COMSOL Analysis of Acoustic Streaming and Microparticle Acoustophoresis

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Abstract: We present a numerical study of the transient acoustophoretic motion of microparticles suspended in a liquid-filled microchannel and driven by the acoustic forces arising from an imposed standing ultrasound wave: the acoustic radiation force from scattering of sound waves on the particles and the Stokes drag force from the induced acoustic streaming flow. The thermoacoustic equations are solved to first order in the imposed ultrasound field taking into account the micrometer-thin but crucial thermoviscous boundary layer near rigid walls. Then, products of these first-order fields are used as source terms in the time-averaged second-order equations, from which the net acoustic forces acting on the particles are determined. The resulting acoustophoretic particle velocities are quantified using the COMSOL particle-tracking scheme. The model shows how the acoustophoretic particle motion changes from being dominated by streaming-induced drag to being dominated by radiation forces as function of particle size, channel geometry, and material properties.

Keywords: Microparticle acoustophoresis, acoustic streaming, acoustic radiation force

1. Introduction

Ultrasound-induced control of motion (acoustophoresis) of microparticles and cells in aqueous solutions is rapidly becoming an important tool in modern bio-chip technology [1,2]. However, the development of optimal device designs is hindered by the lack of full physical understanding of the acoustic driving forces due to acoustic streaming and radiation. One way to advance the field is by combining numerical simulations and experimental characterization [3,4].

Ultrasound acoustics is described by the thermoviscous first-order equations for pressure, density, velocity, and temperature (the continuity equation, the Navier-Stokes equation, and the heat equation). For typical use in bio-chips, the actuation can be regarded as a small density

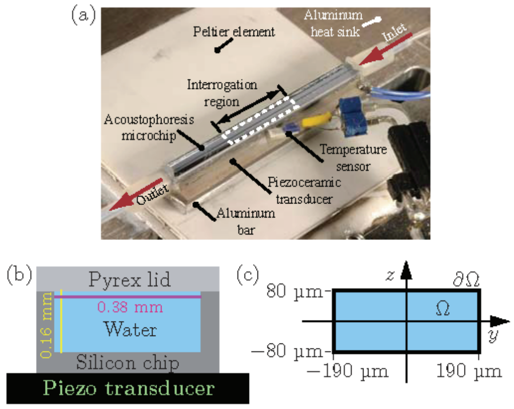

Figure 1. (a) A Photograph of an actual silicon/glass chip for acoustophoresis, which is mounted on a piezo transducer and a Peltier element, from [3]. (b) A sketch of the microchannel cross section showing the water-filled silicon channel with its pyrex lid and piezo transducer. (c) Corresponding computational domain used in the COMSOL simulations, adapted from Ref. [4].

perturbation of the liquid in which the cells are suspended, and it is well-described by boundary conditions on the velocity field with a harmonic time dependence on the rigid walls enclosing the water-filled domain (Figure 1).

The drag force from the acoustic streaming and the acoustic radiation force from acoustic wave scattering are calculated for the microparticles from time-averaged second-order fields for which products of first-order fields act as source terms. Finally, these forces are used as driving forces in the COMSOL Particle Tracing Module to calculate the time-dependent motion of the suspended microparticles.

A more detailed account of this work is given in Ref. [4].

2. Use of COMSOL Multiphysics

Using standard perturbation theory to first order in the amplitude of the oscillating (MHz ultrasound) boundary conditions, we implement the full thermoviscous first-order equations in COMSOL Multiphysics 4.2a using the Thermo-

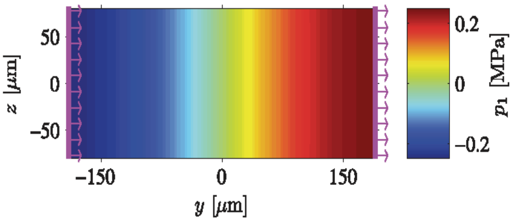

Figure 2. COMSOL color plot of the first-order pressure field p_1 in the domain for the shown 1.95-MHz time-harmonic velocity boundary condition (magenta arrows), exciting a horizontal half-wavelength resonance. Adapted from Ref. [4].

acoustic Physics Interface with a very fine mesh near rigid boundaries to resolve the viscous boundary layer.

