A Systematic Identification Method for Thermodynamic Property Modelling

In this work, a systematic identification method for thermodynamic property modelling is proposed. The aim of the method is to improve the quality of phase equilibria prediction by group contribution based property prediction models. The method is applied to lipid systems where the Original UNIFAC model is used. Using the proposed method for estimating the interaction parameters using only VLE data, a better phase equilibria prediction for both VLE and SLE was obtained. The results were validated and compared with the original model performance.

General information
Publication status: Published
Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, Alfa Laval
Contributors: Ana Perederic, O., Cunico, L., Sarup, B., Woodley, J., Gani, R.
Pages: 205-210
Publication date: 2017

Host publication information
Title of host publication: Proceedings of the 27th European Symposium on Computer Aided Process Engineering
Publisher: Elsevier
(Computer Aided Chemical Engineering, Vol. 40).
Keywords: Lipids, Phase equilibria prediction, Group contribution
DOIs:
10.1016/B978-0-444-63965-3.50036-2
Research output: Chapter in Book/Report/Conference proceeding › Article in proceedings – Annual report year: 2017 › Research › peer-review