MOLECULAR DYNAMICS STUDY OF BINARY SF₆-H₂ SII HYDRATE

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ABSTRACT
Sulfur hexafluoride (SF₆), one of the most potent greenhouse gases, is known as a hydrate former and has been studied at the high pressure up to 1.3 GPa with gas mixtures and with aqueous surfactant. Since we regard SF₆ as a potential promoter molecule that can stabilize hydrate structure more effectively compared to the other promoters, further investigation is required to verify the stabilizing ability of SF₆ in the hydrate structure. However, the insoluble nature of SF₆ in water or gases hinders fine scale analyses. This work discusses the data obtained by using molecular dynamics simulations of structure II (sII) clathrate hydrates containing SF₆ and H₂. The simulations were performed using the TIP4P/Ice model for water molecule and a previously reported SF₆ molecular model (optimized at the pure SF₆ single phase system[1]), and a H₂ molecular model (adapted from the THF+H₂ hydrate system[2]). The simulations were performed to observe the stability of SF₆ and H₂ in the sII clathrate hydrate system with varying temperature and pressure conditions and occupancies of SF₆ and H₂, which cannot be easily tuned experimentally. We observed that stability of H₂ enclathrated in the hydrate structure more affected by the occupancy of SF₆ molecules and temperature than pressure, which ranged from 0.1 to 100 bar.

Keywords: gas hydrates, molecular dynamics simulations, sulfur hexafluoride, hydrogen storage

INTRODUCTION
Gas hydrates have been investigating by many researchers as a potential medium for hydrogen storage. Among many candidates, THF [2-5] was proposed as the most promising promoter molecule to lower the equilibrium pressure and to increase the hydrogen storage capacity.

Sulfur hexafluoride (SF₆) forms a gas hydrate of the cubic structure II at atmospheric pressure [6-8]. Therefore, SF₆ has a great potential as the promoter for the hydrogen storage using hydrate structure. Nevertheless, little is known about SF₆ as a promoter, in particular microscopic mechanism of hydrate stabilization. In this study, we have investigated the hydrogen storing capability of SF₆ hydrates using molecular dynamics simulations.

METHODS
We performed molecular dynamics simulations in the isothermal-isobaric ensemble, using Gromacs[9], with the leap-frog algorithm. Initial configuration was prepared by combining two layers, structure II hydrate of 2×2×2 unit cell, which was 3.46 nm per side, having SF6 and H₂ molecules as guest molecules of large and small