Numerical Analysis of Two-Phase Flow in Porous Media by LBM

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Sequestration of CO₂ to geological formations such as aquifers is considered as one of the possible options for the abatement of CO₂ emission to the atmosphere. Understandings of microscopic two-phase flows in porous media are very important to assess the safety and long-term fate of sequestered CO₂. We had developed a numerical code, which simulates two-phase flow of supercritical CO₂ and water in porous media including the effect of interfacial tension, wettability, buoyancy, and viscosity ratio by means of the lattice Boltzmann method. We investigated effect of capillary number on flow patterns of two-phase flow in a microscopic model of porous media which have highly water-wet surfaces. A present study shows that the interfacial tension affects the relative permeability of CO₂ to deviate from Darcy law at low capillary numbers. The interfacial tension that dominates over the viscous force results in the establishment of secondary flow in a CO₂ bubble.

1. INTRODUCTION

Carbon dioxide is considered to be the greenhouse gas that most contributes to global warming on earth. In response to this problem, several methods have been proposed to remove CO₂ from the atmosphere. Sequestration of CO₂ in geological formations such as aquifers is one such method. In aquifers at depths below 700 to 1000 m, supercritical CO₂ has a liquid like density, but still CO₂ is about 0.6 times lighter than saline in formations. Therefore, buoyancy tends to bring the sequestered CO₂ back to the surface unless there is a confining impermeable stratum (caprock). A potential problem with geological sequestration is the leakage of CO₂ from reservoirs. Carbon dioxide injected into aquifers can be modeled with an immiscible two-phase flow of supercritical CO₂ and water in porous medium. The difference in densities creates strong buoyancy forces that drive the CO₂ upward. On the other hand, at the junction of formations, the capillary pressure of water confined in fine pore structure of water-wet rock prevents the migration of CO₂. Usually, large scale numerical simulations have been used to predict the fate of the injected CO₂ over centuries to millions of years. In such simulations, the two-phase flow is modeled in a macroscopic Darcy scale. Therefore, the accuracy depends on the macroscopic model, namely relative permeabilities of CO₂ and water and capillary pressure function. Understandings of two-phase flow in porous medium from a microscopic point of view are very important to improve the accuracy of the model.

This paper describes numerical research on two-phase flow of supercritical CO₂ and water in porous media from a microscopic point of view. We used a lattice Boltzmann method (LBM) to solve Navier-Stokes equations of two-phase flow at the pore scale. First, we briefly introduce the numerical
model. Next, we discuss the effect of interfacial tension on the relative permeabilities of CO₂ and water. Carbon dioxide reaches its critical state at the depths of 700 to 800 m. Over the critical point, the interfacial tension between CO₂ and water increases and decreases rapidly[9]. Finally, we give some conclusions.

2. NUMERICAL SCHEME

The LBM is a technique to numerically solve the incompressible Navier-Stokes equation. We used the LBM, because it has two major advantages for studies of flow through porous media: the no-slip boundary condition of hydrodynamics is easily implemented for complicated boundaries and the interface between multiple phases can be modeled simply based on thermodynamics. In previous work[6], we used the model proposed by Swift et al[7-9]. In this model, the equilibrium state is associated with a free-energy functional which can be used for the calculation of a pressure tensor using the Cahn-Hilliard description[10]. Potential weaknesses of the original model are the lack of Galilean invariance[11,12] and the non-physical pressure profile across the interface. As a consequence, at relatively high interfacial tensions, non-physical evaporation and condensation, that is, Ostwald ripening phenomenon, reduce the accuracy of numerical simulations. Recently, Inamuro et al.,[13-16] developed a new LBM, which overcomes these weaknesses as well as can treat large density differences by using the projection method. In the present work, we used the model proposed by Inamuro et al. Details of the model have been given in original papers[13-16]. We, therefore, will briefly introduce the model.

In the present work, three-dimensional fifteen velocity $e_i (i = 1, \ldots, 15)$ model is used. The evolution of the particle distribution functions $f_i (\mathbf{x}, t)$ and $g_i (\mathbf{x}, t)$ at the point $\mathbf{x}$ and at time $t$ is computed by the lattice Boltzmann equations with BGK approximation as:

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

(1)

$$g_i (\mathbf{x} + \mathbf{e}_i \Delta x, t + \Delta t) = g_i (\mathbf{x}, t) - \frac{1}{\tau_g} \left[ g_i (\mathbf{x}, t) - g_i^{eq} (\mathbf{x}, t) \right] - \frac{1}{\rho} \left[ \frac{\partial}{\partial \mathbf{x} \cdot} (\mu \frac{\partial u}{\partial \mathbf{x}} + \mu \frac{\partial u}{\partial \mathbf{x}}) \right] \Delta x,$$

