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Molecular Dynamics Study on Coal Matrix Swelling Characteristics by CO2, N2, and CO2–N2 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 CO2 can enhance CBM recovery, meanwhile, CO2 can be stored in the coalbed layer. However, CO2 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, N2 was effective to promote CH4 desorption and improve sweep efficiency [5,6]. However, the major drawback associated with N2 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 CH4 in the coal matrix and the swelling/shrinkage mechanism of the coal matrix are poorly understood.

Methods: In this paper, we studied the CH4 recovery process by injecting CO2, N2, or CO2–N2 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 CH4 was constructed, and the CO2 (N2 or CO2–N2) 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 CO2 (N2 or CO2–N2) molecules enough time to enter the coal matrix and displace the CH4 molecules.

Findings: The calculated recovery factors were 79.9, 54.3, and 70.5% for CO2, N2, and CO2–N2 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 CO2 injection. There are no swell in the pure N2 case and CO2–N2 mixture case, shrinkage may be observed during N2 injection and negligible during the CO2–N2 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 CO2 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 CO2, the permeability will reduce dramatically. For pure N2, it can be helpful to enhance the permeability. If we carefully choose the mole fraction of CO2–N2 mixture, the permeability reduction may be avoided, while keeping enough high CH4 recovery factor.

Time Block Preference

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

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