



An energy map model for colloid transport

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ABSTRACT

When dispersed colloids are flowing, they experience interactions with the fluid (friction) and with other colloids (surface interactions). These phenomena are usually taken into account through a Suspension Balance Model (SBM) that couples mass and momentum balances. However, in many applications, the dispersed particles flow close to an interface or inside a porous media. The flow in such a confined environment leads to significant particle-wall interactions. This paper puts forward an energy map model that accounts for these particle-wall interactions. A way to implement the energy map in the SBM is to introduce an interfacial pressure concept. The new possibilities opened up by the energy map that account for interfacial interaction in the SBM are analysed. A transient 1D case study for the transfer of colloids through a pore illustrates the potentialities of the Suspension Balance Model integrating an Energy Map (SBM-EM). The model enables the description of the transmission of the colloids through the energy map representing the membrane (mass balance) and the consequences in terms of an out-of-equilibrium counter pressure (momentum balance). The counter osmotic pressure is then explained by the interfacial interaction between the colloids and the interface; these interfacial interactions that prevents the colloids from leaving the bulk volume generate forces that are transmitted to the fluid (via the drag force), thus inducing osmosis. The energy map model can enable the incorporation of the physical and chemical heterogeneities of the interacting surfaces. It might be of interest to explore the transfer of colloids along or inside real surfaces (being a mosaic of nano- or micro-scale domains with specific interactions).

1. Introduction

The transport of colloids cannot be described only by classical diffusive and convective mass transport terms. The main reasons are the existence of both surface interactions between the colloids (or between a colloid and its surrounding interface) and hydrodynamic interactions between the particle and the fluid (interactions with the shear rate). These interactions that occurs at a nano- or micro-scale are deeply modifying the way in which colloids are diffusing and/or being advected. For example, processes such as ultrafiltration, nanofiltration or reverse osmosis, which are classically used to purify, eliminate and concentrate colloids or nanoparticles, strongly depend on these interfacial phenomena. The level of fouling, its kinetics or even the way colloids build up (porosity, hydraulic resistance or accumulation reversibility) are driven by colloidal properties (Bacchin et al., 2011). Such an impact of surface interactions is also crucial during the transport of drug and carriers in the crowd environment of cells (Al-Obaidi and Florence, 2015); the nano-scale interactions playing a significant role on the hindered diffusion or advection towards cellular goals.

It is therefore necessary to establish experimental and theoretical

connections between colloidal properties at a local (micro) scale and the efficiency of the mass and momentum transport phenomena; this knowledge is compulsory for the control of numerous processes that deal with concentrated colloids and/or colloids in confined situations.

In a sheared flow, the colloids are submitted to hydrodynamic interactions (due to the fluid velocity-drag force and to the velocity gradient-shear induced diffusion or lateral migration). Additionally, in a concentrated flow, colloids experience multi-body surface interaction (i.e. DLVO forces, etc.). In these flows, it is crucial to account for the momentum coupling or exchange between the fluid and the particle phase. These interactions (and their coupling) can be taken into account by the Lagrangian approach (like the Force Coupling Method or the Monte Carlo procedure) or by the Eulerian approaches (two fluid model, mixture models, suspension balance model). Multiple inter-particle DLVO interactions have been implemented in the Force Coupling Method in order to depict the collective effect induced by the filtration through a pore (Agbangla et al., 2014). However, this method, based on the tracking of individual particles (around 1 μm), remains impossible to apply for describing the process scale (around 1 m). For this reason, the Eulerian approach that considers the variation of spatial averaged variables, is more adapted for the

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description of the transport of concentrated colloidal dispersion. The different hydrodynamic and colloidal forces can be accounted for with two coupled momentum balances for both the particle phase and the fluid phase (called for this reason the two fluid model (Noetinger, 1989)). These momentum balances are coupled by considering momentum exchanges. According to this formulation, the equation can be written for the whole mixture (particles and fluid). It is then called the suspension balance model (Nott and Brady, 1994) or the mixture model (Jackson, 2000, 1997). Both the momentum exchange between the particle and the fluid phases and the slip velocity between the particles and the fluid have to be introduced as closure relationships in order to fully describe the problem. This last Eulerian approach will be introduced in the background section of this paper.

However, the picture is even more complex when the flow of particles takes place in confined conditions, where interactions with the walls are occurring. Furthermore, real surfaces are often chemically heterogeneous on a micro- or a nano-scale (like a biological membrane composed of lipid bilayers with inclusions) and can present local morphological heterogeneity (for example asperities) that can induce different local interaction energies when an object approaches the surface. To account for this complexity, the particle-wall interactions can be accounted for through an energy map. Several authors have defined interaction maps to characterise the approach of colloids near a surface. Interaction maps allows for example, the effect of the roughness, through DLVO calculations (Hoek et al., 2003), to be described. These maps have been used to determine the local equilibrium position that is due to both lateral and normal components of the DLVO force (Kemps and Bhattacharjee, 2005). Comparing the hydrodynamic forces with a DLVO energy map can then help to have a better evaluation of the interactions between colloids and heterogeneous surfaces (Shen et al., 2012). However, this energy map should be integrated in a full transport model in order to account for the coupling with diffusion, advection and hydrodynamic or colloidal interactions.

