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Influence of wettability on interfacial area during immiscible liquid invasion into a 3D self-affine rough fracture: Lattice Boltzmann simulations

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ABSTRACT

In this work, the influence of wettability on the fluid–fluid interfacial area (a_{nw}) in a three-dimensional (3D) self-affine rough fracture during non-wetting phase invasion was studied using the lattice Boltzmann method (LBM). The capillary pressure (P_c)-saturation (S_w)-interfacial area (P_c—S_w—a_{nw}) relationship, irreducible water saturation, and a_{nw} at non-wetting phase breakthrough time and at irreducible water saturation were determined for four different contact angles. The lower contact angles led to increases in both P_c and a_{nw} for a given water saturation. The irreducible water saturation increased as contact angle decreased and the corresponding a_{nw} at irreducible saturation also increased as contact angle decreased. Decreasing the contact angle with the corresponding increase in non-wetting phase entry pressures increased the number of fracture regions in which water became surrounded by NAPL and isolated. This consequently increased a_{nw} for a given water saturation and increased the irreducible water saturation. The a_{nw}—S_w curves from LBM for different contact angles were compared with a thermodynamically based model for the a_{nw}—S_w relationship. The energy dissipation factors varied with contact angle, and were higher than typical values for porous media, indicating predictions of less energy dissipation in the fractures modeled than for previously studied porous media.

1. Introduction

The importance of fluid–fluid interfacial area in porous and fractured media has long been recognized in many fields, such as enhanced oil recovery, geological sequestration of carbon dioxide and polluted groundwater remediation. On one hand, dissolution of non-aqueous phase liquids (NAPL) in fractures will be very sensitive to NAPL–water interfacial area, as mass transfer rates for processes such as adsorption, dissolution and cosolvent flushing are proportional to fluid–fluid and solid–fluid interfacial areas [1,2]. On the other hand, as originally shown by Hassanizadeh and Gray [3] (see also [4]) there is a relationship between capillary pressure, P_c, water saturation, S_w, and specific NAPL-water interfacial area a_{nw}, allowing P_c—S_w hysteretic relationships to be explained by changes in a_{nw}.

For a three-dimensional (3D) fracture, the specific interfacial area between non-wetting and wetting phases (also called effective interfacial area) is defined as $a_{nw} = A_{nw}/v$, where v is the total fluid volume including both phases and A_{nw} is the total NAPL-water interfacial area in v. Similarly, the specific NAPL interfacial area is defined as $a_n = A_n/v$ with A_n being the NAPL interfacial area (see Fig. 1), the specific water interfacial area is defined as $a_w = A_w/v$ with A_w being the water interfacial area, and the specific solid surface area is defined as $a_s = A_s/v$ with being the solid surface area. Many experimental approaches have been used to estimate a_{nw} including interfacial tracer techniques [5], X-ray computed tomography and micro-tomography [6,7]. However, these methods are difficult, expensive, and time-consuming. In addition, the theoretical models, such as thermodynamically-based models, involve estimation of interfacial areas based on an energy-balance approach and measured P_c—S_w curves for drainage [8]. For imbibition, the thermodynamic model underestimated the interfacial area due to the assumption that entrapment occurs only within the largest pores [9]. However, this method was modified to allow estimation of a_{nw} by incorporating consideration of saturation history, energy dissipation during drainage and imbibition [10–12].

In the last decade, a large number of studies have been undertaken to attempt to characterize and validate the constitutive relationship between P_c—S_w—a_{nw}. It is currently of great interest to study the evolution of a_{nw} based on the resulting P_c—S_w curve. Jain et al. [1] studied the influence of wettability on a_{nw} in porous media and observed significant differences in interfacial areas as a

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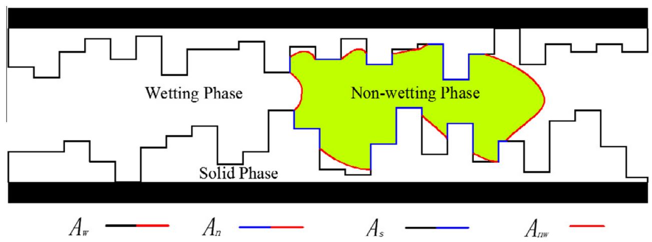

Fig. 1. Illustration of interfacial areas in a rough fracture. A_w includes the black and red lines, A_n includes the blue and red lines, A_s includes the black and blue lines, and the red line represents A_{nw}. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

function of wetting phase saturation as the wettability was changed from water-wet to oil wet. Porter et al. [13] used the Shan–Chen model (which is based on the lattice Boltzmann method (LBM)) to study the hysteresis in the relationship of P_c—S_w—a_{nw} for porous media and found that hysteresis was virtually non-existent in this relationship for multiphase systems. Their results revealed that the Shan–Chen model is capable of simulating the evolution of a_{nw} in a complex 3D multiphase flowing system. Porter et al. [14] used computed microtomography to measure P_c—S_w—a_{nw} relationship for a NAPL-water–glass bead system and showed that the thermodynamic model of Grant and Gerhard [11] predicted the results for a_{nw} within a mean absolute percent error of 15%. Niessner and Hassanizadeh [15] presented a numerical model for macroscale two-phase flow in porous media and emphasized that the constitutive relationship for P_c should involve not only S_w but also a_{nw}. Raeesi and Piri [16] used a 3D mixed-wet random pore-scale network model to investigate the impact of wettability and trapping on the P_c—S_w—a_{nw} relationship during two-phase drainage and imbibition processes. Their results showed that the trapping and contact angle in porous media had a significant effect on the evolution of interfacial area. Recently, Cai et al. [2,17,18] presented a series of studies of immiscible two-phase flow in porous media. They introduced fractal theory to characterize the complexity and self-similarity of solid–fluid interfacial area of stochastic pores in natural porous media and found that the microstructure of pores and wettability had an important influence on the spontaneous imbibition rate. Other studies for porous media have also revealed a strong dependence of the evolution of a_{nw} on porous media texture [19,20]. In particular, corner and film flow may be significant in porous media containing angular pores [21,22].

