# Numerical Analysis of Acoustophoretic Discrete Particle Focusing in Microchannels

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## ABSTRACT

Acoustophoretic particle focusing is a modern and very attractive method of removing a variety of objects from solutions in a microfluidic channel. The process is inherently general and can be readily extended to multiple types of applications such as healthcare (e.g. malignant cell removal), academic research (e.g. nanoparticle separation), industrial (e.g. reclaiming of rare earths) and environmental applications (e.g. sequestration of suspended solids). According to classical understanding, particle separation is realized by the acoustic radiation force. Traditionally, the wavelength of the acoustic wave has to be fine-tuned to the channel width and specified to $\lambda = 2L_{channel.}$ This creates a constant pressure node in the middle of the channel that forces particle motion towards it. Particle motion is theorized to be caused by differences in the pressure gradient acting on the partciles and/or wave scattering. This article also demonstrates that particle focusing can also be achieved under different conditions, provided that the amplitude of the oscillations is sufficiently high. In this study, results from numerical simulations performed in ***FLOW-3D*** help promote understanding of acoustophoretic particle focusing by closely examining the forces that act on the particles. To the best of our knowledge, this is the first explicit study of this phenomenon that focuses on the different force contributions This computational analysis can be generally applied to a multitude of acoustophoretic processes and should prove useful in promoting understanding of the phenomena involved in particle focusing.

***Keywords***: Acoustophoresis, standing acoustic wave, SAW, λ/2 channels, microchannel oscillations, nanoparticles, particle focusing

## 1 INTRODUCTION

The use of acoustic standing wave technology has been increased in the last 10 years for the manipulation, separation or concentration of particulate matter in complex media due to its many advantages, such as non-invasiveness, versatility, simple fabrication, easy operation, and convenient integration with other on-chip units[1]. This "label free" method has allowed the separation of micrometer biological cells from complex biofluids depending on the specific sizes, densities and compressibilities. Among its many advantages, the use of high flow rates (up to L/h) in microfluidic devices makes acoustophoresis more convenient than other sorting methods. For instance, Abdallah et al. [2] were able to transfer particles between different fluids at much higher flow rates (x10) by using acoustophoresis than dielectrophoresis. Also, it was also tested in processing whole human blood and proved capable of transferring blood cells from undiluted whole human blood with an efficiency of 95% at 1 L/h and 82% at 2 L/h [3]. Although it has been employed for the manipulation of micron-sized particles, Laurell's group has recently achieved the separation of submicron particles as small as 500 nm by using two-dimensional acoustic focusing (i.e. focusing of the sub-micrometer particles both horizontally and vertically in the cross section of a microchannel) [4]. Furthermore, the combination of multiple streams flowing under laminar conditions in microchannels, ligand complexed microbeads and acoustic standing wave technology offers a new brand of applications that were not previously possible. For example, Augustsson et al. [5] developed an acoustophoresis-based microfluidic flow-chip as a novel platform to facilitate analysis of proteins and peptides loosely bound to the surface of beads or cells. In this work, the authors demonstrated the elution of surface bound peptides from beads and human spermatozoa by using buffers with different pH levels.

Apart from the wealth of experimental studies, various theoretical and numerical investigations of the process have been reported. For example, Nama et al.[6] have studied the acoustophoresis of particles in PDMS channels. In their work, the system is acoustically actuated via two counter-propagating surface acoustic waves that form a standing wave in a piezoelectric material interfacing the liquid channel, and the particle motion is governed by the viscous drag force from the acoustic streaming as well as the direct acoustic radiation force due to scattering of sound waves on the particles. For their specific model parameters, (600 μm wavelength, 6.65 MHz actuation frequency, and polystyrene particles suspended in water), an approximate critical particle size of 10 μm was obtained for which the particle motion goes from being streaming-drag dominated to being radiation dominated. The numerical study developed by Büyükkocak et al. [7] is also of particular interest since they used a finite element approach for modelling the particle separation under the influence of ultrasonic waves. In their article, the authors solved the fluid flow in a microchannel

