Numerical Modelling of a Microfluidic Ultrasonic Particle Separator

R. J. Townsend*, M. Hill*, N. R. Harris**, N. M. White**, S. P. Beeby**

*School of Engineering Science, University of Southampton,
Southampton, SO17 1BJ, UK, m.hill@soton.ac.uk
**School of Electronics and Computer Science, University of Southampton,
Southampton, SO17 1BJ, UK

ABSTRACT

Particle manipulation can be brought about by using the radiation force experienced by particles in an acoustic standing wave. Where the particles are held in a fluid suspension, particle movement may be predicted analytically for basic descriptions of the fluid and acoustic field, although layered resonators have complex resonant characteristics and, in applications approaching microfluidic scale, flow is typically described by a parabolic laminar flow profile. Numerical techniques are used to successfully describe the acoustic field and determine the resulting particle trajectories and concentration in these more complex cases. This is supplemented with more thorough analyses of the acoustic and fluid fields using finite element analysis and computational fluid dynamics, respectively. These approaches are validated against experimental results for a micro-engineered ultrasonic particle separator.

Keywords: numerical model, ultrasonic, radiation force

1 INTRODUCTION

Particles in suspension and within an acoustic standing wave experience a radiation force, the direction and magnitude of which depends on the position within the field, the strength of the field and the physical properties of the particles and suspending fluid. This phenomenon can be used to manipulate or separate particles and so can be used to enhance cell and spore processing [1].

Devices in which a suitable standing wave can be generated can be designed using analytical models, although as the scale of such devices reduces numerical simulation becomes increasingly useful. Where fluid flow is introduced, and where the fluid chamber depth is of the same order as the wavelength, the acoustic and laminar flow fields have a combined effect which significantly influences particle movement, which can more easily be studied numerically.

The reduced scale also demands alternative fabrication routes. Silicon etching is ideal for the batch creation of microfluidic circuits, although geometric variations are limited and influence fluid flow patterns.

Here, a range of numerical simulation techniques is presented based around a micro-scaled ultrasonic particle separator device and used initially to describe the particle movement, the resulting concentration profiles within an ultrasonic field and the subsequent outlet particle concentrations. The fluid and acoustic fields are investigated more thoroughly using computational approaches and demonstrate the ability to study the effect of the etched geometry. In the case of the fluid flow, geometry has been modified to improve the flow characteristics of the device. Fabricated ultrasonic separator devices have been tested experimental and used to validate simulation work.

2 PARTICLE SIMULATIONS

2.1 Acoustic Radiation Force

Particles within an acoustic standing wave experience a time-averaged force as described by Gröschl [2]. The radiation force is related to the acoustic pressure field, an example of which is shown in figure 1, where it can be seen to be twice the spatial frequency of the acoustic pressure field. For solid phase particles, the radiation force causes them to converge towards the pressure node of the standing wave; beneath the pressure node the force acts in the positive y direction and above in the negative y direction.

The amplitude of the force depends on the acoustic energy density, wave number and properties of the fluid and particle media. The acoustic energy density within the fluid layer of a layered resonator driven by a PZT transducer depends on the transducer voltage and acoustic properties of the various layers.

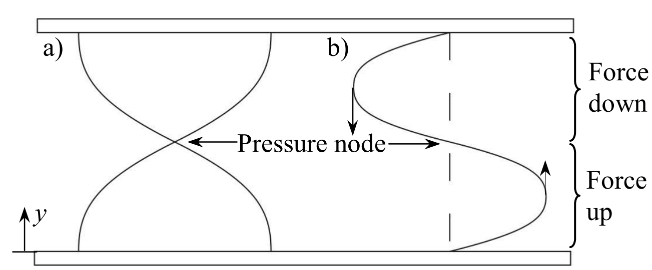

Figure 1: Schematic of a) acoustic pressure profile of a standing wave and b) resulting radiation force profile.

To describe the acoustic field and radiation force more accurately, an acoustic impedance transfer model has been developed which uses an equivalent circuit of the transducer and theoretical acoustic impedance of the resonator. This describes the device response as a function of frequency, predicting the resonant frequencies and the field pattern in 1 dimension through the fluid layer [3]. The acoustic pressure and velocity fields across the fluid chamber are then used to determine the acoustic potential and kinetic energy radiation profiles, respectively, which then relate directly to the radiation force.

