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Automated contact angle estimation for three-dimensional X-ray microtomography data

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ABSTRACT

Multiphase flow in capillary regimes is a fundamental process in a number of geoscience applications. The ability to accurately define wetting characteristics of porous media can have a large impact on numerical models. In this paper, a newly developed automated three-dimensional contact angle algorithm is described and applied to high-resolution X-ray microtomography data from multiphase bead pack experiments with varying wettability characteristics. The algorithm calculates the contact angle by finding the angle between planes fit to each solid/fluid and fluid/fluid interface in the region surrounding each solid/fluid/fluid contact point. Results show that the algorithm is able to reliably compute contact angles using the experimental data. The in situ contact angles are typically larger than flat surface laboratory measurements using the same material. Wetting characteristics in mixed-wet systems also change significantly after displacement cycles.

1. Introduction

Prediction of multiphase flow in geologic materials is crucial to understanding, developing and exploiting subsurface systems including emerging geological activities such as enhanced oil recovery [1,2] and geologic CO_2 storage [3]. Pore-scale understanding is crucial for quantifying multiphase flow considering complex pore geometry, changes in phase saturations, chemical reactions at different phase interfaces, and trapping of residual phases [4–6]. Multiphase flow behaviors in porous media are often characterized using capillary pressure, fluid saturation, and relative permeability [7]. Capillary pressure is a function of pore geometry and wetting properties and is defined as the pressure difference across the interface of two different fluids. Wettability is defined as a fluid's tendency to adhere to a solid surface in the presence of another fluid [8] and can be quantified by the contact angle formed at the interface between two immiscible fluids and the solid surface. Typically, contact angles are measured on a flat surface of solid material using a variety of techniques [9]. The contact angles measured on a flat surface often fail to capture the arrangement of fluids at pore scale due to heterogeneous characteristics such as mineral composition, geometry, and surface roughness [5,10–12]. Additionally, contact angle values change under drainage and imbibition cycles (i.e., contact angle hysteresis) [13–15] and due to chemical reactions [11]. The ability to accurately define wetting characteristics of porous media can have a large impact on predicting multiphase behavior in porous media.

Recent advances in high-resolution imaging techniques such as X-ray microtomography (micro-CT) provide an opportunity to characterize in situ fluid distributions in pore structures under varying pressure, temperature, salinity, and/or wetting conditions [5,16–19]. With micro-CT data obtained in a water-wetting bead packing column, Armstrong et al. [20] demonstrated a curvature-based method to analyze contact angles and linked the capillary pressures calculated from the curvature measurements to those from transducer-based measurements. Their work also shows the importance of connected fluid on curvature measurements. Andrew et al. [21] measured pore-scale contact angles for a supercritical CO_2-brine-carbonate system at reservoir conditions using micro-CT data, showing that the range of contact angles measured for manually selected image sets can be attributed to contact angle hysteresis and surface heterogeneity. Brown et al. [22] use mirco-CT data to demonstrate the importance of segmentation methods when measuring interfacial characteristics. Additionally, they are able to track wetability alteration over the course of mutli-phase flow experiments. These recent studies demonstrate the value of three-dimensional (3D) image datasets to investigate pore-scale contact angle hysteresis under varying conditions.

The objectives of this work are to present a new 3D contact angle algorithm to automatically measure in situ contact angles and apply the algorithm to published results of multiphase flow experiments imaged by micro-CT under different wettability conditions. The

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algorithm avoids manual calculations from selectively chosen image sets or interpolated surface curvature. This work utilizes experimental data from Celauro et al. [18], which includes fluid distributions in uniform and mixed grain core samples of soda lime glass and polyethylene plastic beads. To account for the impact of hysteresis, contact angles are calculated after advancing and receding displacement cycles. Results are related to the wetting properties during each displacement cycle and compared to contact angles measured on a flat surface using the same solid materials. The accuracy of the new algorithm is demonstrated using a synthetic test case and implications of the 3D contact angle analysis are discussed.

2. Materials

Experimental data used in this paper are taken from a study by Celauro et al. [18] which looked at the pore scale effects of variable wettability on multiphase fluid flow. The experiments used core samples that measured approximately 25 mm in diameter and up to 102 mm in length. Each core was packed with beads of varying wettability but uniform grain diameter ranging from 0.710 to 0.850 mm. A micro-CT scanner was used to image solid and fluid distribution during a series of displacement cycles. The voxel resolution for these experiments ranged from 0.0266 to 0.0287 mm in both the horizontal directions. Digital core slices ranged from 0.0268 to 0.0278 mm in thickness. The 3D data is then constructed by stacking the slices in the vertical direction. This results in approximately 2.5 billion data points for each experiment. For this research, contact angles are calculated within a volume of interest measuring 13.7 mm $\times$ 13.7 mm $\times$ 27.4 mm (500 $\times$ 500 $\times$ 1000 voxels = 250 million voxels) in the center of each bead back. A central region of the bead pack was selected to avoid edge effects. The experiments use brine and kerosene as the wetting or non-wetting phase depending on the bead type used in the experiment. Fluid properties correspond to those reported by Landry et al. [23].

