Correlation of Binary Vapor-Liquid Equilibria: Comparison of Least Squares Methods for Parameter Estimation

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Binary vapor liquid equilibrium (VLE) data are needed for the design of distillation equipment and for verification of models of liquid solutions. Most industrial distillation processes involve non ideal multicomponent mixtures and the experimental VLE data for the multicomponent mixtures are rarely found at the desired conditions for the design calculations. Recent developments in liquid models enable us to predict the multicomponent equilibria from the constituent binary data only. The non-ideality in a liquid mixture can be concisely represented by the excess Gibbs energy $\left(G^E/RT = g^E\right)$ which is related in turn to the activity coefficients of the components in the liquid mixture. There are several activity coefficient models proposed in literature .In this paper, the following two parameter models are considered for the correlation of binary VLE data of the system 2–Butanol–Tetrachloroethene using the three least square methods of Gauss Newton, Powell and Marquardt for the estimation of parameters.

- Van Laar
- Wilson
- NRTL
- Effective UNIQUAC
- Orye
- Palmer Smith
- LCG
- Noda – Ishida
- Sigma
- Margules
- Effective Wilson
- LEMF
- Modified UNIQUAC – I
- Extended Van Laar
- Nagata Notoh – I
- LSG
- Gothard
- Modified Wilson
- Redlich Kister
- Enthalpic Wilson
- Heil Prausnitz
- Modified UNIQUAC - II
- Malanowski
- Nagata Notoh - II
- Andiappan McClean
- Hiranuma
- Modified Van Laar
- Scatchard Hamer
- TK Wilson
- UNIQUAC
- CLC
- Zeta
- Nagata Notoh – III
- Nagata Nagashima
- Nagata et al
- Mato

The results of processing and discussion for the data of the example system are presented.

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