Rock Characterisation, Modelling and Engineering Design Methods – Feng, Hudson & Tan (Eds) © 2013 Taylor & Francis Group, London, ISBN 978-1-138-00057-5

CO₂ geological sequestration modelling and injection induced fracturing analysis of the caprock

X.L. Liu, P. Lin, E.Z. Wang & G.H. He

State Key Laboratory of Hydroscience and Engineering, Tsinghua University, Beijing, China

G.F. Han

Institute of Mechanics, Chinese Academy of Sciences, Beijing, China

ABSTRACT: In geological sequestration, CO_2 is injected under high pressure into deep underground rock formations, including deep saline aquifers. This paper presents the invading supercritical CO_2 -brine two-phase numerical model to describe CO_2 flow and transport processes in deep saline aquifers. The effects of anisotropy and different kinds of heterogeneity like horizontal and vertical layers and also existence of barriers between layers on the CO_2 flow and transport in a saturated porous media with brine are investigated using the presented two-phase model. Following to simulation results, it can be obtained that the permeability of the rock formations and the permeability anisotropy should be considered as the most important parameters in CO_2 flow and transport processes and its distribution in the rock formations. Furthermore, the capillary pressure on the buoyancy-driven flow of CO_2 is analyzed, and the XFEM is adopted to simulate the injection induced fracturing process of the naturally fractured caprock.

1 INTRODUCTION

An ever-increasing amount of scientific evidence suggests that anthropogenic release of CO₂ has led to a rise in global temperatures over the past hundreds of years, especially since the Industrial Revolution (Crowley, 2000; Bradley, 2011). Among various greenhouse gases, CO2 is the greatest contributor to global warming. Reducing the concentration of CO2 in the atmosphere is a major challenge to migrate greenhouse gas. Carbon Capture and Sequestration (CCS) is one of the options for mitigating CO₂ emission contributing to global warming (Gale, 2002; Baines and Worden, 2004; Pacala and Socolow, 2004; White et al., 2004; Schrag, 2007). CO_2 emitted by sources such as power plants is separated and captured, and then is stored underground in geological reservoirs in CCS. Three most viable reservoirs for CO2 storage are deep saline formations, unmineable coal bed seems, and oil or gas reservoirs. While from a capacity perspective, deep saline formations offer significant potential. This approach would lock up the CO₂ for thousands of years. Studying the migration behavior of supercritical CO_2 and its leakage risk after it is injected into deep saline formations is the main concern in this paper.

Injection of CO_2 into deep saline formations for the purpose of emission avoidance dates back to the early 1980s. The first large-scale pure CO_2 geological sequestration project, Sleipner, was built in 1996. Since then, CO_2 geological sequestration has gained increasing attention as a carbon mitigation approach

from academia and industry. In the short-term CO₂ injection process, the migration of the injected CO₂ in geological media is mainly controlled by the buoyancy driven volume flow because of its smaller density compared with brine. However, in the long-term or geological time scale storage process, transport of CO₂ by convection and diffusion in brine-saturated porous media plays an important role in determining the long-term fate of the injected CO₂. In addition, the CO₂ movement in the deep saline aquifers may alter the chemo-physical properties of CO₂-brine-rock systems. It is thus clear that the trapping mechanisms to keep CO2 within deep geological formations rely on physical as well as chemical processes (Xu et al., 2003; Dooley et al., 2006; IPCC, 2005; Jaccard, 2005). Physical trapping mechanisms include structural and stratigraphic trapping by caprocks, hydrodynamic trapping by slow aquifer currents, and capillary trapping or residual trapping by interfacial forces. Chemical trapping mechanisms include dissolution of CO₂ in water, mineralization, CO₂ adsorption on coal and rich-organic shales, and CO₂ hydrate formation. Though CO₂ geological sequestration has advanced considerably in the last decade, the technology still is in its infancy and large-scale integrated projects (i.e. capture, transport and storage) do not yet exist. There are a total of about 20 pilot scale projects world-wide (Haszeldine, 2009) that are testing different aspects of the technology. One of the issues that remain uncertain is safety of the trapping mechanisms. The main risks associated with CO₂ geological sequestration lie



Figure 1. Phase diagram for pure CO₂.

in the possible leakage of the injected CO_2 back to the atmosphere or the leakage of CO_2 or brine into other geological formation, such as drinking water formations. Such leakage might harm the environment and health of the human being.

