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A Stokesian dynamics approach for simulation of magnetic particle suspensions

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ABSTRACT

The dynamic behaviour of μm-scale ferromagnetic particles in suspension is of interest for various mineral beneficiation processes. It is, however, difficult to experimentally study such processes at the particle-level. In these instances it can be advantageous to resort to suitable particle simulation methods.

Stokesian dynamics is a mesh-free numerical technique developed for suspensions of nm to mm size particles. The method inherently considers hydrodynamic interactions, but additional interaction models can be included depending on the system under investigation. We here present a Stokesian dynamics (SD) implementation, which allows for simulation of the motion of suspended magnetic particles in presence of an external magnetic field. The magnetic interaction model includes particle-field interactions as well as pairwise interactions between magnetised particles.

Simulations are compared with experiments using a laboratory-scale flow cell. The method is shown to be realistic for studying ferromagnetic suspensions in mineral processing applications, and can be useful in understanding and predicting the efficiency of mineral separation processes.

1. Introduction

The study of magnetic particle suspensions is relevant for better understanding of wet-state separation processes in mineral processing and recycling (Stener et al., 2014; Menad et al., 2014; Svoboda and Fujita, 2003) as well as various other applications or processes based on magnetic properties of particles, for instance magnetorheology, micro-robotics, and medical applications (Costa and Costa Branco, 2009; Lu et al., 2014; Rosengart et al., 2005; Lunov et al., 2011).

Numerical simulation of magnetic particles in suspension have been conducted within a number of probabilistic and deterministic particle dynamics simulation disciplines, including Monte-Carlo simulation (Satoh et al., 1996; Satoh, 2008), Lattice-Boltzmann-Discrete Element Method, LB-DEM (Han et al., 2010a,b), Lattice-Boltzmann-Brownian Dynamics, LB-BD (Satoh, 2012), and Stokesian dynamics (Satoh et al., 1998; Satoh, 2002; Irisa and Yokomine, 2007). The focus of these studies have not been directed specifically towards mineral separation processes, but have rather been phenomenologically oriented or related to novel uses of magnetic effects in applications for instance within nanotechnology, ferrofluids, and drug delivery systems. One of the more accurate methods related to evaluating the combined effect of liquid phase flow and magnetic effects is the LB-LES-DEM approach (Lattice-Boltzmann-Large Eddy Simulation-Discrete Element Method). Work in this direction has been described by Han et al. (2007, 2010a,b). The method is, however, restricted to a very limited number of particles due to the high computational expense.

Some relatively recent studies have been carried out utilising combined DEM-FEM-CFD (Discrete Element Method-Finite Element Method-Computational Fluid Dynamics) simulation approaches for simulating high-gradient magnetic separation (HGMS) and wet low-intensity magnetic separation (LIMS). Such work has been published by Lindner et al. (2013) and Murariu (2013). These types of coupled methods are beneficial in offering one or sometimes two-way coupling between continuum and discrete simulation disciplines by using commercially available simulation tools. The drawbacks mainly come from inherent limitations of each individual method or the coupling between the methods. This can be exemplified by the typical one-way hydrodynamics coupling or otherwise simplified description of the interparticle hydrodynamics, limited possibilities to describe free surface interactions, etc. Although enabling the simulation of fairly large systems and allowing a relatively accurate representation of the macroscopic magnetic field, these methods are not able to fully

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account for the complex mechanisms that can arise as result of combined effects of magnetic, hydrodynamic and possibly other relevant particle-level interactions.

In processes such as wet magnetic separation, single particle properties and interactions play a key role. It is therefore strongly motivated to build such work on predominantly particle-oriented simulation approaches, where particles can be individually designated relevant properties and various mechanisms can be reliably studied at the particle level. A benefit of the Stokesian dynamics technique is that it is developed for particles in suspensions and thus allows for study of high-concentration suspension behaviour without need for the computationally more costly DEM-CFD or DEM-FEM coupling, or less accurate tracer particle simulations by using continuum-type approaches. The Stokesian dynamics technique allows relatively straightforward addition of force models describing various types of particle interactions in liquid media (Toivakka et al., 1997; Nopola, 2004).

In this paper we propose a Stokesian dynamics-based simulation framework, which can combine the accuracy of suspension-oriented particle methods with the efficiency of a simplified mesh-free mathematical approximation of the magnetic field and fluid flow. The model is illustrated and qualitatively evaluated in the context of a number of simulation examples. Furthermore, simulations are compared with experimental results using a laboratory-scale flow cell. We also discuss the wider applicability to the model for numerical simulation-based evaluation of magnetic separation efficiency.

