Modeling Particle-Fluid Coupling and its Impact on Magnetic Particle Transport in Microfluidic Systems

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ABSTRACT

An analysis is presented of the effects of particle-fluid coupling on the transport and capture of magnetic particles in microfluidic systems with magnetophoretic functionality. Magnetic particle transport is modeled using a computational fluid dynamic CFD-based Lagrangian-Eulerian approach that takes into account dominant particle forces as well as two-way particle-fluid coupling. The difference in capture efficiency for one-way versus two-way particle-fluid coupling is analyzed and quantified. The analysis shows that one-way coupling over predicts the magnetic force needed for particle capture as compared to more rigorous fully-coupled analysis. In two-way coupling there is a cooperative effect between the magnetic force and a particle-induced flow towards regions of high field gradient that enhances capture efficiency. While commonly used one-way coupling is useful for rapid parametric screening of particle capture efficiency, more accurate predictions require two-way particle-fluid coupling. This is especially true when higher capture efficiencies and/or particle concentrations are required.

Keywords: Magnetic separation, particle-fluid coupling, magnetophoresis, magnetophoretic microsystem, magnetic particle transport, field-directed particle transport.

1 INTRODUCTION

Applications of magnetic particles are proliferating, especially for emerging applications in the fields of microbiology, nanomedicine and biotechnology. Many of these applications involve the use of microfluidic systems in which magnetic particles are used to sort and separate biomaterials. Magnetic particles are well suited for such applications because they can be functionalized to selectively bind to target biomaterials such as proteins, enzymes, nucleic acids or whole cells, thereby enabling control of these materials in microfluidic channels using an external field as shown in Fig. 1. To date, the analysis of magnetic field-induced particle transport and capture has usually been limited to one-way particle-fluid coupling in which the flow field is uncoupled from particle motion, i.e.

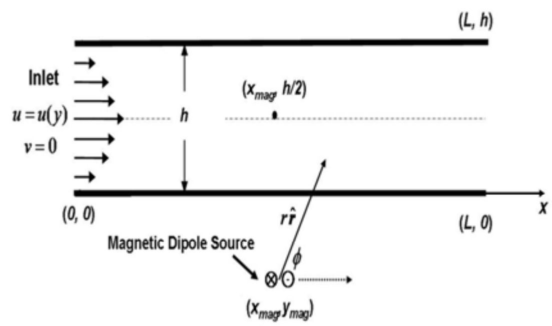

Figure 1. Microfluidic channel above a magnetic dipole field source.

there is no momentum transfer from the particles back to the fluid. In this presentation, a fully coupled analysis is presented. The analysis takes into account the impact of particle motion on the flow field and is used to study the transport and capture of magnetic particles in a microfluidic channel. Particle motion is predicted using a CFD-based Lagrangian-Eulerian approach that takes into account the dominant particle forces as well as two-way particle-fluid coupling. Two dimensionless groups are discussed that characterize particle capture. In addition, the difference in capture efficiency is predicted and quantified using one-way versus two-way particle-fluid coupling. The analysis demonstrates that one-way coupling provides a conservative estimate of capture efficiency in that it over predicts the magnetic force needed to ensure particle capture as compared to the more rigorous fully-coupled analysis. In two-way coupling there is a cooperative effect between the magnetic force and a particle-induced flow towards regions of high field gradient that enhances capture efficiency. This work shows that while one-way particle-fluid coupling analysis is sufficient for an initial estimate of particle capture performance, two-way particle-fluid coupling analysis is needed when considering higher capture efficiencies and/or higher particle concentrations.

NSTI-Nanotech 2012, www.nsti.org, ISBN 978-1-4665-6275-2 Vol. 2, 2012

2 THEORY AND MODELING

The motion of colloidal magnetic particles in fluid under the influence of an applied field is governed by several factors. These include the applied magnetic force, fluidic drag (pressure and viscous), an increase in the effective particle mass due to an entrainment of surrounding fluid, fluid shear, particle/fluid interactions (particle-induced perturbations to the flow field), gravity, buoyancy, Brownian dynamics and interparticle effects such as magnetic dipole-dipole interactions [1-4]. A comprehensive model that takes all these factors into account is highly complex and beyond the scope of this presentation. Here, we make several assumptions that simplify the analysis. We assume that the fluid is incompressible and that the flow is laminar, which is usually the case in microfluidic devices. We further assume that the particle suspension is sufficiently dilute so that particle-particle interactions can be neglected. Particle coagulation as well as build-up and subsequent channel blockage are also neglected. The particle magnetism is assumed to be linear, i.e. below saturation. We also assume that the particles enter the channel with a uniform spatial distribution with respect to the height of the channel.

