CHAPTER 5

SUMMARY
AND
CONCLUSION
5. SUMMARY AND CONCLUSION

Isobaric vapour-liquid equilibrium data at 730 ± 2 mm Hg pressure were obtained for six binary systems, each containing a \( C_8 \) aromatic hydrocarbon (\( p \)-Xylene) as one of the components and the other component was selected on the basis of polarity to ensure varying degree of interactions between the two components. A vapour recirculating type equilibrium still, with bubbling vapours providing thorough mixing of the condensate and the residual liquid, was employed to determine the equilibrium data for the following systems:

- \( p \)-Xylene – \( n \)-Decane
- Triethylamine – \( p \)-Xylene
- \( p \)-Xylene – Isoamyl Acetate
- Vinyl Acetate – \( p \)-Xylene
- \( p \)-Xylene – 1-Octanol
- \( p \)-Xylene – 2-Nitrotoluene

Refractive index method was employed for analysing the equilibrium samples of all the miscible systems. For the systems investigated experimentally in this work, the activity coefficients were calculated taking into consideration the vapour phase non-ideality based on the pure component and mixture properties.

The pure component and mixture properties needed were estimated at system temperatures by carefully selected estimation methods. To represent vapour pressures at the system temperatures, the Antoine equation was used for all the systems. The second virial coefficients and the cross virial coefficients for all the systems were estimated by the Pitzer-Curl correlation modified by Tsonopoulos [403]. The liquid molar volumes were estimated by the Lyckman, Eckerts and Prausnitz method [55, 193] for all the systems.

All the binary systems were observed to be non-azeotropic. \( x \) vs. \( y-x \) plots indicated good internal consistency of the experimental data obtained in this work.
The thermodynamic consistency of the experimental data was verified by the application of Herington, Black and Hirata tests.

The correlations of Margules, Redlich-Kister, Black and Wilson were used to fit the activity coefficient-composition data. The constants in these correlations were evaluated by the method of nonlinear least square minimizing $\ln(\gamma_1/\gamma_2)$ function. This method was found to converge to the final value of constants very rapidly with only one or two iterations in case of Margules, Redlich-Kister and Wilson correlations and three to five iterations in case of Black correlation giving an accuracy of $5.0 \times 10^{-4}$ in the value of the constants.

It was found that in general, the three constant correlations of Margules, Redlich-Kister and Black were found to be better as compared to the two constant correlation of Wilson, though the latter correlation gave comparable fit in most of the cases.

The activity coefficient data for all the six binary systems studied were also predicted using UNIFAC method and a comparison of experimental and UNIFAC method had been made.