



➤ **TITLE: Adsorption behaviors of shale oil in kerogen slit by molecular simulation**

•**ABSTRACT:** Shale oil is widely distributed in organic nanopores, while kerogen plays a complex and key role for adsorption behavior of shale oil, and thus it is crucial to identify the associated storage mechanisms. In this paper, molecular dynamic (MD) simulation had been performed to quantify the adsorption behavior of shale oil in kerogen slits. Both the distribution of shale oil properties and potential of the mean force (PMF) were used to identify the interaction mechanisms between the light and heavy components respectively represented by methane and asphaltene. We also examined the effects of different temperatures and apertures on the adsorption behavior. Owing to the extremely strong adsorption capacity between the asphaltene and kerogen, the adsorbed asphaltene layers reduce the slit width, preventing the light components from adsorbing on the kerogen slits due to the energy barrier formed by heavy components. It is found that, with an increase in temperature, the distribution of hydrocarbons performs more homogeneously. In addition, the adsorption quantity of medium components displays a reduction in kerogen slit, while the heavy component shows a rising as its greater competitiveness, suggesting that the medium components are the most potential fraction in thermal exploitation, and the light components keep a steady quantity with the combined action of medium and heavy components. The small slit (aperture <2 nm) can be blocked by asphaltene molecules, and the adsorption density of hydrocarbons reaches the maximum at 2 nm aperture.

➤ **TITLE: Multicomponent Shale Oil Flow in Real Kerogen Structures via Molecular Dynamic Simulation**

•**ABSTRACT:** As an unconventional energy source, the development of shale oil plays a positive role in global energy, while shale oil is widespread in organic nanopores. Kerogen is the main organic matter component in shale and affects the flow behaviour in nanoscale-confined spaces. In this work, a molecular dynamic simulation was conducted to study the transport behaviour of shale oil within kerogen nanoslits. The segment fitting method was used to characterises the velocity and flow rate. The heterogeneous density distributions of shale oil and its different components were assessed, and the effects of different driving forces and temperatures on its flow behaviours were examined. Due to the scattering effect of the kerogen wall on high-speed fluid, the heavy components (asphaltene) increased in bulk phase regions, and the light components, such as methane, were concentrated in boundary layers. As the driving force increased, the velocity profile demonstrated plug flow in the bulk regions and a half-parabolic distribution in the boundary layers. Increasing the driving force facilitated the desorption of asphaltene on kerogen walls, but increasing the temperature had a negative impact on the flow velocity.

➤ **TITLE: Cellulose nanocrystal structure in the presence of salts**

•**ABSTRACT:** Aggregation and gelation of cellulose nanocrystals (CNCs) induced by magnesium chloride (MgCl₂) are investigated as a function of CNC and MgCl₂ concentrations. Transmission electron microscopy (TEM) and confocal laser scanning microscopy (CLSM) are employed to study the effect of ionic strength and CNC concentration on the extent of aggregation and structure of the CNC network. The location of CNC particles is traced with Fluorescent brightener 28 staining agent. The results show that the addition of different amounts of MgCl₂ causes a cluster formation of CNCs with different fractal dimensions, confirmed by TEM. The fractal dimension of CNC clusters varied from approximately 1.56 ± 0.08 to 1.98 ± 0.01 as the MgCl₂/CNC concentration ratio is increased from 0.17 to 0.42. We use the MgCl₂/CNC concentration ratio as a global parameter to correlate the results of different measurements and imaging data, including TEM, zeta potential and CLSM. Furthermore, we conduct molecular dynamic simulations to quantitatively examine different CNC behavior in MgCl₂ salt–CNC suspension. The results on the potential of mean force (PMF) indicate that the PMF of different ions concentration gravitates to zero where the distance between CNCs is increased from 3.1 nm to 3.5 nm. However, adding ions to the system changes the energy of the system and leads to a different behavior of CNC interactions.