Contribution ID: **110** Contribution code: **Board 17** Type: **Poster Presentation**

Modelling Kerogen Flexibility in Response to Hydrocarbon Adsorption using Hybrid Molecular Dynamics/Monte Carlo

Monday, May 20, 2024 7:10 PM (20 minutes)

Shale gas reservoirs plays a pivotal role in natural gas production in the United States. Organic part of shale is both a source and reservoir of hydrocarbons. Kerogen, an insoluble organic part of shale, exhibits an amorphous structure, and its composition and mechanical properties depend on the level of maturity. It has been shown the kerogen matrix swells upon gas adsorption. It is critical to understand the structure and adsorption characteristics of organic porosity found in kerogen. This knowledge is crucial for predicting the storage capacities of oil and gas, as well as enhancing hydrocarbon recovery.

To begin, we create three-dimensional molecular models of microporous kerogen matrix of type II-A with the same density and pore size distribution as an experimental sample. We also create slit pores of different sizes using the equilibrated kerogen matrix.1 We study adsorption of CH4, CO2, and octane in flexible kerogen matrix and slit pores. To incorporate the effect of adsorption stress exerted by the gas molecules on kerogen matrix, we use the hybrid molecular dynamics/Monte Carlo approach. This involves multiple cycles of grand canonical Monte Carlo simulations and molecular dynamics in NPT ensemble until the convergence in the number of particles and unit cell volume is achieved. Through our hybrid approach, the study aims to gain a deep understanding of deformation of kerogen upon hydrocarbon adsorption. This holds significant implications for advancing techniques for hydrocarbon recovery from shale reservoirs.

This work is supported by the NSF CBET grant 1834339 and ExxonMobil.

1. Parashar, S; Ravikovitch P.I.; Neimark, A.V. Molecular Modeling and Adsorption Characterization of Micro-Mesoporous Kerogen Nanostructures. Energy & Fuels. 2022.

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Session Classification: Poster Session

Track Classification: Poster Presentations