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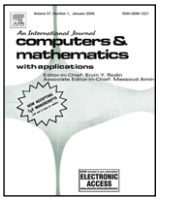

Three-dimensional microscale flow simulation and colloid transport modeling in saturated soil porous media

Hui Gao [a], Charmaine Q. Qiu [a], Dimin Fan [b], Yan Jin [b], Lian-Ping Wang [a,*]

[a] Department of Mechanical Engineering, University of Delaware, Newark, DE 19716, USA

[b] Department of Plant and Soil Sciences, University of Delaware, Newark, DE 19716, USA

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ABSTRACT

Transport of sub-micron colloid particles in soil porous media has been mostly studied numerically with unit-cell-based grain-scale geometries. In this study, we develop a more general approach by combining a multiple-grain pore-scale flow simulation with Lagrangian tracking of individual colloids. First, two numerical methods are applied simultaneously to solve viscous flows in a channel partially or fully packed with spherical grain particles, this allows cross-validation of the numerical methods for considered model geometries. It is demonstrated that the mesoscopic lattice Boltzmann approach can more accurately simulate three-dimensional pore-scale flows with multiple grain–grain and grain–wall contact points. Colloid transport is simulated under the combined influence of hydrodynamic forces, Brownian force, and physicochemical forces. Preliminary results demonstrate the capture of colloids by the secondary energy minimum (SEM) well. The local hydrodynamic retardation is shown to reduce the ability for colloids to move into the SEM well, but does not prevent this. Trajectories before and after the capture are also discussed.

1. Introduction

The attachment of colloids on grain surface and retention of colloids in small soil pores and their subsequent release when the solution or hydrodynamic conditions change determine the distribution and penetration of colloids in groundwater, and are important topics to groundwater contamination and remediation treatments. Most previous studies on colloid retention and transport address issues such as breakthrough curves at the macroscopic column scale. Research in recent years at the soil grain scale reveals that the retention and release depend on the competing effects of physicochemical and hydrodynamic forces acting on the colloids [1–3], indicating a need to better understand and model pore-scale flow in realistic three-dimensional (3D) porous media, particularly under unfavorable conditions as commonly encountered in natural porous media. Additionally, pore geometry affects local flow distribution and can contribute significantly to colloid retention. Important 3D flow features such as large local variations of flow velocity magnitude, direction, and shear rate depend on both grain–grain relative configuration and grain surface heterogeneity.

While the overall objective of our research is to develop an integrated experimental and computational approach focusing on pore-scale processes related to colloid transport [4,5], here we focus on developing a computational method to simulate the interaction of colloids with pore-scale flow and grain surfaces under various physicochemical and hydrodynamic conditions. In general, there are two components to pore-scale computational modeling: simulation of liquid flow and

* Corresponding author.
E-mail addresses: hgao@UDel.Edu (H. Gao), qiuqm@UDel.Edu (C.Q. Qiu), skyrock@udel.edu (D. Fan), yjin@udel.edu (Y. Jin), lwang@udel.edu (L.-P. Wang).

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simulation of transport of colloids by the liquid flow and interactions of colloid with grain surfaces. The second part could be performed in either an Eulerian or a Lagrangian fashion. The Eulerian approach solves a mean-field, extended advection–dispersion equation for colloid concentration [1,6]. The Eulerian approach requires a closure assumption of the driving source/sink terms and it is not certain if the approach can be applicable to unfavorable conditions where colloids and collectors are like-charged and thus are repulsive to one another.

The Lagrangian approach focuses on a single colloid and tracks its position and velocity over time according to Newton's second law. The colloid's equation of motion may include physicochemical, hydrodynamic, Brownian and body forces and torques. The physicochemical forces typically include contributions from the electrostatic, Lifshitz–van der Waals, and Lewis acid/base interactions [7]. The hydrodynamic forces may include Stokes drag, added mass, and fluid acceleration force. The hydrodynamic forces can be modified by a grain surface, nearby presence of other colloids, and local flow shear [8,9]. While the Lagrangian approach is computationally more expensive than the Eulerian approach, it provides a more direct mechanistic description of microscopic colloid transport. Furthermore, the discrete nature of the Lagrangian approach makes it much more feasible to include complex interactions with grain surface. For these reasons, most previous mechanistic modeling studies adopted the Lagrangian trajectory approach.

