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Square-Well Fluid Monomer-Dimer Mixtures: Structural and Thermodynamic Properties JAMES A. PORTER, JANE E.G. LIPSON, Dept. of Chemistry, Dartmouth College — Previous studies of square-well chain fluids using continuum Born-Green-Yvon (BGY) theory have focused solely on the structural and thermodynamic properties of one-component fluids in equilibrium, for which the basic variables are fluid density and temperature. In the case of mixtures, the concentrations of the respective components must also be taken into account, which makes the problem a non-trivial one. In this talk, we propose a method for determining the structure, and thus the thermodynamic properties, of a mixture of monomers and dimers by a series of interconnected BGY equations (to be solved self-consistently). From these, monomer-monomer, monomer-dimer, and dimer-dimer correlation functions are obtained which explicitly account for temperature, the density of each component, and the effects of interactions between the components (concentration dependence). Thermodynamic properties are then calculated and compared with other theoretical approaches and with simulation results. Approximate methods for solving these equations are also discussed, and trends in the refinement of the theory from simpler to more complex approaches are examined.

James A. Porter
Dept. of Chemistry, Dartmouth College

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