A Hybrid Computational Model to Predict Separation of Cells in Hydrodynamic Metamaterials

Wentao Wang[1] and Yi-Kuen Lee[1,2*]
[1*]*Dept of Mechanical Engineering, HKUST, Kowloon, Hong Kong*
[2]*Joint KAUST-HKUST Micro/Nanofluidics Laboratory, HKUST, Kowloon, Hong Kong*

Summary The separation of biological cells or minute particles in hydrodynamic metamaterials, analogous to photonic counterpart, was investigated by a new hybrid model: FVM based computational model in conjunction with an in-house-built computer code. This hybrid model can simulate the interaction of particles in hydrodynamic metamaterials. By examining the streamline of the fluid flow and the collision of particles within the metamaterial, we confirm that separation of particles originates from the hydrodynamic force and interaction between particles and microstructure in the metamaterial. The simulation results were consistent with the experimental data reported in the literature. The proposed model is promising for the design optimization of hydrodynamic metamaterials in the future.

INTRODUCTION

Manipulation of cells or particles, especially separation is one of the fundamental processes in biological and medical applications, such as genomic sequencing, cancer diagnosis, particle counter *et al* [1, 2]. The most conventional separation method is based on a gel sieving matrix or column. Many research works has been devoted to understand the fundamental principles of separation process and optimize the separation efficiency. One promising method is to replace gel-based matrix by hydrodynamic metamaterials (HMs) [3, 4]. It has attracted abundance of interest in this research field because of its unique advantages compared with traditional separation apparatus. However, the mission of designing the HMs using nano/micro structure is still challenging because there are too many design parameters and there is no reliable mathematical model to describe the function of HMs. The complexity of the flow field and geometry make it very difficult to obtain an analytical model. Numerical methods have been used to study the flow in the micro-device to enhance the performance of the device by reducing clogging, lower hydrostatic pressure and increasing the range of lateral displacement [5]. However, it is difficult to reply on numerical models to gain the insight of the overall picture of the underlying separation principle. Analytical models would be useful for us to understand the fundamental physics of the particle separation in HMs. Inglis *et. al*. proposed one simple way to study the separation by investigating the streamline of the flow [6]. Their results show good agreement with the experimental data. However, this analytical model doesn't consider the interaction between particles and microstructure in the HM. In this paper, the flow and particle interaction was first decoupled with help of simple dimensional analysis. A commercial CFD code was used to predict the flow field of pressure-driven HMs. Then the simulation results were imported into an in-house-built computer code using C++ to monitor the trajectory of the micro particles and particle-wall interaction. In this one-direction coupling method, the computation time and complexity were greatly reduced. The final trajectory of particle was consistent with the experimental results in the literature.

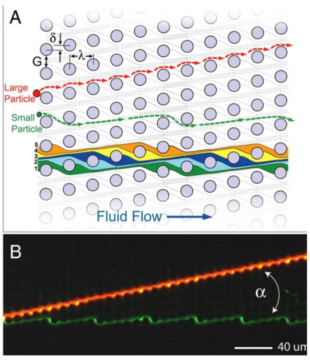

Figure 1. The basic validation model used in the paper [4]. (A). Schematic of a deterministic lateral displacement array; (B). Separation of 2.7 μm red fluorescent beads and 1.0 μm green fluorescent beads by using the array.

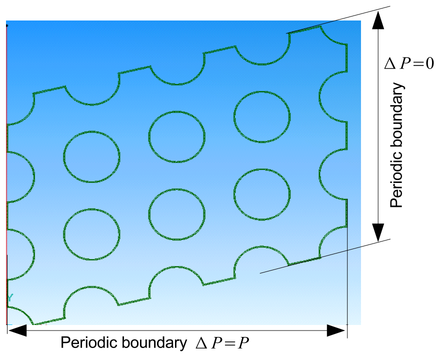

Figure 2. The numerical models for the flow field simulation, the two periodic boundary conditions were applied. Pressure in the vertical direction is zero; Pressure difference in the horizontal direction is 2 Pa. Non-slip wall conditions on the sidewall of micro posts.

MODELING AND SIMULATION

Based on the fabricated microfluidic devices with an array of microposts by Mortan *et al*. [4] as shown in Fig. 1. a commercial CFD code (CFD ACE+, ESI Group, USA) was used to solve the following incompressible Navier-Stokes equations for the flow field inside the HM:

$$\rho(\frac{\partial \vec{V}}{\partial t}+\vec{V}\cdot\nabla\vec{V})=-\nabla P+\eta\nabla^2\vec{V};\quad \nabla\cdot\vec{V}=0 \tag{1}$$

where $\vec{V}$ is a 2D velocity vector, P is the pressure, ρ is the flow density and η is the viscosity.

Because the HM has a periodic micro-post structure, the periodic boundary condition was used in our simulation to reduce the CPU time. For the pressure-driven flow, the boundary condition is shown in the Fig. 2. For the particles with a radius of r_0 and density ρ passing through the HM in low-Reynolds-number condition, the governing equations of the particle motion are:

$$\frac{dx_i}{dt}=v_i;\quad \frac{m_i dv_i}{dt}=f_i^{drag}+f_i^{B} \tag{2}$$

where f_i^{drag} is the hydrodynamic drag force applied by the surrounding fluid and f_i^{B} is the Brownian force.

