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Dynamic data evaluation for solid-liquid equilibria

Larissa P. Cunico[1], Roberta Ceriani[2], Jeong W. Kang[3], Bent Sarup[4], Rafiqul Gani[1]

[1]CAPEC, Dept. of Chemical and Biochemical Engineering, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark
[2]Faculty of Chemical Engineering, State University of Campinas, Av. Albert Einstein 500, Cidade Universitária Zeferino Vaz, 13083-852 Campinas-SP, Brazil.
[3]Department of Chemical and Biological Engineering, Korea University, 5-1 Anam-Dong, Sungbuk-Ku, Seoul 136-701, South Korea
[4]Vegetable Oil Technology Business Unit, Alfa Laval Copenhagen A/S, Maskinvej 5, DK-2860 Soeborg, Denmark

Abstract

The accuracy and reliability of the measured data sets to be used in regression of model parameters is an important issue related to modeling of phase equilibria. It is clear that good parameters for any model cannot be obtained from low quality data. A thermodynamic consistency test for solid-liquid systems using a relation between the solid and liquid activity coefficients for systems containing metals [1], where the data from the two phases are given were proposed. However, as consistency tests based on the Gibbs–Duhem equation are not feasible, new consistency tests have been developed [2]. Some of the developed tests were based in the quality tests proposed for VLE data by Kang et al. [3] and a methodology that combines solute activity coefficients in the liquid phase at infinite dilution and a theoretically based term to account for the non-ideality in dilute solutions are discussed. In this work, case studies considering the methodology proposed for SLE thermodynamic consistency tests and data from open literature and databases such as NIST-TDE®, DIPPR® and DECHEMA® are presented. The SLE consistency test and data evaluation is performed in a software containing option for data analysis, model analysis and parameter regression. The paper will highlight the data collection, the data analysis for SLE data and the thermodynamic model performance (such as NRTL, UNIQUAC and original UNIFAC).

References

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