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CFD SIMULATION OF MAGNETIC SEPARATION IN MICROFLUIDICS SYSTEMS USING MIXTURE MODEL

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ABSTRACT

In this paper, we use mixture model with algebraic slip velocity to simulate the magnetic separation in a microfluidic system. The coupled particle-fluid transport and magnetic field-directed particle capture were analyzed in a 2D microfluidic channel with soft magnetic elements embedded on one of its walls. The High Gradient Magnetic Separation (HGMS) is achieved by the elements while being magnetized by a uniform background magnetic field. The algebraic slip velocity is modeled based on the local equilibrium between drag and the magnetic forces acting on the magnetic particle. For dilute loading and microfluidic scale, the granular and gravitational parameters were found to have a minor effect on the prediction the capture efficiency.

NOMENCLATURE

a	characteristic length
c	mass fraction
d	diameter
F_D	drag function
$f(H)$	magnetization function
$\mathbf{g}$	gravitational field
H	applied magnetic field
M_s	magnetic saturation for the particle
m	mass
p	pressure
V	volume
$\mathbf{v}$	velocity
t	time
α	volume fraction
ρ	density
η	dynamic viscosity
μ_o	vacuum magnetic permeability
χ	apparent magnetic susceptibility

Subscripts

l	liquid
m	mixture
p	particle

INTRODUCTION

The magnetic separation of magnetic targets using microfluidic systems is emerging rapidly with applications involving mineral processing, environmental analysis, toxicology, microbiology, medical diagnostics, and biochemical sensing. In these applications, inherently magnetic or magnetically-labeled targets, such as cells, proteins, genes and pathogens, can be selectively separated from continuously flowing suspensions (Choi et al. 2000; Zborowski et al. 2003; Pamme 2007; Smistrup et al. 2007; Lee et al. 2008; Jung and Han 2009 Ramadan and Gijs 2012). In the microfluidic platform, Ecology is another field in which magnetic separation can serve many agricultural- and water-analysis applications. Furthermore, magnetic microseparator can be used in on-site tests to serve many applications related home security as to detect and monitor biologically and chemically hazardous agents (Mark et al. 2010).

In the context of magnetic separation, using CFD to analyze the coupled particle-fluid transport and the magnetic field-directed particle separation is a very important and cost-effective tool for the development and optimization of related microfluidic systems.

There are several impacts that differentiate the numerical treatment of micro flows from the macro scale counterpart. However, the particles-laden flow in the micro-scale can, still, be viewed as a mixture of phases that interact with each other through an interface and not by a molecular reaction.

With relevance to most of the existing microfluidics applications, the study, here, focuses on the problems involving dilute particle-liquid suspensions. With that, the CFD modeling must adequately depicts the interfacial interaction between the carrier liquid and the dispersed particles. Though it is easy to formulate, the direct numerical simulation for the interfacial dynamics between suspended particles and a carrier liquid is almost impossible to achieve with the current computational resources. Therefore, the interfacial dynamics must be modeled. This is the case with most existing multi-phase models.

In the context of particles-laden flows, multiphase models are characterized, based on the tracking mode of the particulate phase, as either Lagrangian-Eulerian or Eulerian-Eulerian models. In both categories, the carrier fluid is treated in the Eulerian reference. In the Lagrangian tracking approach, the particle motion is solved discretely, i.e. on a particle basis. In its standard form, the model treats the particles as mass points that occupy no volume in the mixture. Such an approach is valid under dilute conditions (volume fractions less that ~5%) and for small Stokes number. It has been employed by many researchers (Han and Bruno Frazier 2004; Han et al. 2005; Smistrup et al.

2005; Torsten Lund-Olesen et al. 2007; Wei et al. 2010; Furlani et al. 2007) to track the magnetophoretic mobility of the particles. In these studies, the velocity field of the carrier flow was simply based on analytical solutions valid for the fully developed flow through microchannels with simple configurations. More refined treatments were achieved by coupling the Lagrangian tracking of the particles with the Eulerian solution for the fluid motion as attained using the full Navier Stokes equations and by which the particle-fluid momentum exchange between phases is accounted for (Khashan and Furlani 2011; Khashan and Furlani 2013; Khashan et al. 2014; Khashan and Furlani 2014; Modak et al. 2008; Modak et al. 2010). Based on our extensive search, the mixture model has not been used for any problem that involved magnetophoresis-based microfluidics. In the absence of magnetic interaction, mixture model was used to simulate blood flow (Wu et al. 2014) and the separation of particles by centrifugal force (Ookawara et al. 2006). In the macro scale and in the contents of magnetic separation, similar Eulerian-Eulerian models were used to investigate the trapping of a slurry containing magnetic particles (Mohanty et al. 2011), and the magnetoconvection in ferrofluids (Bozhko and Tynjälä 2005).

