Final report VISTA 2012

Project title

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1. **En ½ A4 side med populærfremstilling av prosjektet (stipendiat)**

   Gas hydrates are crystalline ice-like structures, which consist of water and some guest gas molecules. The water molecules form cages, in which the guest gas molecules are "trapped". The presence of the gas molecules stabilizes the cages, which are otherwise unstable and will collapse to liquid water or to an ice structure. Gas hydrates are found in the sea bottom and represent a potential source of energy, since the trapped guest molecules are the typical components of the natural gas: methane, ethane, etc. Gas hydrates are also found in outer space (in comets), and are important wherever water exists. Knowledge of hydrates as absorbents is important for several reasons. Many different gases can form hydrates; methane and carbon dioxide are among of them. Thus, hydrates can serve as 1) a potential source of energy, which comes from burning the trapped methane; 2) a potential storage of carbon dioxide, which is found in the atmosphere. The question of tapping hydrates for hydrocarbons is of big interest, because the amount of gas is large. But this tapping cannot occur without destroying the network. An idea is then to exchange methane with carbon dioxide, and use the hydrate to store the greenhouse gas. In order to explore this idea, extensive thermodynamic data of types of gas hydrates are required. This can be done with great accuracy by computer simulations. Such simulations can give knowledge of typical thermodynamic conditions, for a possible exchange of gases in hydrates, and the most efficient way to actually do it. A popular science article was written (Publ. 2).

2. **Har det skjedd endringer i målsetning underveis?/ Oppnådde en det som ble lovet? (stipendiat)**

   Thermodynamic data for hydrates containing either carbon dioxide or methane, or mixtures of the gases were generated as functions of temperature and pressure. This was the main aim of the project, successfully accomplished, leading to articles in the literature, see below. Within the course of the project it was assumed to initiate the research on the kinetics of the gas exchange. This was not achieved since the amount of data required to process this was too large, which required a lot of simulation time. We have, however, prepared background for further work on this topic. This will include two projects with the main focus on hydrate kinetics: nucleation of hydrates and diffusion of guest gases in defected structures.

3. Publikasjoner (stipendiat)

1. F. Ning, K.Glavatskiy, T.J.Vlugt, S.Kjelstrup. *Prep. Pap. Am. Chem. Soc., Div. Fuel Chem.* 2011, 56 (1), 85. “Lattice parameters and corresponding properties of methane and carbon dioxide hydrates: molecular dynamic simulations”.
2. K.Glavatskiy, S.Kjelstrup. *Meta magazine* (Notur project) 3, p. 22 (2011). “Predicting hydrate stabilities”
3. K.S. Glavatskiy, T.J.H. Vlugt, S. Kjelstrup. *J. Phys. Chem*. B 2012, 116, 3745−3753. “Towards a possibility to exchange CO_2 and CH_4 in sI clathrate hydrate”
4. F. Ning, Y. Yibing, S. Kjelstrup, T.J.H. Vlugt, K. Glavatskiy. *Energy Environ. Sci*., 2012, 5, 6779. “Mechanical properties of clathrate hydrates: status and perspectives”.
5. K.S. Glavatskiy, T.J.H. Vlugt, S. Kjelstrup. in preparation. “Gibbs energy of the reaction exchange of CO_2 and CH_4 in sI clathrate hydrates.”
6. K.S. Glavatskiy, T.J.H. Vlugt, S. Kjelstrup. in preparation. “Entropic effect of guest encapsulation”

4. Refleksjoner om videreføring (fra prosjektleder)

The project has been a succes as seen from the Department of Chemistry, Group of Applied Theoretical Chemsitry. It has boosted our competence and activity in computational chemistry, and created synergy between this project and a NFR funded strategy project “From molecules to process applications”. It has served to attain interest from Master students, and led to the reruitment directly of one new PhD, to continue the effort and study the kinetics of hydrate formation (funded by Statoil directly). We are thus looking forward to continued collaboration.