This method is implemented in MATLAB and describes the acoustic field and radiation force, such as that shown in figure 1, for a range of frequencies and at discrete points across the fluid chamber. The mode shape and nodal positions are therefore also determined, indicating to which plane particles will converge.

2.2 Particle Trajectories

The movement of particles can be determined by considering the forces acting on a particle and solving Newton's second law numerically. The principal forces acting on a particle within an acoustic field are the acoustic radiation force, Stokes fluid drag force and gravity and are solved using numerical differentiation using a solver contained within MATLAB [4]. Time, coordinate and velocity data are returned by the solver, which, in the case of continuous fluid flow perpendicular to acoustic propagation, describes particle trajectory as the particle moves along the chamber (x-direction) and relative to the nodal plane (y-direction).

This model is coupled to the acoustic impedance transfer model described above which supplies the data describing the radiation force across the chamber.

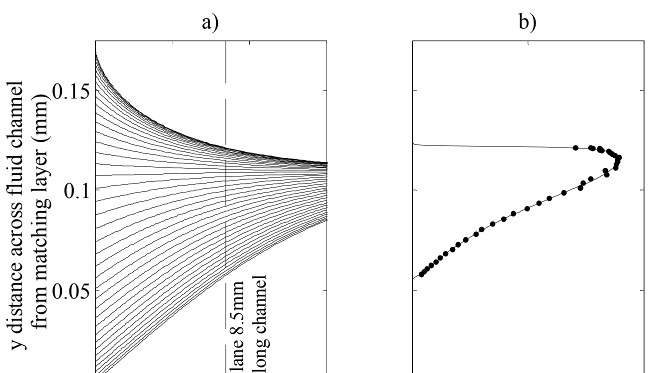

Figure 2: Simulation of particles within an acoustic standing wave showing a) particle trajectories as they are carried by the fluid along the length of the chamber (x-axis) and deflected vertically by the acoustic wave (y-axis) and b) the concentration profile.

To describe the drag force, and so the movement of the particle along the chamber, the fluid velocity profile is assumed to be laminar, therefore similar to flow between parallel plates where the chamber has a high height to width ratio, and varies only as a function of y.

Figure 2a shows an example of the movement of particles passing through an acoustic field where the chamber depth is slightly less than half a wavelength. Similar methods based on particle forces have been used to determine particle movement in acoustic fields [5,6].

2.3 Particle Concentration

Where the concentrated particle stream or cleared fluid is required for subsequent processing, outlets are used to extract the relevant fluid stream. Johnson and Feke [5] and Hawkes and Coakley [6] calculate outlet concentration based on the particle trajectory which marks the split between outlet streams. For applications where particle concentration within the chamber is of importance, it is sometimes more useful to predict the spatial change in concentration, rather than particle trajectories, also from which outlet concentrations can be calculated.

Particle coordinate data, such as that determined by the particle trajectory model, can be used to calculate the change in particle spacing and therefore particle concentration. This requires the simulation of a series of particles, each with different initial positions (figure 2a). In figure 2b, the relative change in concentration based on the adjacent particle trajectories has been plotted (dotted points) and it can be seen that as particles are drawn towards the centre of the chamber the concentration in that region has increased by a factor of 3 upon that at the inlet plane (x=0). It can be seen that the concentration data is slightly noisy and originates from numerical errors in the particle trajectory data.

A more reliable and elegant method is to consider the particles as a continuum described numerically over a grid, reducing computation time by avoiding the need to calculate individual particle trajectories and removing the associated errors. However, care has to be taken in the numerical implementation of this technique in regions where particles do not exist, e.g. either side of the particle stream, and the wall concentration if particles are forced towards the chamber boundary. To avoid these problems whilst still considering particles as a continuum, the method demonstrated here also takes into account particle trajectories and is therefore Lagrangian in nature.

