PhD Proposal

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1 Research Objectives

1.1 Develop fast and robust multi-phase capillary-dominated direct simulation technique

Direct simulation of multi-phase flow in images can be done using numerical approximations to fluid flow equations. Popular methods for doing this are use of the Navier-Stokes (NS) based solvers (like OpenFOAM), and lattice-Boltzmann methods. The Lattice-Boltzmann methods in particular are popular for porous media flow since they can easily handle complex solid boundaries, which is an issue in Navier-Stokes based solvers, which rely on meshing of the fluid domain. The meshing process by itself is fairly complex and can be an issue for a general porous media image. When one encounters capillary-dominated multi-phase flow, tracking the interface becomes important. The most common for doing this in NS solvers are use of the volume of fluid (VOF) method. This technique is often too computationally expensive. Lattice-Boltzmann solvers are easy to implement as they can automatically handle complex solid boundaries. Hence one bypasses a major hurdle for simulation. These are more popular in the porous media community. However, they are also expensive computationally, but are set up to be intrinsically parallelizable. This makes them attractive methods for running on a large cluster. Various mutli-phase models exist for lattice Boltzmann solvers - some better than the others.

Both these broad class of methods suffer from inaccuracies in one form or the other. For example, the VOF method is known to have trouble capturing curvatures of fluid interfaces due to the way phase fractions are handled in the method. The level set method was initially introduced for precisely some of these problems. It works better than the VOF method for problems involving capture of fluid interfaces. It has been combined with the Navier-Stokes equations to yield good results in other works. However, it is also very expensive computationally and is difficult to parallelize.

In their 2006 paper, Prodanovic and Bryant proposed a simple level set model to capture capillary dominated fluid flow in porous media. They bypassed the Navier-Stokes approximations, and instead focused on quasi-static flow, and showed this approximation could be used to obtain good results with much lesser computational cost. Jettestuen and Helland in 2013 extended their work

to impose contact angles at the boundaries. Verma (2014) carried out validation studies for a modified version of their method to validate the technique. If one could make the method more efficient, then large number of pores could be simulated cheaply.

Strategies for speeding up the level set method already exist. One of the obvious steps is parallelization. Another one is implementation of adaptive meshing techniques. Both of these steps are under development.

1.2 Validate techniques against experiments/analytical methods

Validation of the contact angle level set method was already carried out for an experimental data set prepared by Mason and Morrow (1994). That data is for the critical drainage curvatures for a single pore in a rhomboidal packing of four spheres, for different contact angles. A related problem is mixed wettability. If some of the spheres have different contact angles, then one would get different critical curvatures. Mason and Morrow's work also presented an analytical technique for calculation of these curvatures for that geometry, which was essentially a modification of the Mayer-Stowe Princen (MS-P) method to calculate drainage curvature. This method would not work if the spheres have different wettabilities, for reasons elaborated upon later.

Thus, we want to obtain an experimental data set similar to Mason and Morrow against which we could validate numerical techniques. These numerical techniques could then be used for larger porous media samples, and eventually matches against core-scale experimental data sets.

1.3 Upscale results using pore network modeling

Direct simulation techniques would always be computationally expensive, no matter how many speed up strategies we employ. Direct simulation on a sample of size, say of a core, would perhaps defeat the point of a digital approach. It is possible that performing the actual experiment in a laboratory is less time-consuming. However, pore network modeling can be used to simulate cores of large sizes, since it does not attempt to solve the Navier-Stokes equations in the pore space, but relies on simplified relationships for capillary displacement in each pore. However, the approximation usually relies on oversimplified geometries. Usually, this means some key aspects of the flow are not captured properly. Using direct simulation to obtain better rules for displacement of phases in general geometries should give better results for pore networks.

This procedure could be applied for both two and three phase modeling. An example of the application could be the behavior of sandwiched layers of oil between water and gas phases for water-alternating-gas injection processes. The state-of-the-art pore network modeling approaches fail to capture the behavior of the sandwiched layers accurately. It is quite possible the rules for layer stability are inadequate and direct modeling can help to get better rules.

2 ProposedResearch

2.1 Two-phase modeling: Validation of methods and mixed wettability

In the first part of the research, we focus on two-phase flow models for drainage. We implement two different techniques for prediction of critical curvatures in rhomboidal packings: the variational formulation of the level set method, and the OpenFOAM VOF method. Brief descriptions of each method are given later. Subsequently, we use match predictions from the numerical techniques with those from experiments. These experiments are designed to be similar to those conducted by Mason and Morrow (1994).

