

# Numerical simulation of CO<sub>2</sub>-brine-rock interactions on CO<sub>2</sub> sequestration in Shihezi Formation of Ordos Basin in China

Liu B.<sup>1,2</sup>, Li Z.<sup>3</sup>, Fu X.<sup>2,\*</sup>, Lv Y.<sup>3</sup>

<sup>1</sup>Institute of Unconventional Oil-Gas, Northeast Petroleum University, Daqing 163318, China

<sup>2</sup>School of Electrical Engineering and Information, Northeast Petroleum University, Daqing 163318, China

<sup>3</sup>School of Earth Science, Northeast Petroleum University, Daqing 163318, China

\*corresponding author: LIU B.: e-mail: liubin.nepu@hotmail.com

## Abstract

Geochemical reactions play an important role in CO<sub>2</sub> geological storage environments. CO<sub>2</sub>-brine-rock interactions will be enhanced in low pH environment, because of acidity in reservoir being strengthened due to CO<sub>2</sub> dissolution. TOUGHREACT is used conduct kinetic batch modeling and reactive transport modeling in Shihezi formation in Ordos basin, where the first CCS project is carried out in China. Simulations are based on the core data, which are focused on effects of CO<sub>2</sub> for pH, gas saturation, geochemical interactions, porosity and permeability in formation. Results show that K-feldspar and albite, main components of alkaline feldspar, are dissolved, while ankerite and siderite are precipitated. Quartz, calcite and dawsonite are dissolved first and then precipitated, whose reaction mechanisms are associated with environment pH value, temperature and electrolyte existing. These results are consistent with observations in laboratory experiments. For CO<sub>2</sub> sequestration, whether minerals are dissolved and precipitated, amount of CO<sub>2</sub> will be consumed, which will promote CO<sub>2</sub> dissolution in formation resulting in CO<sub>2</sub> sequestered underground. These processes may be very slow, but dissolved and mineralized deposits are ideal CO<sub>2</sub> storage.

**Keywords:** CO<sub>2</sub> geological storage; CO<sub>2</sub>-brine-rock interaction; reactive transport model

## 1. Introduction

CO<sub>2</sub> geological storage is one of the most important technologies in Carbon Capture and Storage (CCS) (Bachu S., et al, 2003, 2007). Characteristics of reservoir and caprock are key factors for long term storage, whereas effects of injected CO<sub>2</sub> in geological site can not be ignored, which play momentous roles for safe sequestration. CO<sub>2</sub> commercial utilization and storage projects have accumulated abundant experiences and real testing data (Bateman K., et al, 2013; Mitiku A. B., et al, 2013), which can provide reference significance.

CO<sub>2</sub>-brine-rock geochemical interactions are focused on as well as geomechanics in CCS. There are two techniques concerned on geochemical reactions: experiments and numerical simulation. In the former, products can be observed directly and analyzed by instruments. However, limitations on core samples

amount, core samples differences, and time scales, will restrict the reliability and generalization of experiments. Furthermore, properties of pore structure, fluid contents variety changed by CO<sub>2</sub> injection will not be verified simply in laboratory. Numerical simulation can reproduce multi-component solute transport process for thousands of years, where integrates several processes including fluid flow, solute transport and geochemical reaction.

## 2. CO<sub>2</sub> Storage Area and Main Interactions

### 2.1. Background

Shenhua group is the largest coal enterprise of China, which is carrying out the first demonstration project of exhaust gas capture and storage in saline aquifer from the process of coal liquefaction (Wu Y., 2013). Simulations are based on the core data from Shihezi formation of Ordos basin including minerals content and brine composition (Wang T., et al, 2013).

### 2.2. main geochemical interactions and their effects

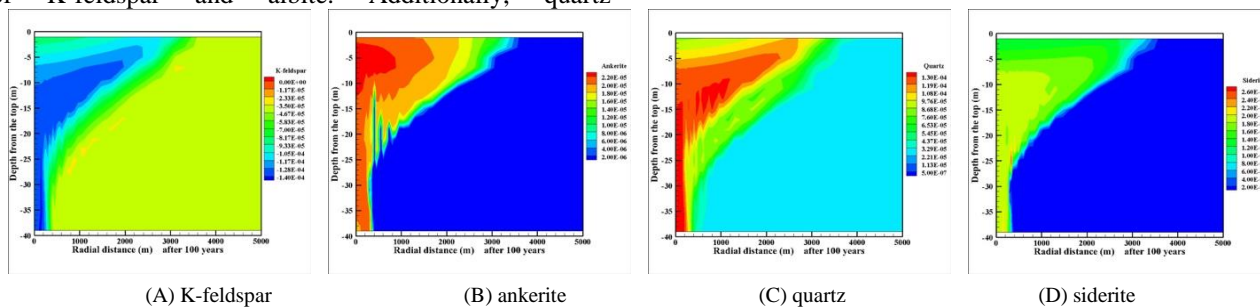
At the initial phase of CO<sub>2</sub> injection, CO<sub>2</sub> will be stored in free state in the reservoir. Hydrogen ion, induced by carbonic acid due to CO<sub>2</sub> dissolution, will reduce the pH value of brine, which will increase the reactivity of rock, and provide initial conditions for the CO<sub>2</sub>-brine-rock reaction. Minerals dissolution and precipitation occur simultaneously. If the former predominates, reservoir porosity will increase as well as its permeability. Otherwise, if minerals precipitation plays a dominant role in reactions, reservoir porosity will reduce as well as its permeability.

