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CO_2/CH_4 Adsorption and Diffusion in Inorganic Nanopores: Effects of Force fields and Mineral Compositions

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CH_4, as one of clean fossil fuels, is the main component of emerging unconventional resources for shale gas. Researchers have confirmed that CO_2 can be adsorbed preferentially over CH_4 onto organic/inorganic surfaces in shale matrix. CO_2 enhanced gas recovery technique (CO_2-EGR), where CO_2 is applied to displace CH_4 for shale gas production and meanwhile to sequestrate CO_2 in shale matrix, is recognized as one of the most potential techniques to produce shale gas.

CO_2/CH_4 adsorption, desorption, diffusion and replacement are key processes to understand migration of shale gas as well as injected CO_2. In the past two years, many researches have been done on these key processes to investigate the characteristics and mechanisms. Most of these studies are focusing on nanopores formed in organic matter or inorganic minerals. The interaction between CO_2/CH_4 and inorganic minerals is strongly affected by mineral compositions. The adsorption, desorption, diffusion and displacement processes in nanopores formed between different inorganic minerals should be strongly controlled by mineral compositions. Several force fields for CO_2 and CH_4 have been applied either united atoms or all atoms styles. However, how much close do these force fields predict adsorption and diffusion characteristics has not been investigated yet. In the present study, the effects of force fields as well as mineral compositions are explored and the results show that they affect much for these key processes.