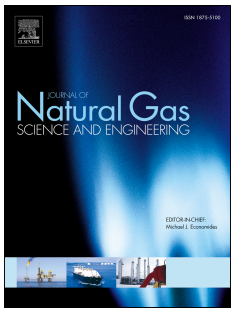
# Accepted Manuscript




Comparison of the thermodynamic, structural and dynamical properties of methane/water and methane/water/hydrate systems using molecular dynamic simulations

Parisa Naeiji, Farshad Varaminian, Mahmoud Rahmati

PII: S1875-5100(17)30179-8

DOI: 10.1016/j.jngse.2017.04.010

Reference: JNGSE 2149

To appear in: *Journal of Natural Gas Science and Engineering*

Received Date: 18 December 2016

Revised Date: 5 April 2017

Accepted Date: 8 April 2017

Please cite this article as: Naeiji, P., Varaminian, F., Rahmati, M., Comparison of the thermodynamic, structural and dynamical properties of methane/water and methane/water/hydrate systems using molecular dynamic simulations, *Journal of Natural Gas Science & Engineering* (2017), doi: 10.1016/j.jngse.2017.04.010.

# Comparison of the Thermodynamic, Structural and Dynamical Properties of Methane/Water and Methane/Water/Hydrate Systems Using Molecular Dynamic Simulations

Parisa Naeiji[a], Farshad Varaminian[a,*] and Mahmoud Rahmati[b]

[a] Department of Chemical, gas and petroleum Engineering, Semnan University, Semnan, Iran.

[b] Chemical Engineering Department, Kerman Graduate University of Advanced Technology, Kerman, Iran.

* Corresponding Author. E-mail: fvaraminian@semnan.ac.ir, Tel.: +982333654120; Fax: +982333654280

## Abstract

In the present work, the thermodynamic, structural and dynamical properties of methane hydrate system were predicted by molecular dynamic simulations. Having knowledge of how methane/water system undergoes thermodynamic, structural and dynamical changes is practical, when methane hydrate is formed. So the aim of this work is to investigate the differences in the properties between two systems; methane/water and methane/water/hydrate systems. The results showed the thermodynamic properties of methane/water/hydrate system are lower than that of another one implying the hydrate structure is more stable and decreases the energy surface of system. The potential energy, density and MSD profiles were determined to distinguish the transition position and width of the interface of hydrate clathrate. Also, the diffusivity reduction proves that the molecular structure varied from liquid-like to the solid-like. A procedure was used to calculate the water/hydrate surface tension that is consistent with the previously reported. Finally, the comparison of oxygen-oxygen, carbon-carbon and carbon-oxygen radial distribution functions indicated that the heights of peaks increase and become narrow in methane hydrate system confirming the regular arrangement of methane and water molecules in the hydrate phase.

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