Goldschmidt 2021 Abstract
https://doi.org/10.7185/gold2021.6780

Asymmetric Competitive Adsorption of CO_2/CH_4 Binary Mixture in Shale Matrix with Heterogeneous Surfaces

JINGYUE SUN, YUE ZHANG, YINGYING CUI, CONG CHEN AND WEIZHONG LI

Dalian University of Technology

Presenting Author: sunjingyue@mail.dlut.edu.cn

Under the background of intensified global energy crisis and greenhouse effect, The CO_2 sequestration and enhanced gas recovery (CS-EGR) technology has gained worldwide attention. Understanding the competitive adsorption mechanism of CO_2/CH_4 in shale matrix and the influence of reservoir parameters on competitive adsorption characteristics plays an important role in increasing shale gas production and CO_2 storage. However, it has not been fully understood, especially in pores composed of organic-inorganic materials. In the CS-EGR process, the mole fraction of CO_2 and CH_4 in the reservoir is an important parameter. The fixed mole fraction of CO_2 and CH_4 in the bulk phase is usually used to study the competitive adsorption characteristics, but it is difficult to control in actual engineering implementation. In this paper, taking the fixed mole ratio of CO_2 and CH_4 in total shale pores as one of the reservoir parameters, a pore model composed of graphene-MMT heterogeneous surface was proposed to study the competitive adsorption characteristics of CO_2/CH_4 mixture in shale matrix by molecular dynamics (MD) simulations.

Absolute adsorption selectivity based on the fixed mole fractions of CO_2 and CH_4 in the total shale pores has been proposed to evaluate the competitive adsorption features with relative adsorption selectivity. A strong asymmetric competitive adsorption behavior of CO_2 and CH_4 has been observed from density distribution, absolute adsorption amount, the proportion of adsorbed gas as well as adsorption selectivities. The competitive adsorption behavior near the MMT surface lags behind that near the graphene surface, especially in pores with a pore size of 3 ~ 8 nm. It is considered that the confinement effect of the pore leads to the competition for the gas source in the pore between the heterogeneous surfaces. The confinement effect near the graphene surface is obvious when the pore size is smaller than a critical pore size of 6 nm. The confinement effect of CO_2 in pores with heterogeneous surfaces is more obvious than that of CH_4. Based on absolute and relative adsorption selectivity under different pressure, gas ratio and pore size, the optimal operation conditions have been discussed and the results may help for CS-EGR project.