

Supporting Information

Measurement and Correlation of Isobaric Vapour Liquid Equilibrium Data for Cyclopentyl Methyl Ether (CPME) + Cyclopentanol (CP)

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Procedure for Calculations

1. Calculate the pressure using the equation , $P_{cal} = \sum x_i \gamma_i P_i^{sat}$.
2. Steps 3 to 5 were repeated for all the data points.
3. Calculate the difference between the experimental pressure and calculated pressure of step 4 (ΔP) for all the data points.
4. Optimize model parameters by minimizing the objective function $RMSD(P) = \sqrt{\sum_{i=1}^n \frac{\Delta P_i^2}{n}}$.
where n is the total number of data points

BUBL T calculation for the estimation of vapor phase mole fraction and RMSD(T) and %AAD(T)

Using these BIP's and experimental T, P and x data, the vapor phase composition was obtained using following BUBL T calculations,

1. Temperature, liquid phase composition (x_i), experimental pressure (P_{exp}) and BIP's were taken as the input parameters.
2. Calculate activity coefficient for both the species for using the activity coefficient model under consideration.
3. Assume the temperature.
4. Calculate vapor pressure of both the species at assumed temperature using Antoine's equation.
5. Calculate the vapor phase composition of both the species using the equation, $y_i = \frac{x_i \gamma_i P_i^{sat}}{P}$.
6. Now change the temperature such that the summation of calculate vapor phase composition is unity, $\sum y_i = 1$.
7. Repeat the above procedure for all the data points.
8. Based on the above calculated T (T_i^{pred}) RMSD (T) and %AAD (T) were calculated as follows,

$$RMSD(T) = \sqrt{\frac{\sum_{i=1}^n (T_i^{exp} - T_i^{pred})^2}{n}}$$

$$\%AAD(T) = \sqrt{\frac{\sum_{i=1}^n 100 \left(\frac{T_i^{exp} - T_i^{pred}}{T_i^{exp}} \right)}{n}}$$

where, n is the number of data points