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Simultaneous correlation of liquid-liquid equilibria for ternary systems and phase equilibria for constitutive binary systems by modified new activity coefficient model

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Abstract (less than 300 words)

In the previous study, new activity coefficient models, Concentration Dependent Surface Area Parameter (CDSAP) model [1] and r-CDSAP model [2,3], were proposed. CDSAP model is based on the quasi-chemical theory, and assumes that the surface area parameters depend on partner molecules and their concentrations. CDSAP model requires iterative calculations for more than 3 component systems. r-CDSAP model is obtained by Taylor expansion at $\Delta E = 0$ for excess Gibbs energy of CDSAP model. The calculated results by r-CDSAP model are very good for binary vapor-liquid and ternary liquid-liquid equilibria. However, the surface area parameter of pure component q_i^0 is assumed to be common to multicomponent systems in r-CDSAP model. This restriction is slightly inconvenient to use r-CDSAP model for multicomponent systems.

In this study, a modified r-CDSAP model, which is called f-CDSAP model, was applied to simultaneous correlation of liquid-liquid equilibria for ternary systems and phase equilibria for constitutive binary systems with the same parameter sets. In f-CDSAP model, the restriction condition that q_i^0 is common to multicomponent systems is removed, and q_i^0 is determined for each binary system ($i + j$ system) as follows.

$$q_i^0 = q_{ji}^*$$

q_i^0 is expressed as follows for more than 3 component systems.

$$q_i^0 = \frac{\sum_{j \neq i} q_{ji}^* x_j}{\sum_{j \neq i} x_j}$$

For isothermal systems, the correlated results by f-CDSAP model are in good agreement with the experimental data for both vapor-liquid and liquid-liquid equilibria with the same parameter set, and better than those by NRTL and UNIQUAC models. By introducing temperature dependence parameters to f-CDSAP model, ternary liquid-liquid equilibria and constitutive binary phase equilibria with different temperatures are simultaneously correlated well with the same parameter set.

References

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