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Lattice Boltzmann simulations of pinched flow fractionation

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ABSTRACT

Direct numerical simulations of microsphere motion through a microfluidic separation device (pinched flow fractionation, PFF, device) were performed using the lattice Boltzmann method. The results were compared with the original experimental work on PFF by Yamada et al. (2004). The effects of the pinched segment width and the ratio between the particle solution and diluent flow rates were studied. Both analyses showed agreement with the experimental trends. Previous modelling of PFF has relied on the assumption that particles follow streamlines, and this assumption was evaluated. The simulations indicated that large particles experience a lift force due to a region of low pressure between the particle and the wall of the pinch. The lift force attracts the particles to the wall as they exit the pinched segment. Smaller particles experience a much weaker force. This force may provide an explanation for the experimental observation that a sharp expansion provides better separation performance than a gradual expansion, an effect that cannot be explained by streamline analyses.

1. Introduction

The motion of solid particles is important in a wide variety of microfluidic devices. In many of these devices, geometric constraints, internal hydrodynamic forces, or external forces are used to control the motion of the particles. Often the goal is to separate the particles by size. The design of such devices requires models for the interactions between the particles and the flow to account for effects such as the lift on particles in shear flow and drag due to Dean flow (Berger et al., 1983). Modelling and simulation are complicated by the fact that next to viscous effects, inertial effects may be important at the moderate Reynolds numbers that can be achieved in microfluidic devices, implying that the simplifying assumption of creeping flow is not applicable. The challenges in understanding the behaviour of particles in microfluidic systems are emphasized by a recent study of microsphere motion in which the assumption that the centre of mass of a particle has the same speed as the particle-free flow was shown to become inaccurate as the width of a microchannel approaches the diameter of the spheres (Di Carlo et al., 2009). Thus, confinement, in addition to finite particle size and mass, causes particle velocities to deviate from the velocity of the undisturbed fluid. Computational studies with fully resolved hydrodynamics and coupled particle motion are a valuable tool for studying complex microfluidic systems when the validity of simplifying assumptions is poor or uncertain. In this work, we present lattice Boltzmann simulations of a device for separating particles by size.

Pinched flow fractionation (PFF), a method for the continuous separation of particles by size, was proposed by Yamada et al. (2004). In PFF, particles with different sizes in a fluid stream are pushed against one wall of a narrow channel, the pinch, by the flow of an injected diluent. Due to their alignment along that wall, the centres of mass of the particles follow different streamlines. When the particles enter a wider channel, they separate as the streamlines spread. The method has been used to separate 15 and 30 μm poly(styrene/divinylbenzene) beads in a viscous aqueous Dextran solution (Yamada et al., 2004), erythrocytes from blood plasma (Takagi et al., 2005), and the droplets of an emulsion (Maenaka et al., 2008). In the latter two examples, the irregular shape and deformability of the dispersed phase introduce additional complexity to performance analyses. Enhanced PFF methods have been proposed (Lee et al., 2011b; Vig and Kristensen, 2008). We study rigid spherical particles in simple PFF.

The analysis and prediction of PFF performance have been primarily based on the assumptions that particles follow the streamlines of the particle-free flow and do not disturb the flow (Jain and Posner, 2008; Vig and Kristensen, 2008; Yamada et al., 2004). The first empirical model for PFF was a linear amplification relationship that was determined from the paths of fluorescent microsphere tracers (1.0 μm diameter) (Yamada et al., 2004)

$$y_o = \left(w_p - \frac{D}{2}\right)\frac{w_o}{w_p} \tag{1}$$

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where w_o is the width of the outlet, w_p is the width of the pinch, y_o is the position of the particle centre at the outlet, and D is the diameter of the particle. This model assumes that particles reach the upper wall while in the pinched segment. If the particles do not reach the upper wall, linear amplification implies that

$$\frac{y_o}{y_p} = \frac{w_o}{w_p} \tag{2}$$

where y_p is the position of the particle centre when it is in the pinched segment. This empirical model assumes that the streamlines, as determined from the tracer trajectories, exhibit linear amplification and that the microspheres being separated follow these streamlines. Mortensen (2007) points out that for low Reynolds number (Stokes) flow, the assumption that particles follow streamlines cannot explain some experimentally-observed phenomena. For example, if particles follow streamlines, then separation performance should be independent of the geometry between the pinch and outlet because the positions of the streamlines in the outlet depend only on the final width of the channel. Yamada et al., however, observed better performance with a sudden expansion (step, 180° boundary angle) than with a gradual expansion (linear, 60° angle). Mortensen indicates a need for more detailed modelling of PFF to better understand and design PFF devices.

