TALKS

Daresbury

REMOVING ACID GASES FROM NATURAL GAS
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Gases like H2S and CO2 are present in natural gas. One way of removing them is by passing the gas within an aqueous solution of ethanolamines. We performed molecular dynamics simulations to determine the force field of those molecules and to calculate thermodynamic properties in the liquid phase and at the liquid-vapor interface on systems containing pure components and mixtures. The solubility of H2S and CO2 is obtained as a function of concentration of ethanolamines and pressure. The simulation results are in good agreement with experimental data.

I would like to thank CCP5 and Professor Bill Smith for the support I received during my visit at UK in August 2010. I appreciate his hospitality and patient to teach me the basics of parallel programming. He told me 'think in parallel' but sometimes it is difficult 'to think' even in serial.

At Dareresbury, I was working with Professor Bill Smith on parallel programming applied to Molecular Dynamics programs using replicated data strategy. We used fortran 77 and fortran 90 languages to speed up some of the routines in programs with classical force fields.

I talked with Michael Seaton about mesoscopic simulations, in particular, the addition on Dissipative Particle Dynamics of electrostatic interactions using the Ewald sums . Laurence Allison explained to me the way he is trying to improve the parallel programming on inhomogeneous systems. I talked with Ilian Todorov about the new version of the molecular dynamics program DL_POLY.

Manchester

PRECIPITATION OF IONS IN WATER

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The molecular description of solubility of ions is water is a fundamental problem that has interest in electrochemistry, geological and biological systems, among other fields. Molecular dynamics simulations allow understand the role that molecular interactions play to describe the solubility of ions in solution. We recently found that precipitation of ions is very sensitive to short ranges interactions and that several force fields of ions do not describe the correct behaviour in solution. Unphysical precipitation of ions can be found at dilute concentrations and some times the ions do not precipitate even at supersaturated conditions. In this talk we will give a molecular description of hydration and precipitation of ions in solution.

I thank Dr. Flor Siperstein for organizing a seminar at the Chemical Engeneering Department at Manchester University. I talked with her and with some of her students about Dissipative Particle Dynamics simulations of polymers and surfactants. We also talked with Laura about ethanolamine aqueous solutions. I talked with Professor Andrew Master and with some of his students about the projects they are developing on nematic phases of liquid crystals. I also talked with Dr. Richard H. Henchman about their calculations of solvation entropy on noble gases and ionic solutions.

Imperial College

Simulation of fluids at interfaces

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The behaviour of fluids close to an interface is different than that observed in a bulk phase. The properties of these systems can be described with theories of inhomogeneous fluids. Computer simulations are also powerful tools to understand the role that molecular forces play on interfacial properties. The properties of inhomogeneous fluids in a simulation strongly depend on the range of the interaction and finite size effects of different variables. Surface tension, adsorption of molecules at the interface and molecular orientation are some of the properties that will be analyzed during this talk. Studied systems include hydrocarbons, water, ionic fluids, ionic solutions and surfactants.

I appreciate Dr. Fernando Bresme of the Chemistry Department at Imperial College-London for organizing a seminar and for the support he gave during my stay at London. We were discussing problems related with ionic solutions at the liquid-vapor interface. I talked with some members of his group. I met also Professor G. Jackson and Dr. Erick Muller and I had some discussion with them about interfacial properties.

I also talked with Dr. D. Dimi and PhD student Edward Smith at the Mechanical Engenering Department who are working with Professor D. Heyes in developing techniques to simulate coupling between molecular dynamics with continuous Navier-Stokes solutions of liquids. They will apply those techniques to calculate the boundary layers flow of real fluids.

Royal Holloway

Ionic fluids and polyeletrolytes

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Charged fluids have interesting properties and they are found in many industrial application. The correct description of their properties using theoretical method is not well understood. In this talk computer simulation results of charged fluids with implicit and explicit solvent are discussed. Interfacial properties and phase equilibrium of ionic fluids with asymmetry in size and charge are analyzed. Electrolytes systems are also studied to understand the solubility of ions as a function of concentration and temperature. Finally, results of large charged polymers in solution are studied using the Dissipative Particles Dynamics method that allows include explicitly the solvent.

I had nice discussions with David Heyes about mesoscopic simulations and I appreciate him for organizing a seminar at the Physics department at Royal Holloway, part of the University of London. I met also Andrew Ho who is in charge of the seminar program. I had discussions with Pet Gardner about the calculation of activity coefficients in electrolytes by using computer simulations.