To first order in the amplitude of the imposed ultrasound field, the thermodynamic heat transfer equation for the temperature T_1, the kinematic continuity equation expressed in terms of the pressure p_1, and the dynamic Navier-Stokes equation for the veloicty field $\boldsymbol{v}_1$, become

$$\partial_t T_1 = D_{\mathrm{th}} \nabla^2 T_1 + \frac{\alpha T_0}{\rho_0 C_p}\, \partial_t p_1, \tag{1a}$$

$$\partial_t p_1 = \frac{1}{\gamma\kappa}\Big[\alpha \partial_t T_1 - \boldsymbol{\nabla}\cdot \boldsymbol{v}_1\Big], \tag{1b}$$

$$\rho_0 \partial_t \boldsymbol{v}_1 = -\boldsymbol{\nabla} p_1 + \eta \nabla^2 \boldsymbol{v}_1 + \beta\eta\, \boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot \boldsymbol{v}_1). \tag{1c}$$

Here, D_{th} is the thermal diffusivity, α the thermal expansion coefficient, γ the ratio of specific heats, κ the compressibility, η the dynamic viscosity, and β the viscosity ratio, which has the value 1/3 for simple liquids. A further simplification can be obtained when assuming that all first-order fields have a harmonic time dependence $e^{-i\omega t}$ inherited from the imposed ultrasound field, because then all time derivates are substituted by a simple multiplicative factor, $\partial_t \rightarrow -i\omega$. The boundary conditions are $T = T_0$ and $\boldsymbol{v} = \boldsymbol{0}$ on all walls but with the addition of a vibrating horizontal velocity component $v_{\mathrm{bc}}\, e^{-i\omega t}$ on the vertical side walls. By proper tuning of the driving frequency to $\omega/2\pi$ = 1.95 MHz, a strong transverse half-wave resonance is induced (Figure 2). This resonance is used in the rest of the paper.

It is a numerical challenge to solve this problem where the thermoviscous boundary layers are resolved. These layers are only 0.5 μm wide, which is a factor of 1000 less than the typical channel width and height of about 500 μm. Ex-

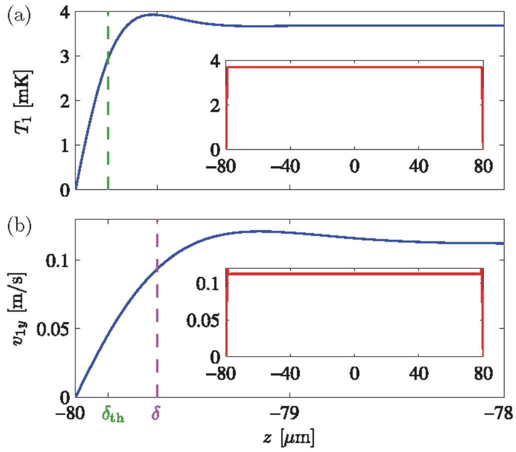

Figure 3. (a) Line plot from the COMSOL simulation of the amplitude of the first-order temperature field T_1 near the wall (blue line) and across the entire channel (red line) along the vertical line at y = 95 μm. (b) Similar plot for the first-order velocity field component v_{1y}. The thickness of the thermal and viscous boundary layers are marked by the vertical dashed lines δ_{th} and δ, respectively. Adapted from Ref. [4].

amples of the thermal boundary layer δ_{th} and the viscous boundary layer δ are shown in Figure 3. The numerical results are in good agreement with the following theoretical predictions [4],

$$\delta_{\mathrm{th}} = \sqrt{\frac{2D_{\mathrm{th}}}{\omega}} = 0.15\ \mathrm{\mu m}, \quad \text{and} \quad \delta = \sqrt{\frac{2\nu}{\omega}} = 0.38\ \mathrm{\mu m}. \tag{2}$$

The values are for 1.95 MHz in water at 25 °C.

