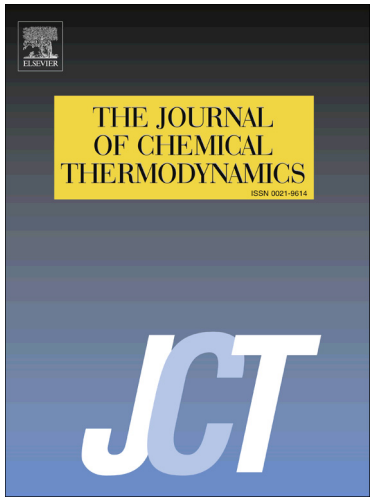

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Experimental and Predicted Vapor−Liquid Equilibrium for Binary Systems with Diethanolamine, m-Cresol and p-Cresol at 20.0 kPa

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ABSTRACT: Isobaric vapour–liquid equilibrium (VLE) data for two binary systems of p-Cresol (PC) + diethanolamine (DEA) and m-Cresol (MC) + DEA were measured at 20.0 kPa. The Herington area method was used to check the binary VLE data, and the results showed good thermodynamic consistency. Meanwhile, the Wilson, NRTL, UNIQUAC models and the chemistry theory proposed by Dolezalek were used to correlate the VLE data. The binary energy interaction parameters for activity models, and reaction equilibrium constants for chemistry theory were obtained. With help of the parameters obtained in this work, the NRTL model was used to predict the VLE data of the two binary systems at the pressure of 8.33 kPa. The predictive results were compared with the literature's data. At same time, the excess Gibbs free energy for the two binary systems, and infinite dilution activity coefficients for MC and PC in DEA were estimated. The calculated results showed that the DEA had slightly stronger interaction with PC than MC.

Keywords: M-cresol; P-cresol; Diethanolamine; Vapour-liquid equilibrium; Chemistry Theory

1. Introduction

M-cresol (MC) and P-cresol (PC) are very important organic materials. MC can be used to synthetize spices, cosmetics, and pharmaceutical products et al.[1]. Furthermore, p-Cresol is mainly adopted in disinfectants and fumigants, in the production of explosives, antioxidants and synthetic resins, et al.[2]. MC and PC are presenting in coal tar and products of chemical synthesis. However, separating these two compounds is difficult because the molecular structure difference and the boiling temperature deference of the two materials are extremely small. At present, the commonly separation methods include crystallization[3], adsorption[4], alkylation reaction[5], et al. Ningoo[6] had proposed the use of extractive distillation with using alkanolamine as entrainer to separate PC and MC, however, Zaretskii et al.[7] believed that this method required more experimental data to verify; At the same time, alkanolamine and cresols are very complex systems. Supplementing the relevant VLE data of the system can provide basic data for the verification and

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