



Molecular Dynamics Study of Carbon Dioxide Storage in Shale



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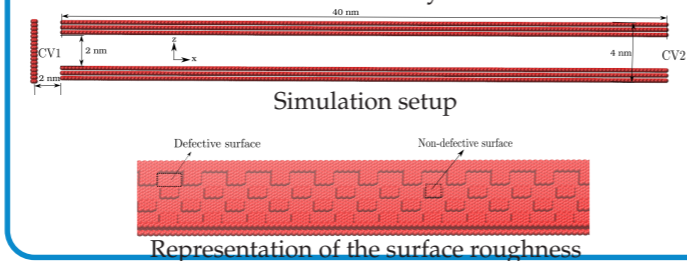
MOTIVATION

With large scale production of gas from shale resources, large volumes of pore space have been recently vacated. Furthermore, due to the higher affinity of the organic matter in shale to CO₂ compared to methane, CO₂ can replace the adsorbed methane and therefore, enhances the recovery of natural gas.

The objective for this study is to investigate the sorption (adsorption of CO₂ and desorption of methane) in carbon-based organic channels using Molecular Dynamics (MD) simulations.

PROBLEM SETUP

The graphite channels consist of three graphite layers. In order to consider the surface roughness, carbon atoms are deleted from the most inner layers.

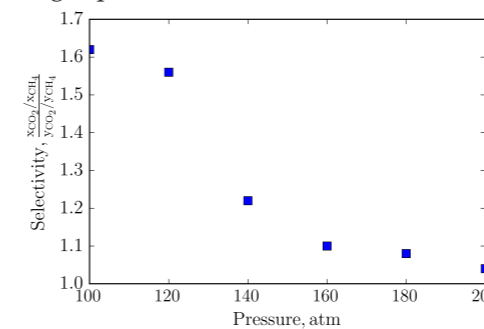


RESULTS

In order to compare the tendency of different components to be adsorbed to the wall, selectivity of CO₂ over methane is determined,

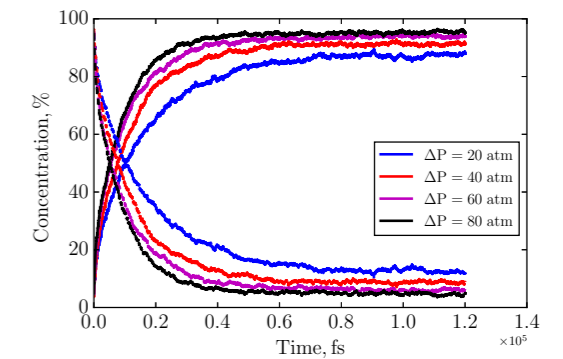
$$S_{CO_2/CH_4} = \frac{x_{CO_2}/x_{CH_4}}{y_{CO_2}/y_{CH_4}}$$

where S is selectivity, x is the mole fraction of the gas in the adsorbed phase, and y represents the gas mole fraction in the bulk gas phase.

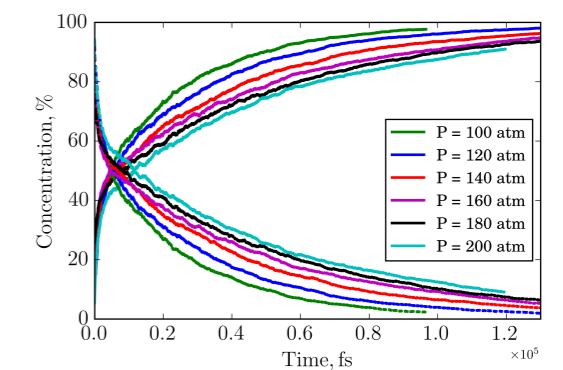


Selectivity of CO₂ over methane at different pressures

For all pressures, methane molecules are displaced by CO₂ molecules. The replacement process is initially very quick for all pressures; approximately 50% of methane molecules are replaced by CO₂ in 10⁴ fs after beginning the simulations. As the pressure increases, the displacement process becomes slower. This is due to the fact that the selectivity of CO₂ over methane decreases as pressure increases.



Displacement with pressure gradients

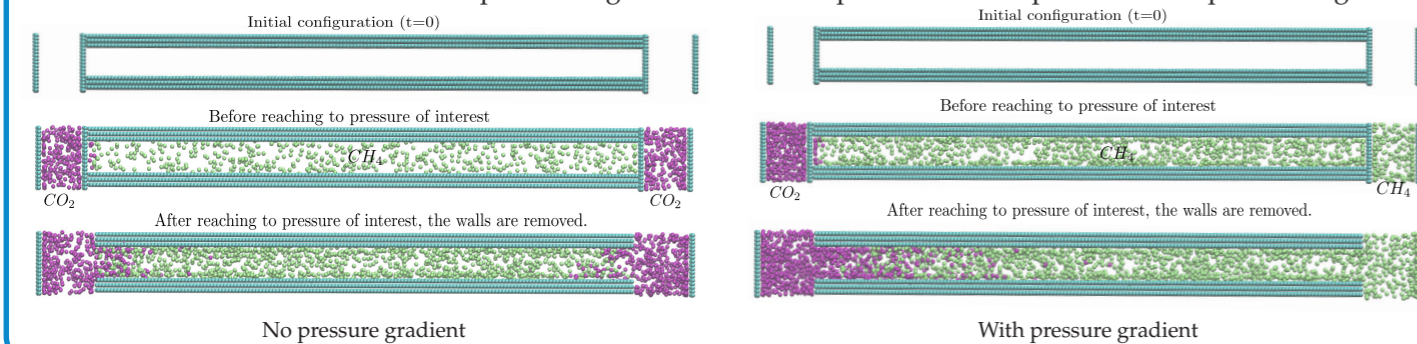


Displacement in the absence of pressure gradients

As the pressure gradient increases, the methane molecules are replaced faster by CO₂ molecules.

