

CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS

Conclusions

1. The present study shows that the use of binary interaction parameters, K_{ij} , is essential in order to obtain better predictions of vapor-liquid equilibria, especially for nitrogen and carbon dioxide systems where the improvement is much greater than that for the methane, ethane and propane systems.

2. The optimum values of K_{ij} should be determined from experimental VLE data using a selected criterion. Comparative studies indicate that the minimization of deviations in predicted bubble point pressure criterion gives better K_{ij} values than the minimization of the deviation between calculated component vapor and liquid fugacity criterion. Furthermore the K_{ij} values varied with the temperature.

3. The K_{ij} values from the former criterion yield the lowest deviations in VLE calculations while the values from the fugacity criterion give only adequate results. However, this second criterion saves considerably on computing time and effort by avoiding iterations in objective function calculations.

4. Of the five equations of state studied in the VLE calculations, the MSRK and the MPR equations are more accurate for bubble point pressure prediction in hydrocarbon systems while the PR and PT equations give better results in non-hydrocarbon systems. However, no major overall difference is found by using the other equations. The overall deviations in all equations are acceptable, with the optimum K_{ij} incorporated.

Recommendations

From a comparison of the predictive powers of the five equations, it is recommended that the MSRK or MPR equations be used in VLE calculation for hydrocarbon systems and the PR or PT equations for non-hydrocarbon systems along with the optimum binary interaction parameters predetermined at specified temperatures and pressures for each system studied.