Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Interpolation between State Points in the Simulated Perturbation Contributions of Polymer Solutions[1] AMIR VAHID, Chemical and Biomolecular Engineering Department, The University of Akron, Akron OH 44325 USA, NEIL H. GRAY, Chemstations Inc., 2901 Wilcrest Dr., Houston TX 77042 USA, J. RICHARD ELLIOTT, Chemical and Biomolecular Engineering Department, The University of Akron, Akron OH 44325 USA — Polymeric mixtures of hydrocarbons, alcohols have been simulated with discontinuous potential models to characterize the Helmholtz energy of the repulsive reference fluids (A0) along with the first and second order perturbation contributions (A1, A2) as functions of density and composition. Taken together, these terms generate a complete equation of state for the mixture, including temperature effects as well as density and composition. The specific hydrocarbons studied were methane, ethane, propane, n-butane, n-hexane, n-heptane, n-decane, and benzene. The specific alcohols were water, methanol, ethanol, n-propanol, and n-octanol. Unfortunately, a slight inconsistency was encountered when the trend observed for these small molecules was extrapolated to the long chain limit. Therefore, we extend the analysis to mixtures of n-alkanes, branched hydrocarbons, and aromatics with polymeric molecules of: n-alkanes, ethyl-styrenes, ethyl-propylenes, and isoprenes. The perturbation contributions can be accurately characterized by van der Waals mixing rules and compared with the MCSL SAFT and Guggenheim-Staverman theories.

[1] The authors gratefully appreciate ChemStations, Houston, TX for financial funding.

Amir Vahid
Chemical and Biomolecular Engineering Department,
The University of Akron, Akron OH 44325 USA

Date submitted: 02 Dec 2008 Electronic form version 1.4