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Influence of Wettability on Constitutive Relations and its Role in Upscaling

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Abstract

The lattice Boltzmann (LB) method is applied to simulating multifluid flow in porous media at sub-pore resolution to determine constitutive behaviors. We address the importance of the LB technique for identifying process based constitutive relationships, and demonstrate its application through analysis of the influence of wettability on interfacial areas and constitutive relationships. Porous media surface wettability is varied from uniformly strongly wetted by the resident fluid through strongly wetted by the displacing fluid. Spatially variable wettability is also demonstrated. Primary imbibition and drainage displacements are run, and interfacial areas (IFA) as a function of time are determined and compared. Results indicate that wettability is an important factor in displacement behavior and resulting interfacial area. Primary imbibition in a strongly wet material under capillary dominated flows produces film flow, resulting in high IFAs that decrease with increasing saturation and viscous forces. Primary drainage produces initially high IFA that decreases slightly with increasing saturation or pressure drop. Surfaces with spatially variable wetting can have a strong influence on resulting fluid distributions and fluid flow.

Introduction

Over the past decade, Gray and Hassanizadeh have developed a new set of multifluid equations, based on thermodynamic principles, that directly account for multiple fluids, and more rigorously account for the effects of microscale phenomena in continuum-level models of multifluid flow (Gray[1], Gray et al.[2]). The theory systematically averages physical behavior represented at the pore scale to an averaged, continuum scale, therein incorporating the specific effects of multifluid phenomena. These new multifluid flow equations produce constitutive relationships that incorporate dependencies on many additional system characteristics, including interfacial areas between phases. Initial results indicate a potential dependence of macroscopic capillary pressure on saturation and the specific interfacial area between two phases in a unit volume of soil. This suggests that the saturation history or state of interfacial energy may be reflected in the interfacial area in the system, a quantity that may differ between wetting and drying conditions.

The challenge in Gray's theory is to characterize the new, and quite numerous, constitutive relationships that arise, and develop a procedure to quantify them. We take up this challenge via application of a numerical lattice Boltzmann (LB) approach. Using this technique, dynamic microscopic quantities such as the pressure and velocity of each phase can be easily measured and integrated over representative medium volumes; volumetric quantities such as saturation or mean interfacial area can be similarly determined. For appropriately-designed simulations, this approach should allow for interfacial areas, pressures, and saturations to be measured at the pore scale such that their hypothesized interdependence at the macroscale can be determined. For example, it should be possible to measure the hypothesized relationship between the macroscopic capillary pressure, saturation, and mean interfacial area. As such, it provides a tool to study the influence of many microscale system variables on resulting bulk scale flow behavior. In this sense, the simulator becomes a surrogate experimental platform from which macroscale parameters, equations of state, and invariance relationships associated with the derived multifluid flow equations and a particular porous medium geometry can be identified.

Description of Computational Approach

The lattice Boltzmann method (LB) is a recently developed approach to modeling the Navier-Stokes equation. It is a discrete in time and space method that is based on representing the fluids via particle movement on a lattice. The LB approach uses the microscopic kinetic equation to describe particle distribution functions (equivalent to an ensemble average of particles over time). Macroscopic quantities are then derived from the distribution functions through moment integrations. The incompressible Navier-Stokes equation is obtained in the nearly incompressible limit of the LB scheme. The LB technique uses purely local particle interactions on the lattice, and is second order accurate in space and time. Extensive reviews and derivations of the method are available in the literature (for example, see Chen et al.[3] and Rothman and Zaleski [4]), and will not be duplicated here.

Lattice Boltzmann algorithms have been successfully applied to a variety of multifluid flow phenomena. Simulations of two-fluid flows have favorably represented observed fluid flow patterns, and have provided very encouraging qualitative agreement with experimental results (Hazlett et al.,[5]; Ferreol and Rothman [6]; Soll et al.,[7]; Grunau[8]). Calculation of intrinsic permeability for a wide variety of media has produced excellent agreement with experimentally measured values (Soll et al.,[7]). Relative permeability curves showing the proper behavior have also been generated [Hazlett, [9]; Grunau,[8]).

In this work we are particularly interested in two characteristics that the LB method has a unique capability to address: the influence of surface wettability, and the role of interfacial areas (IFA). Wettability is typically quantified by equating it with the contact angle between the fluid and the solid in the presence of a second fluid. The contact angle then represents the competition between the molecular attraction of one fluid with the solid to the molecular attraction of the other fluid with the solid. It is possible to simulate contact angles of 0-180 degrees (full range of wettability) as verified by Grunau [8].

IFA plays a significant role in total system energy, and is postulated to be a key to improved constitutive relationships (Gray et al. [2]). Sub-pore resolution of the flow domain results in highly accurate measurements of the contact area between phases. Using the saturation information, it is a simple task to calculate the IFA per unit volume. The temporally discrete nature of the LB method makes it simple to compute changes in IFA over time.

