Pore scale numerical simulation of supercritical CO$_2$ injecting into porous media containing water

Ruina Xu$^{a,1}$*, Shu Luo$^a$, Peixue Jiang$^a$

$^{a}$Key Laboratory for Thermal Science and Power Engineering of Ministry of Education, Department of Thermal Engineering, Tsinghua University, Beijing 100084, CHINA

Abstract

Two phase flow of gases and liquid in porous media is becoming an increasing important area of CO$_2$ storage. The mechanism of the CO$_2$ injected into porous media containing water need to be investigated on the pore scale deeply. In this research, one numerical simulation method was provided to simulate the two phase flow in porous media by solving the Navier-Stokes equation directly. Relative permeability modeling for sands was made using the unsteady-state method. Air and water were first utilized as multiphase fluids, and secondly, supercritical CO$_2$ was used for the same sample. The numerical simulation results of air/water drainage agree well with the experimental data. This modeling also provides insight into the mechanisms in multiphase flow in porous media and a new numerical modeling method to do the pore scale simulation.

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1. Introduction

Carbon dioxide capture and storage in saline aquifer is considered as one of the most important technologies for climate change mitigation. There are many challenges for demonstration and large scale application of CO$_2$ storage. Numerical studies are the useful and important method to simulate the behavior of supercritical CO$_2$ injected into saline aquifer and predict the potential CO$_2$ storage capacities of the selected storage sites.

Currently, CO$_2$ saline aquifer injections have been studied using computer simulations such as ECLIPSE, TOUGH, NUFT and purposely developed software. These large-scale simulations...
which describe the process of CO₂ migration and interactions between CO₂ are important for the purpose of designing and evaluating the capacity and risk management of potential storage site. The important parameters inputting into the large-scale simulations are the empirical trapping models, relative permeability relationships, wettability and/or capillary pressure curves. However, these models yet are poorly understood. Therefore, the fundamental research on trapping mechanism on pore scale is one of the key challenges to CO₂ storage.

In understanding the mechanisms of CO₂ migration in porous media filled with brine and providing correlations such as relative permeability relationships, pore-network modelling has played a significant role\[1,2\]. Experimentally, important progress has been made recently using medical devices such as X-Ray micro-computerized tomography (CT) and magnetic resonance imaging (MRI) to produce detailed descriptions of the two phase flow in core or porous media\[3-5\]. In the large scale numerical simulation, many correlations and modeling are used to simplify the large scale simulation. Therefore, it is important to develop accurate numerical modeling and correlations to govern the movement of supercritical CO₂ in saline aquifer.

In the recent years, pore scale numerical simulations have been used to study single-phase fluid flow and convection heat transfer in porous media\[6,7\]. From their research, it has been proved that this pore scale numerical simulation results agree with the experimental results. Therefore, the pore scale numerical method is used in this paper to investigate the fundamental study of supercritical CO₂ injected into porous media containing liquid water. The numerical simulation results are compared with the experimental data and provide details of supercritical CO₂ and water flow inside the porous media.

2. Physical model, governing equations and numerical method

The commercial software Gambit V2 and FLUENT V6 were respectively used as the grid generator and the CFD solver. The physical model is modelled in a 3D domain in Gambit. FLUENT is a computational fluid dynamics (CFD) software package to simulate fluid flow problems. It uses the finite-volume method to solve the governing equations for a fluid. It provides the capability to use different physical models such as incompressible or compressible, inviscid or viscous, laminar or turbulent, etc. Geometry and grid generation is done using GAMBIT which is the pre-processor bundled with FLUENT.

A fully numerical simulation of the Navier-Stokes equations for the two phase fluid flow in a porous media with the real structure or all the particles is very difficult due to the huge number of calculations. The present paper considers only a limited number of identical particles as the porous media. There are many various arrangements of the particles, such as simple cubic (SC), body centered cubic (BCC) and face centered cubic (FCC). Xu and Jiang\[7\] have discussed the influence of the different arrangement of the particles on the single phase fluid flow in porous media. Their simulation results showed that the differences between the numerical results using SC, BCC and FCC arrangements of the particles with consideration of velocity slip on the solid wall and the experimental data are less than 5%, 10% and 11%, respectively. Therefore, the SC arrangement of the particles as shown in Fig. 1 was used for the numerical simulations.

The physical model, the coordinate system and the grids for the fluid domain are shown in Fig. 2. The calculation region includes an entrance region and an exit region. The nominal particle sizes of the sintered porous channel were 120 μm. These uniform solid particles were assumed to have small but finite contact areas with a simple cubic lattice structure. Different
porosities were obtained by changing the particle sizes and arrangements. In this study, the porosity was 0.4. Constant thermophysical properties at 290 K and 60°C, 15MPa were assumed for the air and supercritical CO2 respectively. Symmetrical boundary conditions were imposed on the boundaries of the computational domain. The inflow into the domain was set as the mass flow rate inlet with the outflow set as the pressure outlet boundary condition.

The dimensions and porosities of the microporous media used in the calculations which were based on the experimental research investigated by Abaci et al (1992). The constant contact areas between the particles were calculated based on the desired porosity. The numerical simulations used two half particles in the x and y directions with 4 particles in the z direction.