We use a combined Lagrangian-Eulerian CFD-based approach to model fully-coupled particle-fluid interactions during the transport and capture of magnetic particles in a microfluidic channel subjected to an applied field. A Lagrangian analysis is used to track the motion of individual particles, and the particle motion is coupled to the fluid by introducing a particle force sink into the Navier-Stokes momentum equations, which are solved using an Eulerian-based CFD analysis. In the Lagrangian formulation particle transport is governed by Newton's second law,

$$m_p \frac{d\mathbf{u}_p}{dt} = \sum \mathbf{F}_{ext} \qquad (1)$$

where m_p and $\mathbf{u}_p$ are the mass and the velocity of the particle and

$$\sum \mathbf{F}_{ext} = 6\pi\eta a\left(\mathbf{u}-\mathbf{u}_p\right)+V_p\left(\rho_p-\rho\right)\mathbf{g}+\mathbf{F}_{mag} \qquad (2)$$

is the sum of the external forces on the particle. The variables $\mathbf{u}$, ρ and η are the velocity, density and viscosity of the carrier fluid, ρ_p, a and V_p are the density, radius and volume of the particle, and $\mathbf{g}$ is the gravitational acceleration. The first term on the right hand side represents the drag as described by Stokes' law. The second term is the lift (buoyant) force, which depends on the mass difference between the particle and the corresponding displaced fluid. The third term is the magnetic force $F_{mag} = \frac{1}{2}\mu_0\chi_m V_p \nabla H^2$, where μ_0 is the free-space magnetic permeability and χ_m (dimensionless) is the susceptibility of the magnetic particle, which is estimated based on its magnetically active volume and relative to the susceptibility of the carrier fluid, H is the magnitude of the applied external magnetic field (A/m), which can be related to the magnetic field induction B (in T) of a particle suspended in a non-magnetic or weakly diamagnetic fluid H = B/μ_0. Taking into account the various force expressions, the equation governing particle motion becomes,

$$m_p \frac{d\mathbf{u}_p}{dt} = b^{-1}\left(\mathbf{u}-\mathbf{u}_p\right)+V_p\left(\rho_p-\rho\right)\mathbf{g}+\frac{1}{2}\mu_o\chi_m V_p\nabla H^2 \qquad (3)$$

The trajectory equations are solved by stepwise integration over discrete time steps. Integration over time of the particle motion equation yields the velocity of the particle at each point along its trajectory

$$\frac{d\mathbf{u}_p}{dt} = \tau^{-1}\left(\mathbf{u}-\mathbf{u}_p\right)+\mathbf{A} \qquad (4)$$

where

$$\mathbf{A} = \frac{V_p\left(\rho_p-\rho\right)\mathbf{g}+\frac{1}{2}\mu_o\chi_m V_p\nabla H^2}{m_p} \qquad (5)$$

and $\tau = m_p b$. The trajectory can be predicted using

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{u}_p \qquad (6)$$

The characteristic time τ is that required for a particle to respond to changes in the base fluid motion, also referred to as the particle relaxation time. Note that Eqs. (4) and (6) are a set of coupled ordinary differential equations that can be integrated using a number of different numerical techniques. We have used a fourth-order Runge-Kutta method for our analysis [2].

We model the fluid phase using an Eulerian approach. The fluid velocity field is described by the Eulerian incompressible Navier-Stokes equations,

$$\nabla\cdot\mathbf{u} = 0 \qquad (7)$$

$$\rho\left(\frac{\partial\mathbf{u}}{\partial t}+\mathbf{u}\nabla\mathbf{u}\right) = -\nabla P+\nabla\cdot\left(\eta\nabla\mathbf{u}\right)-\mathbf{f}_p \qquad (8)$$

The particle volume fraction (particle loading) is assumed to be sufficiently low so that its effect on the fluidic continuity equation and on the inertia and stress flux terms in the fluidic momentum equation can be neglected. The two-way coupling is accounted for through the particle-weighted sink term $\mathbf{f}_p$ that represents the counter drag force density exerted by the particles (located in the continuum cells) on the fluid assuming that the suspension is dilute. In practice, this is realized when the volume fraction of the discrete phase is less than 10–12%. We use the discrete phase model (DPM) provided by ANSYS FLUENT (www.ANSYS.com) to predict particle-fluid coupling and to track particle motion [5-6]. This model employs an Euler-Lagrange approach that treats the fluid phase as a continuum by solving the Navier-Stokes equations, while the dispersed phase is solved by tracking particle parcels, each containing particles with the same properties including diameter, velocity, injection position and trajectory.

