

CHAPTER X

CONCLUSION AND RECOMMENDATIONS

10.1 CONCLUSION

A program has been developed for searching and estimating the properties of gas and liquid on the personal computers. This program has been developed in C++ language using the concept of object-oriented programming(OOP). Relational database model is selected because of advantage, such as not complicated structure and easy access. This model will store data in tables and use keyword for searching those data. A database contains 150 compounds divided into five groups as follows: hydrocarbon, inorganic compound, alcohol, halogenated hydrocarbon, and miscellaneous compounds. Redlich-Kwong, Soave-Redlich-Kwong, and Peng-Robinson equations are used to estimate the properties of gases and liquids. The results of estimation by these equations are compared with those from HYSIM and reference data. The results of estimation properties of gases and liquids is as follows:

1. Vapor pressure, Antoine and Wagner equations are used to predict vapor pressure. The results show that the deviation is less than $\pm 2\%$. Antoine equation should not be used above 2.0 to 2.7 bars(Reid, Prausnitz,and Poling, 1987). Wagner equation is able to use for a wide range of temperature.

2. Heat of vaporization is predicted by Riedel, Chen, Vetere and Pitzer correlation methods. Percent deviation is less than $\pm 7\%$. Chen and Vetere methods yield approximately the same deviation because both methods are derived from the same equation.

3. Compressibility factor is estimated by RK, SRK, and PR equations. The range of the deviation is $\pm 10\%$.

4. Molar volume is predicted by RK, SRK, and PR equations and the deviation is less than $\pm 10\%$.

5. Enthalpy changes and entropy changes can be estimated by SRK and PR equations. The deviation is less than $\pm 5\%$. There are three steps to calculate enthalpy changes as follows: Calculation of enthalpy changes at ideal gas state compared with reference state, Calculation of enthalpy changes between ideal gas state and real state, Calculation of total enthalpy changes (total enthalpy changes equal to summation of enthalpy changes in step 1 and step 2)

6. Fugacity coefficient of vapor phase is predicted by RK, SRK, and PR equations. The range of deviation is $\pm 4.5\%$.

7. Vapor-liquid equilibria is estimated by SRK and PR equations. The deviation is less than $\pm 5\%$. SRK and PR equations. Using mixing rules, both equations are suitable to calculate vapor-liquid equilibria for nonpolar mixtures. But these equations are not appropriate for mixtures containing strongly polar and hydrogen-bonded in addition to common gases and hydrocarbons because strong polarity and hydrogen bonding can produce significant segregation.

10.2 RECOMMENDATIONS

The program can predict the properties of gas phase fairly accurately. But for liquid phase, the program still requires some modification. In liquid phase, P.B. Deshpande (1985) suggested activity coefficient model for estimating the properties of liquid. This program should further be developed by increasing numbers of compound, including activity model, and consideration on the effect of binary interaction parameters for SRK and PR equations. The program has a limitation on estimation of gases and liquids in subcritical only, therefore the following work should be carried out to enable it to estimate these properties in critical region.