2.1.1 Level set method and modification for contact angles

The method introduced by Prodanović and Bryant [21] - called the level set based progressive quasi-static (LSMPQS) method - models displacement of immiscible fluids with zero contact angles in arbitrarily complex geometries.

The method is based on the main level set evolution equation:

$$\partial_t \phi + F|\nabla \phi| = 0 \tag{1}$$

The tracked interface is the zero level set of the function ϕ. The level set function ϕ is defined implicitly such that it is positive "outside", or on the side on convexity, and negative on the concave side. In simpler terms, the function ϕ is defined throughout the domain of interest as the distance from the wetting/non-wetting fluid interface, which is the zero level set. As one advances the interface, the ϕ function is updated throughout the domain according to the level set equation. Therefore, in a two-phase porous media formulation, $\phi < 0$ could denote the wetting phase, and $\phi > 0$ denotes the non-wetting phase and solid grain together (this choice is, of course, arbitrary). For our application, this provides a convenient way of differentiating the wetting and non-wetting fluids, as the wetting fluid is going to be on the convex side of the interface.

Equation (1) governs the evolution of the function ϕ in space during a period of time. F represents the net normal speed of the interface, and in the original LSMPQS algorithm is based on the difference between the current interfacial capillary pressure and the Young-Laplace equation (details omitted here for brevity).

In our application, F is a function defined by the difference between imposed normal speed, a (which can also be viewed as a pressure-like term acting normally to the interface), and normal speed due to curvature of the interface, $b\kappa$. b is a constant which determines how strong the effect of curvature is - it is an interfacial tension-like term, and is always positive for stability of the numerical method. The two speeds are opposite in direction, since the corresponding physical forces balance each other. In addition, we define an external advective velocity field for the interface. This has been used later near the solid boundary to impose the contact angle. Only the velocity components normal

to the interface affect it, and one can include those inside F. Thus, Equation (1) can be written as:

$$\partial_t \phi + (a - b\kappa)|\nabla\phi| + \vec{V} \cdot \nabla\phi = 0 \tag{2}$$

Here, $\vec{V}$ is the external advective velocity field.

Defining the interface implicitly means that changes in the topology of the fluid phases, such as snap-off and merging of fluid menisci, are handled automatically.

The pore-grain boundary is defined by a separate level set function ψ, such that the boundary is where $\psi = 0$, and in this application ψ does not change. In the original formulation, imposing $\phi(x,t) \leq \psi$ prevented fluid-fluid interface from entering the solid phase. This results in a zero contact angle, and we modify it to allow overlap of fluid and solid regions near the boundary that allows for formation of contact angle, see below for details. We refer to this process as "masking".

Initially, we introduce a meniscus of low initial curvature into the domain, and advance it until it reaches an equilibrium position in the given geometry. The speed at which the meniscus approaches the pore throat must be low enough so that it does not simply advance to the opposite end of the simulation volume without reaching an equilibrium position. This is different from the compressible model used by Prodanović & Bryant [21], but it does not affect the ultimate critical curvature.

Once the meniscus has been introduced in the domain, we advance it using a modified form of the level set equation (Equation (1)) from Jettestuen *et al.* [13]. This is done using the variational approach, and we include the normal, curvature and convective velocity terms so that the level set equation becomes:

$$\phi_t + \{H(-\psi)\kappa_0 - S(\psi)H(\psi)Ccos\beta|\nabla\psi|\}|\nabla\phi| + S(\psi)H(\psi)C\nabla\psi\cdot\nabla\phi = H(-\psi)\kappa_\phi|\nabla\phi| \tag{3}$$

Here, $H()$ denotes a Heaviside function, and is given by:

$$H(\psi) = \begin{cases} 0, & \psi < 0 \\ \frac{1}{2} + \frac{\psi}{2\epsilon} + \frac{1}{2\pi} sin\left(\frac{\pi\psi}{\epsilon}\right), & -\epsilon \leq \psi \leq \epsilon \\ 1, & \psi > \epsilon \end{cases} \tag{4}$$

where ϵ is set to $1.5\Delta x$, and Δx is the numerical cell length. It may be noted that ψ in our case is opposite in sign from that used by Jettestuen *et al.* In our application, we multiply $H(-\psi)$ with those velocity terms that are meant to take effect in pore space, whereas the solid phase terms are multiplied by $H(\psi)$. $\theta = \pi - \beta$ is the contact angle imposed on the medium (see Figure **??**), using the direction of the normals $\vec{n}_\phi$ and $\vec{n}_\psi$. Thus, the modified level set equation works by imposing a velocity near the contact line such that the direction of the velocity vector and the gradient vector of the mask make the desired contact angle. Away from the boundary, we impose only Young-Laplace equation. The diffusive term associated with the zero level set curvature κ_ϕ in Equation (3)

