CHAPTER V

CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

The conclusion can be drawn for this work as following:

1. Based on vapor-liquid equilibrium (VLE) data, the fitted parameters of the Wilson equation predicts pressures as accurately as the UNIQUAC equation.
2. Based on heat of mixing data, the fitted parameters of the UNIQUAC equation predicts excess enthalpies more accurately than the Wilson model.
3. The applicability of the binary parameters of the Wilson and UNIQUAC equations based on VLE data for predicting excess enthalpy values, indicates that the Wilson equation is more suitable for heat of mixing calculations for the 1,2-dichloroethane (1) with di-n-butyl ether (2) system than the UNIQUAC model. In all other cases, both models give a poor fit of prediction.
4. The predicting pressures based on parameters from H^E data indicated that the UNIQUAC model gives the better fit for the benzene + cyclohexane, 1-chlorohexane with three n-alkylbenzenes, 1-chloropentane + di-n-butyl ether, 1,2-dichloroethane + di-n-butyl ether systems. On the other hand, the Wilson equation yields better representation of the data than the UNIQUAC model for the 1,2-epoxybutane + alkanols, ethyl formate + benzene, ethyl formate + cyclohexane, butanenitrile + 2-butanol system.
5. The simultaneous correlation of VLE and H^E usually leads to a worsening of the fit to at least one of the data types. This procedure at least doubles the number of parameters, which becomes a serious matter with prediction.
6. The adjustable parameters are rarely sensitive on VLE data and are sensitive on heat of mixing data.

7. Binary parameters based on VLE data should not be used to predict H^E values.

5.2 Recommendations for future studies

1. Additional the activity coefficient model such as the NRTL model should be tested on other binary systems.
2. Assume the energy parameters of the activity coefficient models are dependent on temperature to predict thermodynamic properties for the purpose of accuracy.