

SEMINAR ANNOUNCEMENT

Thermodynamics of Fluid-Phase Benzene Via Molecular Simulation

John Tatarko, MS candidate

Department of Chemical and Biomedical Engineering
Cleveland State University

Abstract: The chemical process industry annually produces about 30,000 different commodities from approximately 500 basic chemicals. Separation processes, contact operations at the core of unit operations account for perhaps 75% of the plant investment and operating costs. The need for accurate thermo-physical data is greater than ever. The estimated laboratory cost for providing properties at one datum; that is one temperature and pressure, is approximately \$3000 and requires two to three man-days to accomplish. Low cost computational power now provides a method for determining thermo-physical properties throughout the fluid phase via molecular simulation. Molecular simulation is computational statistical mechanics. As the bridge between classical mechanics and thermodynamics, statistical mechanics helps us build a *virtual laboratory* unconstrained by manpower and equipment costs.

Benzene is a well-studied and important feedstock for pharmaceuticals and commodity chemicals alike. The beauty of benzene is inherent in its flat, symmetric, and ring-like structure. It is the perfect candidate for property determination via molecular simulation. The discerning thermodynamicist uses molecular simulation, rigorous classical and statistical thermodynamics along with perturbation theory to arrive at a comprehensive mapping of thermo-physical properties through the fluid phase.

This thesis compares the work of three investigators, all who claim that their hexagonal model best describes the benzene molecule. In addition, their claims are compared with the Goodwin equation of state for benzene which was generated from actual laboratory experiments. Finally, the thermodynamic properties generated via virtual laboratory experiments are used to generate a 12 parameter equation of state that accurately describes the thermodynamic properties of benzene throughout the fluid phase region up to 1000 bar. The validity of this equation of state is verified.

Tuesday, April 27th, 2010

12:00 – 1:00 pm

Room SI 117