smooths the level set function so that we get one single smooth interface despite having different speeds of propagation of the interface near and far from the boundary. The curvature κ_ϕ is given by:

$$\kappa_\phi = \nabla \cdot \frac{\nabla \phi}{|\nabla \phi|} \tag{5}$$

For 3D, this becomes:

$$\kappa_\phi = \frac{(\phi_x^2\phi_{yy} - 2\phi_x\phi_y\phi_{xy} + \phi_y^2\phi_{xx} + \phi_x^2\phi_{zz} - 2\phi_x\phi_z\phi_{xz} + \phi_z^2\phi_{xx} + \phi_y^2\phi_{zz} - 2\phi_x\phi_y\phi_{xy})}{|\nabla\phi|^3} \tag{6}$$

κ_0 is the imposed normal speed on the interface in the pore space. This is slightly different from the quantity a in the original level set equation, as a includes terms both in the pore space and near the boundary. S() is the sign function which ensures that the contact angle propagates away from the walls, and hence ensures numerical stability.

$$S(\phi) = \frac{\phi}{\sqrt{\phi^2 + |\nabla\phi|^2(\Delta x)^2}} \tag{7}$$

C is a constant that was used in Jettestuen *et al.* [13] to scale the contact angle and curvature parts of the velocity. By trial and error, we found it enough to set it equal to one. The level set equation must also be periodically reinitialized to make sure that the gradients in ϕ do not become too large. The default reinitialization equation was used, and is given by:

$$\phi_t + S(\phi)(|\nabla\phi| - 1) = 0 \tag{8}$$

By imposing different values of the contact angle at different locations, mixed wettability conditions can be simulated. This has been implemented in Jettestuen *et al.* [13], but we do not use it here.

To simulate a drainage process, at every step, the curvature is increased by $\Delta\kappa$ until the steady state solution is found. Therefore, the "time" t defined in Equation (1) is a parameter without physical meaning.

Masking is enforced at every time step with some overlap, so that, $\phi(x,t) + p \leq \psi$, where p is the overlap, measured in the grid spacing Δx. This is a key difference in our methodology versus that introduced in Jettestuen *et al.* [13]. They also have an overlap in the main equation, but it is not enforced during the masking process. The overlap was found necessary for accuracy as the contact angle became larger. When the contact angle is closer to 0 deg, no overlap was necessary. As the contact angle increased, the overlap between the pore space and the grain space was increased gradually, up to a maximum overlap of one grid cell. For 40 deg, the overlap was 0.3 grid cells, then for contact angle 50 deg it was 0.5, and finally the overlap was increased to one grid cell by contact angle 60 deg, and held constant for greater angles. It may be noted the method is stable without this overlap, but we introduced this as it gave a much better

match to analytical values. Having an overlap is not physical. However, it allows for formation of contact angles between different interfaces (the cusp is not a possible solution to a level set equation that contains a diffusive curvature term) and does not affect the equilibrium solution as long as overlap regions belonging to two portions of grain boundary do not touch. It is intuitive that the contact angle size is related to the size of the overlap.

An imbibition simulation would proceed by taking the endpoint of a drainage simulation as the starting point. Curvature is decreased step by step, just as it was increased for the previous case. In this work, we have not performed any imbibition simulations.

The equation was solved using the MATLAB level set toolbox written by Ian Mitchell [**?**, **?**]. The time derivative is approximated with a total variation diminishing Runge-Kutta integration scheme with an order of accuracy between one and three. The Courant-Friedrichs-Lewy (CFL) conditions restrict the size of the timestep. For the convective term, the gradient is approximated by an upwind finite difference scheme with order of accuracy between one and five. One can get fifth order accuracy if you use the WENO (weighted essentially non-oscillatory) scheme, but fifth order accuracy is achieved only near the zero level set. In our simulations, using the third-order accurate ENO (essentially non-oscillatory) scheme gives satisfactory results. For the curvature velocity term, the mean curvature κ is approximated using a centered second order accurate finite difference approximation. This is also used in post-processing the results when we want to compute the distribution of curvature values on the interface. Finally, as explained earlier, the level set equation is reinitialized every few time steps using the reinitialization equation in order to maintain $|\nabla\phi| = 1$. This is solved using a Godunov scheme. Further details of individual numerical schemes can be found in the book by Osher and Fedkiw [17]. In all of our simulations, we use the "high" accuracy option in the toolbox, which results in third order temporal accuracy, and use of the third order accurate ENO scheme.

