



## Toward direct pore-scale modeling of three-phase displacements



Peyman Mohammadmoradi\*, Apostolos Kantzas

Chemical and Petroleum Engineering Department, University of Calgary, ES902, 5200, University Dr. NW, Calgary, AB, T2N1N4, Canada

### A B S T R A C T

A stable spreading film between water and gas can extract a significant amount of bypassed non-aqueous phase liquid (NAPL) through immiscible three-phase gas/water injection cycles. In this study, the pore-scale displacement mechanisms by which NAPL is mobilized are incorporated into a three-dimensional pore morphology-based model under water-wet and capillary equilibrium conditions. The approach is pixel-based and the sequence of invasions is determined by the fluids' connectivity and the threshold capillary pressure of the advancing interfaces. In addition to the determination of three-phase spatial saturation profiles, residuals, and capillary pressure curves, dynamic finite element simulations are utilized to predict the effective permeabilities of the rock microtomographic images as reasonable representations of the geological formations under study. All the influential features during immiscible fluid flow in pore-level domains including wetting and spreading films, saturation hysteresis, capillary trapping, connectivity, and interface development strategies are taken into account. The capabilities of the model are demonstrated by the successful prediction of saturation functions for Berea sandstone and the accurate reconstruction of three-phase fluid occupancies through a micromodel.

### 1. Introduction

Kantzas et al. (1988a, b) experimentally observed that when inert gas is injected into a water-wet pore containing a non-aqueous phase liquid (NAPL) surrounded by water, the gas occupies the pore and the NAPL is likely to drain via continuous NAPL layers sandwiched between gas and water, called spreading layers. The NAPL flow at a low saturation in the presence of gas and water guarantees the success of tertiary production processes, such as gas flooding or water alternating gas flooding (Fenwick and Blunt 1998a). The thickness of the spreading layer can be in the order of one nanometer across (Hirasaki 1993a) or even one micrometer in the crevices or rough surfaces (Fenwick and Blunt 1998b; Blunt et al., 1995). The conductance of this layer results in low residual NAPL saturations that can even be as low as 0.1% (Dullien et al., 1989). The vast majority of two-dimensional (2D) micromodel studies, conducted at low capillary numbers, report a significant improvement in the ultimate recovery of NAPLs in systems with positive and even negative spreading coefficients (Chatzis et al., 1988; Kantzas et al., 1988a,b; Kalaydjian 1990; Kalaydjian 1992; Vizika 1993; Keller et al., 1997). The spreading layer's stability is controlled by the equilibrium spreading coefficient, which is a function of the contact angles, structure trend, and surface tensions. Depending on the spreading coefficient value, NAPLs can form either a low-volume thin film or isolated lenses and blobs (Hayden and Voice 1993). In the case of spreading NAPLs, upon contact with gas the physical shape of the

immobile NAPL ganglia deforms into mobile NAPL films, and in that of non-spreading NAPLs, the gas pushes out or bypasses the NAPL as discontinuous ganglia (Grattoni and Dawe 2003; Grattoni et al., 2001; van Dijke and Sorbie 2002; van Dijke et al. 2006; Al-Dhahli et al., 2014). A detailed investigation conducted by Øren et al. (1992) shows that such three-phase displacements proceed by means of a double-drainage mechanism, where gas/NAPL displacement is associated with NAPL/water displacement, and NAPL/water displacement leads to the coalescence and merging of NAPL blobs.

The advancement of high-resolution imaging technologies allows fluids' arrangements to be directly investigated from a microscopic standpoint. It is now convenient to capture three-dimensional (3D) phase profiles or image the NAPL layers sandwiched between gas and water (Iglauer et al., 2013; Matthew et al., 2014). However, visualization and direct measurement of the film streams and quantification of the relative permeabilities and capillary pressures in multi-phase systems is still difficult and time-consuming. An infinite number of potential three-phase fluid arrangements and displacement paths exist, and thus it's impossible to provide a comprehensive suite of experimental measurements. Besides, the application of empirical models for estimation of three-phase saturation functions may result in unrealistic predictions. Due to the practical challenges of the experimental observations and the inevitable uncertainty of the conventional models, numerical modeling of pore-scale transport phenomena has received extensive attention in recent years. Pore-level imaging builds an

\* Corresponding author.

E-mail address: [seyedpeyman.mohammad@ucalgary.ca](mailto:seyedpeyman.mohammad@ucalgary.ca) (P. Mohammadmoradi).

