

# Numerical investigation of adsorption and slippage effects on unconventional gas transport in shale reservoirs using molecular dynamics and reservoir simulations

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Gas transport in an unconventional reservoir is a complicated process that is highly subject to nonlinear multi-physics phenomena, such as gas molecule's sorption and slippage effects especially in tiny pores. The quantity of the adsorbed gas release and gas permeability changes due to the complex gas transport phenomena can significantly affect the entire production in unconventional reservoirs. In this research, we analyze these two gas transport mechanisms in shale matrix with different reservoir conditions by molecular dynamics (MD) simulation. A dual control volume grand canonical MD is applied to estimate methane molecular adsorption/desorption and slippage effects in nanometer-scale pores in terms of Langmuir isotherm (pressure and temperature) and Klinkenberg b-factor with different pore sizes and reservoir conditions. Furthermore, these parameters are implemented into a double porosity (DP) reservoir model to determine their effects on the overall gas transport behavior and production efficiency in reservoir-scale. In this paper, we describe the details of the computational models, MD and DP, and example studies to show the applicability and capability of our models to analyze the various fluid transport mechanisms in both pore- and reservoir-scale simulations.

## References

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