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Liquid-liquid equilibria data validation

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Liquid-liquid equilibria are important thermodynamic phenomena in downstream separations such as extraction. Many data exist in the literature and new continue to appear, which implies a need for data validation. Some attempts, which have been made so far, require an abundance of measured data sets, for comparative studies leading to recommended values. Thus, when two independent investigators obtain substantially different results at the same temperature, definitive assessment is difficult. In such cases, data sets may be classified as tentative, even though they are mutually inconsistent. Thus, to make validations, also when fewer data are available, other techniques are needed.

We report steps towards validation of binary LLE based on fluctuation solution theory. The method has the advantage of having a quite reliable concentration dependence provided the measured data are accurate. For binary mixtures, up to three parameters for each coexisting phase were explored for data sets with points not-too-close to the critical region. For closed-loop or hourglass-like phase diagrams, one additional parameter for each phase in expression for limiting activity coefficient is needed. We have later considered a range of criteria for validation, such as goodness-of-fit, prediction intervals based on the parameters uncertainties, influence of outliers, parameter identifiability measures. Identification of derivatives of solution properties, directly from measured data, requires high quality data. This suggest that discrimination of high-accuracy data from others based on identification of derivative properties could be also a criterion in data validation. Thus, the consistency with values of auxiliary solution property data obtained from independent data – not the set considered – has also been explored. We also report initial steps, based on the Kohler model, regarding ternary systems, for cases where pair 2-3 is immiscible and pairs 1-2 and 2-3 miscible, with component 1 distributed differently in the two phases.