Vig (2010) provides a review of recent improvements to the empirical linear model proposed by Yamada et al. (2004). The model of Andersen et al. (2009) employs the analytical solution for the laminar flow profile in a rectangular channel and shows better agreement with experimental results. While this model provides an improvement to the linear streamline amplification model, which is accurate in the limit of high aspect ratio channels, it still relies on the assumption that particles follow streamlines. Vig and Kristensen (2008) and Vig (2010) modelled PFF by assuming that particles follow streamlines, but included a corner effect. This corner effect accounts for the geometric constraints that prevent particles from following streamlines that pass closer to a wall than the radius of the particle. Their 2D computational model used the finite element method (FEM) to obtain the streamlines of the flow. It is based on the assumptions that the particles do not disturb the flow and the walls provide only a geometric constraint and cause no forces on the particles. The model is considered semi-3D because a body force that is inversely proportional to the fluid velocity is used to account for the hydraulic drag of the walls in the omitted dimension (the depth of the channel).

To allow better modelling of PFF, the reasons for the deviation of the particles from the streamlines need to be understood. These deviations appear to be caused by the complex hydrodynamics arising from the confinement of the particles in a narrow channel. The purpose of the present work is to use the lattice Boltzmann method to perform direct three-dimensional simulations of PFF. The flow of single spherical particles of two different diameters through a PFF device was simulated. The simulation results were compared with the experimental performance data reported by Yamada et al. (2004). Such simulations with fully resolved hydrodynamics and full resolution of the solid–liquid interface provide a way to determine the limitations of simplifying assumptions and identify which physical effects are essential for modelling particle behaviour. The simulations could therefore be used to guide the development of simpler yet accurate models.

This paper is organized as follows. First, the mathematical modelling of PFF is described, followed by a description of the required numerical methods. These include the lattice Boltzmann method (LBM), its boundary conditions, the immersed boundary method, and the methods for the numerical integration of particle motion. Several validation benchmarks are described before the full simulations of PFF are presented and discussed. Finally, the research is summarized and main conclusions are provided.

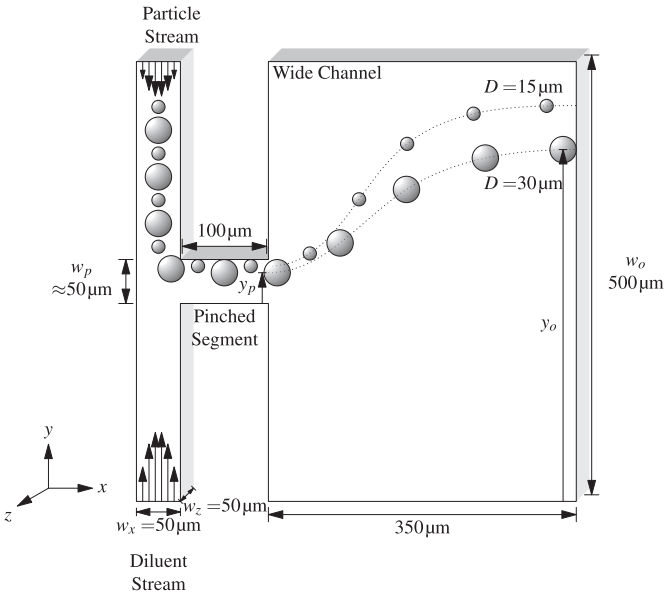

Fig. 1. Schematic of the simulated pinched flow fractionation device.

2. Mathematical modelling and simulation set-up

2.1. Geometry

A schematic of the simulated device geometry is shown in Fig. 1. The geometry employed by Yamada et al. was modified to facilitate the simulations yet allow a comparison between the experiments and simulations to be meaningful. One difference in the geometry is the angle between the inlet channels. While Yamada et al. used an angle of 60°, the simulated geometry has an angle of 180° to simplify the implementation of the boundary conditions on a cubic lattice. This difference in the geometry, though it may affect the position the particles reach in the pinched segment, is considered minor because our main interest is in the behaviour of the particles as they exit the pinched segment. Another difference is the smaller outlet width (500 μm versus 1000 μm). For either width, the ratio between the pinched channel and outlet channel widths is high, and it is expected that the vertical position of particles normalized by the width of the outlet channel would be similar in both cases. The length of the outlet, 350 μm, was chosen to limit simulation time by selecting the shortest length for which FEM simulations with COMSOL (COMSOL AB, 2010) showed a minimal difference in the streamlines when compared with a longer outlet channel.

To allow comparison with the experimental work, the parameters in the simulations were chosen to match the experimental system as closely as possible. In LBM simulations, the distance between lattice nodes Δx is taken to be one, and the time interval Δt of each simulation time step is also one. Quantities used in the simulations, such as length and viscosity, are given in lattice units (l.u.) and the actual units are omitted. For example, a viscosity of 0.1 l.u. means 0.1 $\Delta x^2/\Delta t$. The matching between the simulations and experiments is performed through dimensionless numbers. Based on the ratio of the particle diameter and the pinched segment width, we simulate particles with equivalent physical diameters of 15 and 30 μm, as in the experiments. The particle over fluid density ratio was 1.08. The long computation time imposed by LBM stability constraints prevents running simulations at a Reynolds