CO₂ geological sequestration presents new challenges to geotechnical engineering, such as the identification of target formations, injection engineering, assessment of trapping mechanisms, and final monitoring. In this paper, the mathematical model of CO2-brine two-phase flow in porous media was introduced to describe the transport process of injected CO₂ in deep saline formations, and the corresponding numerical model was present. The effects of anisotropy and different kinds of heterogeneity like horizontal and vertical layers and also existence of barriers between layers on the CO₂ flow and transport in a saturated porous media with brine are investigated. In addition, the capillary pressure on the buoyancy-driven flow of CO₂ is analyzed, and the XFEM is adopted to simulate the injection induced fracturing process of the naturally fractured caprock, which provides the theoretical bases for CO2 leakage risk analysis.

2 CO₂-BRINE TWO-PHASE FLOW IN POROUS MEDIA

When CO_2 is injected into a brine-saturated formation at a sufficiently high pressure, it displaces much of the brine in the pore space. In the process, the CO_2 brine interfaces occur at the pore scale and the two fluids coexist in the pore spaces. The existence of two fluid phases in the pore space significantly complicates the physical and chemical environment of the CO_2 -brine-rock system, and the associated mathematical description becomes concomitantly more complex (Nordbotten, Celia et al., 2008; Nordbotten, Kavetski et al., 2009). These pore-scale (mesoscale) processes will ultimately be represented by variables and parameters defined in REV or macroscale. In this section, the mathematical model for CO_2 -brine two-phase flow in porous media is presented.



Figure 2. Relationship between CO_2 density and viscosity, and temperature and pressure (from Nordbotten et al., 2005).

2.1 Equations of state and mass transfer for the CO₂-brine system

Equations of state for the CO2-brine system relate density and viscosity of a particular phase to pressure. The phase diagram for CO₂ is shown in Fig. 1. Generally, CO2 injection strategies to date involve injection into saline formations that are deep enough to have both temperature and pressure that exceed the critical point for CO_2 , that is, CO_2 will be in a supercritical state, which is at approximately 31°C and 7.4 MPa. The CO2 in this state exhibits both gas-like and liquid-like properties. It can moves through mall spaces in porous media like a gas, and can dissolve materials like a liquid. Given a typical geothermal gradient of 30°C/km and a surface temperature of about 25°C, the critical point is reached at a depth about 800 m. Therefore, most injections of CO₂ are expected to take place below 800 m.

The properties of CO_2 and brine will depend on pressure, temperature, and composition. For CO_2 , the main dependence is on temperature and pressure, while for brine, the temperature and pressure have little effect on its properties, and the composition play an important role. Relationships between the density and viscosity of CO_2 as a function of pressure and temperature are shown in Fig. 2, which illustrate that the properties of CO_2 have very strong variations around the critical point.

In general, the density and viscosity of CO_2 is less than that of brine. So in cases of CO_2 injection into brine-saturated saline formations, the CO_2 will be



Figure 3. Typical forms for relative permeability curves.

much less dense and much less viscous than the resident brine, and the buoyancy will drive CO_2 to upper of the formations.