(2)

where $f_i^{eq} (\mathbf{x}, t)$ and $g_i^{eq} (\mathbf{x}, t)$ are the local equilibrium distribution functions, $\tau$ the dimensionless single relaxation time, $\Delta x$ the spacing of the cubic lattice, $\Delta t$ the time step, $\mu$ the viscosity, $\rho$ the density, $E_i$ the constant. Macroscopic variables of the order parameter $\phi$ distinguishing two phases and the predicted velocity $\mathbf{u}^*$ are defined by using distribution functions as:

$$\phi = \sum_{i=1}^{15} f_i , \quad \mathbf{u}^* = \sum_{i=1}^{15} g_i e_i .$$

(3)

The predicted velocity $\mathbf{u}^*$ does not satisfy the continuity equation $\nabla \cdot \mathbf{u} = 0$, pressure $p$ and velocity should be corrected by using the equation:

$$Sh \frac{\mathbf{u} - \mathbf{u}^*}{\Delta t} = - \frac{\nabla p}{\rho},$$

(4)

$$\nabla \cdot \left( \frac{\nabla p}{\rho} \right) = Sh \frac{\mathbf{v} \cdot \mathbf{u}^*}{\Delta t},$$

(5)

where $Sh$ is a constant satisfies the relation $\Delta t = Sh \Delta x$.

Lattice Boltzmann equations (1) and (2) with pressure and velocity correction (4) and (5) are equivalent to phase advection equation for $\phi$ and incompressible Navier-Stokes equation for two-phase flow with an interfacial tension[13].

The grid size used in simulations is a 64x64x64 cubic lattice. Periodic boundary conditions were
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Table 1: Numerical parameters.

<table>
<thead>
<tr>
<th>parameter</th>
<th>symbol</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>relaxation time for Equation (1)</td>
<td>$\tau_f$</td>
<td>1.000</td>
</tr>
<tr>
<td>relaxation time for Equation (2)</td>
<td>$\tau_g$</td>
<td>1.000</td>
</tr>
<tr>
<td>CO₂ density</td>
<td>$\rho_g$</td>
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</tr>
<tr>
<td>water density</td>
<td>$\rho_l$</td>
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</tr>
<tr>
<td>CO₂ viscosity</td>
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</tr>
<tr>
<td>water viscosity</td>
<td>$\mu_l$</td>
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</tr>
<tr>
<td>constant determining the width of the interface</td>
<td>$\kappa_f$</td>
<td>0.500</td>
</tr>
<tr>
<td>constant determining the interfacial tension</td>
<td>$\kappa_g$</td>
<td>0.100</td>
</tr>
<tr>
<td>constant parameter in Equation (6)</td>
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</tr>
<tr>
<td>constant parameter in Equation (6)</td>
<td>$b$</td>
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</tr>
<tr>
<td>constant parameter in Equation (6)</td>
<td>$T$</td>
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</tr>
<tr>
<td>constant parameter in Equations (4) and (5)</td>
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</tr>
<tr>
<td>grid spacing</td>
<td>$\Delta x$</td>
<td>1.000</td>
</tr>
<tr>
<td>time step</td>
<td>$\Delta t$</td>
<td>1.000</td>
</tr>
</tbody>
</table>

employed in three directions. Numerical parameters are summarized in Table 1. Under the condition of temperature and pressure at the depth of 2000 m, density and kinetic viscosity ratios of supercritical CO₂ and water are about 0.6 and 10, respectively. Dimensionless densities and viscosities of gas and liquid phases were set to satisfy these relations. The pressure tensor of the fluid used for the calculation of the order parameter $\phi$ is given by

$$P_{\alpha\beta} = \left[ \phi T \left( \frac{1}{1-b\phi^2} - \phi \kappa_f \left( \frac{\partial^2 \phi}{\partial x_i^2} - \frac{\kappa_f}{2} \frac{\partial \phi}{\partial x_i} \right)^2 \right) \right] \delta_{\alpha\beta} + \kappa_f \frac{\partial \phi}{\partial x_\alpha} \frac{\partial \phi}{\partial x_\beta},$$

where $a$, $b$, and $T$ are free parameters, and $\kappa_f$ is the parameter determining the width of the interface. The van der Waals theory gives the following expression for the interfacial tension $\sigma$:

![Fig. 1 A pressure profile across an interface.](image1)

![Fig. 2 Laplace law test for various interfacial tension parameters $\kappa_f$. Symbols denote simulation results and lines denote Laplace law for prescribed value of surface tension $\sigma$ as Equation (7).](image2)
\[ \sigma = \kappa_s f_{m \xi} \left( \frac{\partial \rho}{\partial \xi} \right)^2 d\xi, \]

where \( \xi \) is the coordinate normal to the interface and \( \kappa_s \) is the parameter determining the interfacial tension. The values of these parameters used in the simulations are also summarized in Table 1.

