천연 물질을 이용한 이산화탄소 하이드레이트 형성 억제

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Natural Inhibitors for CO_2 Hydrate Formation

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The motivation for this work was the potential of hydrophobic amino acids such as glycine, L-alanine, and L-valine to be applied as thermodynamic hydrate inhibitors (THIs). To confirm their capabilities in inhibiting the formation of gas hydrates, three-phase (liquid-hydrate-vapor) equilibrium conditions for carbon dioxide hydrate formation in the presence of 0.1 to 3.0 mol% amino acid solutions were determined in the range of 273.05 to 281.45 K and 14.1 to 35.2 bar. From quantitative analyses, the inhibiting effects of the amino acids (on a mole concentration basis) decreased in the following order: L-valine > L-alanine > glycine. The application of amino acids as THIs has several potential advantages over conventional methods. First, the environmentally friendly nature of amino acids as compared to conventional inhibitors means that damage to ecological systems and the environment could be minimized. Second, the loss of amino acids in recovery process would be considerably reduced because amino acids are non-volatile. Third, amino acids have great potential as a model system in which to investigate the inhibition mechanism on the molecular level, since the structure and chemical properties of amino acids are well understood.

Key words : Gas Hydrate(가스 하이드레이트), Amino acids(아미노산), Carbon Dioxide(이산화탄소), Thermodynamic Hydrate Inhibitors(열역학적 하이드레이트 억제제), Environmentally Friendly Substances(친환경적인 물질)

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sII SF_6+H_2 하이드레이트의 분자 거동

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Molecular Behavior of SF_6 + H_2 Structure II Hydrates

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Sulfur hexafluoride (SF_6), 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 SF_6 as a potential promoter molecule that can stabilize hydrate structure more effectively compare to the other promoters, further investigation is required to verify the stabilizing ability of SF_6 in the hydrate structure. However, the insoluble nature of SF_6 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 SF_6 and H_2. The simulations were performed using the TIP4P/Ice model for water molecule and a previously reported SF_6 molecular model (optimized at the pure SF_6 single phase system (Olivet and Vega, 2007)), and a H_2 molecular model (adapted from the THF+H_2 hydrate system (Alavi et al., 2006)). The simulations are performed to observe the stability of SF_6 and H_2 in the sII clathrate hydrate system with varying temperature and pressure conditions and occupancies of SF_6 and H_2, which cannot be easily tuned experimentally. We observe that stability of H2 enclathrated in the hydrate structure more affected by the occupancy of SF_6 molecules and temperature than pressure, which ranges from 1 to 100 bar.

Key words : hydrates(하이드레이트), molecular dynamics(분자동역학), SF_6(육불화황), H_2(수소), hydrogen storage (수소저장), promoter(촉진제)

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