2.2 Two-phase extension of Darcy's law

Darcy's law for two-phase flow is written as follows:

$$\mathbf{u}_{\alpha} = -\frac{k_{r,a}\mathbf{k}}{\mu_{a}}(\nabla p_{\alpha} + \rho_{a}g) \quad (\alpha = c, b)$$
(1)

where $\alpha = b$ for brine and $\alpha = c$ for CO₂, \mathbf{u}_{α} denotes the Darcy velocity vector for α phase, $k_{r,\alpha}$ denotes the relative permeability of α fluid phase, μ_{α} denotes the dynamic viscosity of α fluid phase, k is the intrinsic permeability, p_{α} and ρ_{α} denotes the pressure and density of α fluid phase, respectively. A typical form of the relative permeability function is illustrated in Fig. 3, which shows that the relative permeability is nonlinear function of saturation.

2.3 Component mass conservation equations

In CO_2 -brine two-phase system, the mass in each phase is a conserved quantity, satisfying

$$\frac{\partial(\rho_{\alpha}\phi_{\alpha})}{\partial t} + \nabla \cdot (\rho_{\alpha}\mathbf{u}_{\alpha}) = \psi_{\alpha} \quad (\alpha = c, b)$$
(2)

where the term ψ_{α} represents external sources or sinks for α phase, s_{α} denotes the saturation of α phase.

We combine equation (1) (Darcy's law) with equation (2) (the mass balance equation for a phase) to obtain the following

$$\rho_{\alpha}\phi\frac{\partial s_{\alpha}}{\partial t} + s_{\alpha}\rho_{\alpha}c_{\alpha}\frac{\partial p_{\alpha}}{\partial t} - \nabla \cdot \left[\rho_{\alpha}\frac{\mathbf{k}_{r,\alpha}\mathbf{k}}{\mu_{\alpha}}(\nabla p_{\alpha} + \rho_{\alpha}g)\right] = \psi_{\alpha}$$

$$(\alpha = c, b)$$
(3)

Because the pore space is always completely filled with fluid, the following equation is established

$$\sum_{\alpha} s_{\alpha} = s_b + s_c = 1 \tag{4}$$

The relationship between the saturation and the capillary pressure of CO_2 -brine two-phase system can be written as

$$p_c - p_b = p^{cap}(s_b) \tag{5}$$



Figure 4. A capillary pressure-saturation relationship curve.

where $p^{cap}(s_b)$ denotes the capillary pressure, illustrated in Fig. 4.

These four equations, equation (3) written for $\alpha = c$ and $\alpha = b$, equation (1), and equation (2) constitute the governing equations for CO₂-brine two-phase flow in porous media.

3 NUMERICAL MODELLING OF CO₂ GEOLOGICAL SEQUESTRATION IN DEEP SALINE FORMATIONS

Due to the complexity of the problem, numerical modelling is used to study the CO₂ geological sequestration process. Numerical methods for problems in porous media are the subject of rich and interesting research. In this section, we aim to study the effects of anisotropy and different kinds of heterogeneity like horizontal and vertical layers on the CO₂ injection. As an example, we define a saline formation to have a thickness of 100 m, porosity of 15%, and permeability of 10^{-12} m². The fluid properties are as follow, densities of 1099 kg/m³ and 733 kg/m³ for brine and CO₂, respectively, and viscosities of 0.5 mPa·s and 0.06 mPa·s. The residual brine and CO₂ saturations both are specified as 0.3. With these data, the numerical solution is calculated using the 2D axisymmetric model.

For isotropous and homogeneous formations, the CO_2 plumes are shown in Fig. 5, which described the distribution of this buoyancy-driven flow.

Assuming there are impermeable layers in this saline formation, the movement process of CO_2 changes due to the anisotropy and heterogeneity, just as shown in Fig. 6.

4 CO₂ INJECTION INDUCED FRACTURING ANALYSIS

The interaction between mechanical and fluid flow in fractured porous media gives rise to a host of coupled hydromechanical processes fundamental to rock formation instability, induced seismicity and associated fluid migration, including multiphase flow migration.

