Contribution ID: **195** Type: **Poster Presentation**

A molecular simulation study on adsorption and diffusion behaviors of hydrogen, methane and carbon dioxide

Monday, 13 May 2024 09:55 (1h 30m)

Because underground hydrogen storage offers the potential for large-scale, long-term storage of hydrogen, understanding the adsorption and diffusion behaviors of hydrogen and cushion gas in the reservoir is critical to understanding the underlying mechanisms that control hydrogen storage and transport. Using molecular simulation methods, we investigated the adsorption and diffusion behaviors of hydrogen, methane and carbon dioxide in kaolinite slit pores (10 MPa and 303 K), respectively. The distribution characteristics, excess adsorption amounts, diffusion coefficients and gas-solid interaction energies of the three gases in the slit pores were analyzed. Near the pore wall surface, carbon dioxide formed a distinct double adsorption layer, methane formed a smaller second adsorption layer, and hydrogen formed a single adsorption layer. The order of excess adsorption amount is carbon dioxide > methane > hydrogen. The rank of diffusivity of gases under the same conditions is hydrogen > methane > carbon dioxide. The interactions between gases and pore walls are in the following order: carbon dioxide>hydrogen>methane. Van der Waals interactions dominate. However, hydrogen and carbon dioxide have significant coulombic interactions with the pore walls, while methane has negligible coulombic interactions with the pore walls. The minerology of the formation results in different charges on the pore surfaces, which has a significant effect on gas storage. This study provides better insights into the mechanisms of hydrogen and cushion gas storage, thus providing a theoretical basis for underground hydrogen storage site selection.

Acceptance of the Terms & Conditions

Click here to agree

Student Awards

Country

China

Porous Media & Biology Focused Abstracts

This abstract is related to Porous Media & Biology

References

Conference Proceedings

I am interested in having my paper published in the proceedings.

Primary author: SHANG, Zhenxiao (China University of Petroleum (East China))

Co-author: Prof. YANG, Yongfei (China University of Petroleum (East China))

Presenter: SHANG, Zhenxiao (China University of Petroleum (East China))

Session Classification: Poster

Track Classification: (MS13) Fluids in Nanoporous Media