

Determination of Equation of State Parameters by Molecular Simulation and Application to Systems Containing Polymers

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The Sanchez-Lacombe equation of state (SL-EOS) has been employed to calculate the phase behavior of several polymer-solvent systems over a wide range of pressure and temperatures. The characteristic parameters of the SL-EOS have well-defined physical meanings, making it possible to directly estimate these parameters from molecular dynamic (MD) simulation. In this study the characteristic parameters for the involved pure components were estimated using a recently proposed MD method. For systems examined a binary interaction parameter, accounting for interaction between the different species, was used to fit the model prediction to newly available polymer-solvent equilibrium data. The evaluation of the binary interaction parameter unveiled significant temperature dependence, which has been accounted for in the description of the interaction parameter. The calculation results were found to be in good agreement with the experimentally measured data.