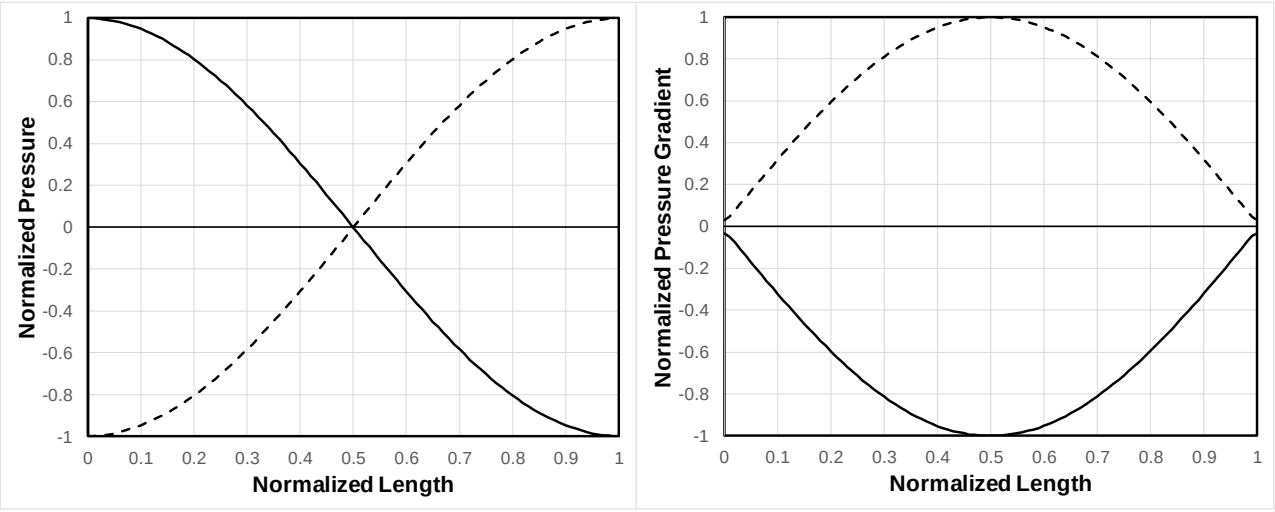


**Figure 1**. Numerical λ/2 channel stable pressure field analysis at φ=0 (solid lined) and at φ=π (dashed line). (a) Normalized pressure vs normalized channel length, (b) Normalized pressure gradient at the direction of wave propagation vs normalized length.

numerically, whereas analytical relations were employed for the calculation of ultrasonic radiation forces (which were coupled to the fluidic analysis). Furthermore, they simulated the cell washing process by taking into account the diffusion of contaminants between colaminar streams flowing side by side inside the channel, and the results were compared with experimental works showing good agreement. In all of the studies listed above, the authors used an analytical expression to for the radiation force coupled with the CFD simulations. To the best of our knowledge, this is the first study that examines particle focusing as a direct result of flow parameters. Explicitly modeling the acoustophoretic process provides additional insight that may prove useful in the development of novel acoustophoretic applications.

## 2 THEORY

Acoustophoresis can be defined as the movement of particles using acoustic radiation pressure from resonant sound waves. The phenomenon has shown promising applications in microfluidics, namely for the separation of free flowing particles [8]. In microfluidics, acoustophoresis is commonly achieved by using a piezoelectric actuator to create a standing ultrasound wave lateral to the direction of the channel. In general, a standing wave can be described as:

$$y = A * \cos\left(\frac{2\pi x}{\lambda} + \frac{\phi}{2}\right) * \sin\left(\frac{2\pi t}{T} + \frac{\phi}{2}\right) \qquad (1)$$

where y is the displacement of a point in the wave at position x and time t, A is the amplitude, λ is the wavelength, T is the period, and ϕ is the phase difference. For the majority of microfluidics applications, the wavelength is set to be twice the width of the channel. This creates a pressure node in the center of the channel with antinodes of fluctuating pressure on either side. The scenario allows for Eq. 1 to also be defined in terms of pressure. It can now be written as:

$$p = p_0 * \sin\left(\frac{2\pi}{\lambda}x\right) * \cos\left(\frac{2\pi}{T}t\right) \qquad (2)$$

where $p$ is the pressure at distance $x$ from the pressure node at time $t$, $p_0$ is the pressure amplitude, $\lambda$ is the wavelength, and $T$ is the period. Since there is only one standing wave in this situation, the phase difference terms could be removed. Based on Eq. 2, one can see that the pressure gradient and, more specifically, the differences in pressure $\delta p$ within the medium play a pivotal role in the acoustophoresis particle focusing phenomenon [9]. Hence, the radiation force $\boldsymbol{F_{rad}}$ on suspended body with surface S can be calculated using the following surface integral:

$$\boldsymbol{F_{rad}} = \int_S (-\boldsymbol{n})\delta p d\alpha \qquad (3)$$

where **n** is the vector normal to the surface [10]. As it can be readily observed from the above derivations, particle motion is possible in the presence of a pressure field.

