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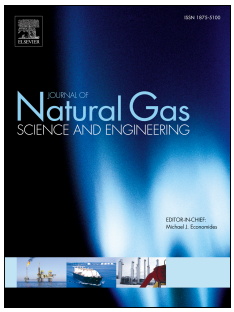

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Thermodynamic and Structural Properties of Methane/Water Systems at the Threshold of Hydrate Formation Predicted by Molecular Dynamic Simulations

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Abstract

Molecular dynamic simulations have been served to investigate various properties of methane/water system at two extreme conditions: away from hydrate formation and threshold it. The results that compare the two conditions have been discussed in the terms of surface tension, mean square displacement (MSD), diffusion coefficient, radial distribution function and thermodynamic functions. Investigation over a timescale of 500 ps demonstrated that the thermodynamic functions at 275 K and high pressures (corresponding to the hydrate formation threshold) are smaller than that of at 298 K, implying that the hydrate formation threshold is more stable. An increase in the system pressure and temperature leads to a decrease in the surface tension because of decreasing the intermolecular attractive forces. Besides, the comparison of oxygen-oxygen, carbon-carbon and carbon-oxygen radial distribution functions at temperatures of 275 and 298 K has been indicated that the height of peaks decreases due to increasing the temperature, demonstrating that the system become more stable at the threshold of hydrate formation.

Keywords: Methane; Hydrate; Molecular dynamic simulation; Diffusion coefficient; Surface tension.