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Smoothed particle hydrodynamics pore-scale simulations of unstable immiscible flow in porous media

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ABSTRACT

We have conducted a series of high-resolution numerical experiments using the Pair-Wise Force Smoothed Particle Hydrodynamics (PF-SPH) multiphase flow model. First, we derived analytical expressions relating parameters in the PF-SPH model to the surface tension and static contact angle. Next, we used the model to study viscous fingering, capillary fingering, and stable displacement of immiscible fluids in porous media for a wide range of capillary numbers and viscosity ratios. We demonstrated that the steady state saturation profiles and the boundaries of viscous fingering, capillary fingering, and stable displacement regions compare favorably with micromodel laboratory experimental results. For a displacing fluid with low viscosity, we observed that the displacement pattern changes from viscous fingering to stable displacement with increasing injection rate. When a high viscosity fluid is injected, transition behavior from capillary fingering to stable displacement occurred as the flow rate was increased. These observations are also in agreement with the results of the micromodel laboratory experiments.

1. Introduction

The efficiency of many engineering applications such as oil recovery, remediation of DNAPL, and geological CO_2 sequestration can be adversely affected by unstable immiscible flows [10]. As a result, unstable immiscible displacement has been a subject of extensive pore-scale theoretical, experimental, and numerical research [1,3,5,6,9–11,16,18,29,32]. A clear understanding of the macro-scale consequences of pore-scale displacement instabilities in porous media is therefore vital for such applications. Despite the attention paid to unstable displacement at the pore-scale, a macro-scale description of the resulting behavior remains a challenge to date [28]. Macro-scale models often use empirical constitutive relationships between capillary pressure, saturation, and relative permeability, which neglect the effects of unstable behaviors such as fingering [4,7,12,21]. Therefore, it is important to incorporate the effects of unstable flow behaviors in constitutive relationships in order to improve the predictive capability of the macro-scale models.

In general, the displacement behavior in porous media is determined by the balance between capillary, viscous, and gravity forces. Here we consider a horizontal flow in a two-dimensional porous medium. Such flows have been studied experimentally using quasi-two-dimensional micromodels, in which (when placed horizontally) the effect of gravity is negligible compared to capillary and viscous forces. The flow displacement in the absence of gravity can be described by two non-dimensional numbers: the capillary number $Ca = v\mu_d/\sigma$ and viscosity ratio $M = \mu_d/\mu_r$, where v is the average pore-scale velocity of the displacing fluid, μ_d is the viscosity of the displacing fluid, σ is the interfacial tension, and μ_r is the viscosity of the resident fluid. Lenormand et al. [16] did pioneering work on studying and visualizing pore-scale displacement phenomenon using micromodels. They established three basic displacement regimes: capillary fingering, viscous fingering, and stable displacement. Viscous fingering occurs at high flow rates (high Ca), when a low viscosity (high mobility) fluid invades a high viscosity (low mobility) fluid and is characterized by narrow forward progressing flow paths. Capillary fingering occurs at low flow rates (low Ca) over a wide range of viscosity ratios. Capillary fingering takes place in the form of wide forward and lateral nonwetting phase flow paths. Stable displacement occurs at high flow rates when a high viscosity fluid displaces a low viscosity fluid and has the form of a flat moving front with no fingering behaviors. As M increases, flow crosses over from viscous fingering to the stable displacement region. As Ca increases, flow crosses over from capillary fingering to the stable displacement region. The existence of such regions was later confirmed by many authors using micromodel experiments [6,10,11,32] and numerical models [1,5,6,10,16,17].

Due to the complexity of pore geometries and the non-linearity of the multiphase flow equations, most of the pore-scale numerical models rely on various simplifications of the pore geometry and/or

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flow equations, potentially affecting the predictive capability of the models. For example, pore-network models use a simplified representation of pore geometry and approximate transient flow with a steady-state Poiseuille law (e.g., [1,5,16]). Statistical models are able to capture certain displacement regimes. For example, Diffusion-Limited Aggregation (DLA) models have been used to model viscous fingering, anti-DLA models – stable displacement, and Invasion Percolation with Trapping (IPT) models have been used to simulate capillary fingering [6,10,17]. The main deficiency of such "specialized" models is that they cannot capture transitions from one regime to another.

Meso-scale methods such as the Lattice Boltzmann method [8,14] and Dissipative Particle Dynamics [2,30] can be used to model complex multiphase flows in domains with realistic pore geometries. While these models have been shown to capture many qualitative features of the multiphase pore-scale flow, they do not solve Navier–Stokes equations directly, complicating the interpretation of the numerical results. Grid-based methods with implicit front tracking schemes such as the Level Set method and Volume of Fluid method have been recently proposed for pore-scale simulations of multiphase flow. However, due to a relatively high computational cost, they have only been applied to simple pore geometries. A detailed review of these and other numerical methods for pore-scale flow can be found in Meakin and Tartakovsky [20].

