COMSOL Analysis of Acoustic Streaming and Microparticle Acoustophoresis

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Abstract

Ultrasound-induced control of motion (acoustophoresis) of microparticles and cells in aqueous solutions is rapidly becoming an important tool in modern bio-chip technology (Figure 1). 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 [1,2]. Ultrasound acoustics is described by the non-linear thermoviscous 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 perturbation of the water 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 (Figures 1 and 2). 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 Thermoacoustic physics interface with a very fine mesh near rigid boundaries to resolve the viscous boundary layer. This poses a numerical challenge, as the width of this layer is only 0.5 um, which is a factor of 1000 less than the typical channel width and height of about 500 um (Figure 3). The acoustophoretic motion of microparticles takes place on a time-scale of ms or more, much slower than the short us-ultrasound time-scale, and 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. This is done using the Laminar Flow Physics Interface, modified to include the time-averaged products of first-order fields as source fields. The resulting drag force from the acoustic streaming and the acoustic radiation force from acoustic wave scattering are then calculated from the second-order fields. Finally, these forces are used as driving forces in the COMSOL Particle Tracing Module to calculate the time-dependent motion of the suspended microparticles (Figure 4). We have performed a mesh-convergence analysis to ensure the convergence of our simulation results. We show (Figure 2) examples of a resulting first-order field in the rectangular, vertical channel cross-section. These are supplemented by line plots emphasizing the viscous and thermal boundary layers (Figure 3). Finally, examples of acoustophoretic microparticle trajectories are shown (Figure 4). In conclusion, we have simulated the ultrasound-induced acoustophoretic motion of microparticles suspended in an aqueous solution. In particular, we have characterized the cross-over from streaming-dominated vortex motion of small particles (< 2 um) to radiation-dominated linear motion of larger particles (> 2 um) (Figure 4). The results of our
COMSOL simulation allow for direct comparison of modeling with experimental observation in the near future, thus paving the way for developing optimal designs of devices for efficient on-chip handling of cells.

Reference


Figures used in the abstract

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 Ref. [1]. (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. [2].

Figure 2: COMSOL color plot of the first-order pressure field 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. [2].
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 $y = 95$ um. (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 $\delta_{th}$ and $\delta$, respectively. Adapted from Ref. [2].
**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 $2a = 0.5 \, \mu\text{m}$. (b) Intermediate pattern of motion for medium-sized particles with $2a = 2.0 \, \mu\text{m}$. (c) Radiation-dominated linear motion for large particles with $2a = 5.0 \, \mu\text{m}$. Adapted from Ref. [2].