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Quantitative Predictions of the Enthalpic Component of the Interaction Parameter in Mixtures: An Assessment of the Accuracy and Precision Required From Molecular Simulations DAVID RIGBY, Accelrys, Inc — The use of force field based atomistic simulation methods to calculate the enthalpic part of the interaction parameter in mixtures containing small molecules or polymers is both conceptually simple and appealing in view of the enormous potential savings in the cost of synthesis and experimental measurements (e.g. when one is seeking a new or modified polymer mixture system). In order for such simulations to be ultimately successful however, it is necessary that they be capable of routinely making accurate predictions of excess thermodynamic properties. This in turn requires both that a force field be capable of high accuracy and that the associated simulation protocol be capable of high precision. This presentation will examine the factors that affect precision and accuracy in typical simulations of experimentally well-studied small molecule mixture systems containing aliphatic and aromatic hydrocarbons, and will further discuss additional sources of uncertainty when the simulations are extended to mixtures of oligomers or polymers comprised of similar aliphatic and aromatic moieties.

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