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Modeling variability in porescale multiphase flow experiments

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ABSTRACT

Microfluidic devices and porescale numerical models are commonly used to study multiphase flow in biological, geological, and engineered porous materials. In this work, we perform a set of drainage and imbibition experiments in six identical microfluidic cells to study the reproducibility of multiphase flow experiments. We observe significant variations in the experimental results, which are smaller during the drainage stage and larger during the imbibition stage. We demonstrate that these variations are due to sub-porescale geometry differences in microcells (because of manufacturing defects) and variations in the boundary condition (i.e., fluctuations in the injection rate inherent to syringe pumps). Computational simulations are conducted using commercial software STAR-CCM+, both with constant and randomly varying injection rates. Stochastic simulations are able to capture variability in the experiments associated with the varying pump injection rate.

1. Introduction

In the last several decades, porescale two-phase flow has attracted significant attention (Blunt, 2001; Hassanizadeh and Gray, 1990; Lenormand et al., 1988; 1983; Sahimi, 2011). At the pore scale, multiphase flow is governed by the Navier–Stokes (NS) equations subject to the Young–Laplace boundary condition at the fluid-fluid interface and the Young condition at the fluid-fluid-solid interface (Young, 1805). These equations are highly non-linear because of the moving fluid-fluid and fluid-fluid-solid boundaries, which presents a significant challenge for obtaining accurate numerical solutions (Miller et al., 1998; Tartakovsky and Panchenko, 2016). A number of mathematical formulations have been proposed to simplify the solution of these equations, including methods that describe interface dynamics implicitly by means of a "color" function (Wachem and Almstedt, 2003) (e.g., the volume of fluid (Hirt and Nichols, 1981), density functional method, and phase-field method (Steinbach et al., 1996)). Various formulations have been used to describe the dynamics of a fluid-fluid-solid interface, including static and dynamic contact angles, energy-balance considerations, and pairwise forces. Various numerical methods, including mesh-based finite volume and mesh-less Smoothed Particle Hydrodynamics, have been used to solve the resulting Navier–Stokes equations. Other (so-called "mesoscale") methods (e.g., Lattice-Boltzmann and Dissipative Particle Dynamics) also have been applied to model multiphase flow in porous media. The resulting models have different degrees of complexity in representing fluid-fluid-solid interactions, numerical accuracy, and the computational cost (for a review of numerical methods for multiphase porescale flow, see Meakin and Tartakovsky, 2009).

A natural question to ask is, what model complexity and numerical accuracy are sufficient to correctly model multiphase flow on the pore scale? The qualifier "correctly" in this question is important because, in many studies, the porescale models are verified and validated only in a "weak" sense, i.e., by comparing the average solution (or its properties, such as pressure-saturation relationship) obtained from a numerical model and the corresponding experiment (e.g., Bandara et al., 2013; Liu et al., 2014; Pan et al., 2004). Not that the comparison of average properties of solutions lacks merit; however, it is also reasonable to require a porescale numerical model to reproduce porescale properties of the solution accurately. Comparison with well-controlled, porescale multiphase flow experiments is a reasonable way to validate and verify a numerical model. The answer to the preceeding question is complicated by, at least, three factors: 1) depending on the initial and boundary conditions, the equations describing multiphase flow could be unstable, i.e., small perturbations in initial and boundary conditions may lead to large differences in the solution; 2) the exact geometry and roughness of the flow domain boundaries (i.e., the pore geometry), even when possible to precisely measure, are

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usually impractical to fully resolve; and 3) initial conditions are difficult to control in an experiment and exactly reproduce in the numerical model. Still, even if these challenges could be overcome, reproducible experimental results are needed to conduct a validation study.

Quasi-two-dimensional microfluidic cells are often used to experimentally study porescale flow (Cottin et al., 2010; Zhang et al., 2011a; 2011b). They afford better control and monitoring of flow dynamics than three-dimensional small-column experiments. Therefore, the microcell experiments are perfect candidates to generate results for a validation study. Often, microfluidic studies use a pore geometry made of a uniform array of cylinders (e.g., Zhang et al., 2011b). Multiphase flows in such pore structures are particularly difficult to reproduce in both experiments and numerical simulations for several reasons: 1) small manufacturing defects break "symmetry" and significantly affect the multiphase flow; 2) even if the actual manufactured geometry could be exactly measured, the differences between the prescribed (design) and actual geometry could be impractical to resolve in a numerical model; and 3) small time-variations in the flux rate generated by syringe pumps may lead to significant changes in the final distribution of fluid phases. In Ferrari et al. (2015), multiphase flow in both heterogeneous and homogeneous pore structures was studied, and the "point-by-point" difference in displacement patterns, obtained experimentally and numerically, was found to be from 17 to 30% in the heterogeneous porous structure and from 30 to 40% in the homogeneous domain, depending on a numerical model used. The reproducibility of experimental results was not addressed in Ferrari et al. (2015).

