

Effects of nanobubble on natural gas hydrate growth revealed from molecular simulation

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Natural gas hydrate, known as fire ice, is a clathrate hydrate in which a large amount of methane is trapped within hydrogen bond network of water. Natural gas hydrate is regarded as a strategic energy resource due to its huge capacity and clean energy nature. To efficiently develop natural gas hydrate resource, the mechanisms of hydrate nucleation, growth and decomposition must be fully understood. However, due to the complexity of heat and mass transfer with phase transition in multiscale, there are still large knowledge gaps.

During decomposition, natural gas hydrate changes to methane gas and water. As the ratio of methane to water is many times larger than the maximum solubility of methane in water, nanobubbles form near the decomposition interface. The forming and evolution of nanobubbles affects heat and mass transfer behavior and has been found to decrease gas diffusion. Nanobubble has also been related with natural gas hydrate reformation, however, no direct proof has been found. In this manuscript, molecular dynamics simulation method was selected to investigate the effects of nanobubbles on natural gas hydrate growth. A system was constructed with natural gas hydrate and water solution containing methane nanobubbles. The nanobubble was found to be stable and stay a certain distance away from the hydrate surface at phase equilibrium condition. When the temperature decreases, natural gas hydrate growth happens. It's interesting that the natural gas hydrate grows around the nanobubble. The methane density profiles were calculated and no special high methane density was found around the nanobubble. The natural gas hydrate growth features as well as nanobubble evolution characteristics were analyzed. The natural gas hydrate growth features include growth rate, hydrogen bond network changing, source of atoms forming natural gas hydrate, water diffusion, methane diffusion. The nanobubble evolution characteristics include size variation, shape changing, methane number decreasing, methane diffusion. The role that nanobubble plays in natural gas hydrate growth was discussed.