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Numerical study of submicroparticle acoustophoresis using higher-order modes in a rectangular microchannel

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ABSTRACT

Manipulation of submicrometer particles in Lab-on-a-Chip systems using acoustophoresis is challenging due to the effect of acoustic streaming. We numerically study the transition from radiation force dominated to streaming-induced drag force dominated acoustophoresis using the fundamental and higher-order resonances of a water-filled rectangular microchannel. We consider the cases of single mode excitation and simultaneous double mode excitation. The acoustic fields at resonance are calculated using a second-order perturbation expansion of the thermoviscous acoustic problem. We show that the acoustophoretic forces using simultaneous mode excitation can be obtained from a linear combination of the single mode forces. We find that the critical size of suspended particles at the transition scales inversely with the square root of the resonance frequency. Particle tracing shows radiation-dominated concentration of 800 nm diameter polystyrene particles using the fifth-order resonance at 9.8 MHz. For smaller particles we find a streaming-assisted concentration regime where particles are concentrated into the streaming regions close to the walls. In case of double mode excitation, the particle concentrations increase a factor 4 to 18 times for 200 nm to 800 nm particles respectively. We include the numerical model, consisting of a COMSOL implementation and MATLAB control script, as supplemental material.

1. Introduction

One of the operations in a Lab-on-a-Chip is the manipulation of suspended microparticles (such as bacteria, fat droplets, plastic microbeads or human cells) in a bulk fluid (like water, milk or blood) [1]. A popular method is ultrasonic acoustophoresis which uses sound waves for the particle manipulation. Over the last decade there have been significant developments in the theory, implementation and application of ultrasonic acoustophoresis in Lab-on-a-Chip systems [2–5]. The processing of submicrometer particles (with a diameter smaller than a micrometer) is of great interest for applications in microbiological analysis, food and drinking water quality analysis and biomedicine. However, the application of acoustophoretic focusing of submicrometer particles is limited due to acoustic streaming flow [6,7], which typically becomes the dominant effect for particles smaller than a few micrometer. Accordingly, there is an ongoing interest in engineering streaming flow patterns which allow focusing of smaller particles.

Significant theoretical and experimental work has been done on the fundamental, half-wavelength ($\lambda/2$) resonance in a rectangular geometry by Bruus and coworkers [3,8–11]. The fundamental resonance often provides an optimal geometry with low complexity for acoustic focusing. It generates a single concentration node in the center of the channel for acoustically

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hard particles (with a positive acoustic contrast factor), preventing clogging or adsorption on the walls and allows straightforward separation of the concentrated stream using a trifurcation at the end of the channel. The lower size limit of such systems for polystyrene (PS) beads in water is around 1 μm for a resonance frequency around 2 MHz (corresponding to a rectangular microchannel of approximately 375 μm wide). A higher operation frequency increases the strength of the acoustic radiation force relative to the Stokes drag force, and subsequently lowers the size limit, but also leads to a smaller width w of the channel due to the resonance condition for the fundamental resonance, $w = n \cdot \lambda/2$ with mode number n equal to one. To compensate for the lower throughput one could use multiple parallel channels [12].

Higher-order modes at higher frequencies allow combination of a wider channel with a stronger radiation force compared with the fundamental resonance [13]. Nilsson et al. used the first harmonic mode ($2\lambda/2$) at 1.96 MHz to achieve focusability of 5 μm diameter polyamide beads in water, as the acoustic radiation force at fundamental resonance was too weak [14]. They also showed operation at the second harmonic ($3\lambda/2$) and third harmonic ($4\lambda/2$) modes but did not measure the performance of these modes as this would require a more complex chip design for separation using the increased number of concentration nodes. Most other research done on higher-order modes work in the limit of dominant acoustic radiation force, i.e. above the lower size limit. Grenvall et al. used the first and second-harmonic mode to separate acoustically hard and soft components and cells from raw milk [15,16]. They show that the fundamental resonance causes severe clogging because the soft lipids are concentrated in the two anti-nodes close to the walls where they adhere and accumulate. The fundamental and the two harmonic modes are all excited around 2 MHz and were implemented by using various channel widths. The higher-order modes provide an improved geometry for separation of hard and soft particles. However, because the excitation frequency is the same for all modes, there is no relative increase of the strength of the acoustic radiation force by using a higher frequency. Kothapalli et al. also used the first-harmonic mode for simultaneous concentration of polymer beads and polymer-shelled microbubbles [17].

