Estimation of the transport properties of fluids confined in a complex structure of kerogen by molecular simulations

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Achieving a sustainable fluid (gas/oil) production rate from unconventional reservoirs, such as shales, has become a great challenge of our time. The process of fluid recovery is hindered by complex structure of organic matter, so called kerogen, where fluids are strongly confined. Thus, the behavior of fluid flow is heavily affected by kerogen's structure. It has been determined that microporous phase plays a significant role on fluid dynamics although kerogen is a multiscale organic material [1]. However, solid-fluid couplings at the microporosity are poorly understood. To shed some light on these mechanisms at the nanoscale, I have studied, using molecular dynamics simulations, the fluid transport properties within two prototypical kerogen matrices, which vary strongly according to their origin, size and pore network. Since the development of more realistic molecular models is required, relatively small matrix (~4×5×4 nm^3) of kerogen has been considered for investigation [2]. The study has been performed while accounting for anisotropy because the matrix size can affect the fluid transport. Strongly anisotropic diffusion has been observed for this kerogen model. Moreover, we have found that the diffusivity increases when accounting for the flexibility effects (swelling) in the preparation of the matrix. Relatively small values have been determined in the case where there are no interactions between the solid and the fluid. In addition, I have verified if this finite size effect (anisotropy) also applies for a larger molecular model (~6×6×6 nm^3) of kerogen initially developed to examine the flexibility effects of the solid. I have found that even for this size the molecular model is still not fully isotropic. However, since the trends of diffusion along three directions with respect to loading are similar, the estimate of the diffusion coefficients for this kerogen model might be considered as approximately isotropic. Knowledge of the characteristics of solid-fluid couplings at the nanoscale may contribute to the enhancement of fluid recovery from shales.

References

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