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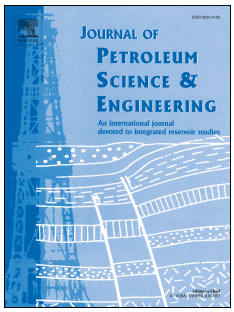

Molecular simulation of methane adsorption on type II kerogen with the impact of water content

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Molecular simulation of methane adsorption on type II kerogen with the impact of water content

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Abstract:

Based on realistic kerogen model, the effects of water content on methane (CH_4) adsorption capacity were studied qualitatively and quantitatively using the molecular dynamics (MD) and Monte Carlo (MC) simulation methods. The methane single component adsorption process under the dry condition, methane and water two components competitive adsorption on dry kerogen, and methane single component adsorption on moist conditions (0.6, 1.2, 1.8, 2.4, and 3.0 wt.%) were simulated. Adsorption processes under different temperatures (298, 323, and 348 K) were modeled, and the pressure was up to 20 MPa. Simulation results show that the absolute adsorption capacity of CH_4 on the dry kerogen increases with the increasing pressure but decreases with the increasing temperature. The excess adsorption capacity increases up to a specific pressure and then declines with the increasing pressure. The competitive adsorption simulation results indicate that kerogen prefers to adsorb water (H_2O) than CH_4. At the pressure of 20 MPa and temperature of 298 K, the competitive adsorption capacity of CH_4 (0.53 mmol/g) is only a seventh of the single component adsorption capacity of CH_4 (3.92 mmol/g) on dry kerogen. The CH_4 adsorption capacity on moist kerogen also decreases with the increasing moist content. Compared with the absolute adsorption capacity on the dry kerogen (3.92 mmol/g), the adsorption capacity on the moist kerogen reduces about 16%, 30%, 40%, 47%, and 55% at 20 MPa, respectively. The reduction of the adsorption capacity is attributed to the strong attraction