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Simulation of colloidal fouling by coupling a dynamically updating velocity profile and electric field interactions with Force Bias Monte Carlo methods for membrane filtration

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ABSTRACT

Pressure-driven flow through a channel with membrane walls is modeled for high particulate volume fractions of 10%. Particle transport is influenced by Brownian diffusion, shear-induced diffusion, and convection due to the axial crossflow. The particles are also subject to electrostatic double layer repulsion and van der Waals attraction, from both particle–particle and particle-membrane interactions. Force Bias Monte Carlo (FBMC) simulations predict the deposition of the particles onto the membranes, where both hydrodynamics and the change in particle potentials determine the probability that a proposed move is accepted. The particle volume fraction is used to determine an apparent local viscosity observed by the continuum flow. As particles migrate, the crossflow velocity field evolves in quasi-steady fashion with each time instance appearing fully developed in the downstream direction. Particles subject to combined hydrodynamic and electric effects (electrostatic double layer repulsion and van der Waals attraction) reach a more stable steady-state as compared to systems with only hydrodynamic effects considered. As expected, at higher crossflow Reynolds numbers more particles remain in the crossflow free stream.

1. Introduction

Water quality and availability are pressing issues with over 1 billion people worldwide lacking access to safe, reliable drinking water. As many as five million die each year of waterborne diseases due to unclean water sources and poor sanitation and hygiene [1]. A range of filtration methods including reverse osmosis (RO), microfiltration and nanofiltration, offer promise in providing potable water. In addition to debris and large contaminants, some membrane filtration can remove biological contaminants such as viruses and bacteria. RO membranes can even be used to remove salts, generating potable water from saline or brackish water. However, all filtration techniques are all susceptible to fouling. Once fouling begins, the systems must be operated at higher pressure to maintain a constant permeate flux, requiring increased power consumption.

Before full-scale, mulit-contaminant systems can be fully understood, it is necessary to investigate the physics of single species fouling in simple geometries. The motivation of this study is to demonstrate coupling of a continuum crossflow to a discrete Monte Carlo simulation and evaluate the validity of such a method for a relatively high (10%) volume fraction of foulant, such as might be present before any pretreatment. Future simulations will predict fouling observed in small-scale laboratory systems such as those of Contreras et al. [2a,b] Faibish et al. [3] and Wang and Tarabara [4]. The geometry of the flow cell, membrane characteristics and foulants described here mimic the geometry of these experiments, but with a high volume fraction of particulates to better demonstrate the impact on the flow and particle migration. Here results are presented for symmetric cells with membranes on both the top and bottom boundaries. In future simulations, fouling of just one surface will be investigated to better compare to experiments.

Force Bias Monte Carlo (FBMC) methods are used to model particle movement. The hydrodynamics that govern particle motion are well documented [5–7], and several components contribute to the total effect. These include Brownian and shear-induced diffusion, as well as hydrodynamic drag forces. Leighton and Acrivos [7] noted that shear-induced diffusion "arises from the random motion of the particles across streamlines due to the inter-particle interactions which occur as a suspension is sheared". These diffusive effects have been considered in previous work [6] and are refined here to provide more accurate predictions. Additionally, the

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velocity profile is updated after each Monte Carlo (MC) step, accounting for the impact of local particle concentration on apparent viscosity.

In addition to the hydrodynamic forces, particle–particle and particle-membrane electric interactions are also considered and influence the migration of the particles in the flow cell. The two interactions examined include van der Waals and electrostatic double layer potentials. The electrostatic potentials are repulsive between objects of the same sign charge (as assumed here). Van der Waals potentials are attractive forces, drawing particles together and toward the membranes and partially offsetting the electrostatic repulsion. In general, the two interactions do not necessarily cancel. It will be shown that these electric interactions damp the randomness in the MC steps.

Here extreme parameters are investigated to describe the impact due to very high contaminant concentrations (10% volume fraction of particles). First cases with just electrostatic and van der Waals forces are considered, without flow. Then a case with no electrostatic or van der Waals interactions is considered to investigate purely hydrodynamic effects. Finally, electrostatic, van der Waals and hydrodynamics are considered. With these limiting cases as benchmarks, future studies will treat more realistic volume fractions for membrane filtration after pretreatment and will attempt to parameterize the impact over a range of charges (for particles and membranes), membrane surface roughness, and particle size distributions.