In the first part of this work, we study the question of reproducibility of experiments by repeating simulations in six microcells with the same (up to the manufacturing error) geometry. We use a highly non-uniform pore-size distribution to minimize the effect of small deviations from the design pore geometry and injection rate on the experimental results. In all experiments, a microcell is initially occupied with a wetting fluid, and a non-wetting fluid is injected through the left boundary for 30 s with a constant flux q using a high-precision pump (variations in the injections rate are less than 5% per manufacturer's specification). Then, a wetting fluid is injected through the right port until the saturation of the non-wetting fluid reaches steady state. Our study shows a significant variability in the porescale distribution of fluid phases, interface area, and saturation. In the second part of our study, we conduct two- and three-dimensional simulations with constant and randomly varying injection rates to capture average behavior and variability observed in the experiments. We use a commercial finite volume code STAR-CCM+ (CD-adapco, Melville, NY, USA) in our numerical study. Our results show that the three-dimensional simulation with a deterministic flux q better captures the mean behavior observed in the experiment than the two-dimensional model (which disregards the effect of the interface curvature in a plane perpendicular to the microcell top and bottom walls) with the constant q. The two-dimensional simulations with randomly varying (around the prescribed in the experiments) flux capture the variability observed in the experiments, but the average behaviors found in the simulations and experiments differ. We also find that the average behavior of stochastic simulations differs from the corresponding deterministic simulations because of strong non-linearity of the governing equations.

2. Microfluidic experiments

2.1. Design and photolithography

The reproducibility of porescale multiphase flow experiments is investigated in a microfluidic device shown in Fig. 1-a. For this

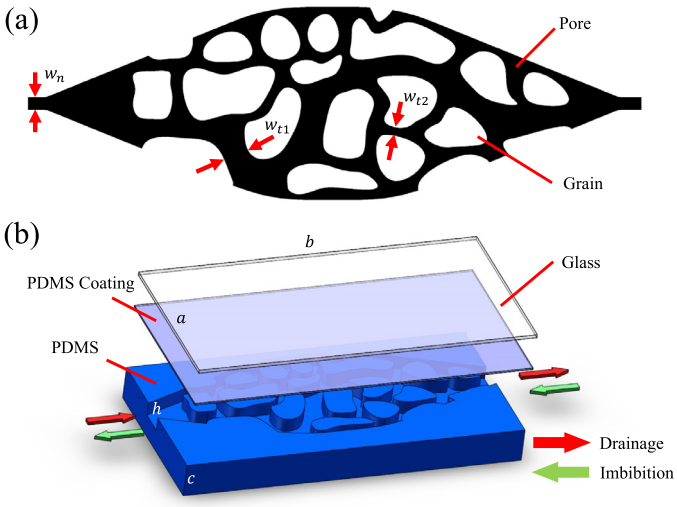

Fig. 1. (a) Pore structure. Pore spaces are shown in black, and the solid phase is in white; (b) Three-dimensional configuration.

Table 1
Micromodel dimensions.

Symbols (Fig. 1)	Length (mm)
$a \times b \times c$	$5 \times 18 \times 5$
h	0.03
w_n	0.1
w_{t1}	$\sim$ 0.4–0.5
w_{t2}	$\sim$ 0.1

study, six replicas of the device are manufactured and up to five experiments are conducted for each replica. To minimize the effect of pore-geometry deviations (manufacturing defects) from the prescribed geometry, porescale heterogeneity is introduced in the form of a preferential flow path with a width w_{t1}. Tubes (or pipes) are connected to the inlet and outlet, which have the width w_{t2}. The design dimensions of the micromodel are provided in Table 1.

The micromodels (Fig. 1-b) are fabricated using standard photolithographic techniques. The six replicas of the design pore geometry are printed on a single photomask. Then, an SU-8 negative photo-resistant material is coated onto a 4-inch diameter silicon wafer. The cell base is made from the hydrophobic polydimethylsiloxane (PDMS) material "baked" in an oven for over 12 h at 75 °C (Fig. 1-b). To make the wetting properties of the cell's glass top the same as that of the PDMS base, the glass is also coated with a thin layer of PDMS. To achieve chemically stable hydrophobic interior surfaces, the assembled cells are placed for an additional 48 h in an oven at 200 °C.

2.2. Experimental design

The fluids are injected and removed from a micromodel using a piping system shown in Fig. 2. To perform drainage and imbibition phases of the experiment, glass syringes (1 mL Glass Syringe, Hamilton) containing the wetting fluid (hexadecane) and the non-wetting fluid (DI-water) are used. A series of valves are used to enable and disable flow paths during these phases (Fig. 2-c). This experimental design allows for a smooth switching from the drainage to the imbibition phase without cross-contamination while preventing formation of air bubbles. A precision syringe pump (NE-4002X, New Era Pump System) is used to produce a constant injection rate.

To conduct an experiment, a micromodel is placed horizontally on a microscope stage (Prior Scientific Instruments LTD.) to