To check the validity of the numerical model, single bubble of CO₂ in stationary water in an equilibrium state is numerically simulated. Figure 1 shows the pressure distribution across the bubble. The difference in pressure between the inside and outside of the bubble is established by interfacial tension. We adjusted the parameter \( \kappa_I \) to let the width of the interface about 6 meshes. Figure 2 demonstrates the agreement between the simulation results and the Laplace law \( \Delta p = 2\alpha/R \), where \( R \) is the radius of a bubble, for prescribed surface tension \( \sigma \) as Equation (7). For various interfacial tension parameters \( \kappa_p \), the calculated values are in excellent agreement with theoretical values.

Wettability of two components is introduced by an external chemical potential at the solid surfaces\(^5\). The thermodynamic force defined as:

\[ F_\alpha = -\frac{\xi_f \phi_a \mu_{ex}}{10 \delta x_\alpha}, \]

is introduced in Equation (1) by replacing \( f_i^{eq}(x,t) \) with \( f_i^{eq}(x,t) + F_\alpha \), where \( \mu_{ex} \) is the chemical potential, which differs from zero only at the surfaces. Preliminary simulation study shows that for the present system, the contact angle of water droplet surrounded by supercritical CO₂ on a flat surface decrease from 90° at \( \mu_{ex}=1.0 \) to 0° at \( \mu_{ex}=1.5 \times 10^{-2} \). Since the quartz-like rocks of aquifers is highly water-wet, the chemical potential \( \mu_{ex} \) is set to be \( 1.5 \times 10^{-2} \).

Porous rock is modeled by solid spheres arranged uniformly on the face-centered cubic lattice. The diameter of spheres was adjusted so as the porosity of porous medium to be 0.75, though the porosity of aquifers is much denser (0.2). To resolve the much denser porous media, the finer grid systems are required, but it is beyond our computer resources.

Uniform body force, which corresponds to the pressure gradient, is applied to each phase in a certain direction parallel to the grid systems. Since the periodic boundary condition is imposed in all directions, the pressure drop is balanced with the body force at the steady state instead of the establishment of pressure gradient. Using the average phase velocities \( U_\alpha \) \( (\alpha = \text{water}, g \text{ (CO₂)}) \) that are calculated from the simulation results, Reynolds number and capillary number for each phase are defined as:

\[ Re_\alpha = \frac{\rho_\alpha U_\alpha L}{\mu_\alpha}, \quad Ca_\alpha = \frac{\mu_\alpha U_\alpha}{\sigma}, \]

respectively, where \( L \) is the characteristic length; it is the minimum distance between spheres in the present study.

3. NUMERICAL RESULTS AND DISCUSSION

In large-scale reservoir simulations, as mentioned above, rock properties are modeled with the relative permeabilities and capillary pressure curve as a function of CO₂ saturation \( (S_\alpha) \). Thus, form a microscopic viewpoint the effect of CO₂ saturation on flow patterns of two-phase flow in porous media is investigated numerically. For any CO₂ saturation, Darcy law says that the pressure loss along the flow direction is proportional to the velocity. However, at the lower capillary numbers the body force balanced with the interfacial tension as well as viscous force is required to drive the flow in porous media. Next, accordingly, we will focus on the effect of the interfacial tension on flow patterns and relative permeabilities.

Figure 3 shows the typical result of numerical simulations at low CO₂ saturations. Even though the
Fig. 3 An example of the migration of a CO$_2$ bubble through the porous medium at the CO$_2$ saturation $S_e$ of 0.2. Right figures show the cross-sectional views of CO$_2$ distributions. Body forces are applied upward.

Front of a CO$_2$ bubble is split into pore spaces to go round the solid spheres, single bubble in shape is maintained by the interfacial tension. In the main flow direction, CO$_2$ and water alternates each other.
Since the surface of solid spheres is set to be highly water-wet, a CO₂ bubble is out of contact with the surface that is covered with thin water films.