The acoustophoretic motion of microparticles takes place on a time-scale of ms or more, much slower than the short μs-ultrasound time-scale. It is therefore calculated as the time-averaged response of one oscillation period. As such a time-average of purely harmonic first-order fields is zero, we employ second-order perturbation theory and calculate the time-averaged second-order velocity and pressure fields field $\langle \boldsymbol{v}_2 \rangle$ and $\langle p_2 \rangle$, respectively,

$$\rho_0 \boldsymbol{\nabla}\cdot\langle \boldsymbol{v}_2\rangle = -\boldsymbol{\nabla}\cdot\langle \rho_1 \boldsymbol{v}_1\rangle, \tag{3a}$$

$$\eta\nabla^2\langle \boldsymbol{v}_2\rangle + \beta\eta\boldsymbol{\nabla}\Big(\boldsymbol{\nabla}\cdot\langle \boldsymbol{v}_2\rangle\Big) - \langle \boldsymbol{\nabla} p_2\rangle = \langle \rho_1 \partial_t \boldsymbol{v}_1\rangle + \rho_0\big\langle(\boldsymbol{v}_1\cdot\boldsymbol{\nabla})\boldsymbol{v}_1\big\rangle. \tag{3b}$$

These equations are solved using the Laminar Flow Physics Interface, modified to include the time-averaged products of first-order fields as source fields. The time-averaged second-order velocity field $\langle \boldsymbol{v}_2 \rangle$ is the so-called acoustic streaming velocity, a bulk flow induced by the shear stresses in the viscous boundary layer.

Throughout our work we have performed a mesh-convergence analysis to ensure the convergence of our simulation results.

3. Resulting acoustophoretic motion

To calculate the time-dependent motion of the suspended microparticles forces we use the COMSOL Particle Tracing Module including the two acoustically induced force on the microparticles, the radiation force $\boldsymbol{F}^{\mathrm{rad}}$ and the Stokes drag force $\boldsymbol{F}^{\mathrm{drag}}$ from the streaming velocity.

For a single small spherical particle of radius a, density ρ_p, and compressibility κ_p in a viscous liquid the former force is given by [5]

$$\boldsymbol{F}^{\mathrm{rad}} = -\pi a^3 \left[\frac{2\kappa_0}{3}\,\mathrm{Re}\big[f_1^* p_1^* \boldsymbol{\nabla} p_1\big] - \rho_0\,\mathrm{Re}\big[f_2^* \boldsymbol{v}_1^* \cdot \boldsymbol{\nabla} \boldsymbol{v}_1\big]\right], \tag{4}$$

where κ_0 is the compressibility of the liquid, and where the pre-factors f_1 and f_2 are given by

$$f_1(\tilde{\kappa}) = 1 - \tilde{\kappa}, \quad \text{with } \tilde{\kappa} = \frac{\kappa_\mathrm{p}}{\kappa_0}, \tag{5a}$$

$$f_2(\tilde{\rho},\tilde{\delta}) = \frac{2\big[1-\gamma(\tilde{\delta})\big](\tilde{\rho}-1)}{2\tilde{\rho}+1-3\gamma(\tilde{\delta})}, \quad \text{with } \tilde{\rho} = \frac{\rho_\mathrm{p}}{\rho_0}, \tag{5b}$$

$$\gamma(\tilde{\delta}) = -\frac{3}{2}\Big[1+\mathrm{i}(1+\tilde{\delta})\Big]\tilde{\delta}, \quad \text{with } \tilde{\delta} = \frac{\delta}{a}. \tag{5c}$$

For a particle moving with veloicty $\boldsymbol{u}$ the Stokes drag force becomes

$$\boldsymbol{F}^{\mathrm{drag}} = 6\pi\eta a\big(\langle \boldsymbol{v}_2 \rangle - \boldsymbol{u}\big), \tag{6}$$

which is valid for particles sufficiently far away from the rigid walls.

The resulting acoustophoretic microparticle trajectories resulting from the action of these two acoustically induced forces on each single particle are shown in Figure 4.

