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Investigation of the vapor-liquid phase equilibrium of a binary mixture of eucalyptol and various alcohols

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Keywords: alcohols, vapor liquid equilibrium, theoretical and computational chemistry

The development and selection of alternative, sustainable solvents have become a key focus in modern chemical engineering, driven by the need to replace volatile, toxic, and fossil-based organic solvents.[1] In this context, naturally derived compounds such as eucalyptol have gained increasing attention due to their favorable environmental and safety profiles.[2] However, the practical application of such solvents requires a thorough understanding of their thermodynamic behavior, particularly in mixtures with common polar solvents such as short-chain alcohols.

The aim of this work was to investigate the thermodynamic and separation behavior of binary liquid mixtures, specifically those composed of eucalyptol and three alcohols: methanol, ethanol, and n-propanol. Various activity coefficient models (Wilson, UNIQUAC, NRTL, UNIFAC) were applied to describe the interactions between components and to evaluate the applicability of each model for these systems.

Experimental measurements were performed at atmospheric pressure, covering a wide concentration range. The data, based on refractive index measurements, were processed using regression methods to fit the different thermodynamic models, and the binary interaction parameters required for vapor–liquid equilibrium calculations were determined.

In the case of the methanol–eucalyptol mixture, the UNIQUAC model showed the best fit for temperature data, while the Wilson model gave the most accurate results for the y_1 values. For the ethanol–eucalyptol system, the Wilson model matched the temperature trends more closely, whereas the NRTL model provided more accurate composition predictions. For the n-propanol mixture, the Wilson model again performed best in terms of temperature, while the UNIQUAC model gave better results for y_1.

Notable differences were observed among the applied models. In the case of the methanol–eucalyptol system, azeotropic behavior was indicated, which proved challenging for accurate representation by the models. In contrast, a better agreement between experimental and calculated data was achieved for the other mixtures. None of the systems could be described as ideal mixtures. Overall, the NRTL and UNIQUAC models provided the most reliable correlations.

1 Shuba, E. S.; Kifle, D.; *Renew. Sustain. Energy Rev.* **2018**, *81*, 743-755.
2 Campos, J. F.; Berteina-Raboin, S.; *Catalysis Today,* **2020**, *358*, 138-142.

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