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A molecular simulation and laboratory characterization study of micropore and sorption sites impact on methane adsorption in kerogen

Wei Li¹, Lee Stevens¹, Dingye Zheng², and Colin Snape¹

¹University of Nottingham, Faculty of Engineering, Chemical and Environmental Engineering, Nottingham, United Kingdom of Great Britain – England, Scotland, Wales (wei.li2@nottingham.ac.uk)

²State Key Laboratory of Petroleum Resources and Prospecting, China University of Petroleum (Beijing), Beijing, 102249, China

The evaluation of shale gas in place by adsorption and free gas is critical for future shale gas reserves development. Laboratory experiments suggest that approximately 50% of the stored shale gas is adsorbed onto the kerogen. Molecular simulation researches suggest methane adsorption capacity increases with the increasing maturity of kerogen. Understanding how thermal maturity controls methane adsorption in kerogen is crucial for predicting shale gas resources. Although porosity and chemical surface functionalities (sorption sites) are the main difference between kerogens with different maturity, the study of their impact on methane adsorption via both simulation and experiment methods is in the preliminary stage.

The comparison of molecular simulations on Type II kerogen matrix with slit models and laboratory experiments on isolated kerogens are carried out to illustrate their impact on methane adsorption in kerogen with different maturity, and reveal the predominant controlling factor. Grand Canonical Monte Carlo (GCMC) and molecular dynamic (MD) simulations are applied to obtain simulation results, including the micropore texture, methane adsorption capacity, and adsorption behavior. Laboratory experiments, high-pressure methane adsorption, low-pressure gas sorption, scanning electron microscopy, and Transmission Electron Microscope, are carried out on isolated kerogens for verifying and comparing with simulation results.

The results indicate micropore volume (V_{micro}) and equilibrium methane adsorption amount (Q_m) of isolated kerogens (10-75 mm³/g TOC, and 21.3-75.8 mg/g TOC) are comparable with simulated overmature (KIID) matrix and slit kerogens (19-261 mm³/g TOC, and 36.5-148 mg/g TOC). The higher results from the simulation are due to the pore interconnectivity is not considered in simulated kerogens. Both experiment and simulation suggest Type I (a) isotherms are contributed by small micropores, and Type I (b) isotherms are contributed by larger micropores. The methane adsorption capacity of the kerogen matrix increases with increased maturity and decreases with increased temperature. A positive correlation between V_{micro} and Q_m is observed with $R^2 > 0.96$. The relative number density and relative coordination number of methane around functional groups at 25 and 100 °C from molecular dynamic (MD) simulation show methane only have

selectivity with few functional groups at very low pressure (<1.6 bar at 25 °C), and the affinity becomes close and weaker at higher pressure. Moreover, similar adsorption heats (23.2, 23.1, 23.5, 22.8 kJ/mol) of methane with different maturity kerogens are observed, showing the interactions between methane and different kerogens are close. Therefore, the impact of functional groups on the methane adsorption capacity is minimal, especially in high-pressure conditions, and micropore is regarded as the key control for methane adsorption.