# A comprehensive review of pore scale modeling methodologies for multiphase flow in porous media

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Invited review

# A comprehensive review of pore scale modeling methodologies for multiphase flow in porous media

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**Abstract:**
Multiphase flow in porous media is relevant to amount of engineering processes, such as hydrocarbon extraction from reservoir rock, water contamination, $CO_2$ geological storage and sequestration. Pore scale modeling, as an alternative approach to lab measurement, firstly serves as an effective bridge to link the pore scale properties (pore geometry and wettability) and displacement mechanisms to continuous scale multiphase flow in porous media; and secondly allows us to determine essential flow functions, such as capillary pressure and relative permeability curves, which are required for continuous scale modeling. In the literature, three methodologies, Bundle of Capillary Tube Modeling (BCTM), Direct Pore Scale Modeling (DPSM) and Pore Network Modeling (PNM), have appeared to be mostly widely adopted in the investigation of the pore-scale mechanics of fluid-fluid and fluid-solid interactions in porous media by numerical simulation. In this review article, a comprehensive review is provided to show their strengths and weaknesses and to highlight challenges that are faced in modelling of multiphase flow, key challenges include: are contact angle characterization, validation and upscale pore scale findings to core, or even field scale.

## 1. Introduction

Multiphase flow and transport processes in porous media play an essential role in the extraction of hydrocarbon from subsurface, environmental issues (e.g., water contamination and $CO_2$ storage and sequestration) and the remediation of non-aqueous phase liquid in the subsurface. The spatial variability of these processes ranges from single pores to geological basin, and thereby spanning from nm (unconventional tight formation) or $\mu$m (conventional formation) to km on length scales. In general pore scale modeling aims to simulate multiphase flow in pore space, and it normally simulate multiphase flow from $\mu$m to cm in length scale and thus links the pore scale events to core scale flow functions. A significant amount of efforts have been dedicated to develop and improve analytical and/or numerical modeling techniques for simulating pore-scale multiphase fluid flow in porous media in past decades; consequently, many computational methods and models have been proposed and developed. Of them, Bundle of Capillary Tube Modeling (BCTM), Direct Pore Scale Modeling (DPSM) and Pore Network Modeling (PNM), have been used extensively to determine fluid configuration together with flow function (mainly capillary pressure and relative permeability curves) under various fluid-rock systems. They differ in their ways of representing the pore space under variable degrees of physically plausible simplification and modelling the behaviors of fluid flow on the simplified pore space defined by plausible physics.

BCTM represents the porous space with a bundle of capillary tubes of variable shape and size cross-section; this type of models provide a simple, yet physically-sound approach to simulate multiphase flow in porous media. In the early days, the cross section of the capillary tubes were described analytically with a pore size distribution (Kovscek et al., 1993; Ma et al., 1996; Van Dijke et al., 2004; Helland and Skjæveland, 2006b; Cai et al., 2010). Recently, capillary tubes with irregular cross section extracted directly from rock images were used to simulate fluid configuration together with flow function (Lindquist, 2006; Virnovsky et al., 2009; Frette and

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Helland, 2010; Helland and Frette, 2010; Glantz and Hilpert, 2011; Kim and Lindquist, 2012; Zhou et al., 2012, 2014, 2016).

The main shortage of BCTM is that a bundled capillary cannot really capture true pore connectivity of a sample that can be obtained by advanced tomographic imaging, making BCTM incapable of modelling key displacement phenomena, such as Haines jump, trapping and ganglia mobilization. With micro-x-ray computerized tomography (micro-CT) and SEM, it is possible to reconstruct 3D pore space of a sample at a high resolution (Wu et al, 2006). Instead of simplifying the pore space of a sample into a set of capillaries, DPSM takes a reconstructed 3D image, typically in binary form, as a pore space model and simulate fluid flow on it. Currently, several Computational Fluid Dynamic methods has been adopted to simulate multiphase flow in these 3D pore space, and they could be classified as either particle- or grid-based. Examples of particle-based methods are the Lattice-Boltzmann (LB) which uses particle probability distribution function (Ahrenholz et al., 2006; Boek and Venturoli, 2010; Ramstad et al., 2010; Bandara et al., 2011) and the smoothed particle hydrodynamics (SPH) methods (Hu and Adams, 2006; Tartakovsky and Meakin, 2006; Kordilla et al., 2013). The main grid-based methods include the level set (LS) (Prodanović and Bryant, 2006; Jettestuen et al., 2013), Volume of Fluid (VoF) method (Raeini et al., 2012). In addition, the Morphology-based methods (Ahrenholz et al., 2008; Silin et al., 2011) were applied to estimate capillary dominated fluid configuration and to derive capillary pressure curves.

Unlike BCTM and DPSM, PNM represents the pore space of a sample by an extracted network of connected pores and throats, and simulates multiphase flow solving flow and transport equations on the network (Øren et al., 1998; Blunt, 2001; Piri and Blunt, 2005; Valvatne et al., 2005; Joekar-Niasar and Hassanizadeh, 2012; Al-Dhahli et al., 2013). Given a binary image, the extracted network has an identical topology of the true pore space and for each network element of pores and throats, its geometry is estimated from the image and approximated so that its cross-section takes one of idealized geometries (e.g., circle, square, star, triangle). PNM was initially proposed to simulate capillary dominated flow, and thus know as quasi-static pore network modeling; recently, it has been extended to model the effect viscous force-dynamic pore network modelling (McDougall and Sorbie, 1993; Dahle and Celia, 1999; Lovoll et al., 2005).

In this review article, we will provide a comprehensive review of all the above mentioned methodologies that have been applied to simulate multiphase flow in pore space; this will allow us to have a good overview of existing methodologies and their strengths/weakness together with the current challenges for performing pore scale modeling.

## 2. Bundle of capillary tube modeling

One of the earliest work in two phase flow modelling is carried out by Purcell (1949), where the porous medium is (ideally) reconstructed from separated parallel tubes which were used to model the capillary pressure-saturation relationship. Later on, an analytical model was proposed by Yuster (1951) to model simultaneous annular flow of oil and water in single as well as multiple capillary tubes. These capillaries can be modelled as interacting; i.e. the fluid can transfer from one to another, or as non-interacting. Both interacting and non-interacting tubes are developed to calculate capillary pressure and relative permeability curves and still attract researchers.

Depending on whether capillary cross-sections are approximated by idealized shapes or not, this approach can be categorized into two categories: 1) Capillary Tube Model based on Analytical Cross Section, and 2) Capillary Tube Model Based on Rock Images.

### 2.1 Capillary tube model based on analytical cross section

Until late 90s, all the capillary tube models considered no flow interchange between capillaries. Bartley and Ruth in two separate works (1999, 2001) had developed a model which could account for the capillaries' interaction. In their model, a frictionless fluid flow between any tubes has been assumed which allows for "perfect-cross-flow" model to be achieved. They compared their model with an extended Darcy Law which showed the later can be substituted with their (simpler) model. Despite the results, the "perfect-cross-flow" is rare to happen in real porous media in which using their methodology would result in misleading interpretations.

$$q_{wi} = \frac{\pi r_i^4 \Delta P}{128 \mu_w L} \tag{1}$$

$$q_t = \frac{\pi \Delta P}{128 \mu_w L} \sum_{i=1}^{N_c} r_i^4 \tag{2}$$

The notation $q$ denotes the flow rate, $\Delta P$ as pressure difference, $r_i$ as the radius of the $i$-th capillary tube, $\mu$ as viscosity and $L$ as the length of the model.

In a separate work, Dong et al. (1998) pioneered a model of interacting bundle of capillary bundle in which the pressure equilibration was assumed to be equal at any distance $x$ measured in those sections holding either water or oil phase. This as well as the assumption of a pre-defined constant capillary pressure at the oil-water interface in every tube, has led to an idealized model. Dong et al. (2005, 2006) introduced an updated model of interacting bundle of capillary tubes in which 51 capillaries with different diameters (Fig. 1). The flow rate passing through one capillary and the bundle are given in Eq. (1) and Eq. (2) respectively. In non-interacting tubes, the movement of fluid-fluid interface in every capillary tube is governed by Washburn equation (Washburn, 1921) which calculates a higher rate of interface movement in imbibition process in larger capillaries while in interacting model, this is shown to be in the opposite way. Yet from Hagen-Poiseuille equation, average velocities for larger capillaries are calculated to be higher than smaller capillaries which is in contrast with the physics of the capillary dominant flow.

The so called interacting bundle tube model was further developed by Zhou et al. (2013, 2014) to understand the

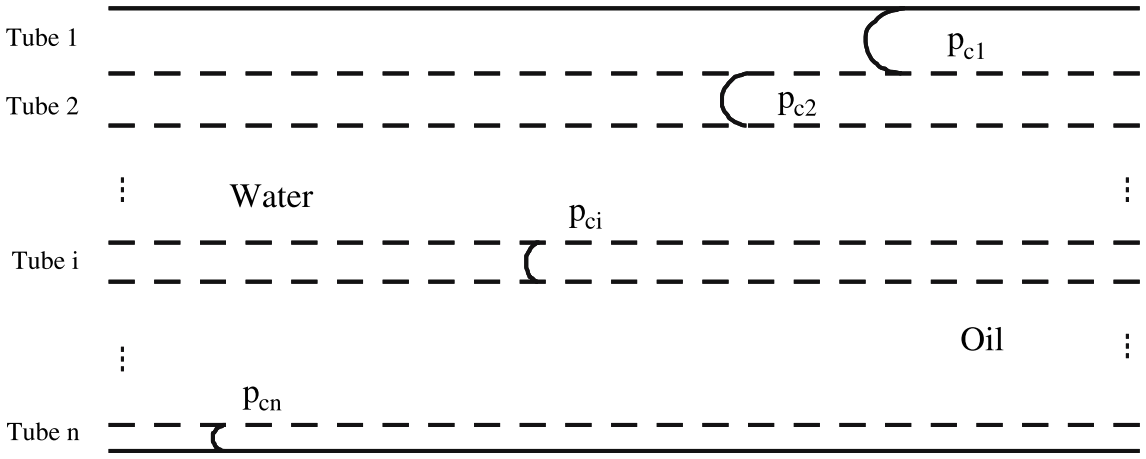



**Fig. 1.** Imbibition process in bundle of interacting capillary tubes adopted in Dong et al. (2006).

imbibition process and dynamic pressure behavior in pore space that extracted directly from 2D rock images under mixed-wet condition.

By assuming to have a system at equilibrium, Mayer and Stowe (1965) and Princen (Princen, 1969a, 1969b, 1970) have derived expressions which relate the capillary pressure and liquid-rise to the cross-sectional geometry, surface tension, and contact angle by minimizing the free energy. Their method later was called the MS-P approach. The idea behind their work was a balance between the work needed to displace a fluid (e.g. non-wetting phase) and changes in surface free energy of the arc menisci. Mason and Morrow (1991) has investigated the curvature of menisci in irregular triangles under perfect wetting condition by using the MS-P method. Entry capillary pressure for arbitrary contact angles were later on investigated by Jia et al. (2007). The interface propagation in triangular tubes between two immiscible fluids has been postulated. Circular, triangular and rectangular capillary tubes has been studied elsewhere in which the flow (as well as curvature) is controlled by capillary force (Kovscek et al., 1993; Man and Jing, 1999, 2000, 2001). In a fairly similar approach to Mason and Mayor, Piri and Blunt (2004) has used the Helmholtz free energy balance and MS-P approach to derive semi-analytical expressions for various drainage and imbibition processes. It's worth mentioning that Arns et al. (2005) has argued based on 3D images from high resolution microtomography, the real porous medium is way more complicated to be modelled through bundle of capillary models. Designing bundle of capillary tubes based on pore size distribution starts to capture the nature of heterogeneous porous media. Garcia-Bengochea et al. (1979) represented the porous media with a bundle of capillary tubes with different diameters reflecting the pore size distribution captured from mercury injection. Amiri et al. (2005) modelled statistically the porous medium using the experimentally available pore size distributions. These models which were based on pore size distribution were first idealized and then were used to calculate permeability.

A bundle of capillary tubes may be constructed to capture the nature of a heterogeneous porous medium with respect to certain macroscopic characteristics. Garcia-Bengochea et al. (1979) represented the porous media with a bundle of capillary tubes whose diameters are tuned to match measured mercury injections. Aït-Mokhtar et al., (1999, 2002) and Amir et al. (2005) modelled statistically the porous medium using the experimentally available pore size distributions derived from mercury injection capillary pressure curves. These models which were based on pore size distribution were first idealized and then were used to calculate permeability.

Another interesting application of capillary tube model is to simulate the streaming potential within porous media by coupling the multiphase flow and electrical properties (Jackson, 2008, 2010; Vinogradov and Jackson, 2011; Cheng et al., 2018).

Also recently the concept of fractals have been widely used in order to study the fluid flow in the porous medium. Reportedly many properties of porous media are related to the fractals (Jacquin and Adler, 1985; Adler, 1991). An important property of fractal objects is that they are free of scale of the measurements. Yu and Cheng (2002) described the cumulative size distribution of pores in porous medium by the fractal scaling law:

$$N(L \geq \lambda) = (\frac{\lambda_{max}}{\lambda})^{D_f} \tag{3}$$

where $\lambda$ is the pore size, $\lambda_{max}$ implies maximum pore diameter and $D_f$ is the fractal dimension for pore size distribution. The disordered capillary length ($L_t$) is suggested to be scaled with capillary diameter as:

$$L_t = \lambda^{1-D_t} L_0^{D_T} \tag{4}$$

in which $D_T$ corresponds to tortuousness of the capillaries and $L_0$ is the length of the model (Fig. 2).

