Contribution ID: **82** Type: **Oral Presentation**

Impact of a kerogen network on the behavior of confined hydrocarbon liquids

Tuesday, May 21, 2024 6:10 PM (20 minutes)

Kerogen is an intrinsically complex, heterogeneous, and disordered material [1]. Depending on its geological origin and maturity, the chemical composition of kerogen may vary significantly along with its structural properties, such as the cross-link density of the network and its intrinsic porosity [2]. Furthermore, upon hydrocarbon migration in shales, extraction, and adsorption, the cross-linked networks dynamically change, making the experimental and modelling of this porous media very challenging.

This work presents recent advances in utilizing molecular dynamics simulations to explore the adsorption and transport of high-pressure liquid hydrocarbons such as toluene, cyclohexane, and n-decane and their impact on the dynamic behavior of a kerogen nanostructure. Kerogen structures are developed following a mimetic algorithm using chemically-accurate coarse-grained models. We postulate that kerogen structures can be assembled as a combination of aliphatic and aromatic molecular building blocks such as n-dodecane, triphenylene, benzopyrene, perylene, and coronene [3]. Combining these molecules and adopting the SAFT force field [4] for their coarse-grained models, we generate fully cross-linked structures representative of four types of kerogens of different maturity, including 1A, 2B, and 2D. The models are validated against available experimental data and in-silico data [3]. The developed CG models offer a unique platform for studying thermodynamic and transport properties of hydrocarbon fluids.

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Session Classification: Tuesday

Track Classification: Oral Presentations