MD Study of Clathrate-Like Ordering and Evolution in Supersaturated Water Solutions

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Understanding the process of hydrate nucleation in the liquid phase is crucial for developing effective methods for hydrate formation. The hydration of hydrophobic guest molecules plays a significant role in dissolving these molecules in the water phase, because for hydrate formation a large amount of dissolved gas is necessary. Experimental study on the molecular level is very complicated due to the small sizes and stochastic nature of the process, that resulting in high requirements for equipment and researcher's expertise. Therefore, molecular dynamics methods are particularly suitable for these studies.

This work focuses on investigating the very initial stages of hydrate formation process from a supersaturated gas solution without applying any excess pressure or super-cooling using MD methods. We studied the influence of various surfactant additives, such as methanol and sodium lauryl sulfate, on the nucleation process and the dynamics of hydrogen bond network reconfiguration during hydrate formation. For MD simulation we used the LAMMPS package.

According to our results specific concentrations of methane in the water phase lead to the formation of hydrate-like cavities; the presence of methanol or sodium lauryl sulfate significantly enhancing the rate of hydrate formation. An optimal concentration of methane was identified, which maximizes the growth rate of hydrates. The study also reveals that the growth of hydrate structures occurs rapidly from a supersaturated metastable solution, demonstrating the universality of this effect across different gases. The findings contribute to a deeper understanding of hydrate formation mechanisms and provide insights for practical applications in gas and oil pipeline management.

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