2.1.2 OpenFOAM VOF methods

The volume of fluid method is a numerical technique used in the open source software OpenFOAM to track interfaces in multiphase flows. In this implementation the location and velocity of the fluid/fluid interface is updated by using the Navier-Stokes equations, in a coupled manner. The motion of a single incompressible fluid can be described completely by the Navier-Stokes equation along with conservation of mass. For incompressible fluids, conservation of mass is given by:

$$\nabla \cdot (\vec{u}\rho) = 0 \tag{9}$$

The Navier-Stokes equation on the other hand describes conservation of momentum:

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u}\vec{u}) = -\nabla \cdot p + \nabla \cdot (2\mu \vec{E}) + \vec{f_b} \tag{10}$$

Here, ρ, $\vec{u}$ and μ describe the density, velocity field and viscosity of the fluid, respectively. $\vec{E}$ is the rate of strain tensor, while p is the pressure field. $\vec{f_b}$ is the external body force term, which can include gravity. So, if one has two immiscible, incompressible fluids, the Navier-Stokes equation along with mass conservation are to be solved for each fluid separately. One would need to solve the appropriate fluid equation depending on which part of the domain we are in.

At the interface between the fluids, we would need to impose continuity of velocity and tangential stresses and maintain jump in the normal stress (equivalent to the capillary pressure). This can be done by considering the velocity to be continuous across the interface, Γ:

$$\vec{u}_{\Gamma^-} = \vec{u}_{\Gamma^+} \tag{11}$$

The stress field must satisfy:

$$[-p\vec{I} + 2\mu\vec{E}]_\Gamma \cdot \vec{n} = \sigma\kappa\vec{n} \tag{12}$$

σ is the wetting/non-wetting fluid surface tension and $\vec{n}$ is the normal to the interface. The curvature, κ is twice the mean curvature of the interface and is nominally the same as the one used in the level set method.

The above system of equations can be used to solve for the pressure and velocity fields for each of the two fluids. The condition set on the velocity and stress fields at the interface can be used to advect the interface. However, in a numerical implementation this would lead to solving for moving boundary conditions which is very complex and time-consuming, especially as we are dealing with two separate fluid domains [**?**]. To get around this problem, the VOF method was introduced by Hirt and Nichols in 1981 [**?**]. Essentially, instead of solving two sets of Navier-Stokes equations and keeping track of the fluid domain and shapes, we define an indicator function which contains the information of which fluid is contained in a given fluid cell.

If one considers a domain having two phases, wetting(P_w) and non-wetting(P_{nw}), then we can define an indicator function $I(\vec{x}, t)$,

$$I(\vec{x}, t) = \begin{cases} 1, & \vec{x} \in P_w \\ 0, & \vec{x} \in P_{nw} \end{cases}$$

So, for cells which are completely wetting phase, the liquid fraction is 1, while for non-wetting it is 0. The interface is located at $I = 1/2$, and is indicated by the Dirac delta function around the interface, $\delta_\Gamma = \delta(I - 1/2)$. We can then get a modified form of the Navier-Stokes equation in the entire domain:

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u}\vec{u}) = -\nabla \cdot p + \nabla \cdot (2\mu \vec{E}) + \vec{f_b} + \vec{f_s} \tag{13}$$

where we can write for the density and viscosity fields:

$$\rho(\vec{x},t) = \rho_w I(\vec{x},t) + \rho_{nw}(1 - I(\vec{x},t))$$
$$\mu(\vec{x},t) = \mu_w I(\vec{x},t) + \mu_{nw}(1 - I(\vec{x},t))$$

The additional term introduced, $\vec{f_s}$ describes the Laplace pressure acting at the surface of discontinuity and is given by:

$$\vec{f_s} = \sigma\kappa\vec{n}\delta_\Gamma \tag{14}$$

For numerical implementation, the term $\vec{f_s}$ is replaced by a continuum surface force (CSF):

$$\vec{f_v} = \sigma\kappa\nabla I \tag{15}$$

$\vec{f_v}$ tends to $\vec{f_s}$ as the thickness of the interface region tends to zero. The curvature κ is calculated from the indicator function. This can't be done directly as it leads to large spatial oscillations. Recursive smoothing is employed to get a sufficiently smooth indicator function, $\hat{I}$. The curvature can then be calculated from the smoothed function using:

$$\kappa = \nabla \cdot \vec{n} = \nabla \cdot \left(\frac{\nabla \hat{I}}{|\nabla \hat{I}|} \right) \tag{16}$$