With the fractal bundle of capillary tubes' model, numerous physical phenomena can be modeled; Newtonian and non-Newtonian flow (Yu and Liu, 2004; Zhang et al., 2006; Xu et al., 2013; Luo et al., 2014), multiphase flow in unsaturated porous media (Yu et al., 2003; Xu et al., 2013), entry capillary

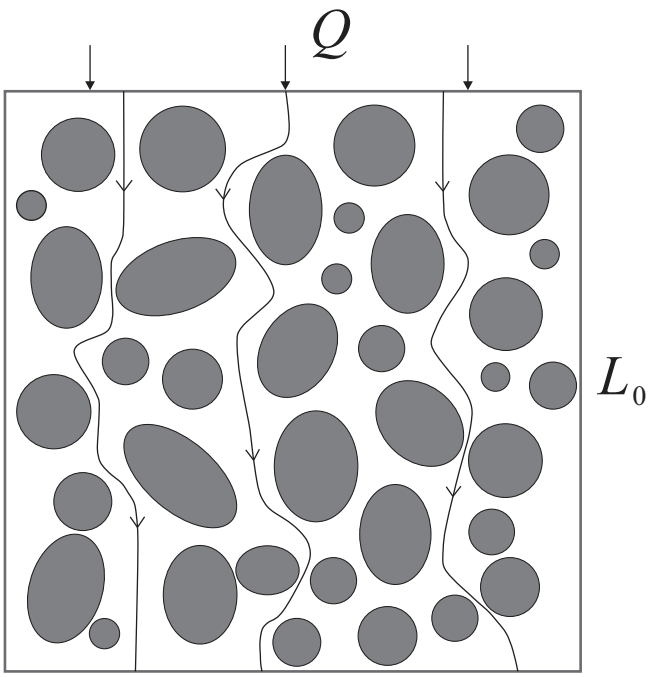



**Fig. 2.** Fractal bundle of capillary tubes (Yu and Cheng, 2002).

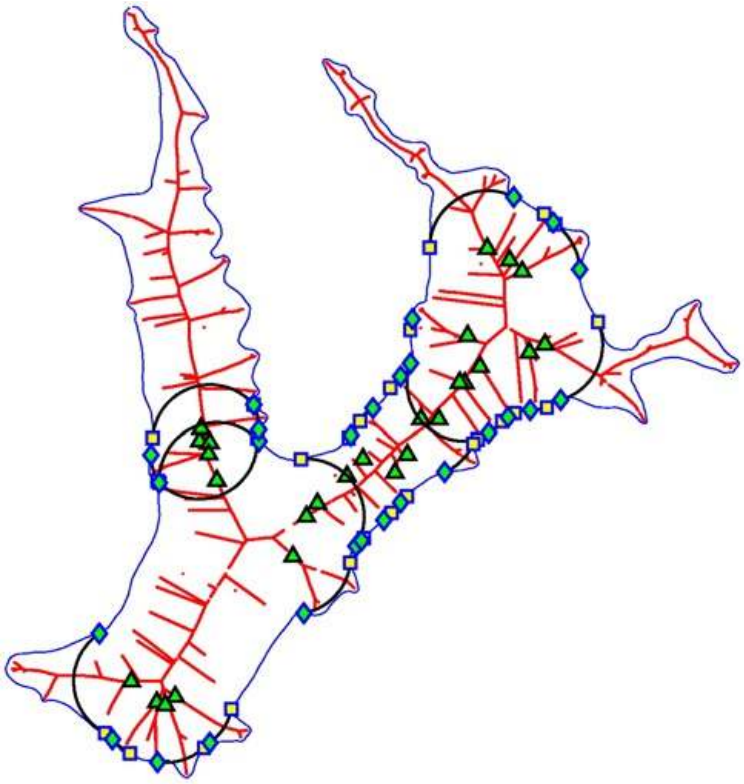


**Fig. 3.** Complete pore space geometry (blue line). Triangles and squares are computational points used for analyzing the entry pressure. Adopted from Frette and Helland (2010).

pressure (Gao et al., 2014) as well as spontaneous imbibition (Cai et al., 2010, 2012, 2014).

### 2.2 Capillary tube model based on rock images

Still the real porous structure can be too complex to be simplified as simply a bundle of capillaries with idealized geometries by techniques above and to produce useful capillary curves due to complex interfacial dynamics. Given a capillary tube whose cross-section takes the shape of a complex pore (see Fig. 3), phase distributions within it at different capillary pressure need to be determined. Several methods have been developed based on the assumption that phases reach instant or quasi-static equilibrium in the pore and therefore the Helmholtz Free Energy of the phases is minimized (Morrow, 1970). For a two phase system of oil, water and solid may be written as:

$$dF = -\sum_{i=o,w} p_i dV_i + \sum_{ij=ow,os,ws} \sigma_{ij} dA_{ij} = 0 \qquad (5)$$

where $p_i$ and $\sigma_{ij}$ are the phase pressure and interfacial tensions respectively, whereas $dV_i$ and $dA_{ij}$ represent the changes in phase volumes and interfacial areas during the displacement. Note that the following Laplace formula holds at each interface of two fluid phases in two-dimensional pore space:

$$r = \frac{\sigma_{ow}}{p_c} \qquad (6)$$

Combining Eq. (5) with Eq. (6) and using Young's equation, $\sigma_{os}$ - $\sigma_{ws}$ = $\sigma_{ow}\cos\theta$, the energy balance is re-written as:

$$r = \frac{dV_o}{dA_{os}\cos\theta + dA_{ow}} \qquad (7)$$

Frette and Helland (2010) established a semi-analytical model based on Eq. (5) to Eq. (7) by assuming the system is at equilibrium. They proposed a scanning algorithm to traverse the entire boundary of any arbitrary 2D cross-section image to determines the two-phase fluid configuration at decreasing entry radii of the invading phase (drainage process) which is directly related to the capillary pressure curve. However, this method is limited to the non-convex 2D cross sections and for drainage process only.

This method was later extended to convex cross-section to compute the capillary pressure of two- and three-phase systems along with imbibition process by Zhou et al. (2012, 2016). They validate this new method against previously developed analytical solutions of known problem, and show their results in consistency with physics and theory of two and three phase capillary pressure curves. They suggest that this method (three-phase capillary pressure correlation) can be used in continuous reservoir simulations and incorporated with pore network modeling to understand the effects of real geometry, pore thought roughness and arbitrary wettability effects on multiphase flow in porous media.

## 3. Directly pore scale modeling

Measuring multiphase flow displacements in space directly in experimental setups is the ideal way to study any physical phenomena; however due to the complexity of pore space in geometry and connectivity, an observed phenomenon might reflect the collective effects of many interacting processes taking place in pores spanning from microscale to macroscale, and this makes it impossible to observe or measure the dynamics of fluid flow taken place in 1-inch core plugs in conventional core flooding experiments (Bedrikovetsky et al., 2013; Yerramilli et al., 2014). Direct observation of multiphase flow has been attempted on smaller samples using advanced imaging techniques. Through 2D micro-models made of glass beads, recent studies have investigated various physical attributes of reactive fluid flow (Kuznar and Elimelech, 2007; Johnson et al., 2010). 3D micro-tomography on the other hand, has provided valuable insight into steady state (Wildenschild and Sheppard, 2013) as well as unsteady state fluid transitions (Armstrong et al., 2014) in porous media at the scale of 5 $\mu$m.

Depending on how the fluids are treated within the mathematical model to be implemented, one can classify pore scale simulation into 1) particle based simulation, 2) grid based simulation, 3) process based simulation, and 4) pore scale network modelling.

### 3.1 Particle based approaches

In the particle based approach, fluids are represented as corresponding sets of particles and their movements are the consequence of interactions with one another in pore space and solid particles. Until now, two types of particle based approaches, LBM and SPH, have been used widely in the application of multiphase flow in porous media.

#### 3.1.1 LBM

LB method is originated from Lattice-Gas Cellular Automata (LGCA) which is similar to molecular dynamics approach, simplified by averaging properties, e.g. velocity or mass, over an ensemble of particles. Since this approach is dealing with the physics of fluid flow at molecular scale, it is considered as a fundamental tool in this research area. Multicomponent, multiphase fluids can be simulated by lattice gas models (Rothman and Zaleski, 1994). They also have been used to simulate dissolution and precipitation (Wells et al., 1991). Capability of undergoing parallel simulations, modelling of complex fluids and porous structures and the simplicity in implementation of corresponding numerical model have all made LGCA an attractive tool for simulation. However, these advantages are offset by stochastic nature of the model which requires averaging over a quite large portion of the sample to obtain an accurate velocity field. This deficiency of LGCA can be overcome by using a mesoscale LBM in which the number of particles associated with any computational node is large enough to suppress the effects of fluctuations through averaging. McNamara and Zanetti (1988) replaced the velocities of individual particles by a velocity distribution

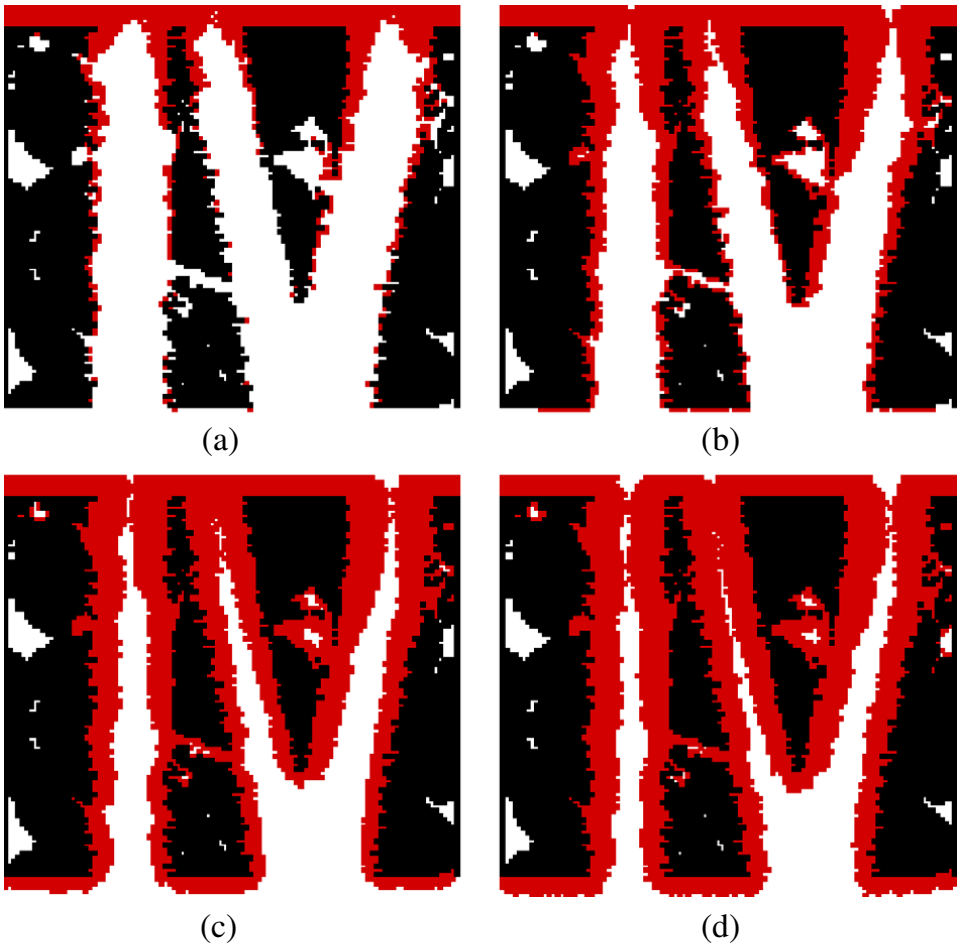



**Fig. 4.** Lattice Boltzmann simulation of progressive precipitation and sealing in micro fracture network (Kang et al., 2005).

function, $f_i(r,t)$, the population of particles moving in the $i$-th direction, with velocity $v_i$ at position $x$ at time $t$. The general form of Lattice Boltzmann equation can be written as:

$$f(r_i + c\delta_t, t + \delta_t) = f(r_i, t) + \Omega[f(r_i, t)] + F(r_i, t) \quad (8)$$

where $\Omega$ is the collision term and $F$ is the external force. A lattice time step includes a streaming process in which the particles (denoted by the distribution function $f$) move from one lattice node to the neighboring node, and a collision step where particles coming from different directions collides with others in a momentum conservative manner. Depending on the configurations of the lattice to be used (e.g. D2Q9 or D3Q27), the macroscopic properties are related the moments of the distribution function:

$$\rho = \sum_{i=1}^{Q} f_i, \;\; u = \frac{1}{\rho} \sum_{i=1}^{Q} f_i c_i \quad (9)$$

In LB simulations the fluid(s) can be driven through a porous structure by using a body force, and/or imposing pressure or velocity boundary conditions at fluid inlets and outlets. At the solid boundary of the pore space, no-slip and no-flow BCs can typically be utilized by "bounce back" implementation. LB models have also been developed to simulate reactive transport of mineral dissolution and precipitation (Kang et al., 2004) (see Fig. 4). Recently a Shan-Chen (Shan and Chen, 1993) type LB model is adopted by Liu and Wu (2016) to include surface tension and wettability effects for modelling of two phase flow in 2D scanned images of a rock sample as well as reconstructed porous which is then compared with a finite-volume VoF method. It is reported that LBM has produced more accurate results in complex porous media. Amount work shows that LBM has been used successfully for pore scale modeling of multiphase flow within flow domain composed by pore and solids. For a detailed review on multiphase LB models and their applicability to the problems in porous media, the reader is referred to review article of Liu et al. (2016).

