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Viscous flow and colloid transport near air–water interface in a microchannel

Xiao-yan Shi [a], Hui Gao [a], Volha I. Lazouskaya [b], Qinjun Kang [c], 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

[c] Los Alamos National Laboratory, Los Alamos, NM 87545, USA

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ABSTRACT

In order to understand the transport behavior of colloids near an air–water interface (AWI), two computational methods are applied to simulate the local water flow field near a moving AWI in a 2D microfluidic channel. The first method is a mesoscopic multicomponent and multiphase lattice Boltzmann (LBM) model and the second is the macroscopic, Navier–Stokes based, volume-of-fluid interface tracking method. In the LBM, it is possible to predict the dynamic contact angles after the static contact angle is correctly set, and the predicted dynamic contact angles are in good agreement with previous observations. It is demonstrated that the two methods can yield a similar flow velocity field if they are applied properly. The flow field relative to AWI depends on the direction of the flow, and exhibits curved streamlines that transport fluid between the center of the channel and the wall region. Using the obtained flow, the motion of sub-micron colloids in a de-ionized water solution is then studied by a Lagrangian approach. The observed colloid trajectories are in qualitative agreement with our visualizations using a confocal microscope.

1. Introduction

An improved understanding of the mechanisms governing colloid retention and transport in soil porous media is crucial to the management of groundwater contamination by strongly sorbing contaminants or by pathogens such as viruses, bacteria, and protozoa [1,2]. Since contaminants and colloids often originate near the land surface, colloid transport and retention in unsaturated soil (i.e., the vadoze zone) are affected by air–water and air–water–solid interfaces. The air–water interface (AWI) may act as a colloid carrier [3,4] or a dynamic physical barrier to transport [5]. The moving contact lines can serve as the site for colloid retention [6,7] or act to re-mobilize colloids previously deposited on grain surface [8]. Lazouskaya et al. [9] reviewed the complex processes associated with colloid transport and retention near AWI, and stressed the need to understand the microscale flow field and the need to examine together the hydrodynamic transport and physicochemical interactions near the moving AWI.

To better understand the mechanisms of colloid transport and retention near AWI and moving contact line, we shall develop a computational approach to address the following aspects: (1) the simulation of viscous flow involving an air–water interface and (2) the tracking of colloids in such a flow field in the presence of AWI and grain surface.

* Corresponding author.
E-mail addresses: graceshi@udel.edu (X.-y. Shi), hgao@udel.edu (H. Gao), volha@udel.edu (V.I. Lazouskaya), qkang@lanl.gov (Q. Kang), yjin@udel.edu (Y. Jin), lwang@udel.edu (L.-P. Wang).

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In recent years, a significant progress has been made in developing computational methods for multiphase interfacial flows. Different methods are available to treat the fluid–fluid interface, including volume-of-fluid interface tracking, front tracking, level set, and lattice Boltzmann method [10–13]. These methods are still undergoing rapid development and severe numerical challenges remain, such as numerical instability for large density/viscosity ratios and spurious currents. Most methods are designed to simulate the shape of fluid–fluid interface. Relatively less attention is paid to the detailed flow velocity field near the fluid–fluid interface.

As a first step, in this paper we consider a viscous flow with a moving fluid–fluid interface in a 2D microfluidic channel. The characteristics of the flow are mostly governed by low capillary number and low flow Reynolds number, namely, the fluid inertial force may be neglected and the flow is mainly governed by viscous force and surface tension. We shall apply simultaneously two computational methods to solve the fluid flow: a mesoscopic multicomponent and multiphase lattice Boltzmann (LBM) model [10] and a macroscopic, Navier–Stokes based, volume-of-fluid interface tracking (VOFIT) method [11]. LBM is better suited for simulating moving contact lines while VOFIT has better numerical stability for large density and viscosity ratios. Our first objective is to simulate the flow field in the fluid–fluid interfacial region as accurately as possible. A good inter-comparison between the two methods would serve as a good indication that such an objective is achievable.