For the smallest particles $2a$ = 0.5 µm, see panel (a), the drag force from the acoustic streaming dominates the particle motion, and the characteristic streaming flow rolls are clearly visualized. For the largest particles $2a$ = 5 µm, panel (c), the acoustic radiation force dominates the particle motion, and the particle velocity is nearly horizontal. This results in a focusing motion of the particles towards the vertical pressure nodal plane at the center of the channel. We note that at the nodal plane the radiation forces are zero, and consequently for times larger than 10 s all particles in panel (c) that have reached the nodal plane are pushed to the top or bottom of the nodal plane due to the weak but non-zero streaming-induced drag forces.

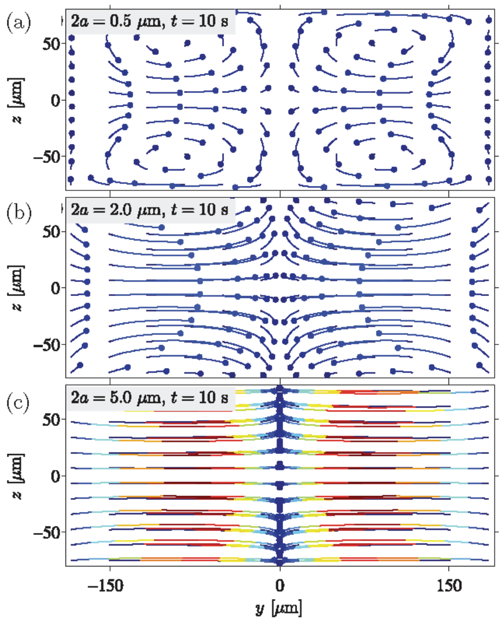

Figure 4: COMSOL simulation of the acoustophoretic motion of polystyrene microparticles resulting from the time-avaraged second-order acoustic fields, which are generated by the first-order field of Figure 2. Starting from an even distribution of 144 particles, the first 10 s of the motion is shown (line segments) as well as the final particle positions (dots). (a) Streaming-dominated vortex motion for small particles of diameter $2a$ = 0.5 µm. (b) Intermediate pattern of motion for medium-sized particles with $2a$ = 2.0 µm. (c) Radiation-dominated linear motion for large particles with $2a$ = 5.0 µm. Adapted from Ref. [4].

For the intermediate particles $2a$ = 2 µm, see panel (b), the drag and radiation forces are of the same order of magnitude. The critical particle diameter $2a_\mathrm{c}$, for which this cross-over takes place, can be estimated by requiring the force balance $\boldsymbol{F}^{\mathrm{drag}} + \boldsymbol{F}^{\mathrm{rad}} = 0$, see details in Ref. [4],

$$2a_c = \sqrt{12\frac{\Psi}{\Phi}}\,\delta \approx 2.0 \text{ µm}. \tag{7}$$

This is in good agreement with Figure 4(b). Here, $\Psi = 3/8$ is the streaming coefficient and $\Phi = f_1/3 + f_2/2$ (= 0.165 for polystyrene particles in water at 25 °C) is the acoustic contrast factor.

4. Conclusion

A finite element method implemented in COMSOL Mulitiphysics 4.2a was successfully used to model the acoustophoretic motion of microparticles in the vertical cross-section of a long, straight, liquid-filled microchannel subject to a horizontal half-wave ultrasound resonance. The particle motion is due to the combined effect of Stokes drag from the second-order time-averaged streaming flow and the acoustic radiation force.

To achieve this, the first-order acoustic field of a standing wave was determined inside a microchannel cavity by solving the linearized compressional Navier-Stokes equation, the continuity equation, and the heat equation, while resolving the boundary layers near the rigid channel walls. Products of the first-order fields was then used as the driving terms in the time-averaged second-order flow equations to determine the streaming flow and the acoustic radiation forces, and from this the time-dependent trajectories of an ensemble of microparticles were calculated. The solutions were checked by a careful mesh-convergence analysis.

A main result shown is the characterization of the cross-over from streaming-dominated to radiation-dominated acoustophoretic microparticle motion as function of particle diameter. In Ref. [4] we have further studied this cross-over as a function of the channel geometry and of the viscosity of the carrier liquid. The clear results of our analysis demonstrate that our numerical model has a huge potential within device design and studies of basic physical aspects of microparticle acoustophoresis.

5. Acknowledgements

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6. References

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