540f Thermodynamics-Based Design of H2 Storage in Clathrates

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The current scenario of diminishing petroleum resources requires us to look for alternate fuel resources. Hydrogen is one such resource with its advantages of clean burning and security of supply. If one needs to use H2, H2 should be stored at reasonable pressures (<100 atm) at ambient temperatures. Our research is aimed at understanding and designing one such sustainable storage medium: Gas hydrates

Gas hydrates are crystalline compounds, also known as clathrates. The H2 molecules are entrapped in a cage like structure of hydrogen bonded water molecules. Their general formula is Mn(H2O)p where M: Gas, n : number of gas molecules, p: number of water molecules. The design of gas hydrate storage systems needs an accurate prediction of dissociation pressures with temperature.

The dissociation pressures are generally predicted using van der Waals and Platteeuw theory. It is applicable to singly occupied cavities. Multiple H2 occupancies in one water cavity are handled by assuming that bi hydrogen and tetra hydrogen molecule clusters are single cluster molecules. Ab initio calculations are performed for determining binary interaction potential of one H2 cluster with one water molecule for various inter molecular distances and various spatial cluster configurations using GAMESS. The interaction energies are fit to various forms: Exp 6, Lennard-Jones and Kihara. The best fit form is used to calculate the Langmuir constant. At equilibrium, the chemical potential of water in liquid / ice phase will be equal to that of water in hydrate phase. The other phase present is the gas phase. The reference chemical potential will be adjusted, if necessary, to get close agreement between the experimental dissociation pressure and the calculated dissociation pressure using a cell distortion model. This model can be used to explore the possibility of producing low-pressure H2 hydrates in confined media.