A standard equation of conservation of mass [7] is used where u and v are the x and y components of particle velocity and c is the concentration (analogous to density).

$$\frac{\partial c}{\partial t} = \frac{c\partial u}{\partial x} + \frac{u\partial c}{\partial x} + \frac{c\partial v}{\partial y} + \frac{v\partial c}{\partial y} \qquad (1)$$

This is simplified by assuming the following: concentration varies spatially only, reducing the left hand side term to zero; u does not change as a function of x removing the first term of the RHS; there is no particle flux across a particle path, which has the effect of removing the forth RHS term. This reduced equation is then solved by replacing the partial differential terms with simple difference equations and finding successive solutions along the chamber in the x direction. Figure 2b illustrates the concentration calculated using this method (solid line) and is compared against the approach based on particle trajectory data. It can be seen that this latter approach creates a smoother, more convincing profile. Despite providing a more refined dataset, the computation time is reduced.

3 2-DIMENSIONAL FIELD SIMULATIONS

3.1 FEA of Acoustic Field

The above analysis has considered the acoustic field in 1 dimension only. However, striated patterns have been observed in resonators used for particle manipulation, where the acoustic field varies in a direction perpendicular to propagation due to acoustic enclosure modes, creating radiation force components in 3-dimensions.

Finite element analysis (ANSYS) has been used to investigate the 2-d field in two layers of the resonator, the fluid (water) and reflector (Pyrex) layers. Modal analyses predict that in the operating frequency range there are resonance patterns where the acoustic field varies significantly across the width of the chamber (z-direction).

Figure 3 shows the modelled acoustic pressure field at a 2-d resonant frequency of 3.4MHz for fluid and reflector thicknesses of 175µm and 1525µm respectively. Within the fluid chamber there is a series of distinct pressure variations in the z direction. Solid particles converge towards the pressure nodes (zero pressure), which referring to figure 3 suggests that particles will converge towards a series of bands across the width of the fluid chamber, with an average spacing of 0.25mm.

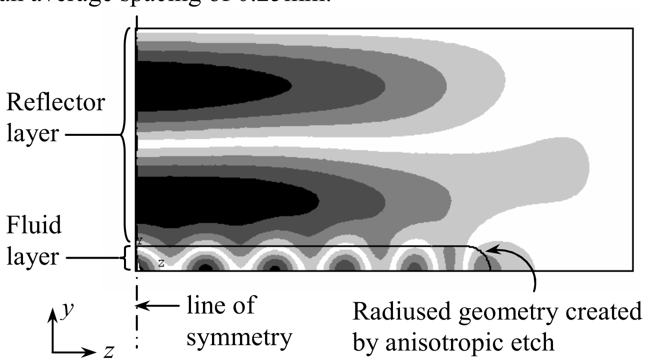

Figure 3: Acoustic finite element analysis of fluid and reflector layers. Contours indicate high magnitude (black) and low magnitude (white) regions of acoustic pressure.

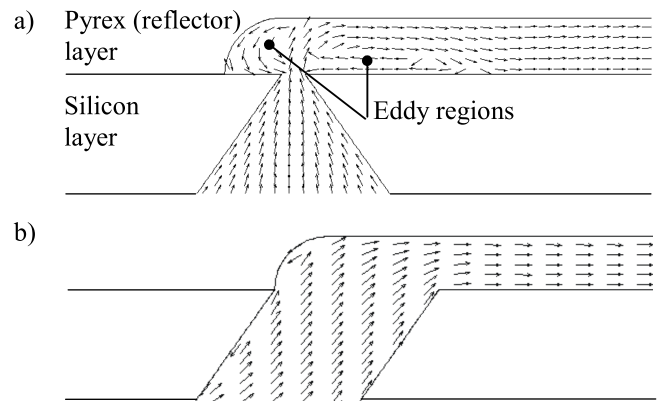

Figure 4: CFD simulation of fluid flow through anisotropic etched ducts leading to main chamber, showing a) eddy regions within a single etch duct design and b) a significant reduction of eddy regions within the revised geometry.

3.2 CFD Analysis of Fluid Flow Field

The fluid flow field is also investigated in 2 dimensions, although in the x-y plane. Dimensions within the fluid chamber and duct are typically 100µm or greater supporting use of the Navier-Stokes equations and macrofluidic methods, as used in commercial computational fluid dynamics packages. The CFD program, CFX, is used to investigate the influence the etched geometry on the fluid flow patterns [8], examples of which are shown in figure 4.

