CHAPTER I

INTRODUCTION

A number of industrially important processes, such as distillation, absorption, and extraction, bring two phases into contact. When the phases are not in equilibrium, mass transfer occurs between the phases. The rate of transfer of each species depends on the departure of the system from equilibrium. Quantitative treatment of mass-transfer rates requires knowledge of the phase equilibrium. Vapor-liquid and liquid-liquid equilibria depend on the nature of the components present, on their concentrations in both phases, and on the temperature and pressure of the system.

In most industrial processes coexisting phases are vapor and liquid, although liquid-liquid, vapor-solid, and liquid-solid systems are also encountered. For vapor liquid equilibrium (VLE), the method may be used at low or moderate pressures commonly encountered in separation operations since vapor-phase nonidealities are taken into account. For liquid-liquid equilibrium (LLE), the effect of pressure is usually not important unless the pressure is very large or unless conditions are near the vapor-liquid critical region.

In any problem concerning the equilibrium distribution of some component i between two phases α and β, the solution is begun with the relation

$$\mu_i^\alpha = \mu_i^\beta \qquad (i = 1,2,...,n) \qquad (1.1)$$

where μ is the chemical potential and n is the number of species present in the system. Although not given here, a similar but more comprehensive derivation shows that temperature and pressure must also be the same for the two phases at equilibrium.

The application of Eq. (1.1) to specific phase-equilibrium problems requires use of models of solution behavior, which provide expressions for the μ_i as functions of

temperature, pressure, and composition. The simplest of these are the ideal-gas mixture and the ideal solution.

Real solutions are non-ideal solutions, which required activity coefficients. In a mixture, the activity coefficient of a component, which is a measure of nonideality of the mixture, is defined as the ratio of the activity of that component in the mixture to that of an ideal solution. In general, activity coefficients are given by vapor liquid equilibrium data.

The purpose of this work is to study comparison of activity coefficients based on heat of mixing data and vapor-liquid equilibrium data. It is expected that this work is capable of widespread application and yet, can lead to very accurate predictions of process calculations.

The scope of this work is as follows:

1. Search and collect the experimental data of binary mixtures (VLE data and excess enthalpy data).
2. Derives the thermodynamic properties based on activity coefficients.
3. Write and compile computer program with a Turbo Pascal Compiler for convenience of calculation.
4. Compare the calculation data with experimental data.