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Numerical simulation of displacement characteristics of CO₂ injected in pore-scale porous media

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ABSTRACT

Pore structure of porous media, including pore size and topology, is rather complex. In immiscible two-phase displacement process, the capillary force affected by pore size dominates the two-phase flow in the porous media, affecting displacement results. Direct observation of the flow patterns in the porous media is difficult, and therefore knowledge about the two-phase displacement flow is insufficient. In this paper, a two-dimensional (2D) pore structure was extracted from a sandstone sample, and the flow process that CO₂ displaces resident brine in the extracted pore structure was simulated using the Navier–Stokes equation combined with the conservative level set method. The simulation results reveal that the pore throat is a crucial factor for determining CO₂ displacement process in the porous media. The two-phase menisci in each pore throat were in a self-adjusting process. In the displacement process, CO₂ preferentially broke through the maximum pore throat. Before breaking through the maximum pore throat, the pressure of CO₂ continually increased, and the curvature and position of two-phase interfaces in the other pore throats adjusted accordingly. Once the maximum pore throat was broken through by the CO₂, the capillary force in the other pore throats released accordingly; subsequently, the interfaces withdrew under the effect of capillary force, preparing for breaking through the next pore throat. Therefore, the two-phase displacement in CO₂ injection is accompanied by the breaking through and adjusting of the two-phase interfaces.

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1. Introduction

The increase of greenhouse gas emissions to the atmosphere during the 20th century is considered to have contributed to global warming. A reduction in the released rate of CO₂ to the atmosphere is essential for mitigating greenhouse effects. One way of achieving this is to inject CO₂ into deep formations (Yang et al., 2015). Such formations include oil and gas reservoirs, saline aquifers and unminable coal seams, of which the deep saline aquifers are widely distributed with the largest CO₂ storage capacity (IPCC, 2005). In China, the storage capacity of deep saline aquifers accounts for 88% of the total geological storage capacity (Li et al., 2009).

CO₂ that is injected into a saline aquifer displaces the resident brine. Different to single-phase flow, the flow process that CO₂

displaces brine is an immiscible two-phase flow, in which the capillary force between the CO₂ and brine plays an important role. The capillary force is inversely proportional to interface curvature and directly proportional to interface tension. Pore diameter of rock is commonly smaller than millimeter-scale, and the rock is commonly hydrophilic. Therefore, the capillary force is an important factor that may control the displacement of the immiscible two-phase flow. However, temporal and spatial variations of two-phase interfaces between the immiscible two-phase fluids are difficult to be observed in porous media (Liu et al., 2012). In addition, methods based on Darcy's law are effective in investigating macroscale two-phase flow but cannot reveal the flow dynamics in the immiscible displacement (Christensen, 2006). Therefore, the dynamics of the immiscible two-phase flow process needs to be understood from a pore-scale viewpoint, which is important but very complicated due to a large number of factors influencing the flow, such as fluid density, fluid viscosity, surface tension, flow rates, surface wettability, pore geometry and medium heterogeneity (Pan, 2003; Liu et al., 2013).

Several approaches have been applied to simulate multiphase flow at pore-scale in porous media, in which the pore-network model is a conventional method. Based on two-dimensional (2D)

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model that is simplified by ball and column connection, [Lenormand and Touboul \(1988\)](#) studied the immiscible two-phase flow using the pore-network model, and established a phase-diagram to identify the flow patterns. In this phase-diagram, the flow patterns were identified by two dimensionless parameters (i.e. capillary number and viscosity ratio) that are determined by fluid viscosity, flow velocity, contact angle and interfacial tension. The capillary number does not refer to the pore structure. Therefore, the phase-diagram is difficult to be applied but plays an instructive role in analysis of two-phase flow in many natural porous media. [Blunt et al. \(2002\)](#) reviewed the pore-network simulation in pore-scale flow. The pore-network model simplifies porous media by connection model of pore body and pore throat with idealized geometries, acquiring certain prediction effects. However, it is difficult to extract a pore-network that topologically and geometrically represents the complex pore geometry and physics, and therefore the pore-network model cannot reveal the fluid dynamics mechanism ([Ramstad et al., 2012](#)). In addition to pore-network model, computational fluid dynamics methods, including the lattice Boltzmann method ([Liu et al., 2012](#)), level set method ([Gunde et al., 2010](#)), volume-of-fluid method ([Raeini et al., 2012](#)) and phase field method ([Anderson et al., 1998](#)), have been developed in pore-scale simulation. Simulating pore-scale two-phase flow by computational fluid dynamics methods can reveal flow characteristics.

In this paper, a computational fluid dynamics method with the level set method is used to simulate movement characteristics of the two-phase interfaces between the CO₂ and resident brine in the displacement process at pore-scale, and the displacement mechanisms are analyzed, which may improve our knowledge on CO₂ displacement flow in porous media.