The standard Lagrangian part of the DPM calculates the trajectory based on the translational force balance that is formulated for a representative particle as in Eq. (1) In the standard DPM, each particle represents a parcel of particles. In our case, a DPM parcel is subjected to a fluidic drag force, a magnetic force and gravity. The magnetic force is programmed based on the particle position and then compiled into FLUENT using a User Defined Function (UDF). The volume loading (per cell) and other variables are monitored using the same UDF. In the DPM, a particle is treated as a point mass, i.e. it does not occupy volume in the computational domain. Thus, interparticle collisions and the volume displacement of the base fluid by the discrete particles are neglected. Due to these assumptions and simplifications, the DPM is deemed to be valid for dilute fluid-particle flow with a volume loading less than 12%. This condition can be tracked throughout the analysis to ensure proper application of the model.

3 RESULTS

We apply the theory to the analysis of particle transport and capture in a two-dimensional microchannel shown in Fig. 1. We perform a parametric analysis of this system about a base configuration in which the microchannel has a height h = 100 μm and a length L = 1000 μm [6]. The width of the channel (into the page) is assumed to be sufficiently large to justify a two-dimensional flow analysis, i.e. we ignore flow variation in that direction. The length of the channel is sufficiently long so that hydrodynamic effects at the inlet and outlet do not impact the magnetic field-directed particle motion near the mid-length of the channel.

A magnetic dipole field source in the form of a pair of anti-parallel current carrying conductors is positioned beneath the lower wall of the microchannel, midway along its length**.** The magnetic field at any location (r,ϕ) with respect to the virtual origin of the line dipole is given by

$$\mathbf{H} = \frac{p}{\mathbf{r}^2}\left(\sin(\phi)\hat{e}_r + \cos(\phi)\hat{e}_\phi\right) \tag{9}$$

where $p = \frac{Id}{2\pi}$, I is the current in each conductor and d is the distance between the conductors. The dipole source is positioned at a distance $y_{mag} = -100\mu m$ beneath the lower wall of the microchannel, midway along its length ($x_{mag} = 500\mu m$).

The performance criterion for magnetic separation is defined in terms of collection efficiency,

$$CE = \frac{\text{number of particles captured}}{\text{total number of particles}}, \tag{10}$$

which is the percentage of incoming particles that are captured in the microchannel by the magnetic force. We introduce two dimensionless groups to study this process [6],

$$\beta = \frac{\frac{1}{2}\mu_o \chi V_p p^2}{6\pi\eta a u_i h^5} \quad \text{and} \quad \gamma = \left(\frac{y_c}{h}\right). \tag{11}$$

The parameter β is independent of the location of the magnetic source, while γ depends on the position of the source (y_c) and therefore the field gradient that it generates within the microchannel. The use of two dimensional groups is motivated by the fact that the magnetic field and its gradient decay rapidly (and in a nonlinear fashion) with distance from the source. Thus the magnetic force is much more sensitive to the placement of the source than any other system parameter.

In our analysis, incompressible Newtonian fluid (water) enters the channel at the left side (inlet) with a fully developed laminar flow profile in which the average velocity is u_i = 200 μm/s. The outlet pressure is set to zero. Spherical magnetic particles are injected into the computational domain at the inlet with a uniform distribution over the entrance plane. The properties of the magnetic particles are chosen to be compatible with the MyOne™ beads produced by Dynal Biotech (www.dynabead.com), which are widely used for bioapplications. The MyOne particle has the following properties: a = 0.525 μm, ρ_p = 1700 kg/m^3 Ms = 4.3× 10^4 and an “effective” susceptibility χ =1.4.

