Adsorption and displacement of methane in graphene-based microstructures: insight from molecular simulations

Dias Bekeshov[1*], Sultan Ashimov[1], Yanwei Wang[1,2*] and Lei Wang [3,4]

[1]*Department of Chemical & Materials Engineering, School of Engineering and Digital Sciences,Nazarbayev University, Nur-Sultan 010000, Kazakhstan*

[2]*Laboratory of Computational Materials Science for Energy Applications, Center for Energy and Advanced Materials Science, National Laboratory Astana, Nur-Sultan 010000, Kazakhstan* [3]*College ofEnergy, Chengdu University of Technology, Chengdu 610059, China*

[4]*School of Mining and Geosciences, Nazarbayev University, Nur-Sultan 010000, Kazakhstan*

*E-mail: dias.bekeshov@nu.edu.kz (D.B); yanwei.wang@nu.edu.kz (Y.W.)

Shale gas and coalbed methane are alternative energy sources that partly or even mainly consist of methane stored in an adsorbed state in pores of organic-rich rock and coal seams. This study employed a combination of Grand Canonical Monte Carlo (GCMC) and Molecular Dynamics (MD) simulations to investigate the mechanisms of gas adsorption and displacement of methane in coal microstructures, which were modeled as slit pores with the slit walls modelled by graphene layers. The adsorption of various gases (CO_2, CH_4, N_2) in such microstructures were quantified at different pore sizes and temperature-pressure conditions. The following findings were obtained: (1) The minimum slit pore size at which molecules can penetrate the pore was found to be ~0.7 nm, and as expected, the amount of methane adsorption increased with the increase of the slit width, and the structure of the adsorbed methane transitioned from a single adsorption layer to multiple adsorption layers; (2) the amount of adsorption for all three cases (CO_2, CH_4, N_2) was found to increase with increasing pressure, and for most cases, the amount of adsorption increased with decreasing temperature; and (3) The comparison of the amount of adsorption of gas molecules provided the following order, $CO_2 > CH_4 > N_2$, at 298 K and atmospheric pressure and a pore size of 1 nm. Enhancing methane recovery was also investigated by injecting CO_2 or N_2 gas to displace the adsorbed methane. This study provides a preliminary understanding of the competitive adsorption mechanisms of methane, carbon dioxide, and nitrogen in organic nanopores common in shale gas and coalbed methane reservoirs

Acknowledgement

This research was supported by the “Simulation of sour gas injection EOR in tight carbonate reservoirs coupling capillarity and geomechanics” project (Grant Award Number 080420FD1918) and the “Development of cryogenic fracturing technology for coalbed methane production in Karaganda Coal Basin, Kazakhstan” project (GrantAward Number 021220CRP2022).