\int (g_{\text{ref}})^2 \, dy \, dz}} \]

Here, \( g_{\text{ref}} \) = most refined solution

- Slower convergence of second-order fields since they depend on the gradients of first-order fields.
**Impedance Sweep**

- Convergence to hard wall solution on increasing impedance of the wall.

- Resonances similar to hard wall system were observed for high values of impedances.

- Hard wall conditions suitable for bulk acoustic wave (BAW) systems but not SAW systems.

\[
C(g) = \sqrt{\frac{\int (g - g_{\text{ref}})^2 \, dy \, dz}{\int (g_{\text{ref}})^2 \, dy \, dz}}
\]

Here, \( g_{\text{ref}} \) = hard wall solution
Acoustic fields

Bulk Acoustic Wave (BAW) Device

\[ n \cdot \nabla p_1 = i \frac{\omega \rho_0}{\rho_m c_m} p_1 \]

Particle tracking

Radiation Force

\[
F^{\text{rad}} = -\pi a^3 \left[ \frac{2\kappa_0}{3} \text{Re}[f_1^* p_1^* \nabla p_1] - \rho_0 \text{Re}[f_2^* v_1^* \cdot \nabla v_1] \right]
\]

\[
f_1 = 1 - \frac{\kappa_p}{\kappa_0} \quad \text{and} \quad f_2 = \frac{2(1 - \gamma)(\rho_p - \rho_0)}{2\rho_p + \rho_0(1 - 3\gamma)}
\]

\[
\gamma = -\frac{3}{2}[1 + \nu(1 + \tilde{\delta})]\tilde{\delta}, \quad \tilde{\delta} = \frac{\delta}{a}, \quad \delta = \sqrt{\frac{\mu}{\pi f \rho_0}}
\]

Hydrodynamic Drag Force

\[
F^{\text{drag}} = 6\pi \mu a (\langle v_2 \rangle - v^{\text{bead}})
\]

\[
m_p a_p = F^{\text{rad}} + F^{\text{drag}}
\]

Newton’s Second Law

\[
v^{\text{bead}} = \langle v_2 \rangle + \frac{F^{\text{rad}}}{6\pi \mu a}
\]
Particle tracking

Vertical focusing: probably due to gravity

Application: Phase Sweep

- Displacement of pressure node by changing the phase of one IDT


\[
\Delta x = \frac{1}{2k} \varphi = \frac{\lambda}{720^\circ} \varphi \quad \varphi \in [0^\circ, 360^\circ]
\]
Conclusion and Outlook

• A numerical model for standing SAW based systems is presented.

• The findings are very different from the BAW systems
  • Traveling wave setup in the channel
  • Different boundary layer
  • Leakage of energy to PDMS

• The boundary layer phenomena is yet to be fully understood.

• Quantitative 3D APTV measurements for the experimental verification are in progress.

• More details about the model in the following article:

Acknowledgments

Rune Barnkob  Christian J. Kähler  Francesco Costanzo  Tony Jun Huang

(CBET-1438126)  (KA 1808/16-1)