Non-equilibrium thermodynamics in hydrocarbon systems

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1.0 Introduction

Non-equilibrium situations are of great importance in many processes in the industry of petroleum. The loss of chemical equilibrium will lead to a spontaneous mass transfer.

Examples of processes in the industry of petroleum, where mass transfer is important, are drying of pipelines for natural gas transport, kinetics in the formation of hydrates, removal of acid gasses (absorption, adsorption, membranes). In a drying process we normally try to achieve a mass transfer as quickly as possible, while in other situations, we wish to achieve slow mass transfer. To keep control of all these non-equilibrium situations, it is important to be able to predict the behaviour of the system accurately.

Computer programs, which are able to handle non-equilibrium situations, have been tried out, and several computer-based programs are under development. To achieve a good result with these, it is important to predict the mass transfer thoroughly and effective. The models for the mass transfer must be validated by experimental data.

A better insight into the physics of mass transfer, will make us able to operate existing processes in a better way, but also develop new and more effective technology.

2.0 Scientific work

Absorption entails the removal of a substance from a gas by contacting it with liquid into which the desired component dissolves. Some typical examples of importance are the removal of sulphur dioxide from stack gases by absorption with alkaline solutions, absorption of carbon di-oxide from combustion product into aqueous amine solutions, and the removal of propane or other heavier components from natural gas by absorption into hydrocarbon oil.

All absorption processes involve the following steps:

- The gas and liquid are brought together in a suitable contacting apparatus.
- The two phases are allowed to approach equilibrium
- The gas-liquid phases are separated.

The desired material is transferred from the gas to the liquid in step 2 at a rate which depends on its concentrations in the gas and liquid, the mass transfer coefficients in each phase, the solubility of the material in the liquid, and the amount of gas-liquid interfacial area made available in the contactor.

This Ph.D work aims to develop precise models for the mass transfer coefficients and kinetics related to the absorption process. The purpose of this research is to be able to process natural gas at very high pressures (200 bar), and my experimental research will therefore be on high pressure systems.

The main experiments will be done in a high pressure wetted wall column, where sour gas (CO_2 and H_2S) and amine solutions will be contacted at pressures up to 200 bar. Experiments will also be done in a two-bulb diffusion cell, which will give important data on the molecular diffusion rates and the coupling effects of CO_2 and H_2S in high pressure natural gas.

At the moment another Ph.D student is doing high pressure phase-equilibrium experiments on gas-amine solutions. The mass transfer- and the equilibrium data will be used to develop a computer-based model for the simulation of a high-pressure absorption processes.

The scientific delivery from this Ph.D work will be:

- Theoretic and experimental based non-equilibrium models (mass-, heat transfer) for a high pressure absorption process.
- A simulation program based on the experimental data from our research on high pressure gas treating.