In this work we use the Pair-Wise Force Smoothed Particle Hydrodynamics (PF-SPH) to simulate multiphase flow in porous media [23,27]. Smoothed Particle Hydrodynamics is a meshless Lagrangian particle technique that has several advantages for modeling multiphase flow. As a fully Lagrangian method, SPH does not suffer from numerical dispersion and does not need complex interface tracking schemes to model interfacial dynamics. Due to its isomorphism with molecular dynamics, complex dynamical wetting behavior can be modeled with relative ease. For example, in the PF-SPH model the surface tension and wetting behavior of fluids is modeled with pair-wise molecular-like forces. The accuracy and consistency of the PF-SPH model for simulating surface angle and static and dynamic contact angles for flows in domains with simple geometries, such as flat surfaces and fractures with uniform apertures have been demonstrated in a number of papers including Tartakovsky and Meakin [26,27]; Kordilla et al. [15].

Traditionally, periodic boundary conditions for fluid pressure and velocity have been used in SPH models, and the flow has been driven by a gravity/body force. In general, two-phase flow is not periodic and periodic boundary conditions cannot be used to describe such flows accurately. Also, in many laboratory experiments the fluids are introduced in a flow cell with a constant flow rate. In the present work, we propose a new method for implementing the prescribed flux boundary condition in SPH.

We use the PF-SPH model to simulate displacement of a fluid initially occupying a micro-cell with another fluid injected into the cell at a constant flow rate under a wide range of Ca and M numbers. We compare the model results with the experimental results of Lenormand et al. [16] and Zhang et al. [32], who conducted a series of displacement experiments in a micromodel representing a uniform two-dimensional porous medium. We demonstrate that the PF-SPH model is capable of capturing different flow regimes including viscous fingering, capillary fingering, and stable displacement and the transition behaviors. We believe that this is an initial step towards developing improved constitutive relationships for macroscale models.

2. Smoothed particle hydrodynamics model

In this section we present PF-SPH equations obtained from discretization of the Navier–Stokes equations governing multiphase flow at the pore-scale. The derivation of the SPH equations can be found in Tartakovsky and Meakin [27] and a parallel solver for the SPH equations is described in Palmer et al. [23]. We also present a novel method for parameterizing the PF-SPH equations and a novel implementation of the constant flux boundary condition (BC) in the SPH method.

2.1. Governing equations

At the pore-scale the flow can be described by the combination of the continuity and momentum conservation equations:

$$\frac{D\rho^\alpha}{Dt} = -\rho^\alpha(\nabla \cdot \mathbf{v}^\alpha), \tag{1}$$

$$\rho^\alpha \frac{D\mathbf{v}^\alpha}{Dt} = -(\nabla P^\alpha) + \nabla.\left[\mu^\alpha(\nabla\mathbf{v}^\alpha + \nabla\mathbf{v}^{\alpha\mathrm{T}})\right] + \rho^\alpha\mathbf{g}, \tag{2}$$

where superscript α refers to properties of the wetting and non-wetting phases; $\mathbf{v}^\alpha$ is the velocity vector; ρ^α is the density; P^α is the pressure; μ^α is the dynamic viscosity; $\mathbf{g}$ is the gravitational acceleration; and $D/Dt = \partial/\partial t + \mathbf{v}\cdot\nabla$ denotes a total derivative.

The Young–Laplace law describes the pressure discontinuity at the fluid–fluid interface due to the interfacial tension, σ,

$$P^n - P^w = S\sigma, \tag{3}$$

where superscripts n and w denote the non-wetting phase and wetting phase, correspondingly; and S is the curvature of the interface. No-slip, no-flow boundary conditions are imposed at the fluid–solid interfaces. At the fluid–fluid–solid interface, the contact angle θ is specified.

In the SPH method it is convenient to approximate incompressible fluids with slightly compressible fluids and to use an artificial equation of state to close Eqs. (1) and (2).

2.2. SPH discretization scheme

In the SPH method, fluid and solid phases are represented by a set of N particles, which carry properties of each phase such as fluid composition, mass, density, viscosity etc. In the following, we refer to particles discretizing the fluid phases as fluid particles and those discretizing the solid phase as solid particles. The SPH method is based on a meshless interpolation scheme that allows estimation of a vector or scalar function $A(\mathbf{r})$ at position $\mathbf{r}$ in terms of the values of the function at the discretization points:

$$A(\mathbf{r}) \approx \sum_{j=1}^{N} m_j \frac{A_j}{\rho_j} W(|\mathbf{r}-\mathbf{r}_j|, h), \tag{4}$$

where subscript j denotes a property associated with particle j, $\mathbf{r}_j$ denotes position of particle j, $A_j = A(\mathbf{r}_j)$, N is the total number of SPH particles, and m_j, m_j/ρ_j, and $\rho_j = \rho(\mathbf{r}_j)$ are the mass, volume, and density of particle j, respectively. The function W is the SPH smoothing weighting function with the compact support h ($W(|\mathbf{r}| > h) = 0$). Due to the compactness of W, the summation in Eq. (4) can be replaced with a summation only over particles within the distance h from $\mathbf{r}$. The weighting function W must have at least a continuous first derivative and satisfy the normalization condition,

$$\int W(|\mathbf{r}-\mathbf{r}'|, h)d\mathbf{r}' = 1, \tag{5}$$

where integration is performed over the entire domain of A. In the $h \to 0$ limit, the weighting function, W, is required to reduce to the Dirac delta function:

$$\lim_{h\to 0} W(\mathbf{r}-r', h) = \delta(\mathbf{r}-\mathbf{r}'). \tag{6}$$

2.2.1. Pair-wise force SPH method

In the Pair-Wise Force SPH (PF-SPH) method, the momentum conservation equation for each fluid phase is discretized as [27],