2. Method

2.1. Stokesian dynamics

The Stokesian dynamics technique was originally developed in the 1980's for the study of many-body interactions in non-equilibrium suspensions (Bossis and Brady, 1984; Brady and Bossis, 1988; Brady, 2001). Due to the possibility to include additional interaction models, efforts have since then been made to enable consideration of various phenomena, e.g. colloidal interactions, Brownian motion, and interparticle effects from added dispersant (Toivakka et al., 1997; Nopola, 2004; Sand et al., 2009). There has also been much work devoted to increasing the computational efficiency of the technique (e.g. Bousfield, 1990; Sierou and Brady, 2001).

Earlier approaches using the Stokesian dynamics technique for studying ferromagnetic particle suspensions have included the definition of the external magnetic field as a homogeneous field covering the full simulation domain, as well as describing particles as being identical and of monodisperse size distribution (Satoh et al., 1998; Irisa and Yokomine, 2007). Efforts have also been made to reduce the computational cost by introduction of a cluster-based simulation approach (Satoh, 2002).

Stokesian dynamics simulations are based on the N-body coupled Langevin equation (Brady and Bossis, 1988), which is a variant of Newton's second law of motion. It can be written in the form

$$\mathbf{m}\frac{d\mathbf{U}(t)}{dt} = \mathbf{F}^{\mathrm{H}} + \mathbf{F}^{\mathrm{P}} + \mathbf{F}^{\mathrm{M}}, \quad (1)$$

where mass, $\mathbf{m}$, times the change in velocity, $\frac{d\mathbf{U}(t)}{dt}$, is a function of the various forces influencing the particles. These forces are commonly divided into three types. Hydrodynamic forces, $\mathbf{F}^{\mathrm{H}}$, includes a drag forces resulting from the macroscopic flow of liquid, pairwise interaction forces between particles or between particles and boundaries mediated through the interstitial liquid. Interparticle forces, $\mathbf{F}^{\mathrm{P}}$, can include e.g. colloidal or steric forces between particles, but also in the case of magnetic properties forces which arise between magnetised particles. Single particle forces, $\mathbf{F}^{\mathrm{M}}$, result from various macroscopic forces that influence the motion of particles. This can for instance include Brownian forces that result from thermal vibration of small particles. In this work, the attraction of magnetic particles to an external stationary magnet is considered as a single particle force. The magnetic interaction models specific to this work are discussed in Section 2.2. All other models are presented and discussed in detail elsewhere (Toivakka 1997; Nopola 2004; Sand et al. 2009).

Due to the additivity of forces in this expression, interactions beyond the typical hydrodynamics and particle interaction models can be included in a relatively straightforward manner. For reducing the computational expense, it is often necessary to conduct an analysis of governing forces through the calculation of non-dimensional numbers. This analysis includes a relative comparison between different forces in order to determine their relative significance. In Stokesian dynamics, the most important non-dimensional number is the particle Reynolds number, Re_p. It describes the relative importance of inertial versus viscous effects as

$$Re_p = \frac{\rho_l a_{\mathrm{char}} u_{\mathrm{char}}}{\mu}, \quad (2)$$

where ρ_l and μ are the density and viscosity of the liquid medium, respectively, a_{char} the characteristic particle size and u_{char} the velocity of particles relative to the liquid. If the particle Reynolds number is small, defined as $Re_p \ll 1$, it can be assumed that viscous effects dominate and particles can be expected to react instantaneously to forces influencing them. This approximation is relevant for small particles that are freely moving with the fluid, and thus suitable for suspension flow simulations. For instance a 1 μm particle moving at a velocity of 0.1 m/s relative to the liquid phase (water) has a particle Reynolds number of 0.1.

While this form of numerical analysis is relatively straightforward in steady-state-type systems, it becomes complicated in systems with rapidly changing conditions or where conditions vary considerably at different locations of the domain. This can for instance be assumed to be the case near the magnetic source in the simulations presented in this work, as in this region magnetic interaction forces will dominate.

The Stokesian dynamics approach utilised in this work includes adaptations to the hydrodynamics model expressions by fitting them to data from CFD simulations. This extensive process is described by Sand et al. (2009) and Nopola (2004). Compared to the standard Stokesian dynamics approach, the modifications significantly improve the accuracy of simulations when studying suspensions of wide particle size distributions and systems where particles are in close contact. This extends the maximum 1/10 size ratio between particles, which is traditionally considered as a limitation in Stokesian dynamics (Kim and Karrila, 1991).

2.2. Magnetic interactions

In this work, we aim at creating a flexible implementation for simulation of ferromagnetic particle suspensions under influence of three-dimensional magnetic fields with an arbitrarily assignable magnetic source. This is advancing the previous state-of-the-art in Stokesian dynamics simulations, where suspension behaviours have been studied in simplified, homogeneous magnetic fields (Satoh et al., 1996; Satoh, 2002; Irisa and Yokomine, 2007).

Particle motion and interactions related to magnetic effects are in this work based on three force models. These include interaction between the particles and a stationary magnetic point source, interparticle magnetisation and orientation of magnetic particle clusters along the magnetic field. There are a number of assumptions made in order to increase the computational efficiency: