A New Excess Gibbs Free Energy Model

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Abstract

A mathematical model for representing the excess Gibbs free energies of multicomponent fluid mixtures is proposed. The model involves the use of one interaction energy parameter, two size parameters, and one size adjustment parameter for each of the constituent binary pairs in a multicomponent mixture. For mixture involving only non-polar substances, the size parameters can be calculated by means of the Peng-Robinson equation of state and the interaction energy parameter can be obtained by means of regression of binary vapor-liquid equilibrium data. In general, the parameters for polar substances cannot be calculated by means of the Peng-Robinson equation of state. However, the size parameters for water and the alkanols ranging from methanol to butanols have been determined. These parameters have been used successfully to correlate the binary vapor-liquid equilibrium data for mixtures of alkanols and aqueous solutions of the above-mentioned alkanols. The capability of the proposed model to predict the vapor-liquid equilibria of multicomponent systems will be illustrated by means of the calculated results for several ternary systems.

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