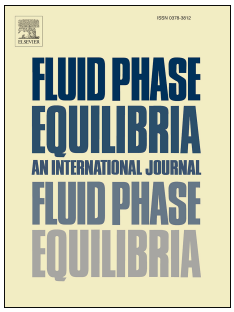

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A Statistical Thermodynamic Model with Strong Adaptability for Liquid Mixtures

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Abstract:

How to accurately predict thermodynamic data of highly irregular liquid mixtures, such as Ca-Pb-Sb and Fe-C-Cr, is always an interesting but knotty problem no matter in the field of metallurgy or chemistry. Based on the same theory foundation (Scott's two-fluid theory and Scatchard-Hildebrand theory) but on different assumptions, a model with two different forms for excess Gibbs energy of liquid mixtures is derived from statistical thermodynamics, in which volume parameter and energy parameter are separated. Under the same conditions, compared with classical local composition models and sub-regular solution model (SRSM), this model not only has a significant increase (more than 30%) in predictive capability, but also shows stronger adaptability to various highly irregular systems, especially to super negative deviation systems (SNDS) whose activity can be as low as 10^{-11} and to low concentration saturated solution (LCSS) with strong asymmetry.

Keywords: MIVM; Scatchard-Hildebrand theory; Asymmetric systems; Activity

1. Introduction

Thermodynamic models can be utilized to predict thermodynamic data as a first approximation or reference, by this means a large amount of manpower and material resources have been saved. Hence, it is no doubt that thermodynamic model provides a promising, efficient and economical approach to obtain reference data.

Generally, the calculating process of thermodynamic models can be briefly expressed as that the predictive results can be achieved by substituting adjustable parameters into corresponding thermodynamic models. So far there are two approaches to obtaining these adjustable parameters: calculating directly from the first principles and fitting from experiments data of binary systems. As early as 1990s, Sam and Sandler tried to calculate