243m Combining Molecular and Chemical Process Simulation Using Step Potential Equilibria and Dynamics (Spead)

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The Step Potential Equilibria And Dynamics (SPEAD) model provides a basis for molecular modeling of thermodynamic and transport properties. It is based on Discontinuous Molecular Dynamics (DMD) and second order Thermodynamic Perturbation Theory (TPT). DMD simulation is applied to the repulsive part of the potential, complete with molecular details like interpenetration of the interaction sites, 110 degree bond angles, branching, and rings.[Cui, and Elliott, 2001; Unlu et al., 2004] The thermodynamic effects of disperse attractions and hydrogen bonding are treated by TPT. This approach accelerates the molecular simulations in general and the parameterization of the transferable potentials in particular. Transferable potentials have been developed and tested for over 200 components comprising 22 families. These families include thiophenes, phosphates, fluorocarbons, alcohols, and amines to name just a few examples.

One challenge to molecular modeling of process and product design is achieving the connection between nano-scale interactions and dynamics and the macroscale process and material properties. This can be achieved by molecular simulation of the key thermodynamic and transport properties and interfacing these properties with a chemical process simulator. This procedure is demonstrated for a typical compound and the ChemCAD process simulator. The properties determined from molecular simulation are vapor pressure, density, diffusivity, viscosity, and thermal conductivity.

A different challenge is the efficient development of transferable potentials to describe molecular interaction for many compounds, mixtures, and properties in globally optimal fashion. We present a systems based approach to solving this problem based on a random recursive search. The global optimum is sought based on minimizing the error in vapor pressure for a large database with interdependent site types while minimizing the number of discrete wells in each potential.

Keywords: Physical properties, molecular simulation, diffusivity, thermal conductivity, viscosity.

References Cui, J.; Elliott, J.R.; J. Chem. Phys., 114:7283 (2001). Unlu, O.; Gray, N.H.; Gerek, Z.N.; Elliott, J.R.; Ind Eng. Chem. Res., 43:1788 (2004).