A comparison of predicted particle trajectories with one-way and two-way coupling for the base problem is shown in Fig. 2 for various values of the dipole field strength p. From this figure, we find that the one-way coupling analysis under-predicts particle capture relative to the two-way fully-coupled analysis. That is, the magnetic force required to achieve a given capture efficiency is predicted to be higher using one-way coupling as compared to the fully-coupled analysis. The p=215 μAm calculations (Fig. 2d) are illustrative of this effect. Specifically, for one-way coupling, this field strength renders critial particle capture, i.e. all particles are captured, albeit some at locations beyond the dipole field source. However, it is obvious that the critial particle capture occurs for at a lower field strength (i.e. for p between 192-215 μAm) in the two-way coupling analysis. This is because near the dipole source, the magnetic force accelerates the particles

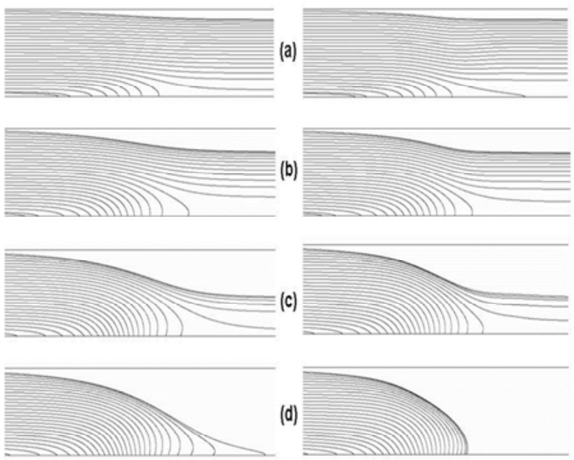

Figure **2.** Comparison of predicted particle trajectories using one-way (left) and two-way (right) coupling vs. dipole strength p: (a) p = 64 μAm, (b) p = 128 μAm, (c) p = 192 μAm, and (d) p =215 μAm [6].

downward. This in turn, induces a downward (vertical) component in the fluid velocity due to the two-way momentum transfer between the particles and the fluid, which is proportional to the instantaneous difference between their respective velocities. This effect can be seen in Fig. 3, which shows the particle trajectories

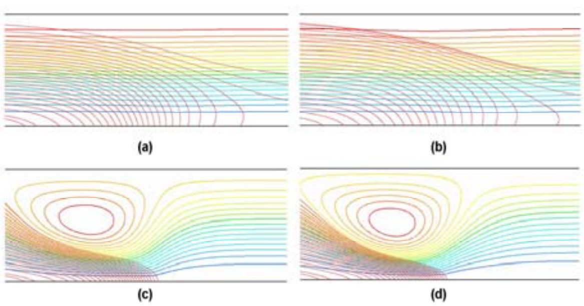

Figure 3. Two-way coupled particle trajectories superimposed with fluid stream lines for different inlet particle volume fractions: (a) ϕ_i =0.0588%, (b) ϕ_i = 0.3%, (c) ϕ_i =0.588%, (d) ϕ_i =0.882% [6]

superimposed with the corresponding fluid stream-lines as a function of the injetcted inlet volume fraction of particles ϕ_i. The downward distortion of the stream-lines due to two-way particle-fluid coupling is clear and is more pronounced at higher volume fractions as expected. Figure 4 shows a comparison of *CE* using one-way vs. two-way coupling analysis. Note that the one-way and two-way values are approximately the same for β such that CE $\leq$ 0.6 However, the former under predicts the latter for larger vales of β.

4 CONCLUSIONS

We have used a CFD-based Lagrangian-Eulerian approach to predict particle motion and its impact on the

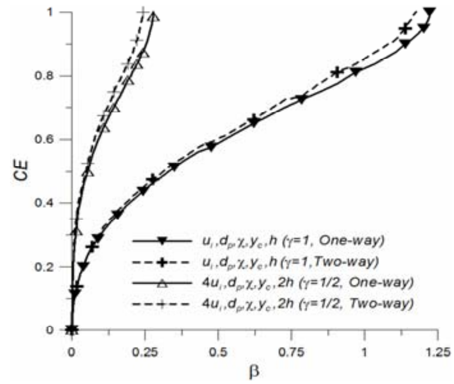

Figure 4. Capture efficiency *CE* vs. β : γ=1.0. and 0.5 for one-way and two-way coupling (ϕ_i =0.3%,) [6].

flow field in a magnetophoretic microfluidic system. We have shown that predictions based on one-way coupling over predict the magnetic force needed for particle capture as compared to those based on two-way coupling. This is due to the fact that in two-way coupling there is a cooperative effect between the magnetic force and a particle-induced flow that acts to enhance the capture efficiency. This shows that while one-way particle-fluid coupling analysis enables rapid parametric screening of viable system parameters, two-way coupling is needed for more accurate analysis, especially when considering higher capture efficiencies and higher particle concentrations. The model presented here should be of substantial use in the development of a broad range of novel magnetophoretic processes and devices.

Acknowledgments The first author acknowledges the financial support received from the Research Affairs at the UAE University under contract number 01-05-7-12/10.

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