## 3 RESULTS AND DISCUSSION

In the following sections, we model particle motion under the influence of an acoustic wave using a CFD analysis performed in ***FLOW-3D***. In section 3.1, we demonstrate discrete particle motion caused solely by the pressure gradient. Whereas, in section 3.2, it is shown that particle focusing may also be possible due to oscillations of the entire microchannel at off-resonance frequencies.

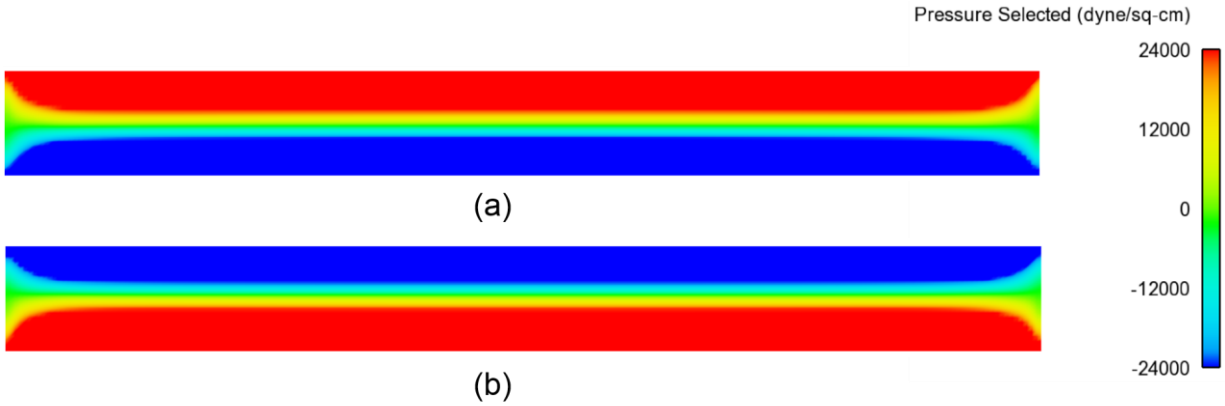


**Figure 2**. Microchannel pressure field at a) Maximum upward acceleration b) Maximum downward acceleration. Both results refer to the case of maximum length amplitude (50 μm) where the maximum pressure was found to be approximately 0.24 Atm. Similarly, to λ/2 channels, a constant pressure node is located in the center of the channel.

### 3.1 Half Wavelength (λ/2) Channel Pressure Field Analysis

We perform a 3D numerical analysis of the impact of an oscillating pressure field to the motion of particle suspended in fluid. For the purposes of this analysis, an elastic membrane is placed at the bottom of the computational domain (Normalized Length = 0) where it follows a prescribed oscillating motion which results in the generation of a standing acoustic wave. The oscillation frequency is carefully chosen so that the wavelength is twice the length of the channel. The force amplitude for the membrane's oscillation is set arbitrarily high so that a pressure field maximum of the order of 1 Atm can be observed. A wall boundary condition that allows for total wave reflection is placed at the top of the domain (Normalized Length = 1). Symmetry boundary conditions are placed on all the remaining boundaries. Initially, the fluid is at rest and its pressure is initialized at 0 Atm. At the onset of the simulation, the membrane begins to oscillate, generating amplifying pressure waves. It was observed that the pressure extrema reach stable values after approximately 1000 oscillations. **Figure 1** shows the pressure field and pressure gradient once these stable operating conditions have been reached. As it can be observed from **Fig 1a**., the simulation results verify the existence of a pressure node at the middle of the channel. It is important to note that the absolute values of the pressure maxima at $\varphi=0$ and $\varphi=\pi$ are higher that the absolute values of their respective minima. Therefore, since the pressure waves do not cancel each other out, particle focusing is possible. Moreover, the pressure gradient along the direction of propagation, shown in **Fig 1b**, reaches a peak value at the location of the pressure node A probe particle was also placed at a random location in the computational domain. The particle appears to move, in phase, with each membrane oscillation while approaching the center of the domain. This simulation required 14 hours on a standard 24-core workstation for a total of 10000 oscillations.

