Prediction of Isobaric Phase Equilibria for Binary Systems from Excess Molar Enthalpies

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The prediction of isobaric binary vapor-liquid eqilibria using only excess molar enthalpies(heats of mixing,) and vapor pressure of pure component has been presented. The binaries of this study are { n-hexane(1) + cyclohexane(2), methanol(1) + 1,2-dichloropropane(2), ethanol(1) + 1,2-dichloropropane(2) at 1 atm} and their experimetal excess molar enthalpies were reported previously. The method consists of calculating the parameters of NRTL model from isothermal heat of mixing data for the corresponding binary system. NRTL parameters derived from the heat of mixing data at one temperature can be used to predict vapor-liquid equilibrium at other tempertures up to the boiling temperature of the liquid mixture.

This method could predict the composition of the vapor phase with average deviation ranging from 2.8-7.5% for selected binary systems.