The spatially discrete nature of the LB method lends easy identification and measurement of parameters called for by the theoretical formulation of the thermodynamically correct multifluid flow equations. Of the seemingly infinite list of parameters that arise in these equations, the LB model can provide: exact fluid distributions, interfacial area between all pairs of phases (fluids and solids), interfacial velocities, line length between three phases, fluid densities, local and averaged velocities, local and averaged pressures, pressures across interfaces, local and averaged momenta, and potentially even free energies. Simulations can range from fully capillary dominated to fully viscous driven providing the tool needed to obtain various bulk quantities. Bulk quantities produced include: saturation, intrinsic and relative permeabilities, and traditional capillary pressure - saturation relationships. Also, the pressure on either side of an interface can be calculated from the local lattice pressures, and related to the apparent curvature of the interface, on a pore by pore basis.

Wettability and Interfacial Area - Simulations

We ran a set of simulations in a simple pore geometry configuration to test the influence of wettability on flow, IFA, and constitutive relationships. The pore geometry selected was a 3-D sinusoidal, converging / diverging tube, symmetric about the center line. Overall system dimension was 90x28x28 lattice units, with maximum radius of 24 and minimum radius of 4. This configuration was chosen because it is complex enough to capture some of the significant behaviors of fluids in porous media (i.e. capillary trapping and snap off) while retaining sufficient simplicity for direct comparison with semi-analytic solutions. Displacement simulations were run for a range of wettability conditions, from strongly wetted by the resident fluid to strongly wetted by the displacing fluid. We are currently in the process of running simulations with spatially variable wetting conditions. One case of non-uniform wetting is a tube where the top half of the solid is wetted by one fluid and the bottom half is wetted by the other. In the following discussion, the initially resident fluid is referred to as water, and is shown as gray in the figures, while the displacing fluid is referred to as oil, and is shown as white. The solid is black.

Figures 1-4 show snapshots of fluid distributions during displacements under each of the wetting scenarios. Each wettability scenario produces quite different displacement characteristics. Displacement under strongly water wet conditions (drainage, Figure 1) produces snap off at low capillary pressures, changing to more of a plug flow at higher pressures. Throughout the displacement, however, a film of wetting fluid remained between the oil and the walls.

Displacement under strongly oil wet conditions (imbibition, Figure 2) initially creeps along the walls as a wetting film under low capillary pressure, with the pore interiors filling in as pressure difference increases. The pore throats fill almost completely at the earliest stages, as a result of narrow throats and thickening films. Note that Figure 2 is somewhat misleading because of the narrowness of the pore throats and the limitations of LB in displaying the saturation information. Although not evident from Figure 2, there are two mechanisms driving displacement of the resident fluid during this

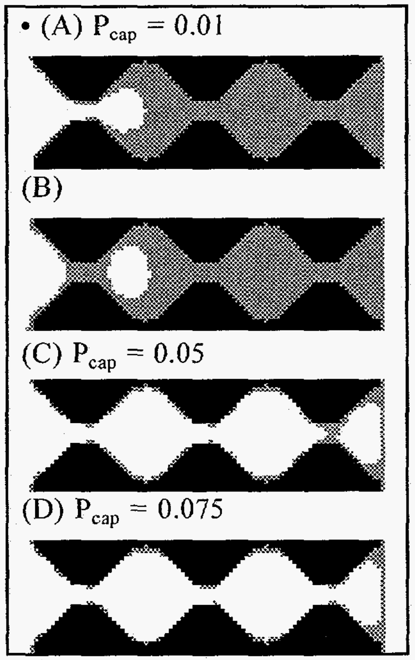

Figure 1: Strongly water wetted solid. Four equilibrium states in the displacement cycle.

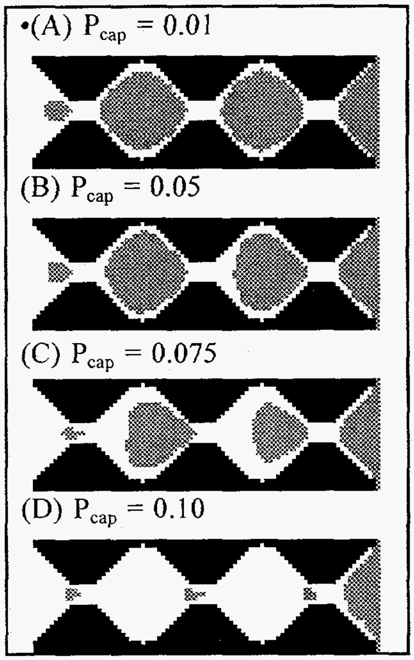

Figure 2: Displacement in a strongly oil wetted solid.

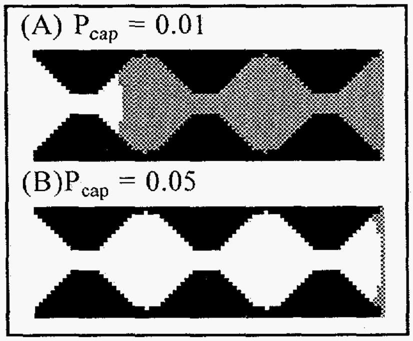

Figure 3: Two fluid displacement in a neutrally wetted solid.

