

Kinetic selectivity of SF<sub>6</sub> during formation and dissociation of SF<sub>6</sub> + N<sub>2</sub> hydrates for hydrate-based gas separation

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This study investigated the time-dependent kinetic selectivity of SF<sub>6</sub> in the hydrate-based gas separation process through both experimental and computational approaches. The enclathrating and releasing behaviors of SF<sub>6</sub> in SF<sub>6</sub> + N<sub>2</sub> hydrates were analyzed using in-situ Raman spectroscopy, gas chromatography, and micro-second molecular dynamics (MD) simulations. During hydrate formation, the growth pattern of the Raman peak for enclathrated SF<sub>6</sub> was similar to that for enclathrated N<sub>2</sub>, and the SF<sub>6</sub> composition in the hydrate phase was almost constant. Furthermore, the captured SF<sub>6</sub>/N<sub>2</sub> ratio in the hydrate structure obtained from the MD simulation was almost constant during hydrate formation. These results demonstrated that there was no significant kinetic selectivity of SF<sub>6</sub> during hydrate formation. In addition, the in-situ Raman spectra and MD simulation results demonstrated that SF<sub>6</sub> was not kinetically selective during hydrate dissociation. These overall results will be helpful for determining the optimal operation time for the hydrate formation and dissociation process and thus for designing and operating the hydrate-based SF<sub>6</sub> separation process.