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Prediction of phase behavior, Henry's constants and infinite dilution partial molar volumes for methane, ethane and hydrogen in *n*-paraffins

M.S.H. Bader *, K.A.M. Gasem

School of Chemical Engineering, Oklahoma State University, 423 Engineering North, Stillwater, OK 74078, USA

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Abstract

A database for methane, ethane, and hydrogen in *n*-paraffins is compiled to evaluate the Soave–Redlich–Kwong (SRK) and Peng–Robinson (PR) equations of state (EOS) in predicting the phase behavior, Henry's constant (H_i), and infinite dilution partial molar volume ($\tilde{V}_i^{\infty}$) for these systems. Five cases are employed in EOS evaluations through the use of bubble point pressure calculations. For each case, interaction parameters along with H_i and $\tilde{V}_i^{\infty}$ are obtained for both EOS. The SRK and PR EOS are adequately capable of predicting the phase behavior of tested systems. The ability of both EOS in predicting H_i and $\tilde{V}_i^{\infty}$ are assessed employing the optimum predictive case (two interaction parameters for each isotherm of each binary system). The SRK and PR EOS are nearly equivalent in predicting H_i, and in good agreement with the available experimental data for the tested systems. However, the SRK and PR EOS are over-predicting the $\tilde{V}_i^{\infty}$, particularly at higher temperatures. © 1998 Elsevier Science B.V.

Keywords: Cubic equations of state; Henry's constant; Infinite dilution partial molar volume; Phase behavior; Supercritical

1. Introduction

The prediction of the phase behavior and thermodynamic properties (e.g. H_i, γ_i^{∞} and $\tilde{V}_i^{\infty}$) of hydrocarbon mixtures containing supercritical fluids is important in chemical and petroleum industries, and receives particular attention in the field of analytical chemistry. Hence, efforts have been directed to provide predictive and correlative models for supercritical systems. Among the available models, cubic EOS such as the SRK and PR are the most successful and widely used for supercritical systems.

In this work, a comprehensive database consisting of binary data acquired at Oklahoma State University on methane, ethane, and hydrogen with *n*-paraffin binary systems, along with data from the literature is compiled and employed to:

(1) evaluate the ability of the SRK and PR EOS to describe the phase behavior of the gathered systems and provide optimum interaction parameters;
(2) test the reliability of the SRK and PR EOS in predicting H_i and $\tilde{V}_i^{\infty}$.

* Corresponding author. Bader Inc., P.O. Box 130248, The Woodlands, TX 77393, USA.

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