The molecular mechanism of nano-bubbles formation and its effect on decomposition of hydrate

WENFENG HU,[12] CONG CHEN,[12] WEIZHONG LI,[12] YONGCHEN SONG[12]

[1] Key Laboratory of Ocean Energy Utilization and Energy Conservation of Ministry of Education, Dalian University of Technology, Dalian 116024, P. R. China. E-mail: congchen@dlut.edu.cn

[2] School of Energy and Power Engineering, Dalian University of Technology, Dalian 116024, P. R. China. E-mail: congchen@dlut.edu.cn

Nano-bubbles have been shown to play an important role in affecting the decomposition kinetics of hydrate and the migration of guest molecules. Although many studies have found the formation of nano-bubbles during hydrate decomposition, whether the nanobubbles promotes or inhibites the decomposition still remains controversial, and the evolution mechanism and the physical properties of the nanobubbles are unclear currently. In this paper, we establish the hydrate-water system and analyse the decomposition characteristics of the hydrate under heating condition by using molecular dynamic simulations. We investigate the change of system potential energy, the order paremeter of H_2O, the statistics of hydrogen bond, the movement of solid-liquid interface, the radial distribution funtion, the density distribution of methane molecules and the diffusion cofficient of methane molecules in liquid water. It is found that the decomposition of hydrate is carried out layer by layer, and with the decomposition of hydrate, the number of hydrogen bonds decreases and the potential energy of the system increases gradually. The formation of nano-bubbles not only reduces the concentration of methane in the liquid phase, but also decreases the diffusion rate of methane molecule in the liquid phase. Moreover, the decomposition rate is defined more accurately by real-time analysis of hydrate cage sturcture in the decomposition process. The paper also provides a way to select nano-bubbles accurately. According to our analysis, it is found that there are two kinds of formation mechanisms of nano-bubbles. The above research aims to clarify the microscopic mechanism of natural gas hydrate decomposition and the formation of nano-bubbles, providing theoretical guidance for the efficient exploitation of hydrates.