

Microscopic Investigation on Adsorption of Shale Gas in Nanopores

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Abstract

With the decrease of oil reserves and the severity of climate problem, shale gas has been paid more and more attention due to its numerous advantages such as wide distribution, abundant resource and long production cycle. Shale gas, which is primarily composed of methane, has a variety of storage methods such as adsorbed gas, free gas and has multi-scale flow mechanisms such as gas desorption, gas diffusion, Non-Darcy flow and Darcy flow. Among them, the adsorbed methane has a great influence on the prediction and exploitation of shale gas.

In this study, the microscopic mechanism about adsorption of methane in nanopores is investigated through molecular dynamics (MD) simulations. Due to the adsorption of the pore walls, the storage capacity of the slit pore is higher and the potential energy of methane in the adsorption layer is lower compared to the bulk phase. The adsorption structures and adsorption isotherms of different slit pores are simulated and compared. As the width of slit pore increases, the structure of adsorbed methane transforms from a single-layer chain to four adsorption layers. Moreover, it is found that more methane can be stored in small pores under relatively lower pressure. Our work can be of great significance for revealing the mechanism of adsorption and guiding the exploitation of shale gas.

Keywords: Shale gas, Molecular dynamics simulation, Adsorption structure, Adsorption isotherm