Standard LB models can be applied successfully to simulate a drainage process where pore surfaces are wet to the wetting phase and to determine correct relative permeability as long as a binary image can resolve pores that together capture main pore connectivity. However, they fail in all other cases when sub-resolution pores exist and are not wetted to the wetting alone. This requires LB models to take sub-resolution pores into account. Recently, gray Lattice Boltzmann models (GLBM) have been proposed to address this need by intro-

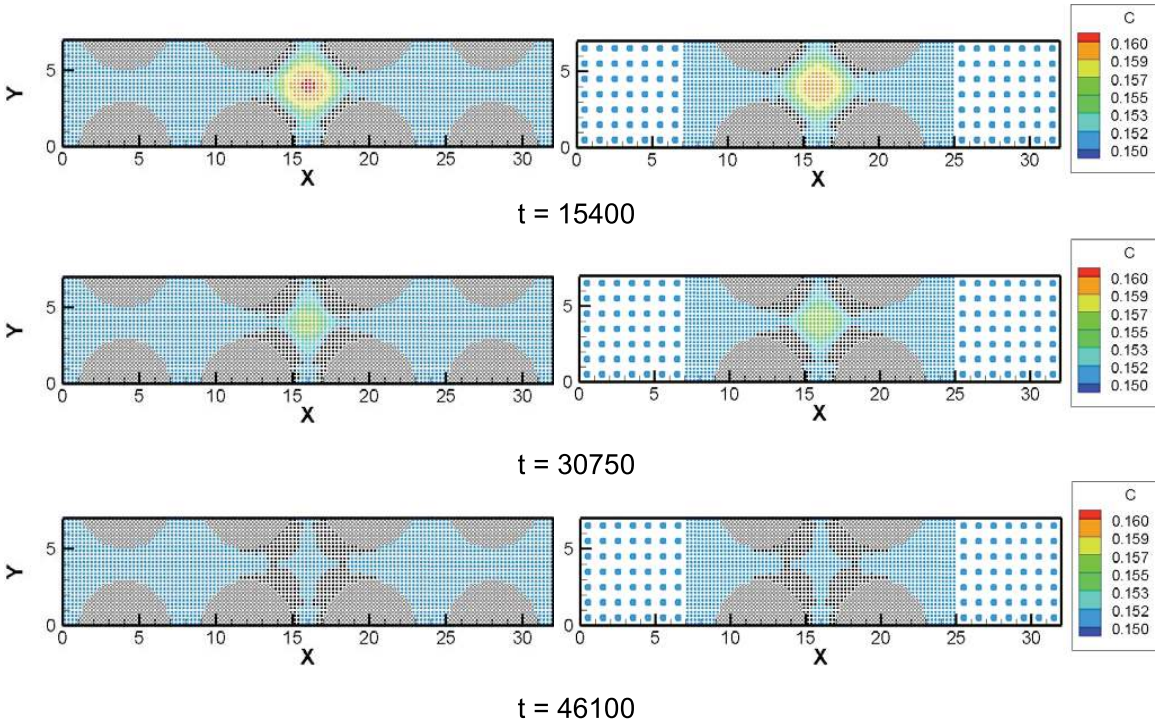



**Fig. 5.** Two dimensional SPH simulations of precipitation resulting from mixing of two reactive solutions in a porous medium. Solute A (red particles) and solute B (blue particles) are injected and the precipitant (green particles) are produced on the mineral surface (Tartakovsky et al., 2008).

ducing gray nodes to represent unsolved pores, in addition to fluid and solid nodes, and to model their resistance to the flow by allowing a fraction of fluids to be reflected back-partial bounding back (Zhu and Ma, 2013, 2018; Ma et al., 2014). Other models are introduced to model flow resistance. Guo and Zhao (2002) introduces a LBM in which the flow resistance is modelled by an additional Darcy body force term. This model solves a generalized NS flow. Kang et al. (2002) introduce a model that replaces the velocity in the equilibrium function with a superficial velocity that is related to the pre-/post-collision velocity through a resistance mapping that considers aggregate permeability and porosity. Recently, the partial bouncing-back idea has been further extended to model multiphase flow (Mcdonald and Turner, 2015).

### *3.1.2 SPH*

Mesh-free approaches, e.g. smooth particle hydrodynamics, are widely used recently in solid and fluid mechanics. These methods are providing with the features to easily simulate problems associated with free surface boundaries. Any continues field, $A(r)$, can be restored from superimposing different smooth Gaussian functions (bell-shaped curves), $W(|r - r_i|)$, centered on a set of positions, $r_i$, and hence the gradient of the field is reconstructed by the superposition of the same Gaussian functions (Monaghan, 1992). Each computational point is associated with a set of extensive properties, e.g. mass, which further on is used to determine the density field:

$$\rho(r) = \sum_i \rho^i(r) = \sum_i m_i W(r - r_i, h) \tag{10}$$

where the summation is taking into account the contribution of each particle at position $i$ to the general density profile.

Within SPH formulation, inter-particle forces are defined to mitigate implementation of physical phenomena like surface tension and capillary forces. This though, comes with increasing in the computational time required for a complete and yet a simple simulation (Liu and Liu, 2010). In a recent study, a pairwise force SPH is implemented to study the effect of surface roughness on contact angle (Shigorina et al., 2017). The contact angle is determined explicitly through defining particle-particle and particle-solid interaction forces. However, Tartakovsky et al. (2008) has argued that since continuum-scale simulations would provide misleading results in reactive transport processes and the fact that pore-scale simulations cannot be applied to simulate large-scale process, they proposed a multiscale multiresolution model that uses small SPH particles to simulate the precipitation zone and large SPH particles to simulate solute dispersion (an example is given in Fig. 5).

Molecular Dynamics incorporates the Newton's law of motion:

$$\frac{dv_i}{dt} = \frac{f_i}{m_i} \tag{11}$$

in which $v_i$ is the particle velocity, $f_i$ the force acting on the particle with mass $m_i$.

In case of typical MD modelling with realistic particle-particle interactions, the time step must be on the order of femtosecond to obtain accurate results which in comparison with any typical process (order of micro or millisecond) is quite small. This is the most important limitation of the molecular

dynamics application to multiphase flow on the pore-scale. Yet to be said, Hybrid molecular dynamics approaches have been developed where continuum models fail to provide accurate predictions for some specific problems. As an example, a coupled LBM with MD approach is proposed by Ning et al. (2016) to compute the transport properties of natural gas in shales. It initially calculates the nano transport properties using MD approach, then upscale them stochastically to microscale digitized voxel-based 3D images and, finally compute the effective permeability using a generalized LB method in which they reported they have produced a reasonable result for a micro-fractured porous medium.

## 3.2 Grid-based computational fluid dynamics

In subsurface flow in which we have simultaneous flow of two or more fluids, the NS equation should be developed in a way that can capture essential features of such conditions, e.g. fluid fragmentation or coalescence. Also, traditionally NS equation has been solved numerically using grid-based methods like finite-difference, finite-volume or finite-element formulation which still these approaches are favorable due to their numerical efficiency and capability of handling a full range of density and viscosity ratios.

Regardless of fluid composition, flow of all simple fluids can be described by the NS equation which makes it an important fundamental for flow of fluids. Meanwhile under certain conditions, e.g. sharp changes in fluid structure due to rapid changes in pressure and/or temperature, NS cannot be applied. Simple fluid flow problems can be tackled analytically but as for more complex problems, we should be looking for numerical solutions. This method is less computationally efficient compared to PNM but with recent increased capability of computing systems, it is becoming more attractive.

Yet to be mentioned, there are two major problems associated with traditional NS equation when it comes down to multiphase fluid flow which limit one to directly apply this method: First is lack of a contact-line/contact angle model that is essential to the multiphase flow concept, and second is the challenge of capturing/tracking the dynamic of fluid-fluid interface.

Tracking the dynamic topology of the interface is categorized as: 1) interface tracking methods (Lagrangian), and 2) interface capturing methods (Eulerian). In first group, the computational mesh used to discretize the interface according to changes in interface topology. Each element of the mesh is recognized by several points. New location of each point (tagged as "interface") are determined during the numerical simulation. Explicitly the new interface in each time step is re-meshed. A good application of this front tracking method in homogeneous bubbly flows, atomization, flows with variable surface tension, solidification, and boiling can be found in Tryggvason et al. (2001). To get a higher accuracy, they used higher order numerical schemes to discretize the NS equation which makes this method computationally expensive. In second category, the mesh is stationary; i.e. the interface undergoing topology changes is analyzed within the static computational mesh. Implementation of this algorithm is simpler and the computations needed are relatively less.

### 3.2.1 Volume of fluids method

The earliest and still most applied approaches to the simulation of multiphase flow is Volume of Fluid (VoF) method (Noh and Woodward, 1976) in which an indicator function (or a marker function, or scalar transport equation are found in context bearing the same meaning) or $n$ - 1 indicator functions for $n$ available phases, are introduced to distinguish between two (or more) immiscible fluids. First implemented VoF suffered from the lack of a model which could describe the interface accurately. But later on, a technique including surface tension was introduced by Brackbill et al. (1992) using integration of a body force over the interface as well as a Piecewise-Linear Interface Calculation (PLIC) scheme that can account for the topological changes of interface.

Raeini et al. (2012) and Raeini et al. (2014) have developed a VoF approach which can be applied to porous medium. They have decomposed the pressure term into capillary and dynamic pressure which later on, the capillary pressure is used to remove the spurious data/current. In order to improve the surface tension force, a new filtered surface force has been introduced and replaced the continuum surface force (CSF). Also relaxation factors have been extensively used to smooth the solution of velocity and pressure coupling. Drainage capillary pressure has been computed using this approach over a star shaped symmetrical three dimensional pore space. Their model is able to predict snap-off mechanisms at certain capillary numbers in drainage process. They have adopted equivalent resistivity approach to derive formulae of analytical entry capillary pressure for imbibition process. They have parameterized the effect of pore geometry on the snap-off and blub-mobilization criteria. The have reported though that their model is only working for uniform cross-sectional area and deviates for non-uniform ones.

Other researchers have tried to represent a sharp contact line and contact angle models which can improve the accuracy of CFD approaches. The contact line propagation is a complex function of contact angle, saturation history, fluid properties and more. However the mass-conservativeness of this approach gives it superiority over other approaches. Just recently, Rabbani et al. (2016) has modeled a two phase flow in straight tubes with square and triangular cross-sections using VoF method (Fig. 6). Their simulation shows a poor prediction of capillary entry pressure comparing to the analytical solution (the error ranges from 10% to roughly 25%).

Another frequently used interface capturing technique is developed by (Osher and Sethian, 1988) which is similar to that of indicator function of VoF. It has increased capability of capturing interface (as a sharp boundary rather than a bandwidth of fluid mixtures in VoF method) but yet it significantly violates mass-conservativeness. Olsson and Kreiss (2005) as well as Olsson et al. (2007) make use of a smeared out Heaviside function which could keep the shape and width of the interface profile constant. Mass conservativeness has been reported to be greatly improved but not completely solved.

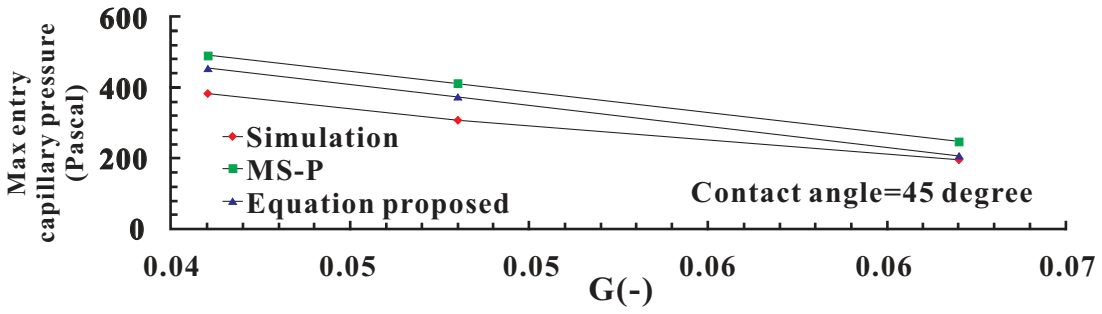



**Fig. 6.** Comparison between theoretical and simulation results for 45 degrees contact angles (Rabbani et al., 2016). G is shape factor of different cross-sections.

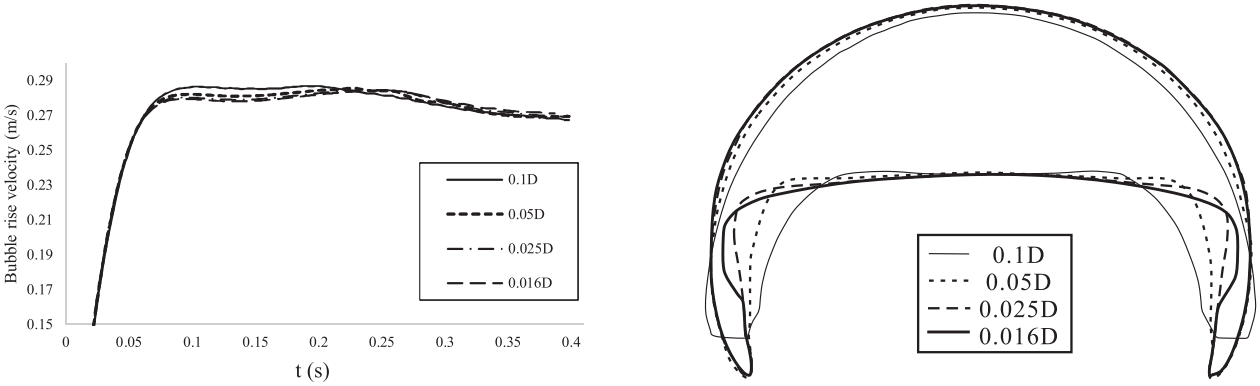



**Fig. 7.** (a) Bubble rise velocities, (b) bubble terminal shape at different grid-size resolution (Ansari et al., 2016).

Other approaches are proposed to take the advantage of the smoothness of level-set function representing the interface while redacting the mass conservation by including another terms.

### *3.2.2 Level set method*

One of the early works in this scope is done by Sussman and Puckett (2000). They proposed a coupled level set and VoF methods for computation of incompressible two phase flows. Within their methodology, they introduced numerical schemes in order to be able to conserve the mass around the interface as well as representing a smoothed gradient of level-set function which was further used to account for surface tension force. In their approach, three advection equations solved simultaneously. They have successfully generated coalescence and phase break-ups for air/water systems. However, this method is highly time consuming when using higher order discretization schemes to get accurate results. Also this method is applied to problems where no flow boundary condition for the level-set function is considered; i.e. wettability effects are excluded.

Sun and Tao (2010) have proposed a coupled method which relies on the solution of the VoF advection equation in which the level-set function is reconstructed geometrically from the solution to VoF equation. They have used this approach to model dam-break problem. They've reported the computational time required to perform this simulation is significantly lower than that of fully coupled level-set method by Sussman and Puckett (2000) but yet argued that a three-dimensional simulation can be much more time consuming. Further on, Ansari et al. (2016) has improved the geometrical reconstruction process of the level-set function and simulated the gas bubble free rise process in a liquid column (Fig. 7). It is concluded there that their approach predicts the interface topology pretty well. Yet no contact angle boundary condition is imposed.

A coupling of level-set and the volume penalization methods for a two phase flow is proposed by Pinilla et al. (2016). Navier-Stokes equation is solved to get the velocity profile which is then fed to the level-set function. They implemented the Cox model (boundary condition) to get the velocity of the interface. The accuracy of their model is tested against a benchmarked capillary-rise problem which shows a great agreement. However, their model deviates from the analytical solution for asymptotic values of contact angle as a function of $\ln(Ca)$. They have argued that this error is due to the numerical approximation of the penalization term. In addition, they haven't shown any particular results of fluid coalescence or break-up.

