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A Dual-site Simplified Local Density Model for Shale Gas Adsorption under Reservoir Conditions

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Direct measurement of shale gas adsorption isotherms at high pressures and high temperatures (HPHT) is intricate and requires expensive apparatuses. Most of the documented studies only report shale gas adsorption data at pressures below 12 MPa, which is much smaller than the reservoir pressure, e.g., up to 36 MPa in Eagle Ford shale. Recent studies also suggest that the excess adsorption isotherm of shale gas exhibits distinct features from that observed at low pressures. Therefore, predicting gas adsorption isotherms at reservoir conditions may be useful.

On the basis of the simplified local density (SLD) theory, we developed a novel dual-site adsorption model for shale gas. Shale matrix composed of both organic matter and inorganic minerals and the pores located within kerogen can be smaller than inorganic pores. Our grand canonical Monte Caro (GCMC) simulations also confirm that the adsorption capacity of organic matter is much greater than those of inorganic minerals. Therefore, the model for shale gas adsorption isotherms should distinguishes methane adsorption in kerogen surface from that of the inorganic substrates. Our proposed dual-site SLD model takes into account the different pore sizes and fluid-solid interaction energy parameters of organic matter and inorganic minerals.

We first used conventional SLD model to match the excess adsorption isotherms of CH4 in graphene and montmorillonite slit (pressure: 0-40 MPa). Excellent agreements are observed, which manifest that the SLD model is able to describe gas adsorption in a slit at both subcritical and supercritical states. Then we examined the validity of our proposed dual-site model using high-pressure CH4 adsorption isotherms on shale reported in the literatures. These experimental data were measured at pressures up to 25 MPa and temperatures up to 150 ℃. Our proposed model fit these adsorption isotherms very well. If we use the experimental results measured at low pressures (<12 MPa) to make the fit, the high-pressure isotherms predicted using the fitted parameters are very close to the measured data, which demonstrated the validation of our model.

We also probed the differences of original gas-in-place (OGIP) and production performance estimated using low-pressure adsorption isotherms (always characterized using the Langmuir adsorption isotherms) and high-pressure adsorption isotherms. The great derivations suggest that reliable adsorption isotherms of shale gas under reservoir conditions are very essential. Our proposed dual-site SLD model provides an alternative method to predict shale gas adsorption isotherms under reservoir conditions using low-pressure experimental measurement.

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