

On the Development of a Group-Interaction-Contribution-Based UNIFAC Model

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A modification of the UNIFAC method is proposed, replacing the concept of group contributions by the group-interaction contributions (interactions between bonding groups: GIC theory). The effects of the environment of each group are captured by the group-interaction contributions in which it takes place, based on the GIC estimation theory. This structure contribution method has a precise physical background and works with a smaller number of model parameters (than the usual UNIFAC) for the description of excess functions. On the basis of these parameters the phase equilibria of hydrocarbon mixtures, - as an example -, has been estimated. The scope of the GIC theory is demonstrated through the well-known UNIFAC model in terms of improved correlation/estimation capabilities, distinction between isomers and ability to overcome proximity effects. It is shown how the new model was developed to estimate vapor-liquid equilibria mixtures of hydrocarbons.