



Contribution ID: 514

Type: Oral Presentation

Diffusion of methane and carbon dioxide within flexible kerogen from molecular dynamics simulations

Tuesday, 31 May 2022 15:05 (15 minutes)

The growing interest in shales stems from the presence of significant hydrocarbon reserves and the possibility of storing carbon dioxide in source rock's organic matter (kerogen). However, the impact of kerogen's microporosity on fluid dynamics is not fully understood yet. Phenomena such as strong adsorption effects have to be taken into account on fluid transport investigations due to the high surface to volume ratio in kerogen. Most of the previous molecular scale studies on the fluid dynamics in kerogen have been performed in the rigid solid approximation [1,2], which is a rather crude assumption in most cases. Thus, in this study, molecular dynamics and free volume theory have been applied to shed light on diffusion of methane (CH₄) and carbon dioxide (CO₂) in a flexible kerogen microporous structure. The molecular kerogen model described in the paper [3] has been reused to extend the methane diffusion study to the carbon dioxide transport properties and collective effects in fluid diffusion. Despite an anisotropy of the transport properties induced by the size of our immature kerogen model (~6×6×6 nm³), analysis of the diffusivity trends has shown that the anisotropic factor is approximately constant and remains small. This allows us to average over the three directions to obtain effective transport properties. In addition, we prove that fluid (CH₄/CO₂) transport in flexible kerogen microstructures is purely diffusive, as the dynamics of the host matrix does not promote collective effects through solid-fluid couplings. Thus, the self-diffusion coefficient is a sufficient measure of the transport properties of fluids confined in both rigid and flexible kerogen microporosity. Moreover, the diffusivity of a fluid in deformable kerogen increases with fluid loading due to adsorption-induced swelling, as opposed to the rigid solid case. Interestingly, this increasing trend is well captured by the Fujita-Kishimoto free volume model. In contrast to fluid adsorption, the replacement of CH₄ with CO₂ led to kerogen matrix shrinkage and decreased CO₂ diffusivity compared to that of CH₄ at certain conditions due to the stronger intermolecular forces of attraction in CO₂ reinforcing fluid-solid couplings. These results raise new issues of the impact of chemical and mechanical diversity of kerogen on fluid diffusion.

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References

- [1] K. Falk, et al., Nature communications, 6: 6949, 2015.
[2] J. Collell et al., The Journal of Physical Chemistry C, 119(39): 22587–22595, 2015.
[3] A. Obliger et al., Journal of Physical Chemistry B, 123(26):5635–5640, 2019.

Time Block Preference

Time Block A (09:00-12:00 CET)

Participation

In person

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