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Three dimensional simulation of negative-magnetophoretic filtration of non-magnetic nanoparticles

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ABSTRACT

Negative magnetophoresis of non-magnetic particles is the induced motion of non-magnetic particles suspended in magnetic media on the application of a magnetic field gradient. Negative magnetophoresis can be used to separate nanoparticles based on their size. An integrated finite-element model was developed using COMSOL to study the transport and separation of nonmagnetic particles in a negative magnetophoresis device. The model solves the magnetic field, fluid flow, and mass transfer equations in three dimensions. The model was used to successfully simulate an experimental separation device and was also used as a tool to develop modified designs that resulted in a substantial enhancement of the separation efficiency. In addition, the model successfully predicted the different phenomena that typically occur in a magnetophoretic device: trapping, focusing, and deflection.

1. Introduction

Magnetophoresis is successfully used to separate particles based on their magnetic properties. Current application of magnetophoresis for separation of nano-sized particulates include radioactive waste separation (Kaur et al., 2013), arsenate removal from water (Tuutijärvi, 2013), microfluidic bacterial separation from blood (Lee et al., 2014), and many other applications. If the nanoparticles to be separated do not have different magnetic properties, magnetophoresis can also be used by tagging magnetic particles to target species in the mixture through suitable handles. After tagging, the application of a magnetic field can be utilized for separation. Developing methods for magnetic tagging and separation continues to be an active area of research (Chen et al., 2013; Cerff et al., 2013; Tang et al., 2013; Pospiskova et al., 2013).

If the nanoparticles only differ in their size, their separation can be quite challenging. Negative magnetophoresis, which is the motion of non-magnetic particles immersed in a magnetic fluid resulting from the application of a magnetic field gradient, can be used to achieve such separation (Fateen, 2002). In negative magnetophoresis, the difference in magnetic susceptibility between the particles and the surrounding medium is negative as opposed to positive magnetophoresis in which the difference is positive. This phenomenon is analogous to buoyancy of objects that are less dense than the surrounding fluid. In the case of buoyancy, gravity acts on the more dense fluid stronger than it acts on the lighter object, causing this object to experience a hydrostatic force opposite to the usual direction of gravity. Similarly, in the case of negative magnetophoresis, the magnetic field acts on the magnetized fluid surrounding the non-magnetic particle, pushing the particle in the opposite direction. This concept can be implemented as a size classification tool that can be used to separate nano-sized particles that are difficult to separate otherwise (Kose et al., 2009).

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Nomenclature

a_1	radius of the non-magnetic particle
$\underline{B}$	magnetic flux density
C	total concentration of the fluid
D_{12}	diffusivity of the non-magnetic particles in the magnetic field
D_p	diameter of the spherical particle
$\underline{F}$	applied force
$\underline{F}_m$	magnetic force
$\underline{F}_d$	drag force
$\underline{H}$	agnetic field
i	index for the components in the mixture: 1 for non-magnetic particles and 2 for the magnetic fluid
$\underline{J}_p$	molar flux of the nonmagnetic particles relative to the mass average velocity $\underline{v}$
k	Boltzmann constant
k^{-1}	Debye length
$\underline{M}$	magnetization
M_s	saturation magnetization
N_A	Avogadro's number
p	pressure field
R	universal gas constant
R_p	hydrodynamic radius of the non-magnetic particles
u	fluid velocity
$\underline{v}_f$	velocity vector of the magnetic fluid
$\underline{v}_p$	velocity vector of the non-magnetic particle
$\underline{v}$	mass average velocity
V	volume of the particle
V_m	magnetic scalar potential
w_i	weight fraction of component i
W	molecular weight

Greek Letters

ε	electric permittivity of the fluid
ψ^2	electric potential
Ψ_o^2	electric potential at the surface of the non-magnetic particle
μ	fluid viscosity
μ_o	permeability of vacuum = $4\pi \times 10^{-7}$ H/m
μ_r	relative permeability
ϕ_i	volume fraction of component i
η	fluid viscosity
ρ	density of the fluid
ρ_p	density of the particle