Jadidi et al. (2014) have proposed a coupled method which can model compressible flows by adding a pressure-dependent density term to the VoF advection equation. They've simulated bubble growth and detachment experiment which shows a good agreement with experimental results (Fig. 8).

Albadawi et al. (2013) used the same methodology as Sussman and Puckett (2000) with the difference of considering

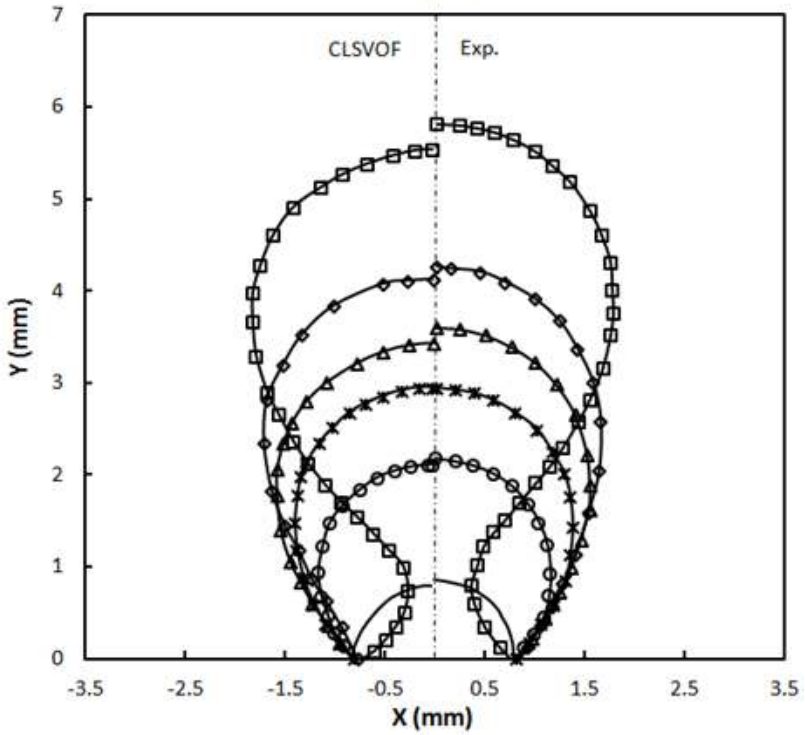



**Fig. 8.** Bubble shape deformation with respect to time comparing simulation with experimental results (Jadidi et al., 2014).

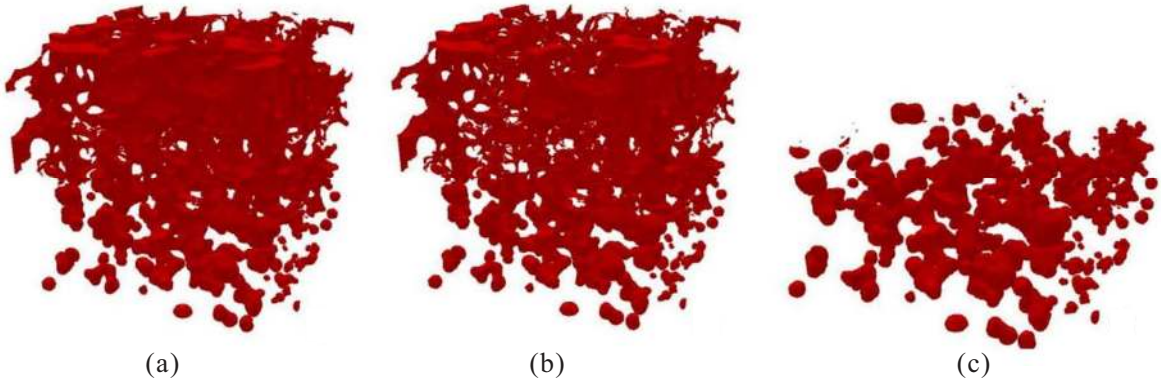



**Fig. 9.** Oil phase distribution after forced water imbibition. (a) So=0.55, (b) So=0.43, (c) So=0.23 (Mohammadmoradi and Kantzas, 2016).

the effect of contact angle for two incompressible fluids. They have considered the different experiments by considering the effect of contact angle of the orifice on the shape of the bubble. However, large three-dimensional gas bubble growth fails to produce correct bubble aspect ratio. In addition, their approach is not subjected to model fluid flow in porous medium.

Studying flow of fluids dynamically is highly challenging especially in porous media. Researchers have tried to bypass the dynamics of flow by introducing terms which are valid under certain conditions. They replace the time-dependent terms in any CFD formulation with force-dependent terms which in turn can be controlled and imposed to the system manually. Mohammadmoradi and Kantzas (2016) proposed a quasi-static level set based approach to investigate the impact of wettability effect on waterflood performance, an example of oil distribution during forced imbibition at different oil saturation is given shown in Fig. 9, and the phase permeability and relative permeability were calculated by volume of fluid method.

Level-set function was basically developed to capture curvature-dependent interfaces (Osher and Sethian, 1988). Prodanović and Bryant (2006) proposed a quasi-static method based on level-set function on fixed, structured Euclidean grids. In their approach, a prescribed curvature model is adopted to evolve the interface. The prescribed velocity model takes the form of:

$$F(\vec{x},t) = \kappa_0 - \kappa(\vec{x},t) \tag{12}$$

where $\kappa_0$ is a given constant, and $\kappa(\vec{x},t)$ is curvature of the level-set function which the interface is being relaxed towards

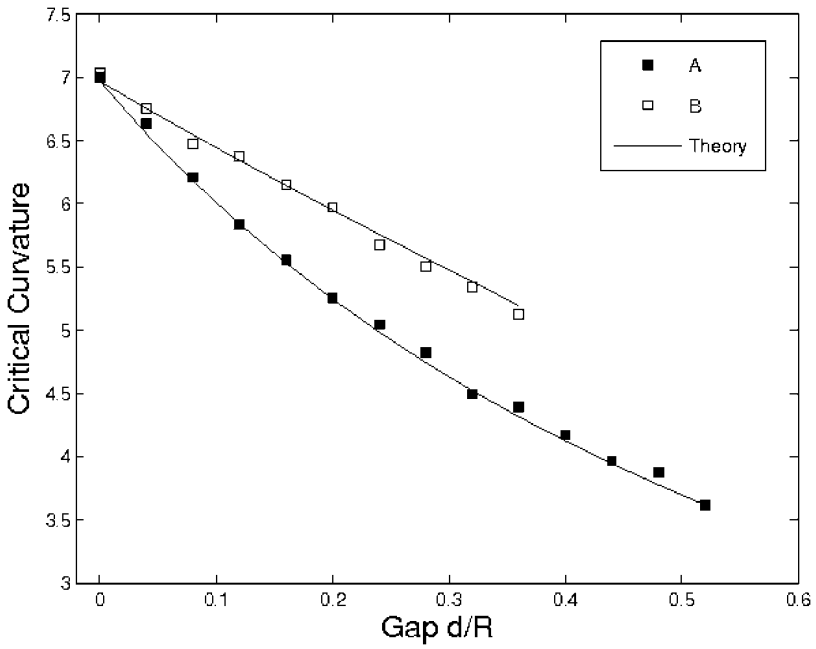



**Fig. 10.** Level-set method progressive quasi-static (LSMPQS) prediction of different geometries versus theoretical results (Prodanović and Bryant, 2006).

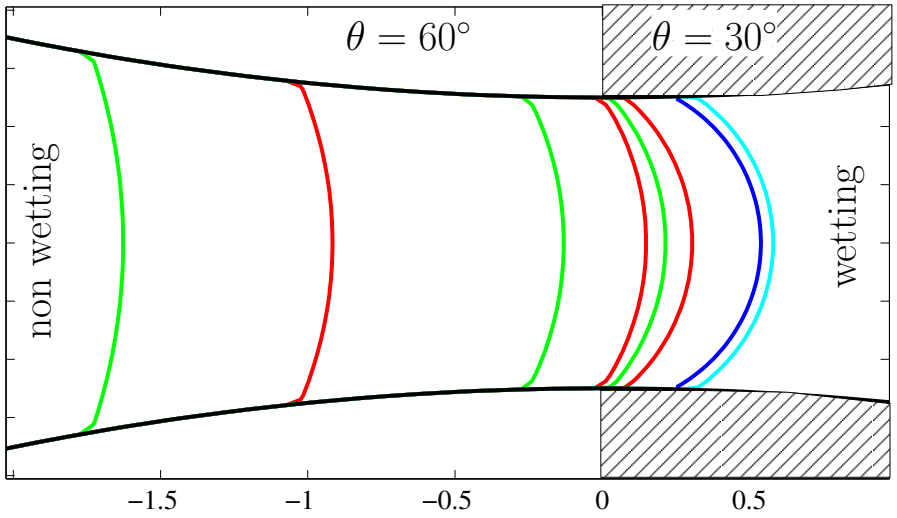
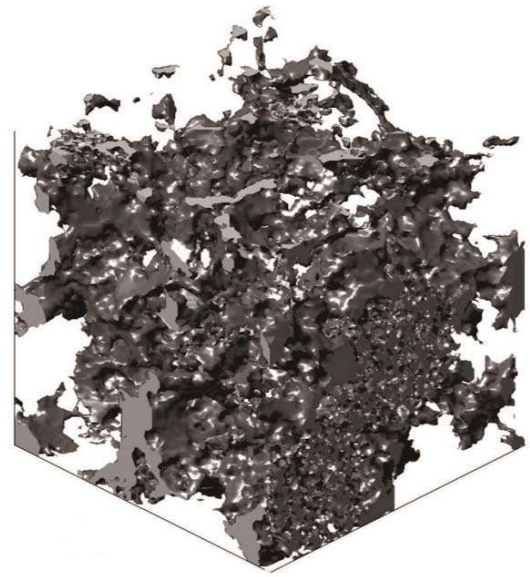



**Fig. 11.** Simulation of varying contact angle with respect to position which changes from 60 degrees to 30 degrees. The solid black line is the solid wall and the interface is shown as different colors (Jettestuen et al. 2013).

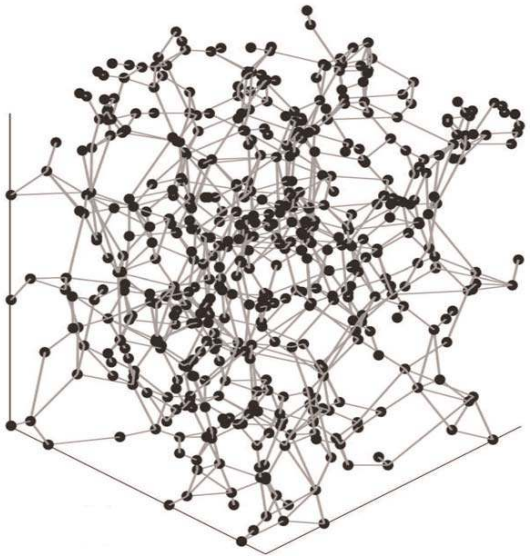
to. As shown in Fig. 10, a series of drainage simulation were conducted and compared to Mayer-Stowe-Princen (MS-P) theory as well as a few experiments which was shown to have a good agreement.

A major drawback to this approach is lack of any boundary condition to the level-set function which could account for a contact angle. This enforcement of the mask that defines the grain space has the side-effect of causing the zero level-set to be tangent to grain surfaces which means the contact angle is zero. Jettestuen et al. (2013) introduced a velocity dependent contact angle boundary condition to the force term (Eq. (12)) inside the solid matrix. For this purpose, they include a second set of level-set function to distinguish between the pore volume and grains. They have conducted several simulations and have shown the capability of their model to predict different mechanisms of phase trapping without enforcing any assumptions onto the model itself (see Fig. 11).

The LSMPQS approach is also developed to investigate the matrix/fracture transfer in drainage and imbibition processes. Prodanović et al. (2013) has modelled the fractured porous medium by changing the grain-size of fractures from the micro-structure. They assigned one set of level-set function to each of grain and pore volumes. Same procedure was applied to model numerical cementation in rough fractures which showed to have poor prediction of relative permeability (Tokan-Lawal et al., 2016).



(a)



(b)

**Fig. 12.** An equivalent network of pore and throats to a real rock sample (Valvatne and Blunt, 2013). (a) is the digitized core sample and (b) is the network model representing the pore volume of the real rock.

### *3.3 Morphology based modelling*

A completely different, yet, discrete approach for modeling capillary dominated flow is the morphology-based method. Maximal inscribed ball (or sphere) (MIS) algorithm is one of the most popular morphology-based methods to model capillary equilibrium fluid configurations at the pore scale (Silin et al., 2003; Silin and Patzek, 2006). The MIS method has the capability to compute capillary pressure curves and fluid configurations in 3D rock images and the results show a reasonable agreement with results obtained from mercury injection experiments (Silin et al., 2003, 2011; Silin and Patzek, 2006). Silin and Patzek (2006) also formulated a new dimensionless capillary pressure function to improve the traditional J-function.

## 4. Pore-scale network modelling

In pore-scale network modelling, the pore volume is simplified into two distinct elements: Pores, which are responsible for holding the bulk volume of the fluids, and throats which are considered as fluid conduits from one pore to the next (Fatt, 1956; Van Dijk et al., 2004; Al-dhahli et al., 2012), an example of the equivalent pore network of a real rock sample is given in Fig. 12. Any pore scale network modelling can be divided into two major steps: Network construction and fluid flow simulation. At early stages, regular networks with elements having only circular cross-sections were considered. Later on,

more sophisticated randomly generated networks based on statistical data obtained from thin sections were used (Jiang et al., 2013). Angular cross-sectional shapes like triangles and stars were added to the pore-network models to account for the highly angular porous medium (Blunt, 2001).

Depending on if the capillary force dominates the viscous force or vice versa, quasi-static model or dynamic model can be applied respectively. Semi-empirical correlations (for entry pressure of invading phase for example) are derived from solving dimensionless NS equation for a known range of aspect ratios, and different cross sections. Fluid-fluid interface and the fluid-solid contact line are tracked using simple procedures which account for displacing and displaced fluids, contact angle and corner angle at each time step. As the fluids flow, a search algorithm is implemented to capture the current state of fluid configuration at each element. Elements are checked for possibility of adding a new set displacements to a new fluid configuration and for validity of previously added displacement mechanisms. Criteria and equations are also developed which can model the normal percolation phenomena (film/layer flow, layer formation/collapse and snap-off for example) as well as invasion percolation phenomena (piston-like displacement).

