

Unified Model of Paramagnetic Particle Transport

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A general mathematical model for the transport of paramagnetic particles in liquid solutions is proposed. The model describes the magnetic particles and the solvent as two interpenetrating continua and takes into consideration magnetophoresis and Brownian motion of magnetic particles, inertial and gravitation effects for both particles and fluid, as well as interaction between the magnetic particles and solvent continua. After developing our model, we show how various approximations made to the model equations lead to simplified approaches, some of them currently being used in the literature. A comparison with experimental data, the conditions under which these approximations can be made, advantages and disadvantages of using various model derivations, and details about their numerical implementation will be discussed in the full paper.

Index Terms—paramagnetic ions, magnetic separation, Navier-Stokes, drift-diffusion.

I. INTRODUCTION

ACCURATELY PREDICTING the dynamics of the paramagnetic particles in liquid solutions under the influence of a nonuniform magnetic field remains a challenging problem as shown by the many (and sometimes contradicting) publications in this field [1]–[6]. However, an accurate description of transport phenomena is essential in many areas related to magnetic separation, such as cell separation [7], [8], mineral processing [9], water purification [10] and others [11], [12], [13]. In this presentation we develop a general model for the simulation of paramagnetic ions and particles in liquid solutions. The model is relatively general as it considers multiple phenomena and material-dependent parameters including diffusion and Brownian motion, magnetophoresis, drag, inertia of both the magnetic particles and liquid, viscosity and pressure of fluid, and gravitation. The model can be applied to the transport of magnetic particles at both low and high Reynolds numbers. The interaction between the magnetic particles (MPs) is modeled phenomenologically through the introduction of the thermodynamic factor (which is appropriate in our case because the magnetic susceptibility of our particles is very low).

In the next section we summarize the model equations, then describe how the proposed model can be simplified to recover models currently published in the literature.

II. TRANSPORT MODEL

Following the same of reasoning as in a recently submitted publication [14], we consider a system of MPs dispersed in an liquid solvent and under the influence of an external magnetic field. The particles are paramagnetic and their magnetization is assumed to depend linearly on the external magnetic field for the range of external fields considered in this study; this fact is usually satisfied for metal ions or cluster of such ions, such as rare earth elements that have a magnetic susceptibility of the order of 10^{-3} and their magnetic moment increase linearly with the value of the magnetic field up to external fields of tens of T (which is the focus of our study). The MPs and the solvent are modeled as two interpenetrating continua, which we call to the MP continuum and the solvent continuum and assume. The MP continuum moves through the solvent continuum while

experiencing a force density of resistance equal to $-6\pi r_p^* \hat{\mu} n(\mathbf{v} - \mathbf{u})$ where $\mathbf{u}$ is the velocity of the solvent, $\mathbf{v}$ and n are the velocity and concentration of MPs, $\hat{\mu}$ is the dynamic viscosity and r_p^* is the hydrodynamic radius of the particles. The external magnetic field ($\mathbf{B}$) is assumed to act only on the MP continuum

$$\mathbf{f}_{mag} = nV_p \frac{3(\mu_p - \mu_0)}{2\mu_0(\mu_p + 2\mu_0)} \nabla B^2 \quad (1)$$

where μ_0 is the magnetic permeability of the solvent, μ_p is the magnetic permeability of the MPs, and $V_p = \frac{4\pi r_p^3}{3}$ is the volume of a MP, while the force due to thermal diffusion is given by

$$\mathbf{f}_{diff} = -kT \left(1 + \frac{\partial \ln \gamma}{\partial \ln n} \right) \nabla n \quad (2)$$

where kT is thermal energy and γ is the chemical activity coefficient. In the case of Boltzmann statistics $\gamma = 1$. However, since the MPs can interact with each other either magnetostatically or through Van der Waals forces and, as in most magnetic separation systems, γ can be relatively large, we need to consider the non-ideal case in this mathematical description. If in addition to the above force densities, we also include buoyancy and inertia, the momentum conservation equation for the MP continuum becomes

$$n\rho_p V_p \frac{d\mathbf{v}}{dt} = -6\pi r_p^* \hat{\mu} n(\mathbf{v} - \mathbf{u}) + nV_p \frac{3(\mu_p - \mu_0)}{2\mu_0(\mu_p + 2\mu_0)} \nabla B^2 - kT \left(1 + \frac{\partial \ln \gamma}{\partial \ln n} \right) \nabla n + nV_p (\rho_p - \rho) \mathbf{g} \quad (3)$$

where ρ_p is the mass density of the MPs. The last equation can be coupled with the equation for mass conservation of MPs

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}) = 0 \quad (4)$$

and solved to compute the velocity and concentration of MPs if the velocity of the solvent ($\mathbf{u}$) is known. To compute $\mathbf{u}$, we model the solvent continuum using the mass and momentum conservation equations

$$\begin{aligned}\nabla \cdot \mathbf{u} &= 0 \\ \rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla) \mathbf{u} &= -\nabla p + \hat{\mu} \cdot \nabla^2 \mathbf{u} + \rho \mathbf{g} \\ &\quad + 6\pi r_p^* \hat{\mu} n(\mathbf{v} - \mathbf{u})\end{aligned}\tag{5}$$

where ρ is the mass density of the solvent, p is the hydrostatic pressure, and $\hat{\mu}$ is the dynamic viscosity. Eqs. (3)-(6) form a system of differential equations that can be solved to compute the velocities of the solvent and MPs, the concentration of the MPs and the pressure of the fluid.

III. COMPARISON WITH EXISTING MODELS

In this paper a continuum model describing the transport of MPs is presented. The model is general in the sense that it includes all of the important physics: the magnetostatic drift and diffusion of the MPs, the particle interactions as described by a chemical potential, and the solvent hydrodynamics. Various models presented in the literature can be shown to be approximations of our general equations, and therefore our unified treatment provides a common understanding of these models and can allow for systematic evaluation of their underlying assumptions.

Among the prior models that we examine are one from Xue et al [15] that neglected the inertia and thermal diffusion of the MPs and another from Gonella et al [16] that also ignored thermal diffusion effects.

Leong et al [17] used similar equations to (3)-(6) to study the magnetophoresis of magnetic nanoparticles in the magnetic field produced by an external NbFeB magnet, however, they also neglected the inertial term and the terms containing ∇n and $\nabla \mathbf{B}^2$ in momentum equation for the fluid. Similarly, Lei et al [18] have included the magnetic force density in eq. (6), however, they have neglected the inertial term of the MPs and the force due to the gradient of the chemical activity and the magnetic and gravitation flux in the drift-diffusion equation for MPs.

Finally, Larbi et al [19] have recently developed a two-fluid model for the transport of ferromagnetic particles in the liquid solutions that is appropriate for the description of ferrofluids in rotating magnetic fields. The fundamental assumptions in [19] are relatively similar to the assumptions made in our work, however, there are few important differences related to the fact that here we model a system of paramagnetic particles, while [19] models a ferrofluid.

IV. CONCLUSION

The general model introduced in eqs. (3)-(6) can be used to describe the transport of paramagnetic particles in liquid solutions (a comparison with experimental data will be presented in the full paper). By making different approximations to this model (that will also be discussed in detail at the conference) the proposed model leads to various models that have been already published in the literature. The model can also be easily extended to diamagnetic particles, in which case the magnetic susceptibility is negative. Since the magnetic susceptibility of diamagnetic particles is very low (of

the order of -10^{-4}), their magnetic moment varies linearly with the magnetic field for a wide range of the applied fields (of the order of tens of tesla).

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