The bead packs used in this study consist of varying amounts of polyethylene plastic beads (oil-wetting) and soda lime glass beads (water wetting). The first bead pack was made up entirely of plastic beads. A flat plate of the same plastic material was used to measure the contact angle using the sessile drop method. Results showed the plastic material was intermediately wetting with a measured contact angle of 100.9°. The second bead pack was made up entirely of glass beads. The dynamic sessile drop technique was used to determine the contact angle on a flat plate of glass. The contact angle varied from 77.1° to 44.8° in the space of 2 min and had a median contact angle of 47.7°. The third bead pack was filled with a mix of plastic and glass beads. This sample consisted of 57.1% glass and 42.9% plastic beads by volume. While the beads were uniformly mixed before packing the core, the plastic beads tended to group together along the outer edge of the core sample due to static charge. Considering the percent of each type of bead and the contact angle measurements on flat surfaces, the bead pack is expected to be slightly water-wet on average.

Each bead packed core was set in the micro-CT scanner. The scanner was used to map the interior structure of the bead pack, as well as the residual fluid distribution in the pore space. After placement in the scanner, an initial dry scan was taken to observe the grain distribution within the core. Next, each core was saturated with either brine or kerosene. The glass bead pack and the plastic bead pack were saturated with their respective wetting fluid (brine and kerosene, respectively). The mixed glass/plastic bead pack was saturated with brine. Each bead pack then underwent a 1st displacement, where the brine was displaced by kerosene (or vice versa in the case of the plastic bead pack). After the system reached steady state, a micro-CT scan was taken to determine the distribution of brine and kerosene in the core. Finally, the system underwent a 2nd displacement where kerosene was displaced by brine (or vice versa in the case of the plastic bead pack). When the system reached steady state, a final scan was taken to measure the distribution of brine and kerosene. Contact angle calculations in this study come from micro-CT scans after both the 1st and 2nd displacements. For the uniform glass and plastic bead packs, the displacement cycles are setup to replicate the standard process of drainage for the 1st displacement and imbibition for the 2nd displacement.

Fig. 1 illustrates residual saturation and vertical cross-section for the central volume of interest for each of the three bead packs. The direction and fluid type for displacement is shown for each cross-section. For each experiment, the 1st and 2nd displacements result in fairly even residual saturation profiles. In the uniform systems, it is expected that the residual wetting phase will be trapped in small pores after drainage and the residual non-wetting phase will be trapped in large pores after imbibition. With the uniform glass and plastic bead packs, the cross-sectional view after drainage and imbibition show this characteristic. With the mixed glass/plastic bead pack, the cross-sectional view after 1st displacement shows that the residual fluid (brine) is often in contact with glass beads and fills small pore spaces. After the 2nd displacement, the residual fluid (kerosene) is in contact with glass and plastic beads and fills a range of pore configurations. The ability to measure contact angles within 3D experimental data could help explain this phenomenon.

Micro-CT data records a CT registration value at each voxel. The CT registration value depends on the radiodensity of the material which depends largely on density [24]. To use this type of data to measure contact angles, each voxel in the data set must be categorized as one of four possible phases: glass, plastic, brine, or kerosene (as shown in Fig. 1). To segment the data into distinct phases, threshold values were determined using frequency distributions for each experiment [18]. The initial scan, taken when the core was dry, was first segmented into glass, plastic, and pore space using simple thresholding. Once the glass and plastic phases were defined, the brine and kerosene phases were superimposed on the segmented pore structure according to the fluid distributions revealed by CT scans after 1st and 2nd displacements. The results are volumetric datasets of each bead pack, at the end of each displacement, showing the spatial location of plastic, glass, kerosene, and brine voxels. In cases of ambiguous phase identification (i.e. the same voxel was defined as glass and brine), voxels are left as undefined. Such undefined voxels only occurred in the mixed glass/plastic bead pack and accounted for less than 0.70% of the analyzed data. For this reason, very few undefined voxels are visible in Fig. 1. The experimental data will be made available upon request.

3. Methods

In this section, the algorithm for the 3D contact angle calculation is described and its use with the experimental data is explained. Additionally, a synthetic test case is used to validate the algorithm.

3.1. 3D contact angle algorithm

The 3D contact angle algorithm used in this work is a new method developed to directly use 3D segmented data without post-processing. Due to the large volume of image datasets, which typically contain over 100 million voxels in a core sample, the automation of the algorithm is key to avoid manual calculations from selectively chosen image sets. The 3D data is typically obtained from segmented micro-CT images as in this work, but not limited to any particular system. To calculate contact angles, a solid phase and a light and dense liquid phase must be defined. Using this algorithm, the angle is calculated through the denser fluid phase. In the algorithm description below, the dense fluid phase is brine and the light fluid phase is kerosene, in keeping with the experimental data described in Section 2. The experimental data includes two solid phases: glass and plastic. The algorithm can track multiple solid

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