For two incompressible fluids, the Kirchhoff's rule (Kirchhoff, 1845) can be written (which simply defines a mass balance equation) on any computational grid points as:

$$\sum_i Q_{ij} = 0 \tag{13}$$

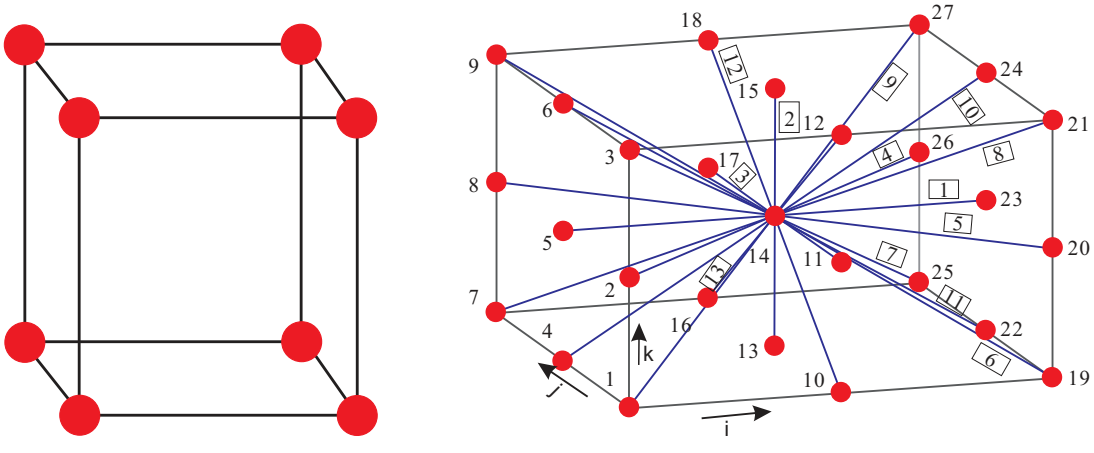
where $Q$ is the fluid flow rate. As Hagen-Poiseuille equation describes, flow rate across a constant cross-section channel can be written as a function of fluid conductivity (also known as permeability), fluid viscosity and pressure gradient. Given Eq. (5) and writing it for each computational node (pore or throat), a system of linear equations is to be solved in order to find the pressure of each phase. Explicit expressions have been devised for fluid conductance for elements with different cross sections (Piri and Blunt, 2005a).

Comprehensive reviews of pore scale network model fundamentals and recent advances can be found in the literature (Blunt, 2017). Blunt (2001) and Blunt et al. (2002) have discussed different pore network models and their applications in details. One great advantage of PNMs are their computational efficiency which makes them ideal to work on pore-scale phenomena in large samples. However, this simplification of geometry and hence the superiority in computational cost comes at the price of losing physical details of fluid flow. In case of unconventional reservoirs like carbonates in which a system of fractures coexist with the micro pores, it is hard to apply the concept of network modelling to this type of reservoirs (Ovaysi and Piri, 2010). Given the limitations of previously stated approaches to fluid flow in porous media, here we discuss other computational methods developed for the purpose of fluid flow modelling in porous media.

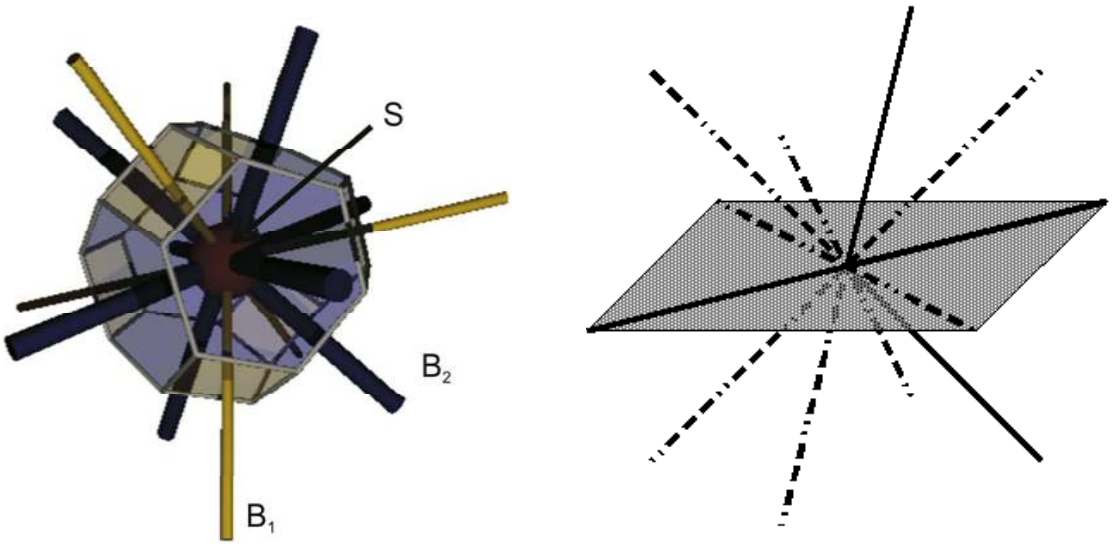
## 4.1 Pore network representation methodologies

Two major algorithms, the maximal ball (Silin et al., 2003) and medial axis based method (Lindquist and Venkatarangan, 1999), have been developed to extract pore networks from arbitrary 3D images. The maximal ball algorithm pioneered by Silin et al. (2003) and Silin and Patzek (2006), is based on generating balls in the center position of each voxel representing void in the image that just fit in the pore space; the largest maximal balls that are surrounded by smaller balls define the pores. Al-Kharusi and Blunt (2007) developed a more comprehensive set of criteria that include sphere clusters to handle equally sized balls. However, this extended algorithm is limited to relatively small systems containing fewer than a thousand pores, and it tends to form pores with lots of connected throats. Instead of growing a ball layer by layer, Dong and Blunt (2009) defined a void ball by developing a two-step searching algorithm to find the nearest solid; they also invented a clustering process to define pores and throats by affiliating the maximal balls into family trees according to their size and rank.

Any pore network simulation can be divided into two separate stages: 1) network construction, and 2) fluid flow simulation. In statistical recreation of pore network model, the objective is to build an equivalent representative model using




(a) (b)




(c) (d)

**Fig. 13.** Regular lattices with preset coordination number; (a) max coordination number of 6 (Ioannidis and Chatzis, 1996), (b) max coordination number of 26 (Raoof and Hassanizadeh, 2010), (c) truncated octahedron (Jivkov et al., 2013), (d) rhombic dodecahedron (Vogel and Roth, 2001).

basic morphological parameters (i.e. pore size distribution and/or average coordination number). Another approach is to directly map the network elements onto available 3D images of a core sample. Fundamentally the two approaches are different in the sense that the later approach tends to represent the real porous structure through some simplifications in which the dynamic part is built on while the first one is statically identical.

Earliest constructed networks were 2D and/or 3D regular (or cubical) lattices with predefined coordination number (Ioannidis and Chatzis, 1993; Reeves and Celia, 1996). It was shown that the real porous medium has higher coordination number (Dong and Blunt, 2009) which led to development of models handling connectivity greater than 6 (Raoof and Hassanizadeh, 2010) (see Fig. 13).

2D images can be used (along with their statistics) to reconstruct 3D images and eventually 3D models. Truncated random Gaussian field (Adler and Thovert, 1998) coupled with the statistical properties derived from the thin sections are usually used to build the 3D images. The combination of correlation functions along with geometrical descriptors have proved to be a valuable tool for generating 3D images from which macroscopic properties are calculated on (Levitz, 1998; Roberts and Torquato, 1999). On another approach, Okabe and Blunt (2004) created a multipoint statistical framework to recreate 3D voxels from 2D thin sections.

On another separate approach pioneered by Bryant et al. in early 1990s, 3D models were recreated through randomly packed spheres of equal size (Bryant and Blunt, 1992; Bryant et al., 1993; Bryant et al., 1993). The idea was to move centers of each sphere allowing overlapping in order to replicate the correct porosity. They have successfully predicted relative permeability and capillary pressure as well as electrical properties of sand packs which was regarded as a breakthrough in pore scale modeling. The major drawback of this work was its limited applicability; it only worked for pore structure made from spherical grains. Further improvement was made by Øren et al. (Bakke and Øren, 1997) where they took into account grain size distribution extracted from 2D images. In an extended research, Øren and Bakke (2002) have reconstructed a geological representative model which has replicated a good connectivity of the pore structure. Despite the success of such approaches in predicting morphological and single phase properties, applying them to more heterogeneous system like carbonates, seems to be a challenging task.

Piri and Blunt (2005a) have started rolling the rock down the road of working directly on the real porous medium by mapping a network on the real sample which results in irregular lattice. In this case, pores (a.k.a. nodes) and throats (a.k.a. bonds) are distinguished by finding the local minima along the medial axis which was introduced by Lindquist et al. (1996). On a different approach, Silin and Patzek (2006) incorporated the maximal ball method to find the biggest inscribed sphere within the voxelized images. Later on, Dong and Blunt (2009) extended the work done by Al-Kharusi and Blunt (2007) by introducing a clustering process to define trees of connected pores and throats. The problem with network constructed from medial axis method is that explicit definition of pores is difficult while the maximal ball algorithm within highly complicated geometries, it is hard to come up with a criterion to differentiate between the network elements (i.e. pores and throats). The next step in fluid flow simulation is to fit the related mathematical model into the network model generated above.

The knowledge of displacement mechanisms at pore scale as well as the mathematical expressions derived for modelling purpose in the context of pore scale network modelling have been expanded hugely in recent years. There are generally two separate sets of fluid flow model in network modelling: 1) quasi-static, and 2) dynamic.

### 4.2 Quasi-static pore network modelling

If the capillary number is smaller than $10^{-5}$, based on the fluid displacement mechanisms a quasi-static pore network modeling could be applied to simulate the equilibrium positions of fluid-fluid interfaces, and thus determine the capillary pressure and relative permeability curves in the pore space.

Majority of pore scale network models that were previously developed are within the context of quasi static which deals only with the capillary dominant flow. In quasi static modelling, "time" is not explicitly introduced but rather the fluids are displaced through a finite number of capillary pressure steps. Generally the quasi static modelling has the assumption of Newtonian, incompressible, immiscible and capillary dominant flow along with neglecting the gravity effect.

Øren et al. (1992) computed oil recovery in spreading and nonspreading systems via a two dimensional network model with spherical pores and rectangular throats. They have successfully reproduced the oil recoveries from the micromodel experiment. They introduced a double drainage process (i.e. displacement of one phase by another phase where it displaced by a third phase) in which gas displaces trapped oil that displaces water, allowing for the coalescence of oil ganglia, resulting in higher oil recovery. They have reported a lower oil recovery for lower spreading coefficient.

Soll and Celia (1993) studied the two phase and three phase movement along with the capillary pressure-saturation relationships in a water wet medium using regular 2D and 3D networks of pores. Each node could hold only one phase in the center of the pore as well as a wetting layer. They compared their results with the micromodel experiment (Soll et al., 1993) as well as the fluid distributions from the 2D and 3D experiments. Although the model was incapable to successfully match three phase data, but it was the first model to accommodate for layer flow in three phase modelling.

Fenwick and Blunt (1998) described details of three phase flow for strongly water wet systems through a regular, cubic, 3D network model composed of equilateral triangular and/or square cross sections. Contact angles between oil/water and gas/water were considered to be zero. The model was capable of any sequential injection of gas/oil/water. Mathematical expressions were derived to accommodate for the stability criterion of layers formed during the injection process. Geometrical parameters such as corner half angle as well as other fluid and solid properties (e.g. interfacial tension and contact angle) were taken into consideration. They used such expressions to estimate the conductance of each phase present in each element which later on was used to calculate relative permeability.

Hui and Blunt (2000) introduced a mixed wet model with triangular throats. Changes in wettability were modeled through changing the contact angle of the solid surface came into contact with oil phase explicitly. Different fluid configuration as well the criteria for the formation of each were discussed. They investigated the effect of initial oil saturation, spreading coefficient and contact angle on relative permeability curve.

Piri and Blunt (2005b) extended Hui's approach which included 30 different possible fluid configurations in three phase 3D flow in a random network model based on Berea Sandstone. They introduced a new clustering algorithm which was based on the displacement mechanisms. They computed relative permeability, saturation path and capillary pressure for any given set of displacement sequence.

Most recently, Raeini et al. (2018) has introduced a quasi-static network model in which the pressure drop caused by the viscous force is considered as "perturbation to the local capillary pressure along the length of the system". They have subdivided the throat into two separate compartments in order to overcome the simplifications made in building the network (Raeini et al., 2017). They calculated entry capillary pressure for all displacements based on the new levels of discretization and compared their results with a finite volume two phase flow solver. They showed a fair number of successful predictions of entry capillary pressure for different sets of contact angle, aspect ratio and geometry.

### 4.3 Dynamic pore network modeling

Dynamic pore-network models are normally applied when the capillary number is larger than $10^{-5}$, as the viscous forces cannot be neglected. In the dynamic pore scale models, at each time step the pressure distribution in the network is calculated first followed by the fluid-fluid interfaces based on pressure difference criteria. The dynamic pore scale models were used to investigate the effects of capillary number and viscosity ratios on the relative permeability, residual oil saturation and pore scale displacement mechanisms (Blunt and King, 1991; Dahle and Celia, 1999). The balance between piston-like and snap-off displacement, and its effect on residual oil could be examined if the flow through thin wetting films is also included in the dynamic pore-network models (Blunt and Scher, 1995; Hughes and Blunt, 2000; Joekar-Niasar et al., 2010).

In quasi static approach, the viscous and gravity terms are taken into account through some approximations if they are to be considered. Viscous and gravity effects might become significant during different situations; for example polymer or surfactant flooding, or high velocity areas around wellbore (Sahimi, 2011). In dynamic network models, on the other hand, the viscous and gravity terms are included to simulate fluid flow where these forces are of relevance. A comprehensive review of dynamic models can be found in Joekar-Niasar and Hassanizadeh (2012).

The first dynamic pore network model is developed by Koplik and Lasseter (1985) where they studied the effect of pore structure on macroscopic phenomena. They picked up on the problems associated with computational time and difficulties dealing with large models. Their model was only based on a number of 100 pores. Lee et al. (1996) developed a parallel model capable of performing water flooding and miscible flooding simulations in quite big networks (~530000 pores). The model developed by Aker et al. (1998) was set to study the fluid propagations as well as pressure distribution in a drainage process which later on was modified by Knudsen and Hansen (2002) by adding biperiodic boundary conditions. Lovoll et al. (2005) tested their dynamic model which was a

high velocity drainage process along with stabilized gravity, with glass bead experiments.

