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Numerical investigation of channel blockage by flowing microparticles

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ABSTRACT

The dynamic formation of 3D structures of microparticle aggregates blocking the flow through straight microchannels is investigated by direct numerical simulation of the coupled motion of particles and fluid. We use the Force Coupling Method to handle simultaneously multibody hydrodynamic interactions of confined flowing suspension together with particle–particle and particle–wall surface interactions leading to adhesion and aggregation of particles. The basic idea of the Force Coupling Method relies on a multipole expansion of forcing terms (added to the Navier–Stokes equations) accounting for the velocity perturbation induced by the presence of particles in the fluid flow. When a particle reaches the wall or an attached particle, we consider that the adhesion is irreversible and this particle remains fixed. We investigate the kinetics of the microchannel blockage for several solid volumetric concentrations and different surface interaction forces. Many physical quantities such as the temporal evolution of the bulk permeability, capture efficiency, modification of the fluid flow and forces acting on attached particles are analyzed. We show that physical–chemical interactions, modeled by DLVO forces, are essential features which control the blockage dynamics and aggregate structure.

1. Introduction

The physics of transport, deposition, detachment and re-entrainment of colloidal particles suspended in a fluid are of major interest in many areas of fluids engineering: fouling of heat exchangers, contamination of nuclear reactors, plugging of filtration membranes and occlusion of human veins, deposits in microelectronics and in the paper industry. In many solid/liquid separation processes such as micro-filtration or ultrafiltration of water, the limitation of the process performance is related to the fouling of filtration devices. To prevent or control the occurrence of fouling, it is necessary to achieve a better understanding of the respective roles of physical–chemical phenomena and hydrodynamic interactions in a confined suspension of particles. Non-hydrodynamic surface interactions and the adhesion of particles onto solid surfaces are the essential features to be modeled. However, mainly because of a complex interplay between the hydrodynamics of the flow, the physical–chemical properties of the filtered suspensions (often in a colloidal state) and the nature of the solid material, predicting fouling dynamics is still challenging.

Different experimental techniques and numerical approaches have been developed to achieve new insights on the local structure of particle aggregates and the kinetics of blockage. Sharp and Adrian [4], by means of experiments in microtubes, observed blockage due to arch formation. The experiments were performed using liquids seeded with polystyrene beads at low volumetric concentration. They showed that a stable balance between the hydrodynamic forces and contact forces (mainly solid friction) between particles and the wall provokes the formation of arches. Wyss et al. [5] studied PDMS microchannels clogging by an aqueous suspension of monodisperse polystyrene beads. The formation of plugs at the microchannel entrance occurred when a critical number of particles had flowed through the pore whatever the flowrate and the particle volume fraction. In this case, the mechanism of blockage was mainly due to successive depositions of particles on walls or interceptions by attached particles. This is drastically different from the bridging mechanism occurring in a stable suspension. Bridging phenomenon is characterized by simultaneous adhesion of several particles. A critical flowrate

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Nomenclature

FCM and particle dynamics

a	particle radius, m
V	particle velocity, m s^{-1}
ρ_f	density of the fluid, kg m^{-3}
μ_f	dynamic viscosity of the fluid, Pa s
p	pressure in the fluid, Pa
$\mathbf{u}$	fluid velocity, m s^{-1}
$\mathbf{x}$	position in the fluid, m
Δ and Δ'	Gaussian envelops of momentum source terms, m^{-3}
σ_M and σ_D	width of the Gaussian envelops, m
$\mathbf{S}_{ij}^{(n)}$	symmetric part of the dipole tensor, N m
$\mathbf{A}_{ij}^{(n)}$	anti-symmetric part of the dipole tensor N m
$d^3\mathbf{x}$	elementary volume, m^3
$F^{(n)}$	monopole force due to the nth particle, N
$Y^{(n)}$	position of the nth particle, m
$V^{(n)}$	velocity of the nth particle, m s^{-1}
$\Omega^{(n)}$	rate of rotation of the nth particle, rad s^{-1}
F_a	attractive force between two particles, N
F_r	repulsive force between two particles, N
A_h	Hamaker constant, J
$\epsilon_0\epsilon_r$	fluid permittivity, C^2 J^{-1} m^{-1}
ψ	electrical potential surface, V
k	inverse of the Debye length m^{-1}
z	distance between the center of two particles, m
$F_{\alpha\beta}$	non-overlapping repulsion force, N
F_{adh}	adhesion force, N
T_{adh}	adhesion torque, kg m^{-2} s^{-2}
W	Stokes velocity, m s^{-1}
t_s	diffusion time, s
F_h	hydrodynamic force, N
F_{pp}	repulsive force between particles, N
F_{pw}	particle–wall repulsive force, N