The aim of this paper is to propose a model that describes the transport of colloids in (or close to) porous media and thus to integrate the effect of both particle/particle and particle/wall interactions. The approach taken will be to implement an energy map (for an interacting surface) in a Suspension Balance Model.

2. Theoretical background

The Suspension Balance Model SBM (Nott and Brady, 1994) was initially established to describe the non-Brownian migration of particles in suspension. The shear-induced migration was depicted by considering the effect of particles in the fluid phase through a particle-phase stress previously introduced by Batchelor (1970). This work and further implementations (Morris and Boulay, 1999) allow to relate the rheology of the suspension to the migration flux (mass transfer) of particles. They demonstrated that the SBM approach was encompassing the diffusive flux model (previously introduced by Leighton and Acrivos (1987)), based on an empirical consideration that mass flux is proportional to gradients in particle concentration and shear rate. More recently, Lhuillier (2009) discussed the discrepancies between the two-fluid approach and the SBM and proposed that the force exchange on the particle phase was the sum of the interphase drag forces, F_{drag} (arising from the difference in velocity between the particles and the fluid phases) and a stress-induced force, Σ_p (arising from the gradient in the field of velocity). A review of the mixture models for shear-induced migration in flowing, viscous and concentrated particle suspensions have highlighted the possibility of describing the non-equilibrium osmotic pressure and shear-induced diffusion coefficients in the same model formulation (Vollebregt et al., 2010). All these recent developments have been integrated in a revisited form of the Suspension Balance Model (Nott et al., 2011) that will be the starting point of the analysis done in the paper.

2.1. The suspension balance model (SBM)

The SBM is based on solving field equations written from the volumic averaging of the governing equations (local momentum and mass balances) on the two phases. These field equations resulting from momentum and mass balances, are written below for the fluid phase, the dispersed phase and the mixture (the balance for the mixture being the sum of the two phases):

Momentum balance

For the dispersed phase

$$\phi \rho_p \vec{g} + n \vec{F}_{drag} + \nabla \cdot \Sigma_p = 0 \quad (1)$$

For the fluid

$$(1 - \phi) \rho_f \vec{g} - n \vec{F}_{drag} - \nabla(1 - \phi)p + 2\eta_f \nabla \cdot \langle \epsilon \rangle + \nabla \cdot \Sigma_f = 0 \quad (2)$$

For the mixture

$$\rho_m \vec{g} - \nabla(1 - \phi)p + 2\eta_f \nabla \cdot \langle \epsilon \rangle + \nabla \cdot \Sigma_p + \nabla \cdot \Sigma_f = 0 \quad (3)$$

Mass balance

For the dispersed phase

$$\frac{\partial \phi}{\partial t} = -\nabla \cdot (\phi \vec{u}_p) \quad (4)$$

For the fluid

$$\frac{\partial(1 - \phi)}{\partial t} = -\nabla \cdot ((1 - \phi) \vec{u}_f) \quad (5)$$

For the mixture

$$0 = \nabla \cdot \vec{u}_m \quad (6)$$

The revisited form (Nott et al., 2011) considers a momentum exchange between the dispersed and the fluid phase via a drag force, $n \vec{F}_{drag}$, and a contribution to the mixture momentum through the divergence of a particle stress, $\nabla \cdot \Sigma_p$, and through the divergence of a fluid stress, $\nabla \cdot \Sigma_f$. In the momentum balance, the other terms are the effect of the gravity of each phases, the fluid pressure gradient and the viscosity of the fluid phase (where ϵ is the strain rate tensor linked to the shear rate $\nabla u_f/2 = \dot{\gamma}/2$ for an uniaxial flow). The mass balances introduces the advective flux of the particle, u_p , the fluid velocity, u_f , and the mixture velocity u_m coming from volume averaging, $\phi u_p + (1 - \phi) u_f$.

2.2. A set of closure relationships for colloids

Closure relationships are necessary to close the problem and to be able to determine the fluid properties (the velocity and the volume fraction) from the previous set of equations (Eqs. (1)–(6)). A first closure relationship expresses the drag force as a function of the slip velocity between the particle phase, u_p , and the mixture phase, u_m :

$$n \vec{F}_{drag} = -\frac{\phi}{V_p} \frac{\vec{u}_p - \vec{u}_m}{m(\phi)} \quad (7)$$

where $m(\phi)$ is the mobility of the particles accounting for the effect of the volume fraction, i.e. $K(\phi)/6\pi\mu a$ where $K(\phi)$ is the hindered settling coefficient.

The writing of the stresses Σ_p and Σ_f is more controversial and a different set of closure relationships have been proposed (as reviewed in Vollebregt et al. (2010)). As underlined by Lhuillier (2009), some of these sets of closure presents some inconsistencies. Clausen (2013) proposes a more consistent formulation: this set of modified closure relationship will be the starting point of the one proposed in this paper.

For low Péclet numbers, the particle-phase stress, Σ_p , can be written by considering only the normal stress (NS) contribution (Clausen, 2013). Furthermore, a reasonable premise for colloidal particles at moderate shear rates is to consider the stress as isotropic (Hallez et al.,

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