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Multicomponent alkanes transport through nanoporous shale matrix

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Shale is attracting more and more attention owing to the huge hydrocarbon resources. However, the large number of nanopores and the multiscale pore structure pose great challenges in accurately characterizing the transport behavior of crude oil within the shale matrix. Although most studies suggested that the classical Darcy's law breakdown in the shale matrix, there is a great controversy on the oil transport mechanism: slip flow or the existence of stick layers, which impedes the efficient exploitation of shale oil. To address this issue, we study the transport of multicomponent alkanes through a nanoporous shale matrix by integrating molecular dynamics and digital rock. We consider the multi-component characteristics of shale oil and the typical mineral composition of shale reservoirs. Firstly, we use molecular dynamics to accurately capture the pressure-driven flow behavior of multi-component alkanes within kerogen cylindrical pores and calcite nanoslits, from which a mathematical model is developed to characterize the transport behavior. Then, based on Focused Ion Beam Scanning Electron Microscopy (FIB-SEM) images, we build an ultrahigh-resolution digital rock model using deep learning. A pore network model is extracted from this digital rock and used for the flow simulation of crude oil through the shale matrix. For the molecular studies within a single nanopore, we reach the following conclusions: sticky layers, whose velocity approximates zero, exist during oil flow through kerogen and calcite nanopores. Oil adheres onto the shale surfaces for the smaller driving force, resulting in a sticky layer that impedes flow. As the driving force increases, certain alkane molecules surpass the affinities from the rock surface and facilitate the flow, leading to a thinner sticky layer. The heavier components in shale oil show stronger interactions with rock surfaces, making them highly susceptible to adsorption and the sticky layer. Moreover, the thickness of the sticky layer in kerogen pores is greater than that of calcite nanopores, which can be attributed to the atomic roughness and fluid-solid interactions. Based on these findings, we have developed a mathematical model that describes the variations in the sticky layer thickness within different pores with respect to parameters such as driving force, alkane components, and pore size. Even with the assistance of FIB-SEM, the observation of shale nanopores smaller than 10 nm is challenging, which leads to the unreliable assessment of shale pore network connectivity. We develop a stepwise 3D super-resolution reconstruction method for shale digital rocks based on deep learning, which significantly improves the accuracy of digital rock core and enables successful observations of pores smaller than 10 nm. We then use the pore network model to simulate shale oil flow at the pore scale. Our findings showed that the transport of oil through the shale matrix is nonlinear and has a threshold pressure gradient due to nanoscale sticky layers. When the displacement pressure gradient exceeds the threshold pressure gradient, oil starts to flow and lighter components dominate shale oil transport. This study sheds light on the accurate modeling of shale oil production and more generally, for mass transport in nanoporous materials.

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