Contribution ID: **492** Type: **Poster Presentation**

A molecular dynamics study on CO2 enhanced shale gas recovery in kerogen nanopores

Monday, 30 May 2022 15:10 (1h 10m)

The injection of supercritical CO_2 into shale gas reservoirs, fracturing the reservoir, enhancing shale gas recovery and achieving CO_2 geological storage, is regarded as an optimum scheme in carbon capture, utilisation and storage (CCUS) due to the distinctive physical properties of supercritical CO_2, e.g. a low viscosity, high diffusion coefficient, high adsorption capacity and zero surface tension. A shale reservoir contains inorganic pores such as clay minerals and organic pores like kerogen, among which the gas adsorption characteristics differ dramatically. A deep understanding of the complex transport mechanism of CO_2-CH_4-moistures in kerogen nanopores with diameters < 10 nm is crucial because of the anomalous diffusion phenomenon and nanoconfinement effects in nanoscale. In this study, molecular dynamics with grand canonical Monte Carlo (GCMC) simulation will be performed to study the competitive adoption of CO_2 and CH_4 with the presence of moistures in kerogen nanopores. Kerogen nanopores are built with six representative molecular structures of different maturity characterised by O/C and H/C ratios. The effects of the pore networks including porosity, pore size, surface area, connectivity and tortuosity will be quantified.

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References

Time Block Preference

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

Participation

In person

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