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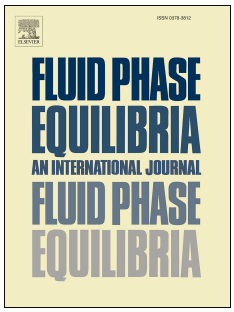

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Niklas Haarmann, Sabine Enders, Gabriele Sadowski

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Modeling Binary Mixtures of *n*-Alkanes and Water using PC-SAFT

Niklas Haarmann[a], Sabine Enders[b], Gabriele Sadowski[a,*,A]

[a]Laboratory of Thermodynamics, TU Dortmund, Emil-Figge-Str. 70, D-44227 Dortmund, Germany

[b]Institute for Technical Thermodynamics and Refrigeration, KIT, Engler-Bunte-Ring 21, D-76131 Karlsruhe, Germany

*Corresponding author: Phone: +49 231-7552635; E-mail address: gabriele.sadowski@tu-dortmund.de

Abstract

Modeling and measuring the mutual solubility in binary *n*-alkane + water mixtures is very challenging due to their low order of magnitude. Consequently, experimental data regarding mutual solubilities of these systems scatter remarkably. In this work, the PC-SAFT equation of state has been applied to model liquid-liquid and vapor-liquid-liquid equilibria of binary *n*-alkane + water mixtures. For this purpose, temperature-dependent binary interaction parameters have been fitted to the *n*-alkane solubility in the aqueous phase for *n*-alkanes ranging from *n*-pentane to *n*-undecane. Furthermore, these binary interaction parameters have been correlated with the carbon number of the *n*-alkane in order to predict phase equilibria of binary *n*-alkane + water mixtures for *n*-alkanes ranging from *n*-propane to *n*-pentadecane. Excellent agreement between modeling results and available experimental data has been observed for the liquid-liquid equilibria including the description of the minimum of *n*-alkane solubility in water as a function of temperature. Even the prediction of the vapor-liquid-liquid equilibria of the respective mixtures showed remarkably good results compared to experimental data.

Keywords: PC-SAFT; water; *n*-alkane; liquid-liquid equilibrium; three-phase equilibrium

1 Introduction

In petrochemical plants like refineries and steam crackers, process water or steam inevitably gets in contact with crude oil or hydrocarbons. As water forms an excess phase, it exceeds its solubility limit in hydrocarbons, e.g. *n*-alkanes, and corrosion of plant equipment can be caused [1]. Thus, knowledge of the solubility limit of water in hydrocarbons is indispensable. Furthermore, wastewater streams are polluted with *n*-alkanes and need to be removed for environmental reasons. Hence, the solubility of *n*-alkanes in water is also of crucial importance.

n-Alkane + water mixtures exhibit large regions of liquid-liquid immiscibility. The solubility of *n*-alkanes in water is several orders of magnitude lower compared to the respective solubility of water in the organic phase. Moreover, the solubility of water in the organic phase increases monotonically with temperature, whereas the solubility of *n*-alkanes in the aqueous phase exhibits a solubility minimum at a temperature of about 305 K [2]. There exist different

[A] The paper is dedicated to Prof. John O'Connell to honor his overwhelming scientific impact.