Inhibition Effects of Hydrophilic and Hydrophobic Ionic Liquids on Methane Hydrates

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Gas hydrate inhibitors have been generally used to prevent plugging risks caused by gas hydrate formation in gas and oil field operations. Recently, ionic liquids (ILs) have been studied as 'dual' function inhibitors, since they can act as both a thermodynamic hydrate inhibitor (THI) and a kinetic hydrate inhibitor (KHI). In this study, we focused on the hydrophobicity of ILs and examined the inhibition effect of ILs on the kinetics and thermodynamic stability of CH4 hydrate by measuring the onset temperature (Tonset) and hydrate phase equilibria. Total 8 ionic pairs (2 cations ([EMIM]+ and [BMIM]+) , 4 anions ([Cl]-, [BF4]-, [PF6]-, and [Tf2N]-)), which have the following hydrophobicity order : [EMIM]+ < [BMIM]+ for cation and [Cl]- < [BF4]- < [PF6]- < [Tf2N]- for anion, were investigated. Moreover, molecular dynamics (MD) simulation was used to figure out the molecular behaviors of ILs for hydrate inhibition by examining radial distribution function (RDF), density profile, and free energy analysis. Our research will provide a better understanding of the inhibition mechanism of various hydrophilic and hydrophobic ILs on CH4 hydrate formation.