Contribution ID: **583** Type: **Oral Presentation**

Experimental and molecular simulation studies of methane adsorption on deep shales

Wednesday, 15 May 2024 14:15 (15 minutes)

Understanding methane adsorption behavior on deep shales is crucial for estimating the original gas in place and enhancing gas recovery in deep shale gas formations. However, the methane adsorption behavior on deep shales under high pressure is challenging, and many uncertainties still exist in the process. In this study, the methane adsorption on deep shales within the Lower Silurian Longmaxi Formation from the Sichuan Basin, South China were conducted at pressures up to 50 MPa. The effects of total organic carbon (TOC), temperatures, clay minerals and moisture content on the adsorption capacity were discussed. Then the molecular models of kerogen nanopores with different shapes and sizes were constructed based on kerogen structure unit of deep shale from the Longmaxi Formation, and the methane occurrence were conducted by coupling a grand canonical Monte Carlo algorithm and a molecular dynamics algorithm. The results indicated that the methane excess adsorption on deep shales increased, then reached its peak and finally decreased with the pressure. The methane adsorption capacities exhibited strong positive correlations with the TOC content and negative relationships with clay minerals. The methane excess adsorption decreased as the temperature while the opposite trend would occur once it exceeded some pressure. The presence of the moisture content on deep shales sharply decreased the methane adsorption capacities, and the reduction of the adsorption capacity decreased with the pressure. The methane adsorption capacity in deep shales is negatively correlated with temperature, and high temperature will inhibit the affinity of methane molecules in pores.

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Session Classification: MS03

Track Classification: (MS03) Flow, transport and mechanics in fractured porous media