Sawtooth structure is formed on the cleavage surface of the clastic albite, indicating albite dissolution during CO<sub>2</sub> sequestration. However, dawsonite, as the main product of the albite dissolution, can not be found. This means it dissolves after precipitation.

K-feldspar is the key component of alkaline feldspar, which dissolves as well as albite, depicted in Fig. 1(A). Kaolinite, product of K-feldspar dissolution, precipitates first and then dissolves in acidic condition. After 100 years, there is almost no kaolinite observed. There is no ankerite observed after CO<sub>2</sub> injection 10 years, either.

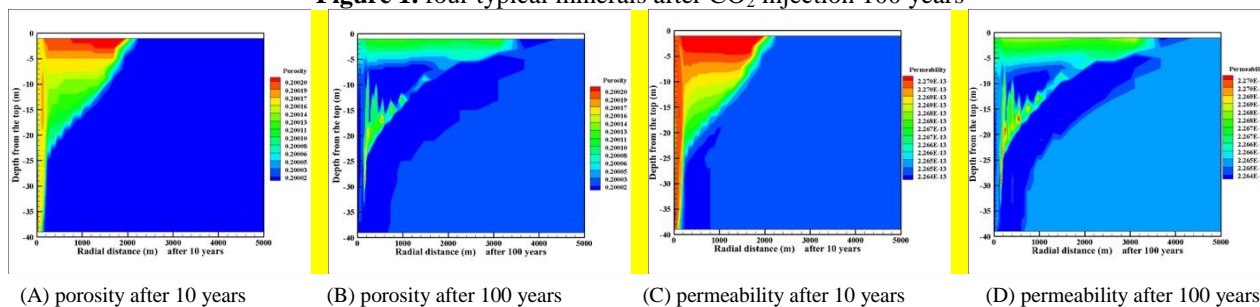
However, amount of ankerite is precipitated after 100 years, depicted in Fig. 1(B). At first, Quartz dissolves predominantly in acidic environment because of salt effect due to electrolyte existing. During CO<sub>2</sub> sequestration, quartz precipitation is related to dissolution of K-feldspar and albite. Additionally, quartz

precipitation strength is also associated with environment pH value, depicted in Fig. 1(C). Siderite, as an insoluble carbonate, is precipitated in great amount after CO<sub>2</sub> injection, depicted in Fig. 1(D), where Fe<sup>2+</sup> comes from composition FeSO<sub>4</sub> in brine.



(A) K-feldspar (B) ankerite (C) quartz (D) siderite

Figure 1. four typical minerals after CO<sub>2</sub> injection 100 years



(A) porosity after 10 years (B) porosity after 100 years (C) permeability after 10 years (D) permeability after 100 years

Figure 2. Variations of porosity and permeability

### 2.3. evolution of pore structure in reservoir

Variations of both porosity and permeability are similar, depicted in Fig. 2, because the relationship between porosity and permeability is chosen as positive correlated. On one hand, large amount of CO<sub>2</sub> will enter into rock pore under the pressure during CO<sub>2</sub> injection, where the predominant CO<sub>2</sub>-brine-rock interactions are minerals dissolution. Reservoir porosity increase is beneficial to expanding storage capacity for reservoir, and the corresponding permeability will improve mobility of multi-phase fluid. On the other hand, CO<sub>2</sub> migration will raise the efficiency of residual CO<sub>2</sub> storage and dissolved CO<sub>2</sub> storage, which has a positive effect on the feasibility of CO<sub>2</sub> storage.

### 3. Conclusion

CO<sub>2</sub>-brine-rock interaction will lead to amount of CO<sub>2</sub> mineralization referred to as mineral trapping after CO<sub>2</sub> injection. Furthermore, variations of porosity and permeability, caused by CO<sub>2</sub>-brine-rock interaction, will promote mineral composition dramatically in reservoir. It has significant influence on CO<sub>2</sub> storage capacity.

### Acknowledgment

This work is supported by National Natural Science Foundation of China under Grant No. 41602134, U1562214, China Postdoctoral Science Foundation under Grant No. 2017T100223, Outstanding Youth Program of Heilongjiang Natural Science Foundation under Grant No. YQ2019D001.

### References

Bachu S. and Adams J. J. (2003), Sequestration of CO<sub>2</sub> in geological media in response to climate change: capacity of deep saline aquifers to sequester CO<sub>2</sub> in solution, *Energy Conversion and Management*, 44, 3151-3175.

Bachu S., Bonijoly D., Bradshaw J., Burruss R., Holloway S., Christensen N. P. and Mathiassen O. M. (2007), CO<sub>2</sub> storage capacity estimation: Methodology and gaps, *International Journal of Greenhouse Gas Control*, 1, 430-443.

Bateman K., Rochelle C. A., Purser G., Kemp S. J. and Wagner D. (2013), Geochemical Interactions Between CO<sub>2</sub> and Minerals within the Utsira Caprock: A 5-year Experimental Study. *Energy Procedia*, 37, 5307-5314.

Mitiku A. B., Li D., Bauer S. and Beyer C. (2013), Geochemical modelling of CO<sub>2</sub>-water-rock interactions in a potential storage formation of the North German sedimentary basin, *Applied Geochemistry*, 36, 168-186.

Wu Y. (2013), Carbon Dioxide Capture and Geological Storage the First Massive Exploration in China, Science Press, Beijing.

Wang T., Wang H., Zhang F. and Xu T. (2013), Simulation of CO<sub>2</sub>-water-rock interactions on geologic CO<sub>2</sub> sequestration under geological conditions of China, *Marine Pollution Bulletin*, 76, 307-314.