Thermophysical Properties Relevant for Gas Hydrate Management Obtained from Atomistic Molecular Simulations

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In this presentation, we will overview our atomistic-level modelling efforts on clathrate hydrates. The initial focus of our research was preventing the formation of clathrate hydrates plugs in oil & gas pipelines, which could lead to environmental accidents (i.e., the flow assurance problem). Using molecular dynamics simulations, we studied molecularly thin films of surfactants adsorbed on methane hydrates. We found that some surfactants yield ordered interfacial structures. Because these surfactants are effective in preventing the formation of hydrate plugs, as observed experimentally, we proposed hypothesis concerning structure-function relations that could help developing new flow-assurance chemicals. The focus of our research then evolved to designing chemicals for promoting the formation of CO_2 hydrates, towards advancing strategies for carbon capture, transport, and sequestration. Of particular interest is the ability of simulations to uncover synergistic and antagonistic effects among chemicals used in practice. These observations will be reviewed, with the objective of promoting sustainable practices.

We will discuss how our atomistic simulations leveraged experimental observations from our collaborators at the Colorado School of Mines (i.e., the group led by Prof. Carolyn Koh), and stochastic simulation studies conducted by our collaborators at the University of Oxford (i.e., the group led by Prof. Michail Stamatakis), as well as comprehensive simulation-based screening of chemical compounds conducted by our collaborators at the University of Surrey (i.e., the group led by Prof. Anh Phan).

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