It can be seen this is the same as the curvature in the level set method, where the indicator function replaces ϕ in Equation (6). Using mass conservation in combination with the modified Navier-Stokes equation (13), we finally get a simple advection equation for the indicator function:

$$\frac{\partial I}{\partial t} + \nabla \cdot (I\vec{u}) = 0 \tag{17}$$

This equation is solved explicitly using the velocity from the previous time step. To counterbalance numerical diffusion, a non-linear convective term is added to the equation, which acts as a shock that balances numerical diffusion.

$$\frac{\partial I}{\partial t} + \nabla \cdot (I\vec{u}) + \nabla \cdot (I(1-I)\vec{u_r}) = 0 \tag{18}$$

where $\vec{u}_r$ is a compression velocity. Its choice does not affect the solution outside the interfacial region. Note that the indicator function defines the interface implicitly as the 1/2 level set of I, and the advection equation for the indicator function is related to the level set equation (Equation (1)). An example smoothed indicator function is the Heaviside function, defined in Equation (4).

At the solid boundaries, the fluids are constrained in the pore space by requiring that the velocity component normal to the solid wall is zero. At the triple-contact line, Young's law determines the contact angle:

$$cos\theta = \frac{\sigma_{nw,s} - \sigma_{w,s}}{\sigma} \tag{19}$$

where $\sigma_{nw,s}$ is the non-wetting fluid/solid interfacial tension, $\sigma_{w,s}$ is the wetting fluid/solid interfacial tension.

For imposing the contact angle in our simulation, this is equivalent to imposing the boundary condition:

$$\vec{n}_{\Gamma_s} = \vec{n}_s cos\theta + \vec{t}_s sin\theta \tag{20}$$

where $\vec{t}_s$ is the unit tangential vector pointing into the wetting phase.

OpenFOAM uses finite volume discretization for the above equations for mass and momentum conservation, and advection of the indicator function. The advection equation (Equation (18)) is used to update the indicator function values throughout the domain. This is then used to update fluid properties throughout the domain, and calculate the CSF force. Finally, the solution of the momentum equation (Equation (13)) is performed by using the Pressure Implicit with Splitting of Operators (PISO) implicit pressure correction procedure. Further details on the implementation of interFoam and the numerical schemes used may be looked up in Deshpande *et al.* [**?**].

To speed up the computations and approach capillary equilibrium faster, a damping term $-K\vec{u}$ has been added to the right-hand side of the momentum equation. The term resembles the Darcy's law with a negative source of momentum given by a constant (e.g. permeability) and the velocity. This stabilizes the interface faster after each increase of pressure and avoids strong oscillations around the equilibrium condition. In this case a unitary viscosity and a very small surface tension have been used, giving rise to negligible parasitic currents. The damping term also helps to kill any arising non-zero velocity. A special version of the solver interFoam, with a local time stepping (LTSInterFoam), has been used to march in pseudo-time without prescribing a pre-defined time step. This technique can maximize the time step (therefore reducing the relaxation time) in each cell. The resulting iterations are therefore not physical and not related to a real evolution in time but simply represent internal iterations to reach the steady state. All these choices make the VOF solver under study equivalent to the quasi-static level set formulation. The remaining differences lay on the different equations solved, on the implementation of curvature and boundary conditions.

2.1.3 Two-phase experiments for mixed wettability

Mason and Morrow (1994) performed experiments for determining the critical curvatures in a rhomboidal packing of four spheres. In their set up, all the spheres had the same wettability. The advantage of that is that one can obtain arc menisci in the same cross section, and one can then use the MS-P method for prediction of critical curvatures. However, if the wettability of the spheres varies, then the wetting fluid would tend to spread differently on some spheres than others. Thus, the critical curvatures are likely to be very different. This is likely much more representative of a real rock, where one can have grains of different mineralogy or roughness packed in the same pore.

Here, we describe the setup for the experiment.

2.1.4 Upscaling: combination with pore network modeling

The results from the two-phase studies indicate that we have at least two reliable techniques for prediction of curvatures in arbitrary geometries. Thus, we can use these methods to predict the critical curvatures in arbitrary shapes used in pore network modeling.

Many different shapes can be employed for a given pore network model. We propose extracting a set of shapes from the three-dimensional image of the porous medium. Instead of defining which shape to extract beforehand, we could modify the image analysis algorithm to find the best possible set of shapes to predict the properties of the porous medium. Alternatively, we could simply use shapes which better approximate the porous medium walls. One common feature of pore network models is that they all rely on a constant cross section for prediction of critical capillary pressures. This is one constraint we could remove from the method.