Our second objective is to simulate the motion of colloids in the interfacial region and to compare the colloid trajectories with our parallel experimental observations reported in [9]. For this purpose, Lagrangian tracking of colloids is developed by numerically integrating the colloid's equation of motion with physicochemical, hydrodynamic, Brownian and body forces. It will be demonstrated that the simulated trajectories are in good agreement with our experimental observations.

2. Flow simulation

Here we describe briefly the two computational methods used to simulate the slow viscous flow in a 2D microscale channel with a moving AWI. In our parallel experimental investigation [9], the flow is governed by a very low flow Reynolds number, about $O(10^{-4})$ on the water side and $O(10^{-5})$ on the air side, based on the mean speed $U(\sim 10\ \mu m/s)$ and the channel width ($\sim 40\ \mu m$). The capillary number $Ca = U\mu/\sigma$ on the water side is $O(10^{-9})$, where μ is the water viscosity and $\sigma = 0.072$ N/m is the surface tension at the air–water interface. Matching exactly these small physical parameters are difficult in the simulations. We shall assume that the flow near the air–water interface is similar as long as $Ca \ll 1$ and the dynamic contact angle is correctly simulated. In this paper, only a 2D model channel with a moving air–water interface is considered (e.g., see Fig. 4).

2.1. The lattice Boltzmann method

The multicomponent, multiphase, mesoscopic lattice Boltzmann method (LBM) developed by Kang et al. [14–16] is used here to simulate the flow with a moving air–water interface. The method is based on the original LBM scheme by Shan and Chen [17,18]. Since the method has been documented fully in [14–16], we only describe the method very briefly. The particular 2D code used here is a modified version of the code used in [15].

The starting point of the Shan–Chen multiphase multicomponent LBM scheme is to introduce a separate particle density distribution function $f_i^k(\mathbf{x}, t)$ for each component k, the LBM equation for the component k is

$$f_i^k(\mathbf{x} + \mathbf{e}_i\delta_t, t + \delta_t) - f_i^k(\mathbf{x}, t) = -\frac{f_i^k(\mathbf{x}, t) - f_i^{k(\mathrm{eq})}(\mathbf{x}, t)}{\tau_k}, \tag{1}$$

where τ_k is the relaxation time of the kth component, $f_i^{k(\mathrm{eq})}(\mathbf{x}, t)$ is the corresponding equilibrium distribution function. We use the standard D2Q9 lattice so $i = 0, 1, 2, \ldots, 8$ and $\mathbf{e}_i$ denotes the corresponding particle velocities in lattice unit: $\mathbf{e}_0 = (0, 0)$, $\mathbf{e}_1 = (1, 0)$, $\mathbf{e}_2 = (0, 1)$, $\mathbf{e}_3 = (-1, 0)$, $\mathbf{e}_4 = (0, -1)$, $\mathbf{e}_5 = (1, 1)$, $\mathbf{e}_6 = (-1, 1)$, $\mathbf{e}_7 = (-1, -1)$, and $\mathbf{e}_8 = (1, -1)$. The density and velocity of the kth component are obtained by

$$\rho_k = \sum_i f_i^k, \qquad \rho_k \mathbf{u}_k = \sum_i f_i^k \mathbf{e}_i. \tag{2}$$

The equilibrium velocity u_k^{eq} is determined by

$$u_k^{\mathrm{eq}} = \frac{\sum_k \rho_k \mathbf{u}_k/\tau_k}{\sum_k \rho_k/\tau_k} + \frac{\tau_k}{\rho_k}\mathbf{F}_k, \tag{3}$$

where $\mathbf{F}_k = \mathbf{F}_{1k} + \mathbf{F}_{2k}$ represents the net force due to mesoscopic fluid–fluid interaction $\mathbf{F}_{1k}$ and mesoscopic fluid–solid interaction $\mathbf{F}_{2k}$.