For flow in fractures, surface roughness in fractures and the influence on flow has been a topic of considerable interest for many years because a description of the surface roughness is essential to the studies of the mechanical and transport properties of rock fractures. Although the roughness in natural fractures is extremely complex, many experimental studies [23,24] have shown that the roughness surface in natural fractures follows self-affine fractal statistics. Due to the flexibility for solving problems with geometrically complex boundaries, the LBM is naturally suitable for simulating the fluid flow in a self-affine fracture [25]. Gutfraind and Hansen [26] studied the permeability of fracture joints using the Lattice-Gas (LG) method. They modeled the fracture as a rough channel bounded by a self-affine surface. Madadi and Sahimi [27] used the LBM to simulate the fluid flow in the 2D fracture networks with self-affine rough surfaces.

While there have been many experimental and modeling studies of saturated and unsaturated water flow in rough fractures (a review of this literature is beyond the scope of this study), there has been limited detailed investigation of two-phase flow in rough walled fractures. In particular, there has not been any study of the effect of contact angle on the evolution of a_{nw} during two-phase flow. Drake et al. [28] reported that the wettability had a significant effect on capillary pressure and saturation curve for porous media. As in porous media, the evolution of a_{nw} in a fracture during non-wetting phase invasion is a complex dynamic process, which is sensitive to flow conditions and fracture geometries. For the non-wetting phase to invade a wetting phase-saturated fracture, the capillary pressure must exceed the displacement pressure. The displacement pressure is related to the interfacial tension, the contact angle, and the local aperture of the fracture [29]. However even a single fracture will have an extremely complex distribution of apertures associated with the roughness of the fracture wall surfaces. This surface roughness in combination with the wettability to the non-wetting phase will have a significant impact on the P_c—S_w—a_{nw} relationship governing two-phase flow and mass transfer in fractured rock. In addition, Reitsma and Kueper [30] measured capillary pressure and saturation curves for a rough-walled rock fracture under different states of normal stress and their results revealed that the behavior of capillary pressure and saturation curve in a rough-wall rock fracture was similar to that observed in unconsolidated porous media.

The main objective of this work is to investigate how wettability influences a_{nw} during non-wetting phase invasion in a single fracture with self-affine rough surfaces. The successive random additions technique and the Shan–Chen model [31,32] were employed to construct self-affine rough fracture wall surfaces and simulate the evolution of a_{nw}, respectively. Two model verifications were used to verify the entry pressure for non-wetting phase invasion and wetting phase drainage in a fracture. Subsequently, the model was applied to investigate the effect of wettability on flow patterns and the P_c—S_w—a_{nw} relationship for four different contact angles. Finally, the correspondence of the results with published a_{nw}—S_w correlations for porous media was examined.

2. Methodology

2.1. Lattice Boltzmann method and multi-component Shan–Chen model

The lattice Boltzmann method is a flexible method for the computational modeling of a wide variety of single and multiphase fluid flow problems in complex geometries [33,34]. This method accommodates a variety of boundary conditions such as the pressure drop across the interface between two fluids and wetting effects at a fluid–solid interface and a constant velocity or pressure boundary condition [35].

The Shan–Chen LBM was developed to simulate multiphase flow. There are two groups of distribution functions in the multi-component Shan–Chen (MCSC) LBM, representing the non-wetting phase and wetting phase, respectively. The evolution equation of each distribution function satisfies the following lattice Boltzmann equation of a single relaxation time model,

$$f_i^\sigma(\mathbf{X}+\mathbf{e}_i\Delta t, t+\Delta t) = f_i^\sigma(\mathbf{X},t) - \frac{\Delta t}{\tau^\sigma}\left[f_i^\sigma(\mathbf{X},t) - f_i^{\sigma(eq)}(\mathbf{X},t)\right], \tag{1}$$

where $f_i^\sigma(\mathbf{X},t)$ is the fluid particle distribution function with velocity $\mathbf{e}_i$ at position $\mathbf{X}$ and time, Δt is the size of the time step, σ denotes either the wetting phase or the non-wetting phase, and τ^σ is the non-dimensional relaxation time which is related to the kinematic viscosity as $\upsilon^\sigma = c_s^2(\tau^\sigma - 0.5\Delta t)$. In the three-dimensional nineteen-speed (D3Q19) model, the nineteen possible particle velocities are given by

$$[\mathbf{e}_0,\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3,\mathbf{e}_4,\mathbf{e}_5,\mathbf{e}_6,\mathbf{e}_7,\mathbf{e}_8,\mathbf{e}_9,\mathbf{e}_{10},\mathbf{e}_{11},\mathbf{e}_{12},\mathbf{e}_{13},\mathbf{e}_{14},\mathbf{e}_{15},\mathbf{e}_{16},\mathbf{e}_{17},\mathbf{e}_{18}]$$
$$= c\begin{bmatrix} 0 & 1 & -1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & 1 & -1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & -1 & 1 & -1 & 1 & -1 \end{bmatrix},$$