Using the updated method for extraction of pore networks, we can use the method on images of cores to test if our hypothesis is correct.

2.2 Three-phase methods: direct modeling and validation

3 Literature Review

3.1 Level Set Methods

The level set method is a mature numerical method first proposed by Osher and Sethian in their seminal work [18]. The method has since been applied for a wide variety of applications: from image-processing and modeling flames to multiphase flows, and was first used for modeling flow in porous media by Prodanović and Bryant [**?**]. The method was used for simulating drainage and imbibition in a porous medium of arbitrary geometry, when the contact angle is zero. By defining the location and propagation of the interface in an implicit manner, the level set method automatically handles operations such as interface splitting and merging. Hence it is ideal for tracking movement of an interface in a porous medium where phenomena like snap-off and trapping take place. Doing this using an explicitly defined interface, such as by front tracking, would be far more time consuming [**?**]. A much more elaborate discussion of the level set method and the algorithms it uses can be found in the books by Osher and Sethian on the topic [17, 22]. The level set method has already been in use for two-phase flow applications for incompressible fluid flow [15].

The level set method has also been modified for media of arbitrary wettability. In the formulation above, a zero contact angle is implicitly assumed. Zhao *et al.* [25] proposed a variational approach for problems involving solid and fluid domains with different surface and bulk energies. The variational formulation for interface movement in porous materials has been implemented in a recent paper by Jettestuen *et al.* [13]. The level set method can also be extended for modeling flow of more than two phases, for example by representing each

interface by its own level set function [8].

Level set methods suffer from problems of mass loss in under resolved regions. Enright *et al.* proposed a new hybrid particle level set method which addresses this problem. This problem has also been tackled by other workers, such as by Sussman and Fatemi [] who constrained the reinitialization step required in level set methods to incorporate area/volume conservation. Rider and Kothe [] devised a set of test problems for determining the reliability of level set and related methods like front tracking. They found that Lagrangian tracking schemes maintain filamentary interface structures better than their Eulerian counterparts. Therefore, one of the objectives in this work is to compare different interface tracking methods and choose the one which is most accurate.

3.2 Navier-Stokes Solvers: OpenFOAM VOF

In this work, we focus on use of the volume of fluid (VOF) method for multiphase flow simulation using the OpenFOAM software tool. The VOF method has been around for some time, and is popular in the computational fluid dynamics (CFD) community to study interface motion in general fluid flow. Essentially, this is based on the idea of solving the Navier-Stokes equations for two fluids simultaneously. However, this would lead to solving for moving boundary conditions - solving which would be a very complex and time-consuming task. To get around this problem, the VOF method was introduced by Hirt and Nichols in 1981 [**?**]. Essentially, instead of solving two sets of Navier-Stokes equations and keeping track of the fluid domain and shapes, we define an indicator function which contains the information of which fluid is contained in a given fluid cell. Huang *et al.* (2005) used this method to study fluid flow in fractures, and were able to obtain qualitative agreements with laboratory experiments. In addition to VOF methods, multiphase flow using Navier-Stokes discretizations may also be done using the level set method [] and phase field variables []. In this work, we will not focus on the phase field variable, and the level set method used is not coupled to the Navier-Stokes equations.

Deshpande *et al.* present details of the numerical implementation of the VOF method in the OpenFOAM module interFoam []. Hoang *et al.* (2013) performed OpenFOAM VOF simulations for confined bubbles and droplets in microfluidics. This is similar to the size range we are interested in. They make recommendations for optimal computational settings for various cases. They model surface tension dominated systems which is what we are interested in. Horgue *et al.* (2013) used the VOF method to model two-phase flow in arrays of cylinders. They studied the spreading of a liquid jet in passages of size close to the capillary length. Ferrari and Lunati (2013) performed numerical drainage experiments to model the transition from stable flow to viscous fingering. They additionally evaluated different definitions of macroscopic and microscopic capillary pressures and conclude a definition based on the total surface energy provides an accurate estimate of the macroscopic capillary pressure.

