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Study of Phase Boundary Change with Cage Occupancy by Molecular Dynamics Simulations

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It has been suggested that carbon dioxide (CO_2) has the potential to replace methane (CH_4) from natural gas hydrates, which is one of the promising methods to recover CH_4 from hydrates and in the meanwhile sequester CO_2 underground. It is important for this method to get the three-phase coexistence lines (solid hydrate, liquid water, and liquid or vapor CH_4/CO_2) of CH_4/CO_2hydrates. In this work, we estimated the phase boundaries of CH_4 hydrate and CO_2 hydrate by molecular dynamics simulations, and discussed the phase behavior of gas hydrates.

In CH_4-hydrate case, the estimated phase boundary is in very good agreement with the experimental data. In CO_2-hydrate case, the experimental data are between the estimated phase boundaries using the full occupancy CO2-hydrate and the partial occupancy CO_2-hydrate. The estimated melting temperature of the full occupancy hydrates is higher than that of the partial occupancy hydrates in both CH_4-hydrate and CO_2hydrate cases, and the gas hydrate stability zone expands. This result implies that the cage occupancy of gas hydrates influences the stability of gas hydrates.

Keywords: methane hydrate, CO_2 hydrate, molecular dynamics, phase boundary, cage occupancy, gas hydrate