Chapter Six

Conclusions and Recommendations

Conclusions

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

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 four equations of state studied in the VLE calculations, the SRK and the PT equations are more accurate for bubble point pressure prediction both in carbon dioxide systems and hydrocarbon systems. However, no major overall difference is found by using the PR and SW equations. The overall deviations in all equations are acceptable, with the optimum K_{ij} incorporated.

Recommendations

From a comparison of the predicting powers of the four equations, it is recommended that the SRK or PT equations be used in VLE calculation along with the optimum binary interaction coefficient predetermined at specified temperatures and pressures of the system studied.