On the other hand, the typical CO₂ distribution at high CO₂ saturations is shown in Figure 4. An almost steady flow of CO₂ occurs at higher CO₂ saturations. At the CO₂ saturations of 0.6 and 0.8, the CO₂ bubbles are combined into CO₂ channels that occupy the center of large pores and connect them through the pore necks along the flow direction. Once the CO₂ channels are established along the flow direction, CO₂ flows easily through the porous media because it does not accompany the viscous water flow. The surfaces of spheres are covered with water films in which water does not migrate well. Quantitatively, these changes in flow patterns with the CO₂ saturation result in the dependence of relative permeabilities of water and CO₂ on the saturation as shown later in Figure 7.

Figure 5 shows the relation between the Reynolds number and the applied body force, which corresponds to the relation between the CO₂ velocity and the pressure loss, because the velocity is

![Figure 5](image)

**Fig. 5** Deviation from the Darcy law at the low capillary numbers at the CO₂ saturation $S_g$ of 0.6. Full squares denote the higher capillary numbers in the range from 0.10 to 0.15, and open squares denote the lower capillary numbers in the range from 2.79×10⁻³ to 2.92×10⁻².

![Figure 6a and 6b](image)

**Fig. 6** Effect of the capillary number on the velocity distribution in a CO₂ bubble. (a) $C_a = 1.33\times10^{-1}$, (b) $C_a = 9.53\times10^{-3}$. Arrows, which denote the direction and magnitude of velocity, are illustrated only in a CO₂ bubble. Body forces are applied upward.
proportional to the Reynolds number due to the definition, and because the applied body force is also proportional to the pressure loss due to the periodic boundary condition as mentioned above. For the capillary number higher than 0.10, the Reynolds number is proportional to the body force. This fact is often referred as the Darcy law. For the capillary number range from $2.79 \times 10^3$ to $2.92 \times 10^2$, the slope deviates from the Darcy law. Since the interfacial tension prevents the migration of CO$_2$ in addition to the viscous force, the Reynolds number, namely the velocity is lower than the Darcy law.

Figure 6 demonstrates the effect of the capillary number on the velocity distribution in a CO$_2$ bubble. For relatively high capillary numbers, the velocity in a CO$_2$ bubble aligns approximately in the mean flow direction. The interaction between CO$_2$ and water by the interfacial tension is lower in comparison with the viscous force. Hence, CO$_2$ flows smoothly in the mean flow direction. On the other hand, for relatively low capillary numbers, the velocity distribution that is attributed to the interfacial tension is clearly observed. Near the interface where its curvature is low due to the constriction by pore necks, the velocity aligns inwards to the CO$_2$ bubble to maintain the area of interface as low as possible. As a result, additional body force is required to migrate CO$_2$ through the pore necks.

Effect of the capillary number on relative permeabilities of CO$_2$ and water is shown in Figure 7. There is only negligible effect of the capillary number on the relative permeability of water, because the velocity due to the interfacial tension is established mainly in CO$_2$ phase. At lower capillary numbers, the interfacial tension lowers the relative permeability of CO$_2$. Because the interfacial tension between CO$_2$ and water increases and decreases rapidly over the critical point$^{[6]}$, the capillary pressure will affect the migration and leakage of CO$_2$. Moreover, for the sedimentary rocks with low porosity, capillary pressure will also result in the residual gas saturation that traps CO$_2$ in pore structure.

4. CONCLUDING REMARKS

We used LBM to numerically simulate immiscible two-phase flow of supercritical CO$_2$ and water in a microscopic model of porous media which have highly water-wet surfaces. We investigated effect of capillary number on flow patterns of two-phase flow. Water and a bubble of CO$_2$ pass through the porous media alternately in a mean flow direction for low CO$_2$ saturations. This fact results in a high relative permeability of water for low CO$_2$ saturations. At high CO$_2$ saturations, CO$_2$ bubbles joined each other establishing CO$_2$ channels along the flow direction. Water covers surfaces of porous material due to its wetting property forming the thin films. Hence, the relative permeabilities of CO$_2$ and water are, respectively, high and low at high CO$_2$ saturations. For low capillary numbers, the interfacial tension that dominates over the viscous force results in the establishment of secondary flow in a CO$_2$ bubble. The interfacial tension lowers the relative permeability of CO$_2$.

In geological sequestration of CO$_2$, capillary force of water at the junction of a caprock and an aquifer inhibits CO$_2$ from migrating due to buoyancy. While the present work shows the effect of the interfacial tension on patterns of two-phase flow of CO$_2$ and water in homogeneous porous media, understandings of the effect of the interfacial tension at the junction of different porous media are an
important task in future.

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