Al-Gharbi and Blunt (2005) developed expressions for layer swelling and snap off displacements in the context of dynamic model to study the effect of viscous force in 2D lattices. Nguyen et al. (2006) included the pressure drop caused by the wetting films to study their effect on the favorable displacement mechanisms (snap off or piston like) in imbibition process. Piri and Karpyn (2007) mapped a network model on a fractured sample and simulated two phase flow in a single fracture using a quasi-dynamic model. Their model was consist of approximately 21000 pores.

In an interesting work, Sheng and Thompson (2013) developed a dynamic pore network model based on the work done by Thompson (2002) and was linked with continuum scale reservoir simulator. The network model was used to predict the continuum scale input parameters such as capillary pressure and relative permeabilities which in turn the simulator provided the boundary conditions for the network model at the given time step to complete the coupling process.

Aghaei and Piri (2015) introduced an entirely new dynamic pore network model which incorporated capillary, viscous and gravity forces. They included the film flow in the corners as well as the mathematical expression for dependencies of local interface in the corners on capillary pressure. They have validated their results with a CT scan core flooding apparatus capable of measuring in situ contact angle dynamically for the first time. Local saturations, relative permeabilities and fractional flow curves were subjected to be compared.

## 5. Challenges

As addressed in the previous sections, amount of various pore scale method have been applied to simulate multiphase phase in porous media. It is indeed that significant achievements have been archived in pore-scale modeling, while many open questions still remain challenging. For example, wettability and pore space characterization, model validation and multiscale problems.

### 5.1 Contact angle characterization

A pre-defined contact angle distribution and pore space are the two essential information required to be used as input for any types of pore scale modeling approaches to mimic multiphase flow at pore scale.

Contact angle is an intermolecular force dependent mesoscale property of a fluid-fluid-solid combination. It is strongly affected by the chemical and physical complexity of the fluids-rock components as well as by pressure and temperature (Derksen, 2015; Iglauer et al., 2017; Yong et al., 2017; Zhou et al., 2017). Contact angle is normally measured on a flat surface at ambient condition through sessile drop and/or captive bubble approaches (Iglauer et al., 2013, 2017; Sun et al., 2018). For pore network modeling, a random in-situ wettability information is normally assigned to pore throat to match the measured capillary pressure drainage curves (Blunt, 2017). Besides that, with the application of advanced imaging techniques, Andrew et al. (2014) initialized the measurements of in situ contact angle using X-ray micro-tomography; the method is based on manual estimation, and thus it might be prone to bias/subjectivity and is time-consuming. Later, Klise et al. (2016) and Scanziani et al. (2017) proposed an automatic method to estimate the effective contact angle at in situ condition.

Besides measurements, few modeling approaches have been applied to simulate contact angle at various temperature-pressure conditions. Such as molecular dynamic simulation (Iglauer et al., 2012; Derksen, 2015; Yong et al., 2017) and extended usage of Frumkin-Derjaguin equation with the application of disjoining pressure (Hirasaki, 1991; Zhou et al., 2017) have been used to estimate contact angle. These two methodologies in general over-simplify the solid surface as flat substrate with uniform component. Besides that, current measurements of gas-water contact angle in silicon capillary tube also demonstrates that contact angle also depends on the size of capillary tube (Li et al., 2013).

So, one open question for pore scale modeling is developing a proper contact angle characterization method that could account for pore size, pore roughness, fluid-rock mineralogy at in-situ condition.

### 5.2 Validation

The pore scale modeling methods deal with the same problems, and most of them are validated either by analytical solution, another numerical approach or experiment measurements.

The first type of validation is performed within single pore channel by analytical solution. For example, the 2D semi-analytical model proposed by Zhou et al. (2013a, 2014, 2016) was validated against analytical solution (Van Dijk et al., 2004) in term of fluid configuration and capillary pressure in star shaped geometry. With the application of volume of fluid method, Rabbani et al. (2016) compared the entry pressure of a non-wetting phase invades a wetting phase filled capillary straight tube with square or triangular cross-section, and they reported almost 10% error between the simulated entry pressure compared with the analytical solution. They is first due to the 2D nature, the longitudinal curvature of the interface has been assumed equals to zero, of analytical solution; and secondly the dynamic effects in volume of fluid couldn't be neglected, even at very small capillary number.

Recently, Verma et al. (2018) performed capillarity dominated quasi-static displacements by level set method and volume of fluid method in a set of converging-diverging pore throat geometries. They founded that both methods perform well for lower contact angles, and a better accuracy for the level set method for contact angles more than 70° is founded, both methods struggle with 90° contact angle. For viscosity and/or gravity force present, the Navier-Stokes based solvers such as volume of fluid are more appropriate.

Besides the entry pressure and fluid configuration comparison in single capillary tube, most of the current existing pore scale modeling approaches have been validated in term of lab measured flow function, such as capillary pressure and

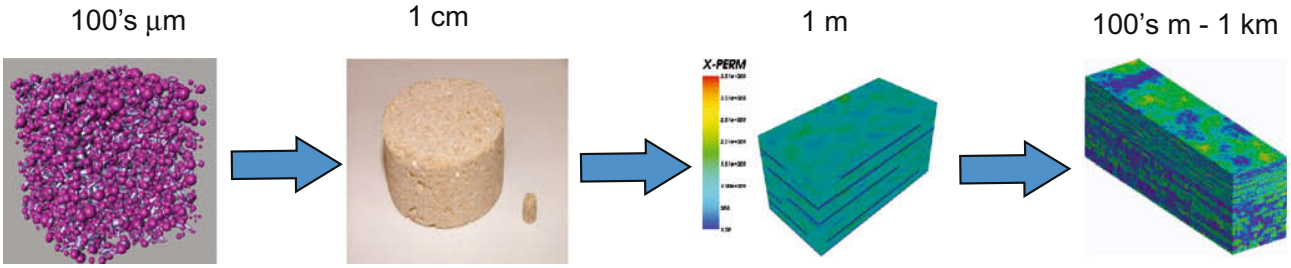



**Fig. 14.** A schematic of a potential upscaling method for flow and transport in porous media, integrating simulation approaches and data at different scales (Rhodes, 2008).

relative permeability curves. Such as pore network modeling (Øren et al., 1998; Blunt, 2001; Valvatne and Blunt, 2003; Piri and Blunt, 2005a), particle based approaches (Ahrenholz et al., 2006; Boek and Venturoli, 2010; Ramstad et al., 2010; Bandara et al., 2011) and grid based approaches (Raeini et al., 2012, 2014).

One essential capability of pore scale modeling is to understand detailed pore scale displacement mechanisms and their contribution to relative larger scale flow performance. While very limited research has been done to compare simulated pore scale fluid configuration with lab measurements. Until recently, Yang et al. (2017) performed a pore to pore validation of a dynamic pore network modeling against micromodel experiment, and they found that the pore-scale matching level is at around 75% for all tested cases between pore network modeling and micromodel measurement. The matching level of core-scale parameters such as initial/connate water saturation and oil-phase permeability varies from case with a relative error from 15 to 60%.

It is true that compressive validation work have been performed for pore scale modeling methods. For simple pore events, numerical methods have showing reasonable agreement with analytical or experimental work in term of fluid configuration. For plug or core scale, pore scale modeling approaches have been validated in term of flow function. While, one critical challenges is validating pore scale fluid configuration and displacement mechanisms, such as pore filling, Haines jump, droplet deformation and droplet re-mobilization directly within complex geometries for and beyond capillary dominated flow.

### *5.3 Multiscale problems*

Fluid flow in subsurface porous media occurs from micro even sub-micro (for example nano-meter) to kilometer scale, and thus it is almost impossible to span the scales using a single tool (Blunt et al., 2013). A common practice is to find averaged properties at different scales with integrated suite of tools, and then properly incorporated into simulations at larger scales. Rhodes et al. (2008) proposed a possible approach, as illustrated schematically in Fig. 14, to simulate multiphase flow across scale for single-phase transport of a non-sorbing and non-reacting tracer. For multiphase flow, the outcomes of pore scale modeling, such as capillary pressure and relative permeability curves, are used as input for continuous scale modeling to understand the pore scale wettability and pore geometries on larger scale flow performance (Jackson et al., 2003; Al-Dhahli et al., 2013). While, one critical issue is whether these effective flow functions are still adequate. How feasible to validate the current existing upscaling approaches against experimental observations at larger scales?

Another scale issue relates to pore scale modeling is how sub-pore scale parameters, such as fluid-rock components, pore and/or throat with sub voxel size, would affect the accuracy of pore scale models.

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## References

Adler, P.M. Fractal Porous Media. Transport Processes in Porous Media 1991: 723-743.

Adler, P.M., Thovert, J.F. Real porous media: Local geometry and macroscopic properties. Appl. Mech. Rev. 1998, 51(9): 537-585.

Aghaei, A., Piri, M. Direct pore-to-core up-scaling of displacement processes: Dynamic pore network modeling and experimentation. J. Hydrol. 2015, 522: 488-509.

Ahrenholz, B., Tölke, J., Krafczyk, M. Lattice-Boltzmann simulations in reconstructed parametrized porous media. Int. J. Comput. Fluid D. 2006, 20(6): 369-377.

Ahrenholz, B., Tölke, J., Lehmann, P., et al. Prediction of capillary hysteresis in a porous material using Lattice-Boltzmann methods and comparison to experimental data and a morphological pore network model. Adv. Water Resour. 2008, 31(9): 1151-1173.

Aker, E., MÅlØy, K.J., Hansen, A., et al. A two-dimensional network simulator for two-phase flow in porous media. Transport Porous Med. 1998, 32(2): 163-186.

Albadawi, A., Donoghue, D.B., Robinson, A.J., et al. Influence of surface tension implementation in volume of fluid and

coupled volume of fluid with level set methods for bubble growth and detachment. Int. J. Multiphase Flow 2013, 53: 11-28.

Al-Dhahli, A., Geiger, S., Dijke, M.I. Accurate modelling of pore-scale film and layer flow for three-phase EOR in carbonate rocks with arbitrary wettability. Paper SPE-154019-MS Preseted at the Improved Oil Recovery Symposium, Tulsa, Oklahoma, USA, 14-18 April, 2012.

Al-Gharbi, M.S., Blunt, M.J. Dynamic network modeling of two-phase drainage in porous media. Phys. Rev. E 2005, 71(1): 016308.

Al-Kharusi, A.S., Blunt, M.J. Network extraction from sandstone and carbonate pore space images. J. Petrol. Sci. Eng. 2007, 56(4): 219-231.

Amiri, O., Aït-Mokhtar, A., Sarhani, M. Tri-dimensional modelling of cementitious materials permeability from polymodal pore size distribution obtained by mercury intrusion porosimetry tests. Adv. Cem. Res. 2005, 17(1): 39-45.

Andrew, M., Bijeljic, B., Blunt, M.J. Pore-scale contact angle measurements at reservoir conditions using X-ray microtomography. Adv. Water Resour. 2014, 68: 24-31.

Ansari, M.R., Azadi, R., Salimi, E. Capturing of interface topological changes in two-phase gasliquid flows using a coupled volume-of-fluid and level-set method (VOSET). Comput. Fluids 2016, 125: 82-100.

Armstrong, R.T., Georgiadis, A., Ott, H., et al. Critical capillary number: Desaturation studied with fast X-ray computed microtomography. Geophys. Res. Lett. 2014, 41(1): 55-60.

Arns, C.H., Bauget, F., Limaye, A., et al. Pore scale characterization of carbonates using X-ray microtomography. SPE J. 2005, 10(4): 475-484.

Aït-Mokhtar, A., Amiri, O., Dumargue, P., et al. A new model to calculate water permeability of cement-based materials from MIP results. Adv. Cem. Res. 2002, 14(2): 43-49.

Aït-Mokhtar, A., Amiri, O., Sammartinoj, S. Analytic modelling and experimental study of the porosity and permeability of a porous. Mag. Concrete Res. 1999, 51(6): 391-396.

Bakke, S., Øren, P.E. 3-D pore-scale modelling of sandstones and flow simulations in the pore networks. SPE J. 1997, 2(2): 136-149.

Bandara, U.C., Tartakovsky, A.M., Palmer, B.J. Pore-scale study of capillary trapping mechanism during $CO_2$ injection in geological formations. Int. J. Greenh. Gas Con. 2011, 5(6): 1566-1577.

Bartley, J.T., Ruth, D.W. Relative permeability analysis of tube bundle models. Transport Porous Med. 1999, 36(2): 161-188.

Bartley, J.T., Ruth, D.W. Relative permeability analysis of tube bundle models, including capillary pressure. Transport Porous Med. 2001, 45(3): 445-478.

Bedrikovetsky, P., Vaz, A.S.L., Furtado, C.J.A., et al. Formation-damage evaluation from nonlinear skin growth during coreflooding. SPE Reser. Eval. Eng. 2011, 14(2): 193-203.

Blunt, M.J. Flow in porous mediapore-network models and multiphase flow. Curr. Opin. Colloid In. 2001, 6(3): 197-207.

Blunt, M.J. Multiphase flow in permeable media: A pore-scale perspective. Oxford, UK, Cambridge University Press, 2017.

Blunt, M.J., Bijeljic, B., Dong, H., et al. Pore-scale imaging and modelling. Adv. Water Resour. 2013, 51: 197-216.

Blunt, M.J., Jackson, M.D., Piri, M., et al. Detailed physics, predictive capabilities and macroscopic consequences for pore-network models of multiphase flow. Adv. Water Resour. 2002, 25(8-12): 1069-1089.

Blunt, M.J., King, P. Relative permeabilities from two- and three-dimensional pore-scale network modelling. Transport Porous Med. 1991, 6(4): 407-433.

Blunt, M.J., Scher, H. Pore-level modeling of wetting. Phys. Rev. E 1995, 52(6): 6387.

Boek, E.S., Venturoli, M. Lattice-Boltzmann studies of fluid flow in porous media with realistic rock geometries. Comput. Math. Appl. 2010, 59(7): 2305-2314.

Brackbill, J.U., Kothe, D.B., Zemach, C. A continuum method for modeling surface tension. J. Comput. Phys. 1992, 100(2): 335-354.

Bryant, S.L., Blunt, M. Prediction of relative permeability in simple porous media. Phys. Rev. A 1992, 46(4): 2004.

