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Effect of Water-Based Fracturing Fluid on Methane Adsorption in Deep Shale Organic Nanopores from the Perspective of Molecular Simulations

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Abstract : Water-based fracturing stimulation is widely used in the shale gas stimulation field. Field data indicate that after fracturing, a significant portion of the fracturing fluid remains in shale gas reservoirs, ultimately affecting methane adsorption behavior. This study aims to investigate the stability of water-based fracturing fluid in the reservoir and its impact on methane adsorption behavior. In this study, ⅡD kerogen was used to construct a shale nanoslit pore model, and three main additives of common water-based fracturing fluids were constructed: polyacrylamide (PAM), hydroxypropyl Guar gum and cetyltrimethylammonium bromide (CTAB). Based on the Grand Regular Monte Carlo method and molecular dynamics equilibrium simulation, the adsorption stability of the additive and kerogen interface was analyzed. The effects of pressure, additive type, and the number of additive molecules on methane adsorption characteristics in deep shale were comprehensively analyzed in conjunction with isothermal adsorption curves, relative concentration distributions, and Langmuir parameters. The results indicate that the main additives in water-based fracturing fluid can adsorb methane to some extent, but they also occupy pore space in shale, thereby reducing methane adsorption capacity. During the low-pressure stage, the effect of additives on adsorption predominated, leading to an increase in the methane adsorption capacity of kerogen. The order of increasing methane adsorption capacity was Guar gum > PAM > CTAB. In the high-pressure phase, the methane adsorption capacity of kerogen decreased due to the predominant effect of additives occupying pore space. The inhibition order was PAM > CTAB > Guar gum. As the number of additive molecules increased from 0 to 15, the Langmuir volume for the PAM system decreased from 24.41 to 20.12 mmol/g, for the Guar gum system to 21.72 mmol/g, and for the CTAB system to 21.37 mmol/g. This suggests that, in deep shale, the impact of slickwater fracturing fluid on methane adsorption is most significant. PAM inhibited methane adsorption at 9 MPa, while Guar gum and CTAB only showed inhibitory effects at 40 MPa. Furthermore, PAM is the most difficult to remove from the reservoir, followed by Guar gum, while CTAB is the easiest to remove. The innovation of this study lies in the use of molecular simulation to comprehensively examine the effects of pressure, types of water-based fracturing fluids, and their volumes on the methane adsorption characteristics in deep shale. This provides theoretical support for mitigating the damage of water-based fracturing fluids to shale reservoirs and enhancing shale gas production.

Keywords : hydraulic fracturing, water-based fracturing fluid, molecular simulation, reservoir damage, adsorption
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