* Corresponding author. Email: meyklee@ust.hk.

By incorporating the drag force and Brownian force into Eqn (2), the motion of the particle can be described as the Langevin equation:

$$m\frac{d^2x}{dt^2} = -6\pi\eta r_0\frac{dx}{dt} + \left(\frac{12\pi r_0\eta k_B T}{\Delta t}\right)^{0.5} f^B \tag{3}$$

With the help of dimensional analysis, we introduce a new set of non-dimensional motion parameters: $\bar{t}$, $\bar{x}$ and $\bar{v}$:

$$x = L\bar{x}; \quad v = \bar{v}L/t_0; \quad t = \bar{t}t_0 \tag{4}$$

to normalized Eqn. (3) as follows:

$$\frac{d^2\bar{x}_i}{d\bar{t}^2} = -\frac{9\pi\eta t_0}{2r_0^2\rho}\left(\frac{d\bar{x}_i}{d\bar{t}} - \bar{V}(x,y)\right) + \frac{t_0^2}{mL}\left(\frac{12\pi r_0\eta k_B T}{t_0}\right)^{0.5}\frac{\bar{f}^B}{\Delta\bar{t}^{0.5}} \tag{5}$$

For typical 3 μm particles, the coefficients in the first and second terms in Eqn. (5) can be evaluated:

$$\frac{9\pi\eta t_0}{2r_0^2\rho} = 1.57\times10^7; \left(\frac{12\pi r_0\eta k_B T}{t_0}\right)^{0.5}\frac{t_0^{\,2}}{m_0 L} = 6.021\times10^3 \tag{6}$$

Obviously, the Brownian and inertia forces are relatively small in comparison with the drag force. Therefore, the governing equation can be reduced to:

$$\frac{d\bar{x}_i}{d\bar{t}} = \bar{V}_x(x,y); \quad \frac{dy_i}{d\bar{t}} = \bar{V}_y(x,y) \tag{7}$$

Assume the initial coordinate of the particle is $\bar{x}(0) = (x_0, y_0)$, the trajectory of the particles is simply the streamline of the fluid flow in the device if the collision is neglected. In order to consider the particle wall collision, simple one-way coupling method was proposed as show in the flow chart of Fig. 3. One C++ code was used to consider the elastic collision [7]. First the flow field was simulated by the commercial code CFD-ACE+, then the predicted velocity field was imported into our C++ code. Finally, through integrating Eqn. (8) as shown in Fig. 3, we can obtain the new trajectory of the particle for different sizes of particles.

$$\frac{d\bar{x}_i}{d\bar{t}} = \bar{V}_x(x,y); \quad \frac{dy_i}{d\bar{t}} = \bar{V}_y(x,y) \tag{8}$$

The results of the particle trajectory for different sizes are shown in the Fig. 4. Compared with the experimental results in the reference [4], the simulation results shows consistent results.

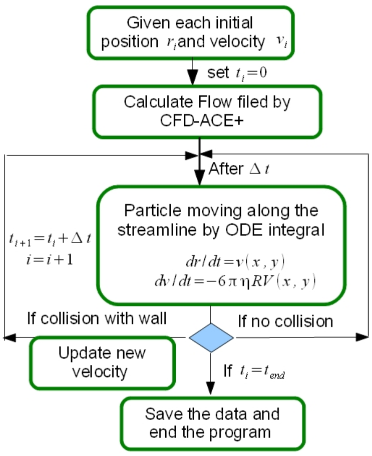

Figure 3. The flow chart for the computer code to determine the trajectory of the particle with different diameters.

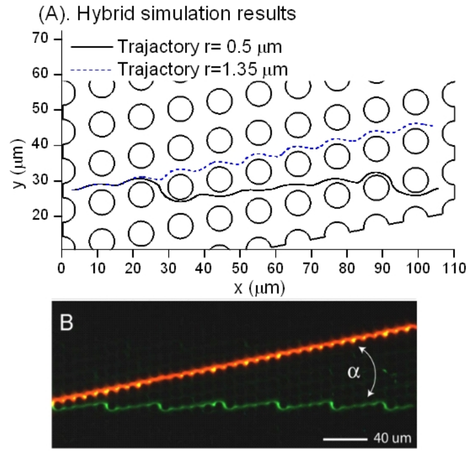

Figure 4. The trajectory of different particles (A) the trajectory of particle with radius of 1.35 μm and 0.7 μm.; (B) the trajectory of a particle with a radius of 0.7 μm.

From Fig. 4, we conclude that the particle and wall interaction is the major separation mechanism. For larger particles, the probability of collision with the microstructure in HM is larger compared with smaller particles.

CONCLUSIONS

In summary, we propose a hybrid model: the FVM based CFD code coupled with a C++ code to simulate particle separation process in HMs. Considering the effects of viscous force and the collision of particle and micro-post boundary, we found that separation originates from the particle and wall collision. The simulation results were verified by the experimental results reported in the literature. The proposed hybrid model is promising for the optimization of different design of HMs with different post diameter, spacing and shape and parametric study of the model in the future.

References

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