Figure 4a illustrates the predicted flow field through the angular geometry of the silicon KOH etched duct and up into the main chamber contained within an etched Pyrex layer. Eddy regions in the fluid easily form either side of the duct, potential sites for particles to lodge. A parabolic flow profile has been assumed to exist the entire length of the fluid chamber, however the eddy regions invalidate this assumption in the duct regions.

In figure 4b and based on the same flow rate, an alternative etched geometry has been simulated demonstrating that the eddy regions have become insignificant in their size and the flow pattern immediately downstream of the duct quickly tends to a parabolic profile.

4 VALIDATION OF MODELS

A series of ultrasonic particle separators have been fabricated and tested to investigate separation performance within a micro-engineered device. Here the experimental results also serve to validate the simulation techniques described above.

The separator is mounted upon an aluminium manifold which facilitates connection to peristaltic pumps (Watson-Marlow) and the accurate control of flow rates. The separator consists of a series of layers; either a bulk or printed PZT transducer, a silicon wafer which acts as a matching layer and into which ducts are etched (figure 4), and a Pyrex wafer into which the main fluid channel is etched. The device is designed such that there are several resonant frequencies which cause particles to move towards the centre or edge of the fluid chamber [9].

The acoustic impedance model is used to predict the resonant frequencies of the devices and the associated modes. In experiment, particles are observed to converge towards certain planes within the fluid chamber when the field is switched on, and supports the predictions made regarding the frequencies and field patterns [9].

Work has begun involving the measurement of outlet particle concentration for yeast and latex particles over a range of transducer voltages [10]. Preliminary application of the concentration model compares well with these results and will contribute to further work comparing the performance of the bulk and printed PZT devices.

A study of particle movement, similar to that used in Harris *et al.* [9] is used to compare against the FEA predictions describing the acoustic field and how it varies across the fluid channel. For the case described in figure 3 predicting band spacing of 0.25mm across the width of the chamber, initial experimental results record an average band spacing of 0.21mm, as seen in figure 5 looking down through the Pyrex layer where the white line are created by the build up of yeast particles along low pressure regions. This initial work is encouraging and further simulation work using more precise geometric measurements of the actual device is expected to reduce discrepancy between modelled and experimental results and demonstrate the influence geometry has on the 2-dimensional acoustic field and also particle movement.

Observation of particle movement due to the fluid flow, rather than the acoustic field, makes it possible to determine the extent of the eddy region downstream of the inlet and within the main chamber. The study of eddy regions created by various duct geometries and measured over a range of flow rates validates the CFD results and demonstrates the significant improvement in the flow field based on the geometry illustrated in figure 4b, minimising eddy development within the micro-fabricated device.

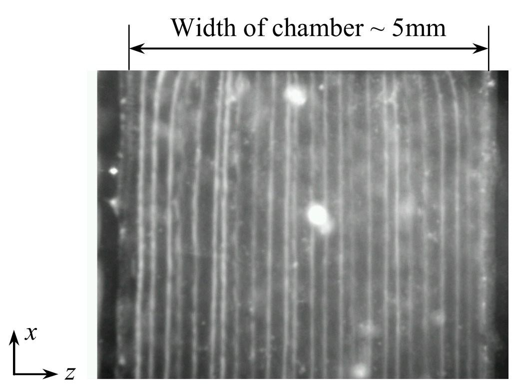

Figure 5: Particle bands formed across the width of the fluid chamber and along it length, caused by variations in the acoustic field. View looking down through Pyrex layer.

5 CONCLUSIONS

A variety of numerical methods have successfully described the behaviour of particles, acoustic field and fluid flow field of a micro-engineered device. The approaches are successful even when limited to a 1-dimension description of the system, although 2-dimensional characteristics can be simulated using alternative, yet commercially available methods with reasonable accuracy at the scale reported. 2-dimensional acoustic and fluid flow field data may be used to expand the more basic 1-dimensional MATLAB numerical model, should a more comprehensive simulation be required.

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