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## Molecular Dynamics Study on Coal Matrix Swelling Characteristics by CO<sub>2</sub>, N<sub>2</sub>, and CO<sub>2</sub>-N<sub>2</sub> Mixture

Tuesday, 1 June 2021 10:00 (1 hour)

**Background:** Coalbed methane (CBM) is an important natural gas resource of growing interest [1,2]. The injection of CO<sub>2</sub> can enhance CBM recovery, meanwhile, CO<sub>2</sub> can be stored in the coalbed layer. However, CO<sub>2</sub> may induce coal matrix swelling, and an inappropriate injection design may result in the cleat closure of the coal system [3,4]. On the other hand, N<sub>2</sub> was effective to promote CH<sub>4</sub> desorption and improve sweep efficiency [5,6]. However, the major drawback associated with N<sub>2</sub> injection is that it tends to lead to an early breakthrough. In the CBM reservoirs, the coal matrix is associated with a large number of micropores that are less than 2 nm. The swelling occurs is due to the adsorption behavior in the micropores [7,8]. Due to limitation of laboratory experiments to the gas adsorption status in the micropores, the replacement process of CH<sub>4</sub> in the coal matrix and the swelling/shrinkage mechanism of the coal matrix are poorly understood.

**Methods:** In this paper, we studied the CH<sub>4</sub> recovery process by injecting CO<sub>2</sub>, N<sub>2</sub>, or CO<sub>2</sub>-N<sub>2</sub> mixture into the coal matrix using molecular dynamics simulations. The relationship between the swelling of coal matrix due to the adsorption, and permeability decline due to swelling, were then discussed. A model of a coal matrix filled with CH<sub>4</sub> was constructed, and the CO<sub>2</sub> (N<sub>2</sub> or CO<sub>2</sub>-N<sub>2</sub>) molecules were added into a large-size fracture of the coal system. This system was equilibrated to investigate coal swelling and the replacement process. A long enough simulation was performed, to allow CO<sub>2</sub> (N<sub>2</sub> or CO<sub>2</sub>-N<sub>2</sub>) molecules enough time to enter the coal matrix and displace the CH<sub>4</sub> molecules.

**Findings:** The calculated recovery factors were 79.9, 54.3, and 70.5% for CO<sub>2</sub>, N<sub>2</sub>, and CO<sub>2</sub>-N<sub>2</sub> mixture injection, respectively. After equilibration, the specific volume (i.e. volume per unit mass) and thickness of the coal matrix were estimated and compared to those at the initial stage for estimation of the coal swelling. There is a swell of 12–17% in the pure liquid CO<sub>2</sub> injection. There are no swell in the pure N<sub>2</sub> case and CO<sub>2</sub>-N<sub>2</sub> mixture case, shrinkage may be observed during N<sub>2</sub> injection and negligible during the CO<sub>2</sub>-N<sub>2</sub> mixture injection. The permeability change was also estimated by using the coal matrix swell data. The swelling estimated by the specific volume for the pure CO<sub>2</sub> case is about 17%. Therefore, the estimated permeability will drop to 0.4% of the original one. The reported porosity of the actual field has some uncertainty, but, if the natural fracture porosity of 0.4% [5] was used, the cleat will be fully closed then. Apart from the micropores, the formation becomes almost impermeable. These findings agrees with previous reports [3,6,7]. In conclusion, in the case of pure liquid CO<sub>2</sub>, the permeability will reduce dramatically. For pure N<sub>2</sub>, it can be helpful to enhance the permeability. If we carefully choose the mole fraction of CO<sub>2</sub>-N<sub>2</sub> mixture, the permeability reduction may be avoided, while keeping enough high CH<sub>4</sub> recovery factor.

### Time Block Preference

Time Block A (09:00-12:00 CET)

### References

1. Moore TA. Coalbed methane: A review. *Int. J. Coal Geol.* 2012; 101: 36–81.
2. White CM, Smith DH, Jones KL, Goodman AL, Jikich SA, LaCount RB, Dubose SB, Ozdemir E, Morsi BI, Schroeder KT. Sequestration of carbon dioxide in coal with enhanced coalbed methane recovery—A review. *Energy Fuels.* 2005; 19: 659–724.

3. Reeves S. Field studies of enhanced methane recovery and CO<sub>2</sub> sequestration in coal seams. *World Oil*. December 2002; 56–60.
4. Fujioka M, Yamaguchi S, Nako M. CO<sub>2</sub>-ECBM field tests in the Ishikari Coal Basin of Japan. *Int. J. Coal Geol.* 2010; 82:287–298.
5. Durucan S, Shi J-Q. Improving the CO<sub>2</sub> well injectivity and enhanced coalbed methane production performance in coal seams. *International Journal of Coal Geology.* 2009; 77: 214–221.
6. Lin W, Tang G-Q, Kovscek AR. Sorption-Induced Permeability Change of Coal During Gas-Injection Processes. *SPE Reservoir Evaluation & Engineering.* 2008; 11: 792–802.
7. Xue Z, Ohsumi T. Experimental studies on coal matrix swelling due to carbon dioxide adsorption and its effect on coal permeability. *Journal of MMIJ.* 2005; 121: 231–239.
8. Pang J, Liang Y., Masuda Y, Matsuoka T, Zhang Y, Xue Z. Swelling phenomena of the nonswelling clay induced by CO<sub>2</sub> and water cooperative adsorption in Janus-surface micropores. *Environ. Sci. Tech.* 2020; 54: 5767–5773.

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