A Fully Consistent Approach for an Associate Solution Model

Dmitry Saulov
GTT-Technologies, Herzogenrath

ABSTRACT

Part 1: Resolving entropy paradox
A modified associate formalism is proposed for thermodynamic modelling of solution phases. The approach is free from the entropy paradox described by Luck et al. The model is considered in its general form for an arbitrary number of solution components and an arbitrary size of associates. Asymptotic behaviour of chemical activities of solution components in binary dilute solutions is also investigated. The suggested model is compared with similar models, such as the classical associate model, the associate species model and the modified quasichemical model. Advantages of the new model are demonstrated.

Part 2: Treatment of polynomial excess functions
The problem of predicting the properties of multicomponent systems from those of corresponding binary systems is considered. Widely used projected methods, including Kohler, Muggianu and Kohler/Toop, are analysed. A probabilistic interpretation of the parameters of the power series polynomial model, which explicitly relates them with the Gibbs free energies of the generalised quasichemical reactions, is proposed. The presented treatment provides a theoretical justification for such parameters. A methodology of estimating the ternary interaction parameter from the binary ones is presented. The methodology provides a way in which the power series multicomponent models, where no projection is required, can be incorporated into the Calphad approach.