

Technical University of Denmark



## Dynamic data evaluation for solid-liquid equilibria

Cunico, Larissa; Ceriani, Roberta; Kang, Jeong Won; Sarup, Bent; Gani, Rafiqul

*Publication date:*  
2014

*Document Version*  
Publisher's PDF, also known as Version of record

[Link back to DTU Orbit](#)

*Citation (APA):*  
Cunico, L., Ceriani, R., Kang, J. W., Sarup, B., & Gani, R. (2014). Dynamic data evaluation for solid-liquid equilibria. Abstract from 27th European Symposium on applied Thermodynamics, Eindhoven, Netherlands.

## DTU Library

Technical Information Center of Denmark

---

### General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

## Dynamic data evaluation for solid-liquid equilibria

Larissa P. Cunico<sup>1</sup>, Roberta Ceriani<sup>2</sup>, Jeong W. Kang<sup>3</sup>, Bent Sarup<sup>4</sup>, Rafiqul Gani<sup>1</sup>

<sup>1</sup>CAPEC, Dept. of Chemical and Biochemical Engineering, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark

<sup>2</sup>Faculty of Chemical Engineering, State University of Campinas, Av. Albert Einstein 500, Cidade Universitária Zeferino Vaz, 13083-852 Campinas-SP, Brazil.

<sup>3</sup>Department of Chemical and Biological Engineering, Korea University, 5-1 Anam-Dong, Sungbuk-Ku, Seoul 136-701, South Korea

<sup>4</sup>Vegetable Oil Technology Business Unit, Alfa Laval Copenhagen A/S, Maskinvej 5, DK-2860 Soeborg, Denmark

Keywords: solid-liquid equilibrium, thermodynamic consistency tests, parameter regression  
Corresponding author: Rafiqul Gani rag@kt.dtu.dk

### 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

- [1] H.R. Null, Thermodynamic consistency test for solid-liquid equilibria, *AIChE J.*, 1965, 11, 780-784.
- [2] L.P. Cunico, R. Ceriani, B. Sarup, J.P. O'Connell, R. Gani, Data, analysis and modeling of physical properties for process design of systems involving lipids, *Fluid Phase Equilib.*, 2014, 362, 318-327.
- [3] J.W. Kang, V. Diky, R.D. Chirico, J.W. Magee, C.D. Muzny, I. Abdulagatov, A.F. Kazakov, M. Frenkel, Quality assessment algorithm for vapor–liquid equilibrium data, *J. Chem. Eng. Data*, 2010, 55, 3631–3640.