Manipulation of non-magnetic nanoparticles in magnetic fluids has been experimentally and theoretically investigated. The Hatton group at MIT has been active in this research area. Fateen (Fateen, 2002) has performed one-dimensional magnetophoretic focusing of submicron polystyrene beads. He also constructed a simple flow separation device with two small permanent magnets for the continuous separation of the particles based on their size. Sharpe (Sharpe, 2004) used a quadruple configuration of permanent magnets in a flow device to continuously separate submicron particles based on their size. Park (Park, 2004) fabricated microsystems for the separation of submicron particles. Gonzalez (Gonzalez, 2009) used a microfabricated device with two external magnets to trap different sized nano-particles at different locations. Annavarapu (Annavarapu, 2010) designed a separation system composed of a regular array of iron obstacle posts which utilized magnetic buoyancy forces to perform size-based separation.

Mao and his coworkers (Cheng et al., 2013; Zhu et al., 2010) and Xuan and his coworkers (Liang et al., 2011; Liang and Xuan, 2012a) experimentally studied the motion of non-magnetic particles immersed in magnetic fluids as they flow through a microchannel with the application of a non-uniform magnetic field. Negative magnetophoresis has been successfully used in mutlilaminar flow to manipulate particles suspended in magnetic fluids (Tarn et al., 2014). Recently, Zhu et al. (Zhu, in press) combined both positive and negative magnetophoresis to separate particles with different magnetic properties.

Different approaches can be used to model the phenomenon of negative magnetophoresis: continuum modeling, Brownian-dynamics simulation and particle trajectory modeling. Fateen (Fateen, 2002) has proposed a one-dimensional continuum transport model that contained no adjustable parameters to represent the concentration profile of the nonmagnetic particles suspended in the magnetic fluid. To represent the available experimental data, the model utilized one-dimensional conservation equation for mass and accounted for the magnetic and electrostatic repulsion forces. The magnetic field profile was measured, fitted to a polynomial and subsequently used in the model. Sharpe (Sharpe, 2004) used the continuum model approach to solve a two-dimensional transport equation for the particle concentration. The magnetic field was generated by solving Maxwell equations for the magnetic field separately and fitting the results to a polynomial, which was then used as input for the transport model. The 2-D results successfully simulated the experimental separation results. Gonzalez (Gonzalez, 2009) used both the continuum model and the Brownian simulation approaches to model his experiments. The continuum model, which contained no adjustable parameters, was able to predict the experimental concentration profiles reasonably well over the range of experimental conditions used. The Brownian simulation was only able to semi-quantitatively predict the experimental results. Fateen and Magdy (Fateen and Magdy, 2010) used COMSOL to solve a two-dimensional continuum model for a negative magnetophoretic separation device.

The particle trajectories approach has been used by Annavarapu (Annavarapu, 2010) to describe the behavior of a single non-magnetic particle in regions of inhomogeneous magnetic field gradients. The trajectory simulations was used to conceptualize and built an experimental setup to perform the required separation. The particle trajectories approach has been also used by Mao and his co-workers (Cheng et al., 2013; Zhu et al., 2010; Liang et al., 2011; Zhu et al., 2011a) and by Zhu (Zhu and Nguyen, 2012) to develop a 2-D and 3-D model for transport of non-magnetic spherical microparticles in magnetic fluids in a microfluidic system that consists of a microchannel and a permanent magnet. The experimental results were compared to the results obtained by the analytical model and reasonable agreement was obtained.

In all the above modeling attempts, the magnetic field was obtained independent of the modeling environment. Any change in the configuration of the permanent magnets would require re-evaluation of the magnetic field through its measurement or through separate solution of Maxwell equation followed by polynomial fitting of the solution. Both approaches have limitations. The aim of this study is to develop an integrated continuum model that captures the multi-physics