CHAPTER I



INTRODUCTION

Calculation of chemical engineering always needs thermodynamic properties of systems. The values of the thermodynamic properties can be calculated from equations of state. An equation of state relates three basic properties: pressure(P), volume(V), and temperature(T). Popular equations of state have parameters such as critical temperature(T_c), critical pressure(P_c), acentric factor(ω), and binary interaction coefficient(k_{ij}).

If there is an error in the experimental data then, the parameters such as interaction coefficient will also have errors. When the equations of state are used to determine the thermodynamic properties, it will give some errors in the answer. Therefore it is interesting to know how much errors in the thermodynamic properties caused by the selected equations of state are.

1.1 Purpose of This Research.

The objectives of this research are: firstly, to study the influence of the parameter values in the selected equations of state on the thermodynamic properties. Secondly, to develop the computer program to study the effect of the parameters in the equations of state on the thermodynamic properties.

1.2 Scope of This Research.

- 1. Select the equations of state and correlations of the paramaters for nonpolar short-chain substances.
- 2. Select the equations of state and correlations of the parameters for nonpolar long-chain substances.
- 3. Select the equations of state and correlations of the parameters for polar substances.
- 4. To develop program that can evaluate the effect of the parameters on the thermodynamic properties.
- 5. The thermodynamic properties to be studied are enthalpy departure, entropy departure, fugacity coefficient, saturation pressure, and liquid and vapor compressibility factors.

1.3 Steps of This Research.

- 1. Collect the data of the equations of state from literatures.
- 2. Select the equations of state to study.
- 3. Write the program for calculating the enthalpy departure, entropy departure, fugacity coefficient, saturation pressure, and liquid and vapor compressibility factors from the equations of state.
- 4. Study the influence of the parameters of the equations of state on the thermodynamic properties.
 - 5. Prepare the report.

1.4 Expected Usefulness of This Research.

- 1. To know the influence of the parameters of the equations of state on the thermodynamic properties.
- 2. To obtain the computer program for calculating the thermodynamic properties from the equations of state.