OpenFOAM has not been very widely used for flow simulation in porous media at the pore scale. A major reason for that is the fact we are interested in

modeling interface motion, which is typically hard to do in Navier-Stokes based solvers. The interfacial tension force may be applied using several approaches: continuous surface stress [], continuous surface force [] or sharp surface force []. Specifically, for very low capillary numbers, large spurious velocities appear on the interface of the two fluids []. Lafaurie *et al.* []proposed a relationship for estimating the magnitude of the spurious currents. Since we are interested in that domain of flow, this is a big problem for us. Many works related to reducing these spurious currents also exist []. One recent work on this is Raeini *et al.* (2012) []. They modeled the volume of fluid (VOF) method in order to simulate two-phase flow. The authors suggest a new filtering technique for removing these velocities from the interface and were able to get a much better resolution of the interface. In Raeni *et al.* [] they followed up their work with another paper applying their new technique to simulate two-phase flow in simple geometries like a star-shaped channel. They studied events like snap-off and layer flow and investigated the effect of geometry and flow rate on trapping and mobilization of disconnected blobs of fluid. In Raeini *et al.* (2014) [] they applied their method in a sandpack and a Berea sandstone. They proposed upscaling relationships for converting pore-scale pressures to Darcy-scale pressures, and derived relative permeability curves from their simulations. They also varied the capillary number in their simulations, in order to study capillary fingering versus viscous fingering.

The problem of spurious velocities for low capillary numbers has been studied for a while, and many authors have proposed different approaches to deal with the problem. Renardy and Renardy (2002) [] proposed a parabolic reconstruction method (PROST) for representation of the body force due to surface tension. Brackbill *et al.* [] also proposed an alternate technique to model surface tension as a body force.

The VOF method shares some similarities with the level set method. In both methods, a separate function indicates the fluid present at a particular point in the domain. For the volume of fluid methods, this would be a binary function - a zero value indicates one fluid, while 1 indicates another. For the level set function, the values change according to the distance from the interface. So, we have a gradation of values. Both methods update the function values using an advection equation. The form and implementation of this is discussed further in the Methods section. For now, suffice it to say that since the form of the equation is similar, similar methods to solve them exist. Direct comparisons of the two methods have also been done. Sussman and Puckett (2000) presented a hybrid level set-VOF method, and detailed problems and advantages for each method. Specifically, VOF methods are problematic for computation of local curvatures, since there is a sharp change in the indicator function value in the region of the interface. Standard VOF methods compute the curvature by smoothing the volume fractions in some way []. This is often problematic. If one does not smooth enough, even a simple circle would have oscillatory curvatures []. If one smooths too much, then the algorithm does not capture changes in curvature. A direct comparison of the level set and VOF methods will be made in this work, and preliminary results are shown in the Results section. Gerlach

et al. performed a direct comparison of three different techniques for surface tension modeling in VOF methods - Brackbill's continuum surface tension force formulation, the combined VOF and level set method proposed by Sussman and Puckett, and the PROST method proposed by Renardy and Renardy. They concluded that the PROST method was the most successful in eliminating these spurious currents.

VOF methods are typically computationally expensive. One strategy for speeding up convergence of this method is use of local time-stepping (LTS). The OpenFOAM module ltsinterFoam performs this function. Local time stepping speeds up convergence by using as large a time step as possible based on the local Courant number. This violates the local physics of the flow, but if one is only interested in equilibrium solutions, as is the case we are interested in, then this can be very useful []. The most restrictive time step in the interface region is spread through the domain by processing the time step field. Some smoothing is also required to prevent instability caused by large conservation errors due to large changes in time steps.

To our knowledge, the VOF method has not been applied for capillary dominated three phase flow. It has been applied for higher Reynold number flows, for example in work by Wardle and Weller [] and Shonibare and Wardle []. This would be one of the objectives of this work. A direct simulation of three phase flow would not only be novel, but could also help verify analytical relationships for simple geometries proposed by other authors based on thermodynamics.

3.3 Pore network models

Representing pore space as a network of pores (openings) connected by throats was introduced by Fatt [**?**] in the 1950s. Later, in the 1980s, percolation theory was used to describe multiphase flow properties [3]. The history and development of the pore network modeling has been reviewed elsewhere [1]. A few representative works are considered here. Jerauld & Salter [12] describe a pore model to simulate two phase relative permeability and capillary pressure of strongly wetting systems (like Berea sandstone). The model was used to calculate scanning loops of hysteresis between primary drainage, imbibition and secondary drainage. Sahimi & Helba [10] was another paper which described the approach of using pore networks for generating flow properties, where they tried to develop a theory of two-phase flow using percolation theory. The earlier models were restricted to very simple geometries. Bryant *et al.* [4], used geologically realistic geometries, and for the first time were able to predict transport and flow properties. They based their models on a random close packing of equally-sized spheres. Diagenesis and compaction were modeled by adjusting the centers and radii of the spheres, thus making the model representative of sandstones. Single and multiphase flow was simulated through the pore space. They were able to predict the absolute and relative permeability, capillary pressure, and electrical and elastic properties of water-wet sand packs, sphere packs, and a Fontainebleau sandstone. Øren *et al.* [16] extended this work to simulate packing of spheres of different sizes. A reconstruction algorithm based on thin

section analysis was used to generate a topologically disordered network. Two-phase flow was simulated and compared with experimental data. The model predicted the relative permeabilities for two water-wet sandstones and for a mixed-wet reservoir sample.