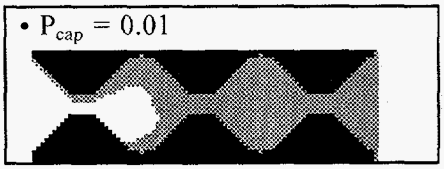

Figure 4: Early time during displacement in a mixed wet solid. Top half is strongly water wet and bottom half is strongly oil wet.

simulation. First, the center of the pore throats does contain continuous, non-wetting fluid. Because this is less than 0.5 in the particle density function, though, the pixels in the saturation map appear as wetting fluid. Second, at higher capillary pressures, closed off throats are forced to periodically reopen, allowing the non-wetting fluid packets to move into the next pore.

Displacement under neutrally wet conditions, shown in Figure 3, occurs as plug flow, without any films evidenced. The curvature of the interface is basically parabolic. The intermediate wet material response (not shown) is most similar to that of the neutrally wet medium.

The simulation run in the mixed wet system with top and bottom walls of alternate wettability (Figure 4) shows a strong preference for flow in the bottom half of the system, which is preferentially wetted by the displacing fluid. The distribution of the displacing fluid is not at all regular, as was observed in the uniformly wetted systems. It is not possible to draw any solid conclusions about the role of mixed wettability based on this single case, however it clearly indicates the need to run a series of simulations under a range of spatially distributed wettability.

For each of the simulations we calculated the time dependent interfacial area between the fluids. A plot of the IFA versus time is provided in Figure 5. The y axis is the computed interfacial area divided by the total pore space volume of the system - the form of the parameter called for by the equations of Gray and Hassanizadeh (Gray et al. [2]). For the strongly oil wet line, data prior to t = 500 was lost, so the line does not begin at t=0. Values computed for a longer system (x=150) show that the characteristic of the curve between t=0 and t=500 is a steeply rising function. This early time covers the period during which the wetting film establishes itself along the solid surface, supporting the indication of rapid growth of the interface up to the t=500 value of approximately 0.13.

The IFA versus time plot is a quantitative representation of the fluid distributions that we observe in Figures 1 - 4. The strongly wetted systems produce early rapid growth of interfacial area at low capillary pressures due to the establishment of wetting films. In the strongly water wet system the interfacial area is maintained due to the presence of the wetting film on the solid surface. In the strongly oil wet system the initially large IFA falls off again, in time, as the resident fluid in the center of the pores is replaced with the displacing fluid. The intermediate wet and neutrally wet systems produce only a small IFA between the two fluids, indicating a plug like displacement front. The sinusoidal characteristic of the neutrally wet curve reflects the sinusoidal cross sectional area of the pore geometry. For the intermediate wet system data is only available at early times, but the trend correlates with neutrally wet system, though somewhat delayed.

The increased amount of time required for displacement in this system is a result of the mild wettability.

The primary information gleaned from the time axis is to notice how much more time is required to reach equilibrium under the strongly wetted conditions than for the more neutral systems. Under strongly wetting conditions, the films reduce the effective area available to flow, resulting in a lower flow rate for the same capillary pressure. Also, the mechanism for flow is made more difficult by the drag at the interfaces.

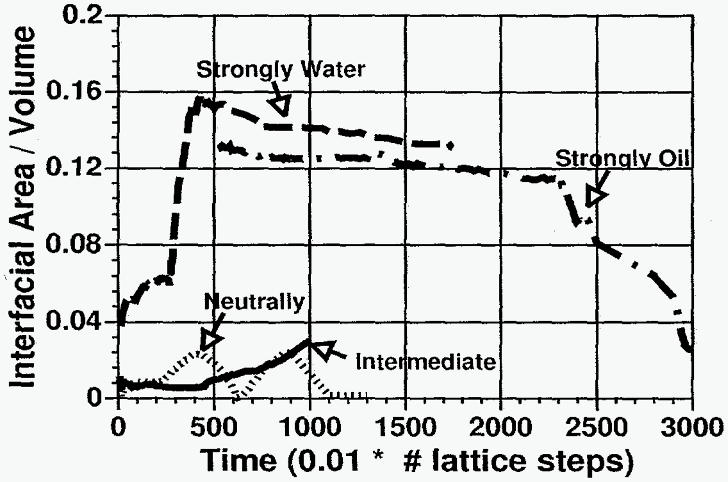

Figure 5: Specific IFA as a function of time for displacement under a range of wettability conditions.

Summary

Preliminary results indicate that wettability is an important factor in fluid displacement behavior and needs to somehow be captured in the multifluid flow equations. Wettability of the solid strongly influences the fluid displacement behavior as well as the temporal variation of interfacial area. Wettability is a characteristic of the particular porous media, and its influences operate at the microscopic scale. As such, it is not possible to directly incorporate wettability into the bulk equations. Rather, it must be accounted for through constitutive relationships describing the system. Tracking interfacial area between fluids is one means of making the role of wettability observable. Gray and Hassanizadeh [2] have developed a new set of thermodynamically correct multifluid flow equations. Within their derivations they postulated an important role of IFA, and have suggested new constitutive relationships that incorporate some of the other important microscopic processes, including temporal variations of IFA and wettability. This work is the first step towards helping to confirm the validity of these equations and alternative constitutive parameters.

Acknowledgments

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