Suspension statistics

A	area of simulation domain, m^2
ϕ, C	volumetric concentration of particles
N_c	number of fixed particles onto one wall of area A
N_p	initial number of particles corresponding to ϕ_0
k	bulk permeability of channel, m^2
$K(\phi)$	dimensionless coefficient

forces the particles to overcome the repulsive potential barrier leading to sudden formation of a plug at the pore entrance. This mechanism has been clearly identified by Ramachandran and Fogler [6] when they studied the conditions under which multilayer deposition occurs in a microchannel. In a previous experimental work [10], we demonstrated with microfluidic experiments that very different clogging structures (arches, deposit, dendrites) can be observed in flows of micrometric particles in microchannels. These different structures depend on the hydrodynamic conditions, the particle concentration and the surface interaction magnitude. These features are possibly related to the collective effect of particles (due to multibody particle interactions) and highlights the need for numerical approaches to depict the complex interplay between transport phenomena and multibody interactions.

Although numerical simulations of these phenomena are not widespread, hydrodynamic forces and physical-chemical interactions are more and more frequently taken into account in the modeling and/or simulation of multiphase flows. For examples, Henry et al. [38] used a new Lagrangian stochastic approach to confirm that clogging may result from the competition between particle–fluid, particle–surface and particle–particle interactions. Particle deposition can lead to the formation of either a single monolayer or multilayers depending on hydrodynamical conditions, fluid characteristics (such as the ionic strength) as well as particle and substrate properties (such as zeta potentials). For direct numerical simulation of small colloidal particle collision and agglomeration in turbulent flow, Mohaupt et al. [39] proposed a new probabilistic approach. This is based on evaluating continuous relative trajectories between possible collision partners to evaluate the probability for this trajectory to reach the minimum distance corresponding to particle collision. This approach can address new physical issues related to two-phase flow modeling and opens interesting avenues for the simulation of particle interactions, aggregates over a wide range of suspension characteristics.

For aerosols, Marshall [7] investigated the adhesion of particle aggregates onto straight channel walls under laminar flow. To show that particle deposition onto walls is dominated by particle–particle and particle–wall surface interactions, he used a Discrete Element Method assuming that the particle density is much larger than the fluid density. The trajectory equation accounts for Van der Waals and collision forces (soft-sphere model). The translational velocity and rotation rate of each particle are obtained by numerical integration of Newton's second law. They neglected the perturbation of the fluid flow due to the presence of attached particles which limits their study to the early instants of blockage when the permeability of the channel is unaffected by the growing plug. This is a serious shortcoming of this approach. Concerning colloidal suspensions, Tanaka and Araki [8] studied the importance of interparticle hydrodynamic interactions during aggregation using the Fluid Particle Dynamics method. In the FPD method, colloidal suspension is modeled as a mixture of viscous undeformable fluid particles and a non-viscous simple liquid, instead of treating colloids as solid particles. This method is based on a hybrid model, which combines a lattice simulation for continuous fields and an off-lattice simulation for particles. The importance of interparticle hydrodynamic interactions in aggregation, gel formation, and phase separation of colloidal suspensions has been highlighted.

In our study of channel blockage by adhesion of spherical particles, we choose to use the Force Coupling Method to simulate the adhesion and aggregation of spherical particles in laminar channel flow accounting for hydrodynamic interactions and DLVO forces related to the presence of fixed and flowing particles. The paper is organized as follows. The Force Coupling Method and its validation are presented in Section 1. In Section 2, we describe the configuration and conditions of the simulation. The kinetics of clogging according to different volume fraction of particles and interaction forces is investigated in Sections 3 and 4, respectively. The evolution of the bulk permeability, the capture efficiency in the microchannel, the particulate microstructure and the modification of the fluid flow around attached particles will be discussed. Conclusions are drawn in Section 5.

2. Numerical modeling of flow particle interactions

Early numerical methods for discrete particle tracking were often based on the restrictive assumption that the presence of particles does not modify the carrying fluid flow (one-way coupling