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PROCEEDINGS

The Study of Shale Energy: Perspective from Molecular Dynamics (MD)

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ABSTRACT

In the last decades, the successful development of hydrofracture has paved the way to replace conventional energy with shale energy, such as shale oil and shale gas. However, shale energy always exists in very tight rock, which has extremely low porosity and permeability, proposing a high requirement for experimental facilities. The rise of molecular dynamics avoids the physical limitation handily, and it can provide a better understanding at the level of mechanism. In our studies, the MD method is used on the adsorption and transport behaviors of shale gas and oil in kerogen nanopores. Regarding the heterogeneous spatial distribution of shale energy in the equilibrium state, the relevant potential of the mean force (PMF) and potential energy surface (PES) are presented to address the explanation of interactive mechanisms dominating corresponding behaviors, such as the interaction between the light and heavy components in shale oil, and the competitive adsorption in shale gas mixed with water and carbon dioxide molecules. The dynamics behaviors are analyzed from different aspects, where the effect of branch chains of kerogen is also taken into consideration. The results show that the adsorbed layer should be an intermediate state between shale fluid and shale nanopores, and it also affects a lot on the slip effect if it is still regarded as the fluid phase. An algorithm is developed for the multi-scale problems from the MD to the MC methods. The shale fluid always presents different states during the adsorption and transport processes, suggesting that these states can be predicted by the MC method as long as the accurate probability transition matrix is identified. Our algorithm carries out this problem base on a simplified toy model and addresses the multi-scale simulations from the special and temporal coarsening methods.

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