 CO_2 injection into deep saline formation using a high injection pressure disturbs inevitably the in-situ stress of the formation and its caprocks. And from section 3 in this paper, the injected CO_2 moves upward to the caprock or impermeable layer because of the driving of buoyancy, and thus the hydraulic pressure of CO_2 alters the stress state of the seal rocks, such as caprocks and impermeable layers. When the injection pressure is too high, the hydraulic pressure of the CO_2 -brine system will be higher correspondingly, and can lead to new fractures occurring or original cracks propagation. The injected CO_2 may have increasing probability of leakage form the formation. Therefore, there are risks of CO_2 leakage in CO_2 geological sequestration.

XFEM has been used very successfully to model fractures because the traditional finite element mesh can be created independent from the fracture geometry (Belytschko, et al., 2009; Richardson, et al., 2011), and in particular the domain does not have to be remeshed as the fracture propagating. In this section, we use extended finite element method (XFEM) to simulate the propagation of fractures induced by CO_2 injection. The propagation of fractures provides new channels for CO_2 to escape. The interaction between fractures propagation and CO_2 -brine two-phase flow migration is investigated.

Fig. 7 shows the hydraulic pressure of CO_2 -brine two-phase flow in an isotropous and homogeneous



Figure 5. Distribution of the injected CO₂.

formation, same with the formation in Fig. 6(b). The hydraulic pressure along line AB is illustrated in Fig. 8.

In every time step, the hydraulic pressure of CO_2 brine system is calculated and applied on the caprock or impermeable layer. If the pressure is high enough to make new fractures occur or original existing fractures propagate, the migration process of CO_2 -brine twophase flow will be calculated again using the updated porous media model. Though the repeating algorithm, the fracture propagation induced by CO_2 injection and CO_2 -brine two-phase flow process can be invested thoroughly.

We assume some fractures exist originally in the impermeable layer. CO_2 injection leads to the fractures to propagate, as shown in Fig. 9.

The propagation of fractures meanwhile provides new space for CO_2 -brine system to transport, which causes the CO_2 plume migrating along the fractures, and thus increases the leakage risk of CO_2 , as shown in Fig. 10.

From Fig. 9 and Fig. 20, the interaction process between caprock (or impermeable layer) and injected CO_2 can be made clear, which provides a theoretical fundamental for CO_2 leakage risk analysis of the CO_2



Figure 6. Distribution of the injected CO_2 in isotropous and homogeneous formations.



(b) a horizontal impermeable layers exist

Figure 6. Continued.



Figure 7. The hydraulic pressure of CO_2 -brine system in an isotropous and homogeneous formation.

geological sequestration projects. Obtaining an understanding of these fundamental processes is crucial to guaranteeing security of the storage sites.

5 CONCLUSIONS

In this paper, the mathematical model describing CO_2 brine two-phase flow in deep saline formations is presented, and the corresponding FEM numerical model is used to calculate the distribution of CO_2 . The numerical results show that the permeability of the rock formations and the permeability anisotropy should be



Figure 8. The hydraulic pressure of $\rm CO_2$ -brine system along line AB.



T=10 year

Figure 9. Fractures propagation induced by CO₂ injection.



Figure 10. CO₂ leakage along the propagated fractures.



Figure 10. Continued.

considered as the most important parameters in CO_2 flow and transport processes and its distribution in the rock formations.

Furthermore, the CO₂-brine two-phase hydraulic pressure has a significant effect on the in-situ stress field of the saline formation and its caprocks. By the calculated fluid hydraulic pressure, XFEM is applied to analyze the CO₂ injection induced fracturing process of the saline formation and its caprocks. The achievement in this paper makes clear the interaction between caprock (or impermeable layer) and CO₂-brine two-phase flow.

The presented mathematical model describing the CO_2 -brine two-phase flow in porous media in this paper does not include the geochemical process of the CO_2 -brine-rock system, which should be investigated further in future.