In the past couple of decades, more sophisticated ways of modeling the pore space have been developed: we can now simulate contact angles (and hence wettability), three-phases, non-Newtonian behavior, reactive flow solute transport and thermodynamically consistent oil layers [**?**, 3, 19, 20, 23]. One key aspect of pore network modeling is the extraction of networks representative of the pore space. The pores and throats are assigned effective properties, such as volume, inscribed radius and shape. Pore connectivity is also tracked, for example by grain-based approaches [**?**]. Grain based approaches work well for clearly granular media and are well suited for pore space representations derived not from images, but from object based simulation of grain packing and diagenesis. They work less well for more complex systems, such as many carbonates, where grain identification is more difficult. There are other techniques for generation of the networks like the maximal ball approach [**?**] and the erosion-dilation technique [**?**, **?**] which work well for pore space geometries derived from images.

In most network modeling approaches, the shape assigned to the pore is of great significance for proper wettability modeling. For demonstrating wetting layers, especially in three-phase flow, the wetting layer is modeled as being trapped in the corners, with the non-wetting phase in the centre of the pore. The simplest shape that captures this is a triangle. In three-phase flow, the intermediate wetting layer is sandwiched in between these two layers. Hence, the way the layers interact influences the relative permeability values. Many different shapes have been tried for simulating multiphase flow physics [19].

Reviewing both direct modeling and network modeling approaches, Blunt *et al.* [2], conclude that network modeling still offers the most efficient and proven way of simulating multiphase flow in porous media, since workflows for network modeling are already mature. Direct simulation on representative samples of rocks (around 5 mm length scale) in some applications like mixed wettability and three-phase simulation is still beyond the reach of computers. Hence, direct simulation can at present only help to elucidate displacement mechanisms, and ultimately network modeling must be used to scale up the results using idealized geometries. Pore network modeling cannot lead to a good understanding of, for instance, overall connectivity of intermediate wetting layers in the network and their unusually high permeability due to somewhat ad-hoc rules of displacement [6, 7].

3.4 Experimental and analytical data sets

A large fraction of experimental observations at the pore scale have been micromodel experiments. Micromodels are idealized two-dimensional representations of porous media typically etched into a glass plate and monitored through a microscope, thus one can observe processes like fingering, snap-off and trapping associated with multiphase flow using them. For examples of micromodel

experiments, see [?, ?, ?, ?, ?]. Micromodels are a very popular method for observing multiphase as well as multicomponent flow behavior, including reactive flow [?, ?]. Most of these models are fabricated, and hence are not exactly representative of real rocks - they need to have porosity of the order of 50% in order to percolate, but are very useful for imaging flow. For instance, two and three phase displacement rules used in pore scale modeling have been devised based on micromodel observation [26].

High resolution X-ray micro-tomography experiments, first performed by Flannery *et al.* [9], have enabled 3D multiphase observation. A review of X-ray computed tomography and its applications and limitations was done in Wildenschild *et al.* [?], and more recently in Wildenschild and Sheppard [?]. Recent flow imaging experiments were performed by Wildenschild and co-workers in a series of papers. Imaging of both 2 and 3 phase flow in packings of glass beads or general porous media is now common [11,20,21,24]. In Culligan *et al.* [5], the authors quantify the fluid-fluid interfacial areas using imaging of flow in bead packs. Mineralogy and dissolution/precipitation processes can be quantified as well [?].

Focusing on the menisci formed during two-phase displacement, Mason and Morrow [?] determined the maximum meniscus curvatures (or critical curvatures) in rhomboidal pore throats formed by four ball bearings. In a later work [14], they worked out critical curvatures for a range of contact angles and rhomboid pore angles, both analytically and experimentally. Their experiments were performed on PTFE ball packings.

There is of course a massive amount of literature present for experiments done at the lab scale [?, ?, ?]. Oak, 1990 [?] measured three-phase relative permeability of Berea sandstone. However, we have not attempted to make any simulations beyond a single pore in this work.

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