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Type: **Poster (+) Presentation**

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

Thursday, 3 June 2021 20:00 (1 hour)

Over the last decades shale gas production from deep rock formations has become increasingly important in the gas industry. This has led to thorough examinations of fluid transport properties by molecular dynamics simulations in the organic part of the porous medium, such as those found in unconventional reservoirs, so called kerogen. 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 a significant increase in the free volume due to the adsorption-induced swelling that increases fluid transport when the fluid loading increases, as opposed to what found in the rigid case. This study has only been performed for a few set of thermodynamics conditions and collective diffusion has not been studied yet. All this calls for the need of in-depth studies of the flexibility effects on transport properties in immature kerogen. Thus, in this work methane diffusion in kerogen 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 increases via fluid loading can be well captured using free volume scaling. Furthermore, we have started studying the carbon dioxide diffusion in the kerogen matrix. These results contribute to the investigation of fluid transport properties in such microporous medium and will be extended to study transport of carbon dioxide and methane mixtures in a near future.

Time Block Preference

Time Block B (14:00-17:00 CET)

References

- [1] J. Collell et al., Energy & Fuels, 28(12):7457–7466, 2014.
- [2] K. Falk et al., Nature communications, 6:6949, 2015.
- [3] A. Obliger et al., Nano Letters, 18(2):832–837, 2018.
- [4] A. Obliger et al., Journal of Physical Chemistry B, 123(26):5635–5640, 2019.

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