### 3.2 Microchannel Oscillations

Particle focusing at the middle of the channel may also be possible in cases where the oscillation wavelength is not set to be half the wavelength of the channel. More specifically, by allowing the entire microchannel to oscillate and by setting the oscillation length amplitude sufficiently high, similar results can be observed. This may be due to the fact that particle motion occurs due to contributions from multiple forces including pressure gradient, added mass, fluidic drag and, potentially, impulse forces due to collisions of the particles with the channel walls, given that the length amplitude microchannel oscillation is sufficiently large. This combination of factors acts to focus the particles undergoing acoustophoretic separation in the middle of the microchannel. To the best of our knowledge, this is the first computational study that takes into account all the force contributions previously mentioned. For the purpose of this analysis, a computational domain defining a microchannel with a square cross-section with 100 μm edges and a total length of 1 mm was used. A total of 1148 particles were initially introduced in the entire computational domain in a random fashion. We opted to oscillate the entire microchannel at a constant frequency of 10 Khz and at multiple amplitudes. The length of the amplitudes ranged from 3.125 μm to 50 μm. As a general rule, larger oscillation amplitudes require smaller time-step sizes in order to account for the rapidly varying temporal variable changes. Results from numerical simulations performed with ***FLOW-3D***, appear to indicate that channel oscillations at increased length amplitude generate a pressure gradient similar to what is observed in λ/2 channels even at off resonance frequencies, albeit much weaker. As seen in **Fig 2.**, depending on the phase of the oscillation, the pressure field changes accordingly, effectively pushing the particles to the center of the microfluidic channel. Moreover, impulse forces caused by collisions with the channel walls act to accelerate the process of particle focusing at high length amplitudes. The simulation results obtained with this method (shown in **Fig. 3**) seem to indicate a level of separation exceeding 90%

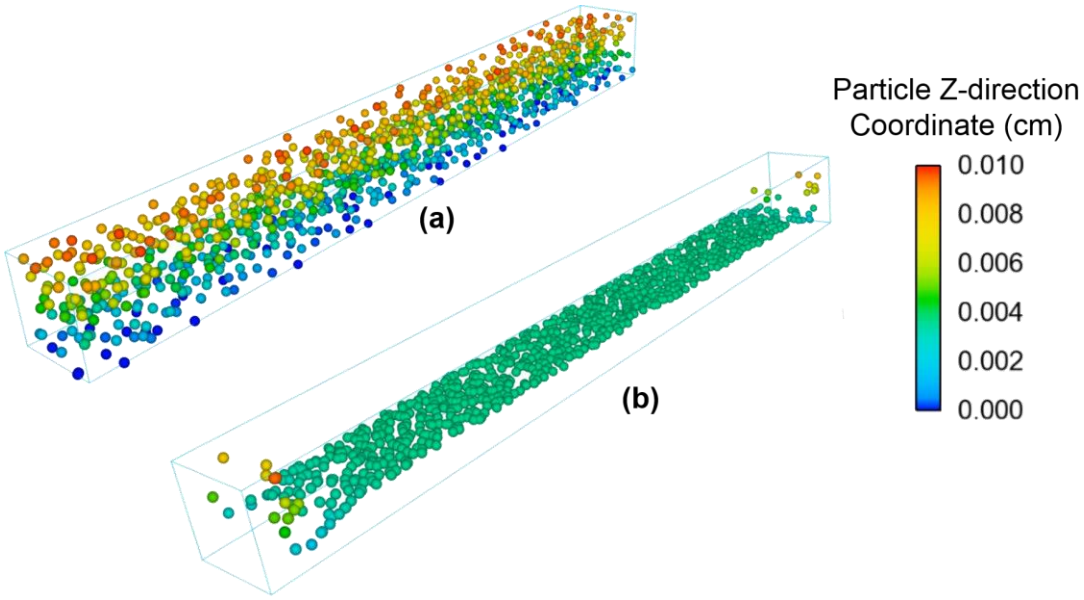


**Figure 3**. Acoustophoretic particle focusing accelerated by wall collisions: (a) Initial particle distribution (b) Final particle locations

for an overall process time of less than 4 ms. However, one drawback of this process is that particle sorting may not be as selective as in λ/2 channels, especially so, if large oscillations are preferred. This is due to the fact that impulse forces due to collisions are more dominant at larger oscillations, effectively forcing all particles to focus in the center of the domain.

## 4 CONCLUSIONS

In this article, we used CFD simulations to model the acoustophoretic process. Particle motion under the influence of acoustic waves was modeled for the case of λ/2 channels and for cases where the amplitude is sufficiently large to cause oscillations of the entire domain. To the best of our knowledge, this is the first numerical investigation of acoustophoresis where the forces acting on the particles are a direct result of the flow characteristics such as pressure gradient and drag force instead of coupling CFD with analytical predictions of the acoustic radiation force. It was demonstrated that particle focusing can be made possible due to the pressure field created by a standing acoustic wave and also by impulse forces caused oscillations of the entire domain.

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