ACKNOWLEDGEMENTS

The financial supports by the National Natural Science Foundation of China (NSFC) (Grant No. 51009079), National Basic Research Program of China (No. 2011CB013500), and Open Research Fund Program of State key Laboratory of Hydroscience and Engineering (Grant No. 2013-KY-6 and 2012-KY-1) are greatly acknowledged.

REFERENCES

- Baines, S. J. and Worden, R. H. 2004. Geological Storage of Carbon Dioxide, 1–6 (The Geological Society of London).
- Belytschko, T., Gracie, R., and Ventura, G. 2009. A review of extended/generalized finite element methods for material modeling. Modelling and Simulation in Materials Science and Engineering 17(1): 1–31.
- Bradley, R. S. 2011. Many Citations Support Global Warming Trend, Science, 292 (5524).
- Crowley, T. J. 2000. Causes of Climate Change Over the Past 1,000 Years, Science, 289: 270–277.
- Dooley, J. J., Dahowski, R., Davidson, C., Wise, M. A., Gupta, N., Kim, S. H., and Malone, E. L. 2006. Carbon Dioxide Capture and Geologic Storage: A core element of a Global Energy Technology Strategy to address climate change, PNNL, Richland, WA.
- Gale, J. 2002. Overview of CO₂ emission sources, potential, transport and geographical distribution of storage possibilities. Intergov-ernmental Panel on Climate Change, Working Group III: mitigation of climate change. In: Workshop on carbon dioxide capture and storage, Regina, Canada, 15–30.
- Gasda, S. E., Bachu, S., and Celia, M. A. 2004. Spatial characterization of the location of potentially leaky wells penetrating a deep saline aquifer in a mature sedimentary basin, Environmental Geology, 46, 707–720.
- Haszeldine, R. S. 2009. Carbon Capture and Storage: How Green can Black Be?, Science, 325(5948), 1647–1652.
- IPCC. 2005. IPCC Special Report on Carbon Dioxide Capture and Storage. Prepared by Working Group III of the Intergovernmental Panel on Climate Change (Metz, B., O. Davidson, H. C. de Coninck, M. Loos, and L. A. Meyer (eds.)). 442 pp., Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA.
- Nordbotten, J. M., Celia, M. A. and Bachu, S. 2005. Injection and Storage of CO₂ in Deep Saline Aquifers: Analytical Solution for CO2 Plume Evolution During Injection, Transport in Porous Media, 58(3), 339–360
- Nordbotten, J. M., Celia, M. A., Dahle, H. K. and Hassanizadeh, S. M. 2008. On the definition of macroscale pressure for multiphase flow in porous media, Water Resour. Res., 44, W06S02.
- Nordbotten J. M., Kavetski, D., Celia, M. A. and Bachu, S. 2009. A semi-analytical model estimating leakage associated with CO₂ storage in large-scale multi-layered geological systems with multiple leaky wells, Environmental Science & Technology, 43(3), 743–749.
- Pacala, S., and Socolow, R. 2004. Stabilization wedges: Solving the climate problem for the next 50 years with current technologies, Science, 305(5686), 968–972.
- Richardson, C. L., Hegemann, J., Sifakis E., Hellrung J., and Teran, J. M. 2011. An XFEM method or modeling geometrically elaborate crack propagation in brittle materials, International Journal for Numerical Methods in Engineering, 88(10), 1042–1065.
- Schrag, D. P. 2007. Preparing to capture carbon, Science, 315, 812–813.
- White, D.J., Burrowes, G., Davis, T., Hajnal, Z., Hirsche, K., Hutcheon, I., Majer, E., Rostron, B. and Whittaker, S. 2004. Greenhouse gas sequestration in abandoned oil reservoirs: The International Energy Agency Weyburn pilot project, GSA Today, 14(7), 4–10.
- Xu, T., Apps, J.A. and Pruess, K. 2003. Reactive geochemical transport simulation to study mineral trapping for CO₂ disposal in deep arenaceous formations, Journal of Geophysical Research 108(B2), 2071–2083.