Investigation of Six Imidazolium-Based Ionic Liquids as Thermo-Kinetic Inhibitors for Methane Hydrate by Molecular Dynamics Simulation

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Abstract

The thermo-kinetic inhibition mechanism of six imidazolium-based ionic liquids (ILs) on methane clathrate hydrate formation and growth is studied in this work using classical molecular dynamics (MD) simulation. The ionic liquids investigated include 1-(2,3-dihydroxypropyl)-3-methylimidazoliumbis(fluorosulfonyl)imide ($[C_3(OH)_2mim][f_2N]$), 1-(2-hydroxyethyl)-3-methylimidazolium bis(fluorosulfonyl)imide ($[C_2OHmim][f_2N]$), 1-ethyl-3-methylimidazolium tetrafluoroborate ($[C_2mim][BF_4]$), 1-butyl-3-methylimidazolium tetrafluoroborate ($[C_4mim][BF_4]$), 1-butyl-3-methylimidazolium acetate ($[C_4mim][OAc]$) and 1-ethyl-3-methylimidazolium ethylsulfate ($[C_2mim][EtSO_4]$). Simulations showed that $[C_2OHmim][f_2N]$ and $[C_3(OH)_2mim][f_2N]$ are strongly hydrated compared to other ILs because of hydrogen bonding between OH groups of the cation and water molecules. They also exhibit high diffusion rates towards crystal surface and bond to it through strong intermolecular interactions. As a result, these two ILs are stronger thermo-kinetic inhibitors for formation and growth of methane hydrates compared to other ILs studied in this work as well as conventional inhibitors like methanol and NaCl. The simulations also revealed that cations of $[C_3(OH)_2mim][f_2N]$ and $[C_2OHmim][f_2N]$ show that the presence of ions near the hydrate crystal causes hindrance for water and guest molecules adsorbing on the hydrate surface, which inhibits the growth of hydrate crystals. In addition, it is shown that $[C_3(OH)_2mim][f_2N]$ and $[C_2OHmim][f_2N]$ are more likely to inhibit hydrate formation.

Keywords: methane hydrate, molecular dynamics simulation, ionic liquid, kinetic inhibitor, thermodynamic inhibitor.

Research Highlights:

- Investigation of kinetic inhibition mechanism of six imidazolium-based ILs on methane hydrates formation and growth using MD simulations.
- Investigation of thermodynamic inhibition mechanism of six imidazolium-based ILs on methane hydrates growth by MD simulations.
- Drawing a comparison between methane hydrate inhibition Effectiveness of ILs.