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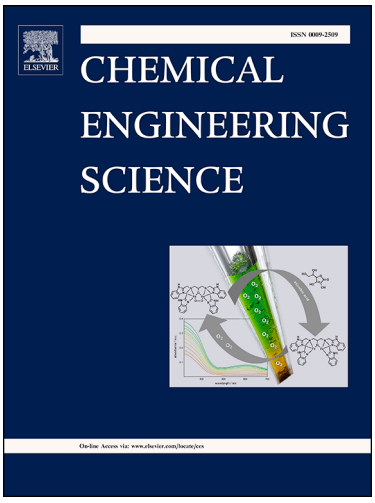

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A simple and reliable procedure to accurately estimate NRTL interaction parameters from liquid-liquid equilibrium data

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Abstract

Fitting liquid-liquid equilibrium (LLE) data to common thermodynamic models (NRTL, UNIQUAC...) has been proved in the past to be a non trivial task. Many times it leads to inconsistent solutions where the Gibbs stability criteria is not satisfied. In this work, a simplified parameter estimation problem is formulated where the Gibbs stability criteria and the minimization of experimental and calculated phase composition distances, are simultaneously applied. This formulation is intended to be implemented in general mathematical computing software. Five isothermal ternary systems are studied and the obtained NRTL binary interaction parameters are compared with both existing published parameters and those obtained from commercial data regression tools. Results show that the combination of the proposed problem formulation with commercial non-linear programming solvers improves the quality of the ternary fittings obtained.

Keywords: Liquid-liquid equilibrium, NRTL, parameter estimation

1. Introduction

There is a common problem for chemical process modellers at the time of incorporating the liquid-liquid equilibrium (LLE) or vapour-liquid-liquid equi-

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