

An investigation of kinetic selectivity of SF₆ during the formation and dissociation of SF₆ + N₂ hydrates

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In this study, hydrate-based gas separation (HBGS) was adopted to capture SF₆ and the kinetic selectivity of SF₆ during the hydrate formation and dissociation process was closely examined via experimental and computation approaches. Time-dependent enclathrating and releasing behaviors of SF₆ and N₂ in the hydrate phase were analyzed using both *in-situ* Raman spectroscopy and gas chromatography. Furthermore, the kinetic selectivity of SF₆ was also investigated using microsecond MD simulations. The SF₆ composition in the hydrate phase was consistently higher than that of N₂ and remained almost constant throughout the hydrate formation and dissociation, indicating that SF₆ was a thermodynamically selective, but not kinetically selective. The results provide a better understanding of formation and dissociation kinetics of SF₆ + N₂ hydrates and will be helpful for designing and operating the hydrate-based SF₆ separation process from SF₆ + N₂ gas mixtures.