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Vapour Liquid Equilibrium Model Testing Based on Activity Coefficient Models Applied to Binary Azeotropic Systems

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Abstract: The isobaric vapour liquid equilibrium data for fourazeotropic systems, viz. acetone-chloroform, benzene-cyclohexane, methylacetate-methanol and tetrahydrafuran-water has been determined experimentally using Othmer VLE still. Activity coefficient models namely NRTL, UNIQUAC, UNIFAC and modified forms of Flory-Huggins equation (SRS and TCRS) were tested for theoretical prediction of VLE for the azeotropes.ASOG method of computation for the UNIFAC model and Newton- Raphson's technique for the other four models was adopted for the estimation of VLE. Validation of the simulated VLE data was made using error analysis. The correlation parameters obtained for these four models and the comparison results are reported. RedlichKister method of thermodynamic consistency test was also made and the results are in accordance with the results yielded by the error analysis.

Keywords: Activity coefficient model,Azeotrope,Nonideality, Thermodynamic consistency,Vapour liquid equilibrium.

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