Bryant, S.L., King, P.R., Mellor, D.W. Network model evaluation of permeability and spatial correlation in a real random sphere packing. Transport Porous Med. 1993, 11(1): 53-70.

Bryant, S.L., Mellor, D.W., Cade, C.A. Physically representative network models of transport in porous media. AIChE J. 1993, 39(3): 387-396.

Cai, J., Hu, X., Standnes, D.C., et al. An analytical model for spontaneous imbibition in fractal porous media including gravity. Colloids Surfaces A 2012, 414: 228-233.

Cai, J., Perfect, E., Cheng, C.L., et al. Generalized modeling of spontaneous imbibition based on Hagen-Poiseuille flow in tortuous capillaries with variably shaped apertures. Langmuir 2014, 30(18): 5142-5151.

Cai, J., Yu, B., Zou, M., et al. Fractal analysis of invasion depth of extraneous fluids in porous media. Chem. Eng. Sci. 2010, 65(18): 5178-5186.

Chao, J., Mei, R., Singh, R., et al. A filterbased, massconserving lattice Boltzmann method for immiscible multiphase flows. Int. J. Numer. Meth. Fl. 2011, 66(5): 622-647.

Cheng, S., Fu, M., Kulacki, F.A. Characterization of a porous transducer using a capillary bundle model: Permeability and streaming potential prediction. Int. J. Heat Mass Tran. 2018, 118: 349-354.

Dahle, H.K., Celia, M.A. A dynamic network model for twophase immiscible flow. Computat. Geosci. 1999, 3(1): 1-22.

Derksen, J.J. Droplets sliding over shearing surfaces studied by molecular dynamics. AIChE J. 2015, 61(11): 4020-4027.

Dong, H., Blunt, M.J. Pore-network extraction from micro-computerized-tomography images. Phys. Rev. E 2009, 80(3): 036307.

Dong, M., Dullien, F.A.L., Dai, L. et al. Immiscible displacement in the interacting capillary bundle model part I. Development of interacting capillary bundle model. Transport Porous Med. 2005, 59(1), 1-18.

Dong, M., Dullien, F.A.L., Dai, L., et al. Immiscible displacement in the interacting capillary bundle model part ii. applications of model and comparison of interacting and non-interacting capillary bundle models. Transport Porous Med. 2006, 63(2): 289-304.

Dong, M., Zhou, J.. Characterization of waterflood saturation profile histories by the completecapillary number. Transport Porous Med. 1998, 31(2): 213-237.

Fatt, I. The network model of porous media. Society of Petroleum Engineers 1956, 207: 144-181

Frette, O.I., Helland, J.O. A semi-analytical model for computation of capillary entry pressures and fluid configurations in uniformly-wet pore spaces from 2D rock images. Adv. Water Resour. 2010, 33(8): 846-866.

Gao, H., Yu, B., Duan, Y., et al. Fractal analysis of dimensionless capillary pressure function. Int. J. Heat Mass Tran. 2014, 69: 26-33.

Garcia-Bengochea, I., Altschaeffl, A.G., Lovell, C.W. Pore distribution and permeability of silty clays. Journal of the Geotechnical Engineering Division 1979, 105(7): 839-856.

Glantz, R., Hilpert, M. Capillary displacement in totally wetting and infinitely long right prisms. Multiscale Model. Sim. 2011, 9(4): 1765-1800.

Guo, Z., Zhao, T.S. Lattice Boltzmann model for incompressible flows through porous media. Phys. Rev. E 2002, 66(3): 036304.

Helland, J.O., Skjaeveland, S.M. Physically based capillary pressure correlation for mixed-wet reservoirs from a bundle-of-tubes model. SPE J. 2006, 11(2): 171-180.

Hirasaki, G.J. Thermodynamics of thin films and three-phase contact regions. Interfacial Phenomena in Petroleum Recovery 1991, 1991: 23-75.

Hughes, R.G., Blunt, M.J. Pore scale modeling of rate effects in imbibition. Transport Porous Med. 2000, 40(3): 295-322.

Hui, M.H., Blunt, M.J. Effects of wettability on three-phase flow in porous media. J. Phys. Chem. B 2000, 104(16): 3833-3845.

Hu, X.Y., Adams, N.A. A multi-phase SPH method for macroscopic and mesoscopic flows. J. Computat. Phys. 2006, 213(2): 844-861.

Iglauer, S. $CO_2$-water-rock wettability: Variability, influencing factors, and implications for $CO_2$ geostorage. Acc. Chem. Res. 2017, 50(5): 1134-1142.

Iglauer, S., Mathew, M.S., Bresme, F. Molecular dynamics computations of brine-$CO_2$ interfacial tensions and brine-$CO_2$-quartz contact angles and their effects on structural and residual trapping mechanisms in carbon geo-sequestration. Journal of Colloid and Interface Science 2012, 386(1): 405-414.

Iglauer, S., Salamah, A., Sarmadivaleh, M., et al. Contamination of silica surfaces: Impact on water-$CO_2$-quartz and glass contact angle measurements. Int. J. Greenh. Gas Con. 2014, 22: 325-328.

Ioannidis, M.A., Kwiecien, M.J., Chatzis, I. Statistical analysis of the porous microstructure as a method for estimating reservoir permeability. J. Petrol. Sci. Eng. 1996, 16(4): 251-261.

Jackson, M.D. Characterization of multiphase electrokinetic coupling using a bundle of capillary tubes model. J. Geophys. Res-Sol. Ea. 2008, 113(B4): B04201.

Jackson, M.D. Multiphase electrokinetic coupling: Insights into the impact of fluid and charge distribution at the pore scale from a bundle of capillary tubes model. J. Geophys. Res-Sol. Ea. 2010, 115(B7): B07206.

Jacquin, C.G., Adler, P.M. The fractal dimension of a gas-liquid interface in a porous medium. J. Colloid Interf. Sci. 1985, 107(2): 405-417.

Jadidi, M., Tembely, M., Moghtadernejad, S., et al. A coupled level set and volume of fluid method with application to compressible two-phase flow. Paper Presented at the Proceedings of the 22nd Annual Conference of the CFD Society of Canada, Toronto, ON, Canada, June, 2014.

Jettestuen, E., Helland, J.O., Prodanović, M. A level set method for simulating capillary-controlled displacements at the pore scale with nonzero contact angles. Water Resour. Res. 2013, 49(8): 4645-4661.

Jiang, Z., Van Dijke, M.I.J., Sorbie, K.S., et al. Representation of multiscale heterogeneity via multiscale pore networks. Water Resour. Res. 2013, 49(9): 5437-5449.

Jia, P., Dong, M., Dai, L. Threshold pressure in arbitrary triangular tubes using RSG concept for all wetting conditions. Colloids Surfaces A 2007, 302(1-3): 88-95.

Jivkov, A.P., Hollis, C., Etiese, F., et al. A novel architecture for pore network modelling with applications to permeability of porous media. J. Hydrol. 2013, 486: 246-258.

Joekar-Niasar, V., Hassanizadeh, S.M. Analysis of fundamentals of two-phase flow in porous media using dynamic pore-network models: A review. Crit. Rev. Env. Sci. Tec. 2012, 42(18): 1895-1976.

Joekar-Niasar, V., Hassanizadeh, S.M., Dahle, H.K. Non-equilibrium effects in capillarity and interfacial area in two-phase flow: Dynamic pore-network modelling. J. Fluid Mech. 2010, 655: 38-71.

Johnson, W.P., Pazmino, E., Ma, H. Direct observations of colloid retention in granular media in the presence of energy barriers, and implications for inferred mechanisms from indirect observations. Water Res. 2010, 44(4): 1158-1169.

Kang, Q., Tsimpanogiannis, I.N., Zhang, D., et al. Numerical modeling of pore-scale phenomena during $CO_2$ sequestration in oceanic sediments. Fuel Process. Technol. 2005, 86(14-15): 1647-1665.

Kang, Q., Zhang, D., Chen, S. Unified lattice Boltzmann method for flow in multiscale porous media. Phys. Rev. E 2002, 66(5): 056307.

Kang, Q., Zhang, D., Lichtner, P.C., et al. Lattice Boltzmann model for crystal growth from supersaturated solution. Geophys. Res. Lett. 2004, 31(21).

Kim, D., Lindquist, W.B. A semianalytic model for the computation of imbibition through polygonal cross

sections. Water Resour. Res. 2012, 48(4): W04529.

Kirchhoff, S. Ueber den Durchgang eines elektrischen Stromes durch eine Ebene, insbesondere durch eine kreisfrmige. Ann. Phys-Berlin. 1845, 140(4): 497-514.

Klise, K.A., Moriarty, D., Yoon, H., et al. Automated contact angle estimation for three-dimensional X-ray microtomography data. Adv. Water Resour. 2016, 95: 152-160.

Knudsen, H.A., Hansen, A. Relation between pressure and fractional flow in two-phase flow in porous media. Phys. Rev. E 2002, 65(5): 056310.

Koplik, J., Lasseter, T.J. Two-phase flow in random network models of porous media. Society of Petroleum Engineers Journal 1985, 25(1): 89-100.

Kordilla, J., Tartakovsky, A.M., Geyer, T. A smoothed particle hydrodynamics model for droplet and film flow on smooth and rough fracture surfaces. Adv. Water Resour. 2013, 59: 1-14.

Kovscek, A.R., Wong, H., Radke, C.J. A porelevel scenario for the development of mixed wettability in oil reservoirs. AIChE J. 1993, 39(6): 1072-1085.

Kuznar, Z.A., Elimelech, M. Direct microscopic observation of particle deposition in porous media: Role of the secondary energy minimum. Colloids Surfaces A 2007, 294(1-3): 156-162.

Levitz, P. Off-lattice reconstruction of porous media: critical evaluation, geometrical confinement and molecular transport. Adv. Colloid Interf. Sci. 1998, 76: 71-106.

Lee, S.H., Padmanabhan, L., Al-Sunaidi, H.A. Simulation of linear displacement experiments on massively parallel computers. SPE J. 1996, 1(3): 327-340.

Lindquist, W.B. The geometry of primary drainage. J. Colloid Interf. Sci. 2006, 296(2): 655-668.

Lindquist, W.B., Venkatarangan, A. Investigating 3D geometry of porous media from high resolution images. Physics and Chemistry of the Earth, Part A: Solid Earth and Geodesy 1999, 24(7): 593-599.

Liu, H., Kang, Q., Leonardi, C.R., et al. Multiphase lattice Boltzmann simulations for porous media applications. Computat. Geosci. 2016, 20(4): 777-805.

Liu, M., Liu, G. Smoothed particle hydrodynamics (SPH): An overview and recent developments. Arch. Computat. Method E 2010, 17(1): 25-76.

Liu, Z., Wu, H. Pore-scale modeling of immiscible two-phase flow in complex porous media. Appl. Therm. Eng. 2016, 93: 1394-1402.

Li, X., Fan, X., Askounis, A., et al. An experimental study on dynamic pore wettability. Chem. Eng. Sci. 2013, 104: 988-997.

Luo, L., Yu, B., Cai, J., et al. Numerical simulation of tortuosity for fluid flow in two-dimensional pore fractal models of porous media. Fractals 2014, 22(4): 1450015.

Løvoll, G., Méheust, Y., Måløy, K.J., et al. Competition of gravity, capillary and viscous forces during drainage in a two-dimensional porous medium, a pore scale study. Energy 2005, 30(6): 861-872.

Ma, J., Couples, G.D., Jiang, Z. et al. A multi-scale framework for digital core analysis of gas shale at millimeter scales. Paper 1063-1070 Presented at Unconventional Resources Technology Conference held in Denver, Colorado, USA, 25-27 August, 2014.

Man, H.N., Jing, X.D. Network modelling of wettability and pore geometry effects on electrical resistivity and capillary pressure. J. Petrol. Sci. Eng. 1999, 24(2-4): 255-267.

Man, H.N., Jing, X.D. Pore network modelling of electrical resistivity and capillary pressure characteristics. Transport Porous Med. 2000, 41(3): 263-285.

Man, H.N., Jing, X.D. Network modelling of strong and intermediate wettability on electrical resistivity and capillary pressure. Adv. Water Resour. 2001, 24(3-4): 345-363.

Ma, S., Mason, G., Morrow, N.R. Effect of contact angle on drainage and imbibition in regular polygonal tubes. Colloids Surfaces A 1996, 117(3): 273-291.

Mason, G., Morrow, N.R. Capillary behavior of a perfectly wetting liquid in irregular triangular tubes. J. Colloid Interf. Sci. 1991, 141(1): 262-274.

Mayer, R.P., Stowe, R.A. Mercury porosimetry-breakthrough pressure for penetration between packed spheres. Journal of Colloid Science 1965, 20(8): 893-911.

McDonald, P.J., Turner, M.N. Combining effective media and multi-phase methods of Lattice Boltzmann modelling for the characterisation of liquid-vapour dynamics in multi-length scale heterogeneous structural materials. Model. Simul. Mater. Sc. 2015, 24(1): 015010.

McDougall, S.R., Sorbie, K.S. The prediction of waterflood performance in mixed-wet systems from pore-scale modelling and simulation. Paper SPE-25271-MS Presented at the SPE Symposium on Reservoir Simulation, New Orleans, LA, USA, 28 February-3 March, 1993.

McNamara, G.R., Zanetti, G. Use of the Boltzmann equation to simulate lattice-gas automata. Phys. Rev. Lett. 1988, 61(20): 2332.

Meakin, P., Tartakovsky, A.M. Modeling and simulation of porescale multiphase fluid flow and reactive transport in fractured and porous media. Rev. Geophys. 2009, 47(3): RG3002.

Mohammadmoradi, P., Kantzas, A. Pore scale investigation of wettability effect on waterflood performance. Paper SPE-181309-MS Presented at the Annual Technical Conference and Exhibition, Dubai, UAE, 26-28 September, 2016.

Monaghan, J.J. Smoothed particle hydrodynamics. Annu. Rev. Astron. Astr. 1992, 30(1): 543-574.

Morrow, N.R. Physics and thermodynamics of capillary action in porous media. Ind. Eng. Chem. 1970, 62(6): 32-56.

Ning, Y., He, S., Liu, H., et al. A rigorous upscaling procedure to predict macro-scale transport properties of natural gas in shales by coupling molecular dynamics with lattice Boltzmann method. Paper SPE-181689-MS Presented at the Annual Technical Conference and Exhibition, Dubai, UAE, 26-28 September, 2016.