**Nomenclature**

$C_G$	Matrix index (-)	$r$	Pore radius ( $\mu\text{m}$ )
$D$	Computational fluid dynamics (-)	$r_d$	Drainage radius ( $\mu\text{m}$ )
$C_p$	Pore index (-)	$r_s$	Radius of inscribed sphere ( $\mu\text{m}$ )
$C_s$	Spreading coefficient (N/m)	$r_{gn}$	Gas invasion radius ( $\mu\text{m}$ )
$C_s^e$	Equilibrium spreading coefficient (N/m)	$r_{wn}$	NAPL invasion radius ( $\mu\text{m}$ )
$DP$	Demerit Point index (-)	$R$	Image resolution ( $\mu\text{m}/\text{pixel}$ )
$d$	Distance Function (-)	$S$	Sphere (-)
$F$	Binary matrix (-)	$SR$	Snap-off ratio (-)
$G$	Grain space (-)	$Sw_i$	Connate water saturation (-)
$H$	Interface Curvature (1/m)	$S_{nr}$	Residual NAPL (-)
$K_e$	Effective permeability (-)	$v$	Velocity (-)
$K$	Permeability (md)	$h$	Thickness (m)
$L$	Node location (-)	$VOF$	Volume of fluid (-)
$M_x$	Accessibility index	$\beta$	Structure trend (Radian )
$P$	Parent matrix (-)	$\sigma$	Interfacial tension (N/m)
$P_c$	Capillary pressure (MPa)	$\emptyset$	Void space (-)
		$\theta$	Contact angle (Radian)
		$\Delta P$	Pressure difference (MPa)

appealing framework for incorporating complex small-scale physics in the prediction of porous media characteristics. The development of digital rock physics packages for conducting numerical simulations using high-resolution images as inputs is a cheap, clean, fast, and reliable option for characterization of saturated and unsaturated porous media. However, because of the pore space geometrical complexity and the interface tracking numerical issues, direct dynamic simulations using CFD or LB are computationally expensive and have not yet been fully achieved. A popular approach is to simplify the pore space geometry, eliminate the viscous and gravity forces, and predict the three-phase properties using pore-network models. Experimental studies on pore network micromodels reveals the displacement mechanisms, and numerical models are then adapted and developed as computer programs (Fenwick and Blunt 1998a; Øren 1994). The pore network models simplify the microstructure, and then based on some predefined fluid configurations, calculate the capillary pressure curves (Piri and Blunt 2002a, b; Suicmez et al., 2006). It is assumed that the entire process is capillary-dominant and quasi-static and that the pressure within each phase is constant and irrespective of its position in the pore space. Each of the infinitesimal displacement steps is conducted serially until the capillary pressure equilibrium is reached. At equilibrium, fluid saturations are calculated and the capillary pressure/saturation curves are plotted. Then, to estimate the relative permeabilities, empirical expressions for the hydraulic conductance of each phase are used to define the flow resistance in terms of pressure differences (Blunt et al., 2002). However, when high-resolution porous media images are available, the application of pore network models results in the miscalculation of the interfacial areas, losing the medium surface complexities, the impossibility of predicting the solid-related parameters such as effective thermal and elastic properties, and the generation of unrealistic and simplified three-phase realizations. It is assumed that interfaces are always located at the throat entrance, all pores and throats contain only a single bulk fluid, and other fluids may be present as wetting and/or spreading films in the corners, which may distort the nature of the three-phase displacements and result in erroneous estimations (Sheppard et al., 2005).

In this paper, a direct three-phase quasi-static pore morphology-based model is described that incorporates the effects of NAPL spreading layers and double displacement process. No medium discretization/simplification is applied and the workflows are directly applied to pixels as computational nodes. A two-phase version of the model is first proposed by Hazlett (1995), and more sophisticated models were then developed to extend its capabilities (Schulz et al., 2015). This paper briefly describes the adapted two-phase algorithms and then extends the previous models to three-phase flows, including a

full range of possible drainage and imbibition mechanisms. The workflows are validated using the available two- and three-phase experimental datasets.

## 2. Two-phase simulation

The Young-Laplace equation and local capillary pressure equilibria are used to rearrange interfaces and develop two-phase fluid configurations for any specified pressure difference. Each pore cross section has its own shape, and surface complexities may be filled with multiple phases in multiple steps. The pressure of the invading phase is allowed to rise/fall and a succession of equilibrium fluid configurations are computed directly within the pore space. The simulation results including fluid occupancies and interfacial arrangements describe the pore-level displacements under capillary equilibrium condition, where the capillary number is too small and the effects of viscosity and gravity forces on the interfacial arrangements can be ignored.

### 2.1. Algorithms

Detailed algorithms for direct quasi-static simulation of two-phase displacements and petrophysical characterization of unsaturated mixed-wet microstructures together with validations of the simulated fluid occupancy profiles and saturation functions are presented in our previous studies (Mohammadmoradi et al. 2016a, b, 2017). In order to predict pore-level effective electrical and thermal conductivities, a physical Cartesian wetting phase film is added to the filling process. The filling process is then adjusted for shale reservoirs and a particle-wised direct simulation Monte Carlo (DSMC) solver is added to the post-processing engine to simulate slippage and transition gas flow regimes accurately. In summary, the main elements for simulation of two-phase displacement scenarios through pore-level domains are as follows:

- Pixel-wised pre-processing of the input binary images to extract the pore size at each pixel using expanding spheres.
- Object-based simulation of filling processes, drainage and imbibition, to predict phase distribution profiles at different pressures.
- Pixel-wised post-processing of the partially saturated media to determine the effective properties, such as the effective permeability, thermal conductivity, electric conductivity, and elastic moduli.

The immature intersection of the expanding spheres during the image preprocessing can develop unrealistic connections between larger pores, and then some restrictions might be ignored by the advancing fluid-fluid interface, Fig. 1. Here, two matrices called Demerit

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