There is some literature on acoustophoresis using temporally and spatially combined modes. Switching between modes can be used to separate beads with different sizes [2,18]. Liu et al. separate 5 and 10 μm PS beads into two parallel streams by switching between the fundamental and second harmonic ($3\lambda/2$) based on the dependence of particle concentration speed on particle size [19]. The same effect is used in free flow acoustophoresis using the fundamental resonance [20]. Cho et al. sweep back and forth between modes $n = 4$ to $n = 7$ by changing the excitation frequency from 1.8 MHz to 3.1 MHz, sweeping 10 μm PS particles towards one side of the channel.

Other researchers combine resonances in two dimensions to increase control over the concentration process. Grenvall et al. show two-dimensional particle focusing with two orthogonal fundamental resonances at 2 and 5.3 MHz for microchip impedance spectroscopy of 3, 5 and 7 μm PS beads and red blood cells [21]. In other work they combined two orthogonal fundamental resonances to improve particle sorting, but these modes were on different location on chip, i.e. spatially separated [22]. Leibacher and coworkers used a two-dimensional (2D) mode at 870 kHz to study acoustophoresis of hollow and core-shell particles [23].

Antfolk and coworkers reported on focusing 500 nm diameter polystyrene beads and E. coli bacteria in water using a 2D half-wavelength mode in a square microchannel [24]. The numerical analysis suggests that, even though the Stokes drag force due to the acoustic streaming is the dominant force, focusing is achieved because the acoustic radiation force causes slight displacements from the otherwise closed streamlines, causing the particles to spiral inwards. This observation provides a path towards lowering the size limit of acoustophoresis.

Little research has been done on acoustophoresis using simultaneous excitation of multiple higher-order modes in the acoustic streaming dominated limit. The rectangular geometry by Bruus and coworkers is well studied, both theoretically as well as experimentally, and therefore serves well as a reference system. In this paper, we shortly discuss the theoretical framework and numerical model developed by Muller et al. [9] for single resonances and explicitly extend it to combinations of modes. Such an extension was mentioned earlier [24,25]. Next we numerically study submicroparticle acoustophoresis in the acoustic streaming dominated limit using the fundamental resonance mode and the next four harmonic modes ($n = 1$ to 5), for the cases of single and simultaneous excitation. We show that a higher excitation frequency as well as simultaneous excitation of two modes significantly improves the lower particle limit for acoustophoretic concentration.

2. Theoretical background

In this section we give theoretical background of the thermoviscous acoustic theory for the fields and forces. As basis we use the study of a single resonance in a water-filled rectangular channel by Muller et al. who used a perturbation series to solve the governing equations [9]. We show that the acoustic fields and time-averaged acoustic forces calculated for single resonances can be added in a linear superposition to find the fields in case of multiple simultaneously excited modes at different frequencies. Finally the acoustic radiation force and Stokes' drag force are then calculated from the linear superposition of fields.

2.1. First and second order acoustic fields

The first and second-order fields are calculated using the continuity equations for mass, momentum and energy. We assume no flow in the absence of the acoustic disturbance, $\mathbf{v}_0 = \mathbf{0}$. Also we assume a harmonic time dependence for all first-order fields, i.e. $g_1(\mathbf{r}, t) = \mathrm{Re}\{g_1(\mathbf{r})e^{-\mathrm{i}\omega t}\}$ with ω being the acoustic frequency. Note that generally $g_1(\mathbf{r})$ is complex, with its argument (i.e.

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