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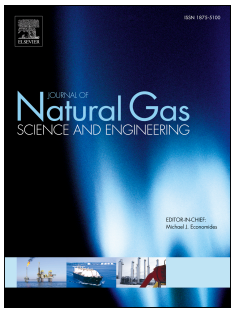

Selective adsorption of supercritical carbon dioxide and methane binary mixture in shale kerogen nanopores

Tianyu Wang, Shouceng Tian, Gensheng Li, Mao Sheng

PII: S1875-5100(17)30472-9

DOI: 10.1016/j.jngse.2017.12.002

Reference: JNGSE 2377

To appear in: *Journal of Natural Gas Science and Engineering*

Received Date: 22 September 2017

Revised Date: 7 December 2017

Accepted Date: 10 December 2017

Please cite this article as: Wang, T., Tian, S., Li, G., Sheng, M., Selective adsorption of supercritical carbon dioxide and methane binary mixture in shale kerogen nanopores, *Journal of Natural Gas Science & Engineering* (2018), doi: 10.1016/j.jngse.2017.12.002.

Selective Adsorption of Supercritical Carbon Dioxide and Methane Binary Mixture in Shale Kerogen Nanopores

Tianyu Wang, Shouceng Tian, Gensheng Li, Mao Sheng

(State Key Laboratory of Petroleum Resources and Prospecting, China University of Petroleum, Beijing 102249, China)

ABSTRACT

The adsorption of carbon dioxide and methane binary mixture in shale kerogen nanopores and the underlying mechanism significantly affect the supercritical carbon dioxide enhanced shale gas development project. In this study, we investigated the adsorption properties of carbon dioxide and methane in shale kerogen using grand canonical Monte Carlo (GCMC) method. Shale kerogen was fabricated based on Ungerer molecular model and its parameters were validated. The effects of temperature, pressure, mole fraction on the adsorption isotherms, average isosteric heat, potential energy distribution, and adsorption selectivity of binary mixture were discussed. The results show that the absolute adsorption capacity of methane in binary mixture decreases as temperature increases, but increases as mole fraction increases. Compared with methane, carbon dioxide is in lower energy absorption sites, which indicates the adsorption capacity of carbon dioxide in shale kerogen is stronger than that of methane. The adsorption selectivity of carbon dioxide over methane first decreases as pressure increases until pressure reaches critical pressure (7.38 MPa for