Since the flow involving the magnetic particles, typically flowing through microfluidic systems, known to have small Stokes number, the particle will respond almost instantaneously to the acting forces. Accordingly, the mixture model can be considered as a feasible substitute to the Lagrangian-Eulerian models. In the mixture models, solving for the momentum conservation is only required for the continuum mixture and not for all phases individually. With that, it can cut on the computational cost greatly.

MODEL DESCRIPTION

The motion of dispersed magnetic particles is subject to many influences such as; the applied magnetic force, drag, gravitational forces, inter-particles interactions and the induced Brownian motions (Fletcher 1991; Gerber et al. 1983). However, it is widely adopted that when a dilute suspension of micro, not nano, particles is occupying a volume fraction of less than 10%, only magnetic, drag and, gravitational forces are important. Furthermore, depending on the particle loading, the fluid-particles interaction, mainly drag and counter drag coupling, can be modeled as either two-way or one-way. One-way coupling is applied when the fluid motion impacts that of the particles and not vice versa, and two-way coupling is applied when the motion of each phase is expected to impact the other's motion.

Based on Newton's second law, the motion of a single particle can be described as

$$m_p \frac{d\mathbf{v_p}}{dt} = m_p F_D(\mathbf{v_l} - \mathbf{v_p}) + V_p(\rho_p - \rho_l)\mathbf{g} + \frac{1}{2}\mu_o V_p f(H)\nabla H^2 \quad (1)$$

The first term on the right hand side of Eq. (1) represents the drag. The second and third terms represent the buoyant and magnetic forces, respectively. Based on the Stokes' drag model, the drag function F_D can be defined as

$$F_D = \frac{18\eta}{\rho_p d_p^2} \quad (2)$$

The function $f(H_a)$ describes the magnetization status of the particle based on the applied magnetic field H_a and the magnetic saturation M_s of the particle. Covering under-saturated and saturated magnetization, the function can be stated for a magnetic particle with an apparent magnetic susceptibility χ as (Khashan and Furlani 2013):

$$f(H) = \begin{cases} \chi & , H_a < \frac{M_s}{\chi} \\ \frac{M_s}{H_a} & , H_a \geq \frac{M_s}{\chi} \end{cases} \quad (3)$$

Under local equilibrium, the inertia force ($m_p \frac{d\mathbf{u_p}}{dt}$) in equation (1) is neglected. Accordingly, the slip velocity ($\mathbf{v}_{slip} = \mathbf{v}_p - \mathbf{v}_l$) takes the algebraic form

$$\mathbf{v}_{slip} = \frac{\mu_o V_p f(H)}{6\pi\eta d_p}\boldsymbol{\nabla} H^2 + \frac{d_p^2(\rho_p - \rho_m)}{18\eta}\mathbf{g} \quad (4)$$

In our numerical implementation, the applied magnetic field H and the corresponding gradients were pre-calculated analytically (Khashan and Furlani 2013) to yield closed-form expressions.

For particle-laden flows, the mixture model is more applicable when the particle loading is dilute and when the particles are known to respond instantaneously to the acting forces. This means that the acting forces establish a local equilibrium causing the particle to move at a constant terminal velocity along the computational cell. The phases are treated as interpenetrating continua. However, unlike the case with the full Eulerian model, only one momentum equation comprising the whole mixture is solved. In the following, we briefly outline the mathematical formulation of the mixture model. If the volume fraction of the particulate phase is denoted by α_p and its mass fraction are defined as $c_p = \alpha_p\rho_p/\rho_m$, the mixture's mass-center velocity takes the form $\mathbf{v_m} = c_p\mathbf{v_p} + (1 - c_p)\mathbf{v_l}$. The mass and momentum conservation for the mixture take the forms

$$\frac{\partial}{\partial t}(\rho_m) + \nabla\cdot(\rho_m\mathbf{v_m}) = 0 \quad (5)$$

$$\frac{\partial}{\partial t}(\rho_m\mathbf{v_m}) + \nabla\cdot(\rho_m\mathbf{v_m}\mathbf{v_m}) = -\nabla p_m + \mu_m\nabla^2\mathbf{v}_m - \nabla\cdot\left(\rho_m c_p(1 - c_p)\mathbf{v}_{slip}\mathbf{v}_{slip}\right) + \rho_m\mathbf{g} + \alpha_p\frac{1}{2}\mu_o f(H)\nabla H^2 \quad (6)$$

