Keynote Lecture KL 07

Prediction of vapor-liquid equilibria for multicomponent systems by a modified concentration dependent surface area parameter model

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Key Word (3 words)

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Abstract (less than 300 words)

Our group proposed a new activity coefficient model which is based on the regular solution theory and composition-dependent surface area parameters. Surface area parameters, which account for the number of interactions between molecules, vary depending on partner molecules and the concentration of mixtures. This is called r-CDSAP model. r-CDSAP model can successfully describe an exceptionally high value or convex behavior of activity coefficient in the dilute region. r-CDSAP model also shows improved performances in correlating the liquid-liquid equilibria for ternary systems and the vapor-liquid equilibria for constituent binary systems with the same parameter sets [1,2].

r-CDSAP model is very flexible, but this flexibility is an obstacle in estimating the activity coefficients of multicomponent systems from the parameters determined with binary systems. Another obstacle is the restriction condition to make the surface area parameters of pure components common to multicomponent system.

In order to use r-CDSAP for estimating the activity coefficients of multicomponent systems, the following modifications have been made.

(1) In r-CDSAP model, there is the restriction condition to make the surface area parameter of pure components common to multicomponent systems, which is removed.

(2) When correlating the activity coefficients of binary systems, a limiting condition is added to the surface area parameters of pure components to avoid taking extreme values.

(3) The surface area parameters of pure components determined by binary systems are used only for the corresponding term in excess Gibbs free energy.

As a result, it is possible to estimate the activity coefficients of multicomponent systems using the parameters determined from binary systems by a modified r-CDSAP model. This is called p-CDSAP model. The calculated results for several ternary and quaternary systems are good by p-CDSAP model.

References

[1] Y. Iwai, Fluid Phase Equilibria 465 (2018) 24-33

[2] Y. Iwai, R. Seki, Y. Tanaka, Fluid Phase Equilibria 488 (2019) 62-71