Prediction of Mixture Interaction Parameters for Multi-Component Mixtures Using Quantitative Structure-Property Relationships (QSPR)

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The state-of-the-art in calculating the thermodynamic properties of mixtures is based on the use of Helmholtz-energy-explicit equations of state for each of the components of the mixture and an excess term that accounts for the non-ideality of the mixture. The excess part requires a few pair-specific fitted parameters. Mixing model parameters are available for a number of binary mixtures, but there are many binary pairs for which little or no experimental thermodynamic data are available. Ultimately we will arrive at a correlation that allows for straightforward predictions of the mixture parameters for an arbitrary mixture of fluids based on information about the molecular structure of each of the fluids (from the Quantitative Structure-Property Relationships (QSPR) framework) forming the binary pair. The first step is to apply the state-of-the-art mixture parameter fitting routines in order to obtain predictions of the binary pair parameters for all the current binary pairs that are included in REFPROP. After the binary pair interaction parameters have been obtained, a correlation will be developed for each of the binary pair interaction parameters as a function of QSPR fluid data. The successful application of this technique will allow the prediction of thermodynamic properties, including vapor-liquid equilibria, critical points, densities, and many other parameters of technical interest for binary pairs of components for which high-accuracy equations of state are available, but where no binary mixing model parameters exist.