In equation (6), the third term in the right hand side accounts for the momentum transfer between the phases and physically represents the diffusive flux due to phasic slip. The diffusion (drift) velocities are defined for particles and liquid phases, respectively, as $\mathbf{v}_{mp} = \mathbf{v}_p - \mathbf{v}_m$ and $\mathbf{v}_{ml} = \mathbf{v}_l - \mathbf{v}_m$. The last term accounts for the applied magnetic force weighted by the particulate volume fraction, that is, the force exerted by a single particle is multiplied by the total number of particles in the Eulerian control volume. Similar to the density, the mixture viscosity can be simply weighted with respect to the phasic volume fractions as $\mu_m = \alpha_l\mu_l + \alpha_p\mu_p$. The volume fraction of the dispersed phase can be described by,

$$\frac{\partial}{\partial t}(\alpha_p\rho_p) + \nabla\cdot\left(\alpha_p\rho_p\left(\mathbf{v_m} + (1 - c_p)\mathbf{v}_{slip}\right)\right) = 0 \quad (7)$$

Without the slip velocity (Eq. (4)) the mixture model would refer to a homogeneous multiphase flow.

RESULTS

As a test problem, we simulate the particle-fluid transport and particle capture in a 2D microchannel with a single soft-magnetic element embedded at its lower wall. The microchannel (shown in Fig. 1) is 300 μm in height, 2 mm in width, and 10 mm long. Such height to width ratio permits 2D analysis. The fully developed laminar flow of the water-particle mixture enters the microchannel at the inlet average velocity v_{in}. The outlet pressure is set to zero (gauge). The particles interaction with walls is accounted for simply by applying no slip condition for the continuous mixture equations.

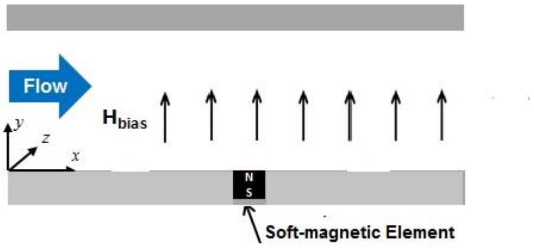
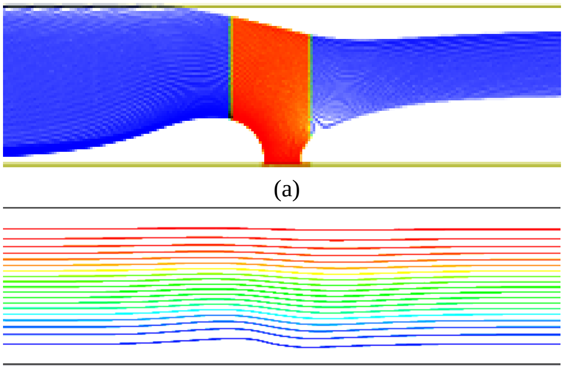


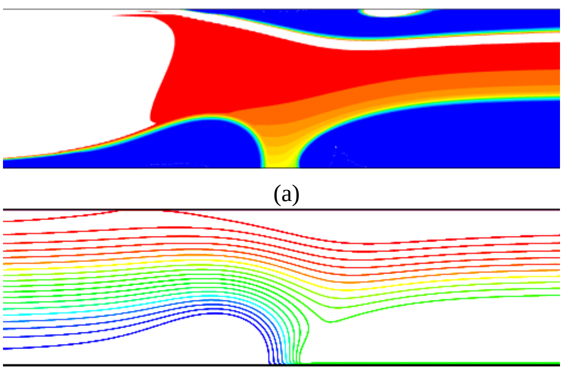
Figure 1: The flow and magnetic arrangement. The external magnetic source, located beneath the channel, produces homogenous magnetic field *H*(y) normal to the flow direction. Only one soft-magnetic element is used.



(a)

(b)

Figure 2: (a) Calculated trajectories, CE= 51% , red colored trajectories just marks the position of the magnetic element beneath and (b) streamlines of the whole mixture using two-way DPM approach. Inlet velocity and injection volume fraction α_{p_i} are 4 mm/s and 0.002 respectively.



(a)

(b)

Figure 3: Mixture model results; (a) Volume fractions (contours clipped to values lower than the value at the inlet), blue refers to particles-free regions (b) streamline of the particulate phase. Inlet velocity and injection volume fraction $\alpha_{p_i}$are 4 mm/s and 0.002, respectively.