2. Methodology

2.1. Geometric model

A sandstone sample is chosen from a shallow saline aquifer at a depth of about 200 m, which is located about 41 km northeast of Tongliao, Inner Mongolia, China. In this saline aquifer, a small-scale CO₂ shallow injection experiment is conducted ([Zhu et al., 2015](#)). The pore structure ([Fig. 1](#)) is extracted from a microgram of sandstone slice.

2.2. Numerical method

According to the continuum assumption of fluid, a crucial issue for numerically simulating immiscible two-phase displacement is to track the movement of interfaces in the two-phase flow. The level set method, an interface capture method, was firstly proposed

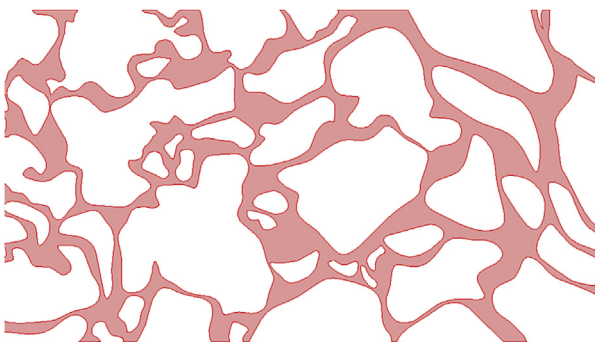


Fig. 1. Pore structure extracted from a sandstone slice.

by [Osher and Sethian \(1988\)](#). In this method, the flow field is covered by a level set function, and the interfaces are expressed with contour lines or surfaces of the level set function. The level set function moves with the flow just as the interfaces do, and the level set function remains a smooth function when it evolves. The level set function performs naturally for problems with singularities, large distortion or interface breakup, etc. Unlike the volume-of-fluid method, the level set function is a continuous function. Therefore, there are more choices for numerical discretization. In addition, some geometric parameters such as the interface normal vector, tangent vector and curvature can be derived from simple derivation.

In standard level set method, the level set function $\phi(\vec{x}, t)$ is defined to be a signed distance function:

$$|\phi(\vec{x}, t)| = d(\vec{x}) = \min_{x_i \in i} (|\vec{x} - \vec{x}_i|) \quad (1)$$

where \vec{x} is the point coordinates, t is the time, i is the interface domain, $\phi(\vec{x}, t) > 0$ on one side of the interface, $\phi(\vec{x}, t) < 0$ on the other side, and $\phi(\vec{x}, t) = 0$ on the interface. The level set function $\phi(\vec{x}, t)$ evolves under advection velocity field as

$$\phi_t + \mathbf{u} \cdot \nabla \phi = 0 \quad (2)$$

where \mathbf{u} is the velocity field, and therefore is the movement velocity on the interface; the subscript t , which denotes the time, represents a partial derivative with respect to time; ∇ is the Laplace operator. In a simulation that uses fluid velocity \mathbf{u} , the level sets close to the zero level set move with velocities that considerably distort the level set function. In this case, the level set function will cease to be an exact signed distance function after a few of time steps, affecting numerical calculation at the next time step ([Sussman and Puckett, 2000](#)). Therefore, a process called re-initialization is needed, which is used to stop the level set calculation at some points in time and to rebuild a level set function corresponding to the signed distance function. There are several ways to accomplish this re-initialization. The most commonly used method among them is the method introduced by [Sussman et al. \(1994\)](#). Its virtue is that the level set function is re-initialized without explicitly finding the zero level set. This re-initialization method is used to solve Eq. (3) to steady state ($\tau \rightarrow \infty$):

$$\phi_\tau = \frac{\phi_0}{\sqrt{\phi_0^2 + h^2}} (1 - |\nabla \phi|) \quad (3)$$

where ϕ_0 is the level set function distribution calculated by Eq. (2) before the re-initialization; h is a parameter of amplitude that is a function of grid size; the subscript τ denotes a partial derivative with respect to the re-initialization time τ that is different from the time t . Calculating Eq. (3) to steady state will provide a new value for ϕ with a property that $|\nabla \phi| = 1$. In addition, this re-initialization calculation ensures that the zero level set does not move ([Sussman et al., 1994](#)). However, a main defect of this level set method is that the advection of ϕ , including the re-initialization steps, is not done in a conservative way, not even for divergence-free velocity fields. This implies that the area bounded by the zero level set is not conserved ([Sussman and Puckett, 2000](#); [Olsson and Kreiss, 2005](#)). In order to ensure mass conserved, [Olsson and Kreiss \(2005\)](#) and [Olsson et al. \(2007\)](#) modified this level set function by replacing the signed distance function with a smeared-out Heaviside function $\tilde{\phi}(\vec{x}, t)$:

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