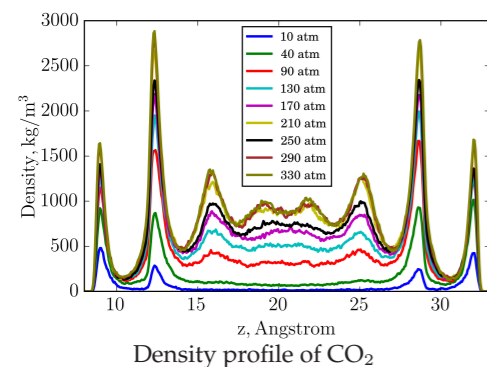
METHODOLOGY

To study the storage of CO₂ in the molecular level, two types of displacements of methane molecules with carbon dioxide are considered: displacements with introducing CO₂ at the channel entrance in the absence of pressure gradient and displacement in presence of pressure gradients.



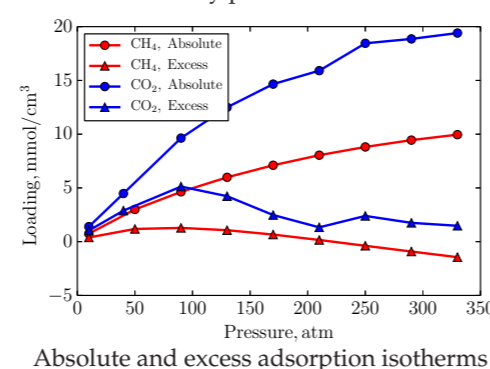
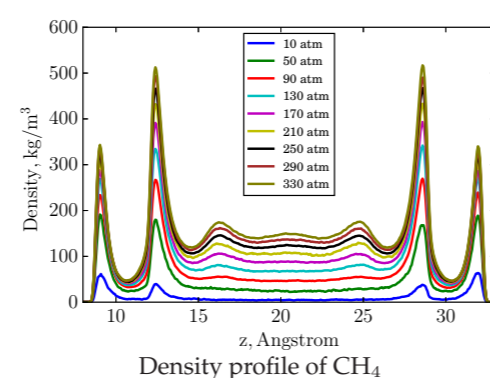
RESULTS: DENSITY PROFILES

To determine density profiles and adsorption isotherms, grand canonical Monte Carlo (GCMC) simulations are performed.



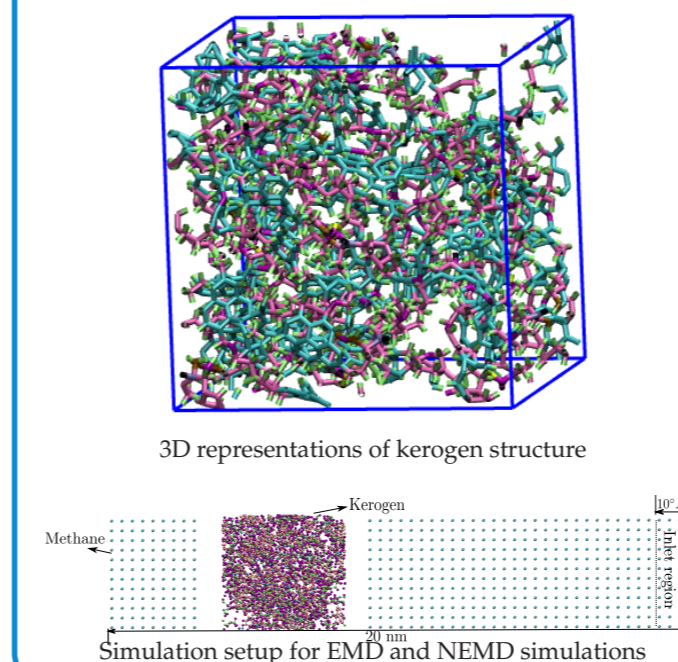
Absolute and excess loading quantities (moles of adsorbed molecules per unit volume of gas (mmol/cm³)) at 350 K are plotted. Absolute adsorption is defined as total amount of gas adsorbed to the solid walls. Excess adsorption is the amount of gas in absence of walls subtracted from amount of gas in adsorbed phase.

For CO₂, a behavior similar to BET isotherms is observed.



CURRENT RESEARCH

Adsorption and transport of methane in a 3D type II kerogen model are being studied.



REFERENCES

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- [2] Kazemi, M. and A. Takbiri-Borujeni (2016). Flow of gases in slit shaped organic nanopores of shale: A boundary-driven molecular simulation study. In *SPE Low Perm Symposium*. Society of Petroleum Engineers.
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