Atomistic Insights on the Coalescence between a Hydrate Particle and a Water Droplet within a Hydrocarbon Mixture

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The formation of hydrates can cause interruptions in the flow of oil from wells to refineries, with a substantial impact both in terms of economics and environment. To prevent the formation of hydrates, thus ensuring the continuous production of a well, the industry employs three types of hydrate inhibitors: thermodynamic inhibitors such as methanol, which shift the stability region of the hydrates, kinetic inhibitors, such as PVCAP, which are thought to both reduce the frequency of hydrate nucleation events and delay the growth of hydrate particles once formed, and anti-agglomerants, AAs, which essentially are surfactants thought to prevent the assembly of growing hydrate particles, thus preventing the formation of large agglomerates. The molecular mechanisms responsible for the performance of AAs are at present not completely understood. In an attempt to fill this knowledge gap we report here atomistic molecular dynamics simulations conducted in a system composed by decane, methane, water, hydrate, and a common surfactant, hexadecyl-trimethyl-ammonium chloride. We prepared one hydrate particle and one water droplet. We then investigated how the surfactant affects the agglomeration between the hydrate and the water droplet as a function of amount of surfactant, amount of water, and a few other thermodynamic parameters. Although the surfactant used in this study is not an effective anti-agglomerant for practical applications, the results presented could be useful for the design of novel compounds that prevent the agglomeration of hydrates in complex hydrocarbon mixtures.