Noh, W.F., Woodward, P. SLIC (simple line interface calculation). Paper 330-340 Presented at the Proceedings of the Fifth International Conference on Numerical

Methods in Fluid Dynamics, Springer, Berlin, Heidelberg, June 28-July 2, 1976.

Okabe, H., Blunt, M.J. Prediction of permeability for porous media reconstructed using multiple-point statistics. Phys. Rev. E 2004, 70(6): 066135.

Olsson, E., Kreiss, G. A conservative level set method for two phase flow. J. Computat. Phys. 2005, 210(1): 225-246.

Olsson, E., Kreiss, G., Zahedi, S. A conservative level set method for two phase flow II. J. Computat. Phys. 2007, 225(1): 785-807.

Osher, S., Sethian, J.A. Fronts propagating with curvature-dependent speed: Algorithms based on Hamilton-Jacobi formulations. J. Computat. Phys. 1988, 79(1): 12-49.

Ovaysi, S., Piri, M. Direct pore-level modeling of incompressible fluid flow in porous media. J. Computat. Phys. 2010, 229(19): 7456-7476.

Øren, P.E., Bakke, S., Arntzen, O.J. Extending predictive capabilities to network models. SPE J. 1998, 3(4): 324-336.

Øren, P.E., Billiotte, J., Pinczewski, W.V. Mobilization of waterflood residual oil by gas injection for water-wet conditions. SPE Formation Evaluation 1992, 7(1): 70-78.

Peng, X., Qiao, X., Qiu, S., et al. Radial permeability of fractured porous media by Monte Carlo simulations. Int. J. Heat Mass Tran. 2013, 57(1): 369-374.

Pinilla, J., Bruneau, C.H., Tancogne, S. Front-tracking by the level-set and the volume penalization methods in a two-phase microfluidic network. Int. J. Numer. Meth. Fl. 2016, 80(1): 23-52.

Piri, M., Blunt, M.J. Three-phase threshold capillary pressures in noncircular capillary tubes with different wettabilities including contact angle hysteresis. Phys. Rev. E 2004, 70(6): 061603.

Piri, M., Blunt, M.J. Three-dimensional mixed-wet random pore-scale network modeling of two- and three-phase flow in porous media. I. Model description. Phys. Rev. E 2005a, 71(2): 026301.

Piri, M., Blunt, M.J. Three-dimensional mixed-wet random pore-scale network modeling of two- and three-phase flow in porous media. II. Results. Phys. Rev. E 2005b, 71(2): 026302.

Piri, M., Karpyn, Z.T. Prediction of fluid occupancy in fractures using network modeling and X-ray microtomography. II: Results. Phys. Rev. E 2007, 76(1): 016316.

Princen, H.M. Capillary phenomena in assemblies of parallel cylinders: I. Capillary rise between two cylinders. J. Colloid Interf. Sci. 1969a, 30(1): 69-75.

Princen, H.M. Capillary phenomena in assemblies of parallel cylinders: II. Capillary rise in systems with more than two cylinders. J. Colloid Interf. Sci. 1969b, 30(3): 359-371.

Princen, H.M. Capillary phenomena in assemblies of parallel cylinders: III. Liquid columns between horizontal parallel cylinders. J. Colloid Interf. Sci. 1970, 34(2): 171-184.

Prodanović, M., Bryant, S.L. A level set method for determining critical curvatures for drainage and imbibition. J. Colloid Interf. Sci. 2006, 304(2): 442-458.

Prodanović, M., Bryant, S.L., Karpyn, Z.T. Investigating matrix/fracture transfer via a level set method for drainage and imbibition. SPE J. 2010, 15(1): 125-136.

Purcell, W.R. Capillary pressures-their measurement using mercury and the calculation of permeability therefrom. Journal of Petroleum Technology 1949, 1(2): 39-48.

Rabbani, H.S., Joekar-Niasar, V., Shokri, N. Effects of intermediate wettability on entry capillary pressure in angular pores. J. Colloid Interf. Sci. 2016, 473: 34-43.

Raeini, A.Q., Bijeljic, B., Blunt, M.J. Numerical modelling of sub-pore scale events in two-phase flow through porous media. Transport Porous Med. 2014, 101(2): 191-213.

Raeini, A.Q., Bijeljic, B., Blunt, M.J. Generalized network modeling: Network extraction as a coarse-scale discretization of the void space of porous media. Phys. Rev. E 2017, 96(1): 013312.

Raeini, A.Q., Bijeljic, B., Blunt, M.J. Generalized network modeling of capillary-dominated two-phase flow. Phys. Rev. E 2018, 97(2): 023308.

Raeini, A.Q., Blunt, M.J., Bijeljic, B. Modelling two-phase flow in porous media at the pore scale using the volume-of-fluid method. J. Computat. Phys. 2012, 231(17): 5653-5668.

Ramstad, T., Øren, P.E., Bakke, S. Simulation of two-phase flow in reservoir rocks using a lattice Boltzmann method. SPE J. 2010, 15(4): 917-927.

Raoof, A., Hassanizadeh, S.M. A new method for generating pore-network models of porous media. Transport Porous Med. 2010, 81(3): 391-407.

Reeves, P.C., Celia, M.A. A functional relationship between capillary pressure, saturation, and interfacial area as revealed by a porescale network model. Water Resour. Res. 1996, 32(8): 2345-2358.

Rhodes, M.E., Bijeljic, B., Blunt, M.J. Pore-to-field simulation of single-phase transport using continuous time random walks. Adv. Water Resour. 2008, 31(12): 1527-1539.

Roberts, A.P., Torquato, S. Chord-distribution functions of three-dimensional random media: Approximate first-passage times of gaussian processes. Phys. Rev. E 1999, 59(5): 4953.

Rothman, D.H., Zaleski, S. Lattice-gas models of phase separation: Interfaces, phase transitions, and multiphase flow. Rev. Mod. Phys. 1994, 66(4): 1417.

Sahimi, M. Flow and transport in porous media and fractured rock: From classical methods to modern approaches. New Jersey, USA: John Wiley and Sons, 2011.

Scanziani, A., Singh, K., Blunt, M.J., et al. Automatic method for estimation of in situ effective contact angle from X-ray micro tomography images of two-phase flow in porous media. J Colloid Interf. Sci. 2017, 496: 51-59.

Shan, X., Chen, H. Lattice Boltzmann model for simulating flows with multiple phases and components. Phys. Rev. E 1993, 47(3): 1815.

Sheng, Q., Thompson, K. Dynamic coupling of porescale and reservoirscale models for multiphase flow. Water Resour. Res. 2013, 49(9): 5973-5988.

Shigorina, E., Kordilla, J., Tartakovsky, A.M. Smoothed particle hydrodynamics study of the roughness effect

on contact angle and droplet flow. Phys. Rev. E 2017, 96(3): 033115.

Silin, D.B., Jin, G., Patzek, T.W. Robust determination of the pore space morphology in sedimentary rocks. Paper SPE-84296-MS Presented at the Annual Technical Conference and Exhibition, Denver, Colorado, 5-8 October, 2003.

Silin, D., Patzek, T. Pore space morphology analysis using maximal inscribed spheres. Physica A 2006, 371(2): 336-360.

Silin, D., Tomutsa, L., Benson, S.M., et al. Microtomography and pore-scale modeling of two-phase fluid distribution. Transport Porous Med. 2011, 86(2): 495-515.

Soll, W.E., Celia, M.A. A modified percolation approach to simulating three-fluid capillary pressure-saturation relationships. Adv. Water Resour. 1993, 16(2): 107-126.

Soll, W.E., Celia, M.A., Wilson, J.L. Micromodel studies of three-fluid porous media systems: Pore-scale processes relating to capillary pressure-saturation relationships. Water Resour. Res. 1993, 29(9): 2963-2974.

Sun, D.L., Tao, W.Q. A coupled volume-of-fluid and level set (VOSET) method for computing incompressible two-phase flows. Int. J. Heat Mass Tran. 2010, 53(4): 645-655.

Sun, X., Yao, Y., Liu, D., et al. Investigations of $CO_2$-water wettability of coal: NMR relaxation method. Int. J. Coal Geol. 2018, 188: 38-50.

Sussman, M., Puckett, E.G. A coupled level set and volume-of-fluid method for computing 3D and axisymmetric incompressible two-phase flows. J. Computat. Phys. 2000, 162(2): 301-337.

Tartakovsky, A.M., Meakin, P. Pore scale modeling of immiscible and miscible fluid flows using smoothed particle hydrodynamics. Adv. Water Resour. 2006, 29(10): 1464-1478.

Tartakovsky, A.M., Tartakovsky, D.M., Scheibe, T.D., et al. Hybrid simulations of reaction-diffusion systems in porous media. SIAM J. Sci. Comput. 2008, 30(6): 2799-2816.

Thompson, K.E. Porescale modeling of fluid transport in disordered fibrous materials. AIChE J. 2002, 48(7): 1369-1389.

Tokan-Lawal, A., Prodanović, M., Landry, C.J., et al. Influence of numerical cementation on multiphase displacement in rough fractures. Transport Porous Med. 2017, 116(1): 275-293.

Tryggvason, G., Bunner, B., Esmaeeli, A., et al. A front-tracking method for the computations of multiphase flow. J. Computat. Phys. 2001, 169(2): 708-759.

Valvatne, P.H., Blunt, M.J. Predictive pore-scale network modeling. Paper SPE-84550-MS Presented at the SPE Annual Technical Conference and Exhibition, Denver, Colorado, 5-8 October, 2003.

Van Dijke, M.I.J., Lago, M., Sorbie, K.S., et al. Free energy balance for three fluid phases in a capillary of arbitrarily shaped cross-section: Capillary entry pressures and layers of the intermediate-wetting phase. J. Colloid Interf. Sci. 2004, 277(1): 184-201.

Verma, R., Icardi, M., Prodanović, M. Effect of wettability on two-phase quasi-static displacement: Validation of two pore scale modeling approaches. J. Contam. Hydrol. 2018, 212: 115-133.

Vinogradov, J., Jackson, M.D. Multiphase streaming potential in sandstones saturated with gas/brine and oil/brine during drainage and imbibition. Geophys. Res. Lett. 2011, 38(1):121-133.

Virnovsky, G.A., Lohne, A., Frette, O.I. Modeling capillary pressure using capillary bundles with arbitrary cross-sections obtained from photomicrographs. J. Petrol. Sci. Eng. 2009, 69(12): 117-128.

Vogel, H.J., Roth, K. Quantitative morphology and network representation of soil pore structure. Adv. Water Resour. 2001, 24(3): 233-242.

Washburn, E.W. The dynamics of capillary flow. Phys. Rev. 1921, 17(3): 273-283.

Wells, J.T., Janecky, D.R., Travis, B.J. A lattice gas automata model for heterogeneous chemical reactions at mineral surfaces and in pore networks. Physica D 1991, 47(1-2): 115-123.

Wildenschild, D., Sheppard, A.P. X-ray imaging and analysis techniques for quantifying pore-scale structure and processes in subsurface porous medium systems. Adv. Water Resour. 2013, 51(1): 217-246.

Xu, P., Qiu, S., Yu, B., et al. Prediction of relative permeability in unsaturated porous media with a fractal approach. Int. J. Heat Mass Tran. 2013, 64(3): 829-837.

Yang, J., Bondino, I., Regaieg, M., et al. Pore to pore validation of pore network modelling against micromodel experiment results. Computat. Geosci. 2017, 21(5-6): 849-862.

Yerramilli, R.C., Zitha, P.L.J., Yerramilli, S.S., et al. A novel water-injectivity model and experimental validation with CT-scanned corefloods. SPE J. 2014, 20(6): 1200-1211.

Yong, W., Zhou, Y., Derksen, J. Molecular dynamic simulation of wettability in the context of EOR process. Msc Dissertation, University of Aberdeen, 2017.

Yu, B., Cheng, P. A fractal permeability model for bi-dispersed porous media. Int. J. Heat Mass Tran. 2002, 45(14): 2983-2993.

Yu, B., Li, J., Li, Z., et al. Permeabilities of unsaturated fractal porous media. Int. J. Multiphase Flow 2003, 29(10): 1625-1642.

Yu, B., Liu, W. Fractal analysis of permeabilities for porous media. Aiche J. 2004, 50(1): 46-57.

Yuster, S.T. Theoretical considerations of multiphase flow in idealized capillary systems. Proceedings of the 3rd World Petroleum Congress, Section II, The Hague, The Hague, the Netherlands, 28 May-6 June, 1951

Zhang, B., Yu, B., Wang, H., et al. A fractal analysis of permeability for power-law fluids in porous media. Fractals 2006, 14(3): 171-177.

Zhou, Y., Hatzignatiou, D.G., Helland, J.O. On the estimation of $CO_2$ capillary entry pressure: Implications on geological $CO_2$ storage. Int. J. Greenh. Gas Con. 2017, 63: 26-36.

Zhou, Y., Helland, J.O., Hatzignatiou, D.G. A dimensionless capillary pressure function for imbibition derived from pore-scale modeling in mixed-wet-rock images. SPE J. 2012, 18(2): 296-308.

Zhou, Y., Helland, J.O., Hatzignatiou, D.G. Pore-scale modeling of waterflooding in mixed-wet-rock images: Effects of initial saturation and wettability. SPE J. 2014, 19(1): 88-100.

Zhou, Y., Helland, J.O., Hatzignatiou, D.G. Computation of three-phase capillary pressure curves and fluid configurations at mixed-wet conditions in 2D rock images. SPE J. 2016, 21(1): 152-169.

Zhou, Y., Helland, J.O., Hatzignatiou, D.G., et al. Experimental validation of a pore-scale derived dimensionless capillary pressure function for imbibition under mixed wet conditions. Paper Presented at the 78th EAGE Conference and Exhibition 2016, Vienna, Austria, 30 May-2 June, 2016.

Zhou, Y., Helland, J.O., Jettestuen, E. Dynamic capillary pressure curves from pore-scale modeling in mixed-wet-rock images. SPE J. 2013, 18(4): 634-645.

Zhu, J., Ma, J. An improved gray lattice Boltzmann model for simulating fluid flow in multi-scale porous media. Adv. Water Resour. 2013, 56: 61-76.

Zhu, J., Ma, J. Extending a gray Lattice Boltzmann model for simulating fluid flow in multi-scale porous media. Sci. Rep-UK. 2018, 8(1): 5826.