The external magnetic field is generated by a rare-earth NdFeB permanent magnet with dimensions much larger than the microchannel size and it is located beneath the microchannel system. Hence, external magnetic arrangement generates a uniform macro-scale field *H*(y) which can be concentrated into a localized micro-scale field in the nearby region of the soft elements. In this study, the external magnetic field is assumed equal to 0.5 Tesla which is sufficient to magnetically saturate the 100 µm ×100 µm soft element (Permalloy 78% Ni 22% Fe). The magnetic saturation of the element M_{es} is equal to 8.6×10^5 A/m.

The properties of the mixture are based on water (η = 0.001 N·s/m^2 and ρ = 1000 kg/m^3) and the Dynal Biotech magnetic beads "*Myone*" (d_p = 1.05 µm, ρ_p= 1800 kg/ m^3, saturation magnetization M_s = 4.3×10^4 A/m and effective magnetic susceptibility χ = 1.4). The mass flow rate of the beads injected through the middle inlet (v_{in} = 4 mm/s) is corresponding to an inlet volume fraction α_p of 0.002.

The gravitational force acting on a bead in water, $\mathbf{F}_g = V_p(\rho_p - \rho_l)\mathbf{g}$, can be calculated to be 0.004 *pico* N. This force can be justly neglected when compared with the magnetic force generated near the magnetic elements, which are on the order of tenths of a *pico* N.
The performance criterion for magnetic separation system is defined in terms of capture efficiency *CE*. The capture efficiency is calculated from the normalized mass difference between the particle's flow at the inlet and outlet as,

$$CE = \frac{\dot{m}_{p,in} - \dot{m}_{p,out}}{\dot{m}_{p,in}} \qquad (8)$$

Experimental work needed for validation is currently in progress by the authors, however, for now, we compare our results against those obtained using the Lagrangian-Eulerian model under two-way coupling approach, usually referred to as Discrete Particle Model (DPM). Both models were implemented numerically using the commercial software ANSYS-FLUENT. The conservation equations were discretized using QUICK approach and the velocity-pressure coupling is established using SIMPLIC method. The magnetic field and the modified slip velocity were incorporated in the code as a User Defined Function (UDF). In the DPM analysis, particle streams are released at the inlet plane then they can be either trapped (captured) at the walls or escaped the capture through the outlet. The trajectories of the representative particles obtained by DPM are shown in Figure 2. The trajectory profiles have red colored bands that define the locations of the magnetic elements. For the same inlet mass flow rate, both of mixture and DPM model resulted in capture efficiency equal to 51%.

The vector field of the induced magnetic force acting on a magnetic bead is discussed in details in a previous study by the authors (Khashan and Furlani 2013; Khashan and Furlani 2014; Khashan et al. 2014). Mainly, the magnetic particles experience an alternating repulsive-attractive forces when pass over the soft element. Since the mixture model deals with the particulate phase as continuum, the trajectories obtained by DPM are not available directly. In the mixture model, the solution of the momentum equation yields only the mass-centered velocity of the continuous mixture. The velocities of the dispersed particles can be obtained via the algebraic slip equations. The regions occupied by non-zero volume fraction and the streamline of the particulate phase are shown in Figures 3(a-b). A comparison between Figure 2 and Figures 3(a-b) shows that both models depict the same flow tracks and the same response to the repulsive-attractive magnetic field.

For such very dilute particles loadings, the results clearly indicate that the granular pressure and temperature are negligibly small throughout the whole channel. The calculated mixture density, viscosity and the shared pressure are greatly dominated by those of the liquid phase. Having $\mathbf{v}_m$ as a mass-averaged quantity, the diffusion velocity $\mathbf{v}_{ml}$ approaches zero ($\mathbf{v}_m \approx \mathbf{v}_l$) and, accordingly, the particulate diffusion velocity will be mainly equivalent to the "equilibrated" slip velocity, i.e. $\mathbf{v}_{mp} \approx \mathbf{v}_{slip} = \mathbf{v}_p - \mathbf{v}_l$.

CONCLUSION

The transport and magnetic capture of magnetic beads flowing through a microchannel is simulated using the mixture model. For dilute loading, the slip velocity is mainly attributed to the local equilibrium between magnetic and drag forces. Other influences, like gravitational forces, are negligible. The granular properties of the mixture models can be neglected without any significant impact on the calculated capture efficiency or particles-fluid coupling. Mixture models returned almost the same results of the Lagrangian-Eulerian model with particle-fluid coupling,

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