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A molecular dynamics study on dissolution and adsorption dynamics of CO2 with H2 impurity in oil reservoir

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CO2 capture and storage (CCS) is one of the indispensable decarbonization technologies to achieve green industrial growth and address the challenge of global climate change. CO2 captured using the Sorption Enhance Water Gas Shift process at steel mills contains H2, with its molar ratio reaching 10% or higher. Since the thermophysical properties of CO2 and H2 are distinctly different, the effects of H2 impurity on CO2 transportation and geostorage in oil reservoir should not be overlooked. Moreover, according to our previous modelling study, the solidification of oil on caprock surface can generate a preferentially orientated molecule structure because of the interfacial crystallization. The solidified oil film can alter the minimum miscible pressure of the gas mixtures, thereby changing the adsorption and dissolution process of CO2 in oil reservoir.
In this study, molecular dynamics simulation will be performed to investigate the effect of injection temperature and pressure on the dissolution behaviour of CO2/H2 mixtures in solidified oil film. The crystalline alkane structure on silica subtract will be constructed, featuring the surface freezing monolayer and the crystalline parallel middle layers. The atomic interaction energy between the gases, function groups of alkane and silica subtract will be quantified to elucidate the mechanism behind the miscibility and surface adsorption. The conclusion of this study will shed guiding light on optimising the operating conditions of injecting CO2 containing H2 as the major impurity species and facilitating the deployment of CCS infrastructures.

Participation

In-Person

References

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