Under the Lagrangian trajectory approach, unit-cell-based flow representation were typically employed due to its computational efficiency. Examples include the sphere-in-cell model [8,10], 2D and 3D constriction tube models [11–14]. These unit-cell models provide a phenomenological representation of soil pore-scale geometry, but are unable to treat adequately grain–grain contact and grain surface irregularities. Cushing and Lawler [15] considered grain–grain contact in a unit cell representing densely packed regular array of spheres and solved the creeping fluid flow using an approximate Galerkin's method. They then studied colloid attachment efficiency using the trajectory approach. Johnson et al. [2] adopted the same unit-cell approach to solve pore-scale flow and a trajectory approach for colloids; they confirmed colloid retention in flow stagnation zones and wedging in grain-to-grain contacts. They also indicated the need to solve viscous flows through pore domains rendered from actual porous media, in order for such approach to become a useful quantitative tool.

Here we intend to study colloid transport and retention involving multiple grain–grain and grain–wall contacts in a model porous channel. To accurately simulate the pore-scale viscous flow, both the mesoscopic lattice Boltzmann method (LBM) and a Navier–Stokes-based hybrid method (i.e., Physalis) [4,16] are applied to same 3D flow configurations. The first part of this paper concerns inter-comparison of simulated 3D viscous flows in a channel. This extends the previous unit-cell flow representations. Simultaneous applications of two numerical methods provide a cross-validation step for simulating flows in the considered model geometry. Such inter-comparison has been performed recently for 2D pore-scale viscous flows by Gao et al. [4].

We then present a preliminary study of colloid transport in a simulated porous channel packed with 25 spherical grain particles (or glass beads). A preliminary study in 2D without considering local hydrodynamic interaction showed that the retention rate of colloids depends on both the mean flow speed and solution ionic strength [5]. Here we will extend our previous work to include local hydrodynamic interactions and 3D flow effects to more realistically model colloid transport and retention.

2. Flow simulation

In this section, we first introduce the two numerical methods for solving viscous flows in complex geometries. Several benchmark cases are then used to compare the results from the two methods. The general problem to be solved is flow through a three-dimensional channel with fixed spherical grain particles occupying part of the channel.

2.1. The mesoscopic lattice Boltzmann approach

The mesoscopic approach is based on a lattice Boltzmann equation with the multiple-relaxation-time (MRT) collision model using 19 discrete particle velocities in three dimensions (*i.e.*, the D3Q19 model), as described in detail in [17]. In the MRT-LBM, the evolution equation for the discrete particle density distribution function, f_i, for $i = 0,\ 1,\ 2, \ldots, 18$, is written as

$$f_i(\mathbf{x} + \mathbf{e}_i\delta_t, t + \delta_t) = f_i(\mathbf{x}, t) - M_{ij}^{-1}S_{jk}\left[m_k - m_k^{(\mathrm{eq})}\right] + \psi_i(\mathbf{x}, t), \tag{1}$$

where the collision operation is performed in a properly defined moment space through the transform matrix M_{ij} of rank 19×19, namely,

$$m_i = M_{ij}f_j, \qquad f_i = M_{ij}^{-1}m_j. \tag{2}$$

The detail of the transform matrix M_{ij} is given in [17]. By construction, the inverse matrix M_{ij}^{-1} can be easily obtained by the transpose of M_{ij} with a renormalization as the product of M_{ij} and its transpose is a diagonal matrix. In Eq. (1), ψ_i is a prescribed forcing field designed to model the driving pressure gradient or body force. In this work, ψ_i is specified as $\psi_i(\mathbf{x}, t) = \mathbf{e}_i \cdot \mathbf{F}_B/10$, where $\mathbf{F}_B$ is the macroscopic force per unit volume acting on the fluid. This forcing implementation is rather simple and does not explicitly consider the potential lattice effects associated with forcing, which has been described