

Perturbing the Stability of Gas Hydrates - Perturbing the Stability of Gas Hydrates - Biannual report VISTA 2011

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Annual and Biannual report VISTA 2011

Stability of gas hydrates

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Project duration: 01.10.09 - 30.09.12

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Division head: Nøier, Lars

Project number: 6343

Object

The main objective of the project is to investigate the stability of clathrate hydrates under different external conditions and with different gas inclusions. The study is done with the help of Monte-Carlo and molecular dynamics simulations. The stability is to be analyzed by building the phase diagram for empty and filled hydrates. Proposed gas inclusions to be studied are the methane, CO₂, ethane and others.

The future work in the project will be related to the effect of different inclusions on the hydrate stability as well as the effect of coexistence of different cage structures.

Status:

The Helmholtz energy of CO₂+CH₄ hydrate has been calculated. These data are the main information needed to build the phase diagram. This resulted in a journal article, which is currently being reviewed. The main result of the article is suggestion of a thermodynamic path to convert a CH₄ hydrate into a CO₂ hydrate without destroying the clathrate structure. The work on calculating the phase diagram of the CO₂+CH₄ mixture is ongoing.

The adsorption isotherms of ethane have been calculated. It will next be used to calculate C₂H₆+CH₄ phase diagram the same way it is done for CO₂+CH₄ hydrate.

The ongoing work is basically within the targeted timeline.

Project meetings:

In January 2011 there was a meeting with the group in Bergen, leaded by Bjørn Kvamme and Arne Graue. They are willing to collaborate on further results.

There was a meeting with Statoil in April 2011. An important input on the project needs has been received.

Publications:

1. *Adsorption of CO₂ and CH₄ and their mixtures in gas hydrates.* K. Glavatskiy, T. Vlugt, S. Kjelstrup. Submitted to J. Phys. Chem. C.

2. *Lattice parameters and corresponding properties of methane and carbon dioxide hydrates: molecular dynamic simulations.* F. Ning, K. Glavatskiy, T.J. Vlugt, S. Kjelstrup. Gas Hydrates Symposium at ACS 241st National Meeting, 17-28 March 2011, Anaheim, CA, USA. Talk (F. Ning)