The VOF model for two phase fluid flow in the porous media was used through FLUENT 6.1. The VOF model can simulate two or more immiscible fluids by solving a single set of momentum equations and tracking the volume fraction of each of the fluids throughout the domain. The detail introduction to this model please refer Fluid help document.

The general equations governing the flow fields for these conditions are:

Continuity equation:

$$\frac{1}{\rho_q} \frac{\partial}{\partial t} \left( \alpha_q \rho_q \right) + \nabla \cdot \left( \alpha_q \rho_q \mathbf{V}_q \right) = S_{\alpha_q} + \sum_{p=1}^{n} \left( \dot{m}_{pq} - \dot{m}_{qp} \right)$$  \hspace{1cm} (1)

Momentum equations:

$$\frac{\partial}{\partial t} \left( \rho \mathbf{V} \right) + \nabla \cdot \left( \rho \mathbf{V} \mathbf{V} \right) = -\nabla \rho + \nabla \cdot \left[ \mu \left( \nabla \mathbf{V} + \nabla \mathbf{V}^{T} \right) \right] + \rho \mathbf{g} + \mathbf{F}$$  \hspace{1cm} (2)

The effect of surface tension along the interface between the two phased are included in the VOF model. The model can be augmented by the additional specification of the contact angles between the phases and the walls. The properties appearing in the transport equations are determined by the presence of the component phases in each control volume.

3. Data processing method

The JBN method is a common method to calculate the relative permeability and it provides calculation of individual relative permeability from displacement data obtained on normal sized reservoir core samples. The theory requires two conditions that must be achieved before applying for use. Upon meeting the requirement, relative permeabilities (water-oil system) are then derived as:
$k_{rg}(S_g) = f_w(S_g) \frac{d}{d\left( \frac{1}{W_i} \right)}$

$\Delta P (\text{Pa})$

$t (s)$

$\eta_{rg} = f_w(\mu_w)/(\mu_w + f_w(\mu_w))$

$= \frac{k_{rg}(S_g)}{k_{rw}(S_g)}$ (3)

$\forall 0, 1 - f_w$

$= k_{rw}(S_g) \frac{\mu_w(1-f_w)}{f_w}$ (4)

where, $W_i$ = cumulative injection of pore volumes, $f_w$ = fraction flow of water, $I$ = relative injectivity.

Through the numerical simulation, the pressure drop, the water saturation, the cumulative injection volume, the fraction flow of water and the relative injectivity and other parameters can all be obtained. Therefore, based on the JBN method, the relative permeability can be analysed.

4. Numerical simulation results and discussions

4.1 Air/water drainage

Relative permeability modeling for sands was made using the unsteady-state method. Air and water were first utilized as multiphase fluids, and secondly, supercritical CO$_2$ was used for the same sample. First, the modeling results of air/water drainage are compared with the other investigator’s experimental results. The aim of doing air/water drainage is to evaluate the accuracy of the numerical simulation model.

Figure 3 shows the pressure drop variation with injection time. Results of the numerical simulation of injecting air into saturated water porous media were plotted in figure 4. The results have been plotted using percent saturation of the porous media versus relative permeability values. The black lines show the experimental results provided by Abaci et al (1992) and the black points show the numerical simulation result. It can be seen that the numerical simulation results agree well with the experimental data.

Figure 5 shows the pressure distribution along the flow direction in the center cross section at $t=5$ s and 12 s. The pressure deceased as the injection time increased.

Figure 3 The pressure drop variation with injection time

Figure 4 Relative permeability – saturation relation using air and water (porosity 40%)
4.2 Supercritical CO\textsubscript{2}/water drainage

In this model, supercritical CO\textsubscript{2} was injected into the porous media containing water. The potential injection site was selected at the depth of 1500m; therefore, the properties of supercritical CO\textsubscript{2} and water at 60\degree C and 15MPa were used in this model. The physical model and the structure in this section are same with the model described in section 4.1.

Figure 6 shows the pressure drop variation with injection time. The pressure drop in CO\textsubscript{2}/water drainage is smaller than air/water drainage at the same injection rate. Results of the numerical simulation of injecting supercritical CO\textsubscript{2} into saturated water porous media were plotted in figure 7. Figure 8 shows the CO\textsubscript{2} volume fraction distribution along the flow direction in the center cross section at t=4 s and 9 s. The volume fraction of CO\textsubscript{2} increased as the injection time increased.
5. Conclusion

Two phase flow of gases and liquid in porous media is becoming an increasing important area of CO₂ storage. The mechanism of the CO₂ injected into porous media containing water need to be investigated on the pore scale deeply. In this research, one numerical simulation method was provided to simulate the two phase flow in porous media by solving the Navier-Stokes equation directly. This modeling also provides insight into the mechanisms in multiphase flow in porous media and a new numerical modeling method to do the pore scale simulation. It is true that this method could not be used in the large scale numerical simulation; however, the pore scale could provide the fundamental understanding of the mechanism of trapping and CO₂ behavior after CO₂ injection into the saline aquifer.

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Reference

