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Editorial

Challenges of Modeling Hydrocarbon Recovery from Shale

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Shale gas is expected to account for 30% of world natural gas production by 2040 [1]. Shale is different from the conventional hydrocarbon resources due to the presence of nanoporous organic matter, known as kerogen, embedded within the inorganic matrix. Although kerogen accounts for a small percentage of total shale volume, almost half of the total hydrocarbons are in the adsorbed state within its pores [2,3]. Due to the extremely small sizes of the pores, the nature of the species transport is different from those predicted by continuum-based theories from which the Navier-Stokes and Darcy equations are derived [4]. Furthermore, depending on the gas type and intermolecular forces between the molecules of gas and solid molecules at the pore walls, the gas molecules cannot escape from the force field at the pore wall, which causes inhomogeneous fluid distribution in the pores [5]. Moreover, due to the differences in the species sorption properties in natural gas, fluids are not uniformly distributed across the pores; heavier components tend to accumulate in the vicinity of the pore walls and may trap within the pore and remain in the reservoir, while the lighter components are extracted [6]. Therefore, the composition of the fluids may change as production progresses. This limits the application of conventional petroleum engineering models to predict the volume of hydrocarbon in place and recovery from these resources.

Quantity and composition of the hydrocarbons accumulated in shale resources depend on chemical composition and structural features of kerogen. To characterize the species transport and storage properties of kerogen based on its chemical compositions and burial history, it must be first extracted from the inorganic matrix, which is a challenging task. In addition, once the kerogen is extracted, performing experimental characterization of storage and transport properties in reservoir conditions is extremely difficult [7]. Molecular simulations are credible alternatives to physical ex-

periments for characterization of the kerogen [8]. An appealing feature of this approach includes the ability to perform an endless set of numerical tests at different pressures and temperatures, and types and compositions of fluids, without degrading or altering the sample.

Due to the adsorption selectivity in organic pores of shale, understanding the competitive adsorption equilibria is of significant importance. Molecular simulations, e.g., Grand Canonical Monte Carlo (GCMC) method, have been extensively used to study the species adsorption in realistic molecular models of coal [9,10] and shale [11-13]. Among the models used for predicting the mixture adsorption isotherms, the Extended Langmuir model [14] and the Ideal Adsorbed Solution model [11] have been shown to be capable of predicting the GCMC simulation result [15].

The mass transfer in shale organic matter is of diffusional nature [16] and therefore, understanding the species diffusion through shale organic pores is of significant importance. The species diffusion manifests itself into different diffusion coefficients, namely self-, corrected (or Maxwell-Stefan), and transport diffusion coefficients. Diffusion of pure fluids in organic pores of coal and shale has been extensively studied using molecular simulations [13]. However, there are only a few studies on molecular simulation of the diffusion coefficients for fluid mixtures. Collell et al [16], studied the transport of hydrocarbon mixtures through kerogen using molecular simulations. They found that the Onsager's autocorrelation coefficients scale linearly with the adsorption loading and inversely with the alkane chain length. They proposed a simple scaling law to predict the transport coefficient of linear alkanes in the mixture. Zhao et al. [17] computed diffusion coefficients of carbon dioxide-methane mixtures at different temperatures, pressures, and mixture compositions in a bituminous coal model. They showed that the dominating mechanism for the mixture diffusion in coal changes from surface diffusion to configurational diffusion

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at high pressure.

Although we have advanced our understanding of the transport and storage phenomena in shale, we are still far from developing predictive models for hydrocarbon recovery. Kerogen is a mixture of organic chemicals and its chemical compositions, pore structure, porosities, etc. vary depending on the geographical location and maturity and sedimentary history [17]. Therefore, due to variability of kerogen, it is never possible to propose a general representative kerogen structures to be used in molecular simulations. Once the kerogen structure is known, it is also important to understand the impact of the interfaces between kerogen and surrounding inorganic matrix on the hydrocarbon recovery from shale. In the absence of such modalities, efficient design of hydrocarbon recovery will remain limited.

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