

Inferring Phase Behavior of Polymer Solutions from Molecular Simulations and Extrapolation to the Long Chain Limit

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Molecular simulation of polymeric systems is impeded by the slow equilibration and large simulations inherent in directly treating these systems. Work by Ghobadi and Elliott (2011) and Elliott and Gray (2005) showed how molecular simulations of the terms contributing to perturbation theory exhibit asymptotic trends in the long chain limit. This observation forms the basis for a general approach to treating polymers of any molecular weight of structure. For polymer solutions, detailed simulations of mixtures over broad ranges of molecular weight, branching, and ring content form the basis for mixing rules to interpolate between state points of various compositions, densities, and molecular weights. This methodology is tested using the database of Elliott and Natarajan (2002) for polymer solutions. The methods are then applied to predict the compatibility of several plasticizers in polyVinylChloride and polyLactide with an emphasis on naturally occurring and sustainable plasticizers.