

Molecular dynamics study of methane diffusion in flexible microporosity of source rock's organic matter

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Over the last decades shale gas production from deep rock formations has become increasingly important in gas industry. This has led to thorough examinations of fluid transport properties in organic-rich unconventional reservoirs by molecular dynamics simulations. Most of these studies have been done by considering the microporous structure of kerogen as a rigid solid [1-3]. However, a recent study [4] has revealed that accounting for the kerogen flexibility while investigating the hydrocarbon transport in an immature kerogen matrix could play a crucial role. Flexibility can lead to significant increase in free volume due to the adsorption-induced swelling that increases fluid transport when the fluid loading increases, as opposed to the rigid case. This study has only been performed for a few conditions and collective diffusion has not been studied yet. All this calls for the need of in-depth studies of the flexibility effects. In this work methane diffusion for a wide range of conditions (pressure, temperature) and fluid loading is investigated. It is proven that the collective effect on fluid transport through a deformable matrix of kerogen can be neglected. It is also shown that the trend of diffusion coefficient increase via fluid loading can be well captured using free volume scaling. These results contribute to the investigation of fluid transport properties in such microporous phase and will be extended to study carbon dioxide transport in the near future.

References

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