2. Problem statement, interactions and assumptions

The channel geometry used in the simulations is shown in Fig. 1. The mesh areas (top and bottom) indicate the membrane surfaces of the flow channel, through which there is small permeate outflow. These act as reflective boundaries for particles, which are assumed to be perfectly rejected. The particle centers can only approach to within a radius to the membrane. Periodic conditions are applied on the remaining boundaries. Particles in the flow are subject to many-body hydrodynamic, electrostatic and van der Waals forces, as well as force bias due to the flow.

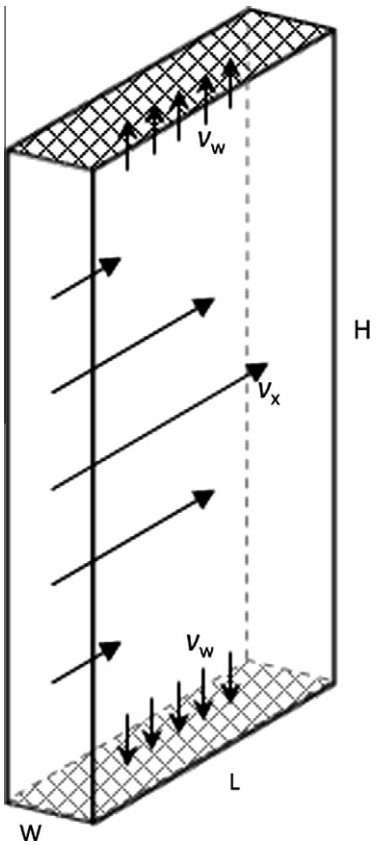

Fig. 1. Channel geometry in dimensional coordinates.

2.1. Hydrodynamic forces

Particles in the flow are subject to hydrodynamic forces. The velocity normal to the membrane v_z is given by Berman [8] as:

$$v_z(z) = v_w\left[\frac{z}{2}(3-z^2) - \frac{Re_\perp}{280}z(2-3z^2+z^6)\right] \tag{1}$$

where $Re_\perp$ is the Reynolds number based on v_z, v_w is the permeate velocity (here taken to be constant), and z is the normalized channel height, scaled such that it is 0 at the center of the channel and +1 and -1 at the top and bottom membrane surfaces, respectively. Assuming that $Re_\perp$ of the permeate flow is sufficiently small, as in previous work [6], the permeate profile which convects particles to the membrane surfaces simplifies to $v_z(z) \simeq v_w(3z-z^3)/2$. This profile also assumes incompressible, laminar, steady state flow, in which the presence of particles on the membrane are neglected. This velocity profile is used in conjunction with Happel's sphere-in-cell model and Brownian and shear-induced diffusivities to generate the hydrodynamic force in z that drags particles toward or pushes particles away from the membranes [5]. The crossflow velocity is treated as an unknown and is solved using the one-dimensional momentum equation as discussed in Section 3.1. The hydrodynamic force normal to the membranes is:

$$\mathbf{F}_h = \frac{k_b T v_z(z) K^{-1}(\phi)}{D_B + D_{SI}}\hat{\mathbf{z}} \tag{2}$$

where D_B is the Brownian diffusivity, D_{SI} is the shear-induced diffusivity in the normal direction, K is the sedimentation coefficient that depends on the volume fraction ϕ of the spherical particles in suspension, and K^{-1} is approximated by Happel's model as:

$$K^{-1}(\phi) = \frac{6+4\phi^{5/3}}{6-9\phi^{1/3}+9\phi^{5/3}-6\phi^2} \tag{3}$$

which varies as shown in Fig. 2a. The hydrodynamic force in the crossflow (x) direction is accounted for by the envelope of possible random moves in the Force Bias Monte Carlo method, discussed in Section 3.3.

The Brownian diffusivity is given as:

$$D_B = \frac{k_b T}{6\pi\mu R}S(\phi) \tag{4}$$

where $S(\phi) = \partial(\phi Z(\phi))/\partial\phi$ and Z represents the osmotic compressibility, which in hard-sphere systems is given by the Carnahan–Starling equation [9]:

$$Z(\phi) = \frac{1+\phi+\phi^2-\phi^3}{(1-\phi)^3} \tag{5}$$

Because of the relatively low volume fraction of particles, S is assumed constant with a value of unity [9]. The shear-induced diffusivity can be expressed as:

$$D_{SI} = \dot{\gamma}(z)R^2\widehat{D}(\phi), \tag{6}$$

where $\dot{\gamma}$ is the shear rate in the channel, and $\widehat{D}$ is the dimensionless shear-induced correction factor experimentally found to be:

$$\widehat{D}(\phi) = \frac{1}{3}\phi^2\left(1+\frac{1}{2}e^{8.8\phi}\right) \tag{7}$$