Contribution ID: **972** Type: **Oral 20 Minutes**

Molecular Simulation of Competitive Adsorption behaviors of CO2/CH4 Mixtures on Shale Clay Minerals

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Objectives:
CO2 injection, as one of the effective techniques for enhancing recovery of shale gas, has been widely used and proved economically available. In shale, clay minerals play an important role on methane adsorption due to its large volume of micropores. So far, however, a few attentions have been paid on competitive adsorption of CO2/CH4 Mixtures on clay minerals. In this study, we conduct molecular simulations of CO2/CH4 mixtures to provide a better understanding of competitive adsorption behaviors on clay minerals with the grand canonical Monte Carlo (GCMC) simulation.
Methods Procedures/Process:
We conduct GCMC simulations of CO2/CH4 mixtures adsorption in various clay minerals. Based on the actual conditions of shale gas reservoir, the competitive adsorptions of CO2/CH4 mixtures are investigated at various temperatures of 303.15K, 333.15K, and 363.15K with the pressure range of 0-35Mpa. For comprehensive comparison, the effects caused by pore size, mole fraction of CO2/CH4, and different clay minerals on competitive adsorption are processed. The competitive adsorption behaviors are characterized by selectivity and such key parameter are employed to evaluate the density profiles of CO2 and CH4, the characteristics of CO2 adsorption over CH4, and the timing of CO2 Injection.
Results/Observes/Conclusions:
Due to strong quadrupole moment and higher van der Waals interactions, CO2 possess a stronger affinity for clay minerals than that of methane, which is nonpolar. CH4 has the characteristic of single-layered adsorption, while the CO2 is able to form multi-layers adsorption with higher adsorption amount. Molecular simulations results show that the selectivity of CO2 in competitive adsorption decrease with decreasing of pressure. In addition, the selectivity of CO2 is independent on temperature. Because of negatively charged silicate layers, CO2 adsorption in nanopores of illite and montmorillonite are stronger than that of in kaolinite. As a result, the selectivity of CO2 in kaolinite models is less than that of in illite and montmorillonite models. When pressure is higher than 10Mpa, however, the selectivity of CO2 in three different clay minerals are similar. Due to the more adsorption sites occupied by CO2, the selectivity increases with mole fraction of CO2. By comparison with different pore size adsorption, the selectivity is insensitive to the mole fraction in micropores, while it increases with the increasing of mole fraction of CO2 in mesopores.
Novelty:
This work is a study on CO2/CH4 Mixtures adsorption behaviors on shale clay minerals. The molecular simulations with GCMC are proposed to give an insight in competitive adsorption mechanism, which is expected to provide a more accurate understanding of CO2 injection for enhancing recovery of shale gas.

References

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