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Solid–liquid phase equilibria of binary indole mixtures with some aromatic compounds using a solid–liquid–vapor equation-of-state

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Abstract

The separation of useful chemicals, such as indole from coal tar, is an important subject of research in the field of fossil energy, renewable energy, and utilization of byproducts and waste materials. High-pressure crystallization is one of the proposed separation methods. To understand the process requires detailed knowledge of solid–liquid phase behaviors. Solid–liquid phase equilibrium data of various binary mixtures of indole have been reported in the literature. In the present report, we analyze some of the experimental data with our unified solid–liquid–vapor equation-of-state to see whether our model can be useful for the calculation of solid–liquid equilibria in these organic systems. Good correlations of the data and predictions of phase behavior, at very high pressures, are demonstrated.

Keywords: Solid–liquid equilibria; Indole; Aromatics; Equation-of-state; Melting curves; Eutectic; High pressure

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1. Introduction

In a previous report [1], we examined phase behaviors of benzene, cyclohexane, and their binary mixtures using a unified solid–liquid–vapor equation-of-state (EOS) [2]. This report is an extension of the previous work, and here we investigate solid–liquid phase equilibria (SLE) of binary indole (2,3-benzopyrrole) mixtures with several aromatic compounds: thianaphtene(benzo[*b*]thiophene); 1-methylnaphthalene; 2-methylnaphthalene; biphenyl; and benzene.

Indole is among the important chemicals, which can be extracted from coal tar and liquids produced by coal pyrolysis, liquefaction, or gasification, and whose derivatives are useful for various applications in medicine, specialty chemicals, perfumery and flavoring. The separation of useful chemicals (various aromatic compounds) from coal tar is still an important area of research. During the past decade, Yokoyama and his coworkers [3–10] have studied experimental SLE of binary mixtures containing indole and other aromatic compounds in order to determine the feasibility of their separation using high-pressure crystallization. An example is the separation of high-purity indole from a model coal-tar mixture containing 1-methylnaphthalene, 2-methylnaphthalene, biphenyl and 2-methylquinoline [4]. In such an application, it is very important to have a reliable thermodynamic model, which can correlate the experimental data well and predict thermodynamic behaviors at various conditions (temperatures, pressures, and compositions).

Low pressure SLE analyses are commonly made with activity (or solution) models [11,12]. Often, the solid phase is treated as the pure compound state, particularly in the case of simple eutectic phase behaviors [6,11,12]. For high-pressure SLE, the liquid phase can be calculated with a fluid EOS and the solid phase is modeled with a *separate* (solid-state) EOS [10,13]. Here, we have applied a unified solid–liquid–vapor EOS [2] to SLE calculations for several indole-containing mixtures. The EOS model is the same form as that used in the benzene–cyclohexane system [1].

However, little information is available on some of the compounds studied here; in some cases, only the triple-point and normal boiling-point temperatures. To set up the pure component EOS parameters requires at least the critical temperature and pressure, and the triple-point temperature and pressure. In this study, we use estimated values when the data are unknown. Thus, it is interesting to see whether EOS with such estimated values works for the binary SLE calculations. In addition, one of the advantages of using the present EOS model is to be able to predict the high-pressure phase behaviors. Such capability will be examined when high-pressure experimental data are available: namely, for indole/1-methylnaphthalene [6] and indole/thianaphtene [5] systems.

2. Thermodynamic model

Although the present EOS model has been presented in a previous paper [1], a brief summary is repeated here for the reader's convenience and for a self-consistent