CHAPTER II
LITERATURE REVIEW

This chapter is donated to research work which relate to this work

2.1 L.Oellrich, U. Plocker, J.M. Prausnitz, and H. Knapp(1981) studied calculation of vapor-liquid equilibrium, enthapy deviations with the aid of equations of state. The results of this study can be concluded as follows:

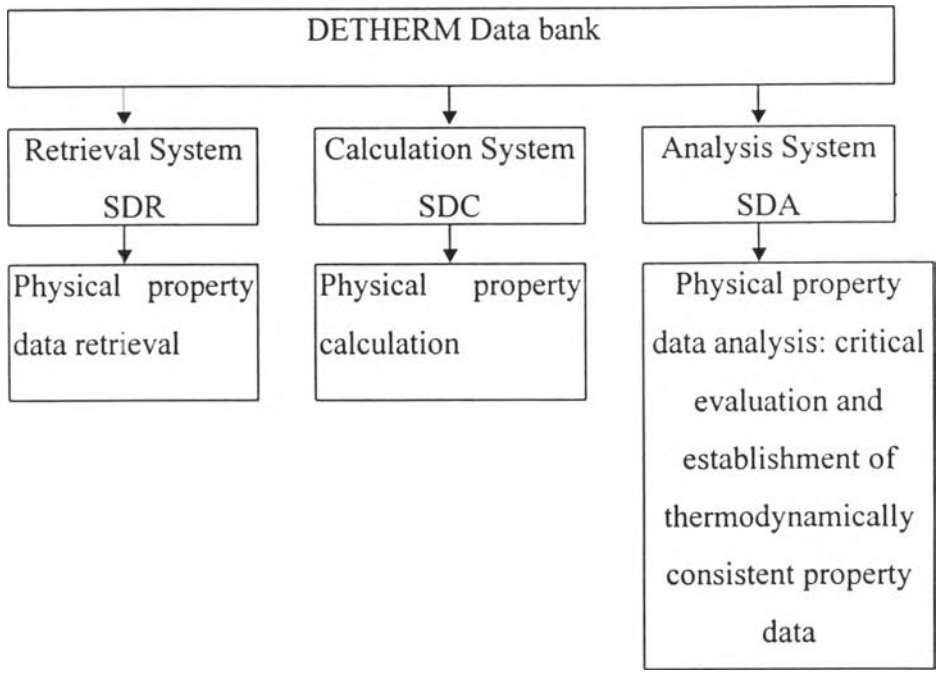
Lee and Kesler with Plocker, Knapp, and Prausnitz(LKP): The comparatively good results for almost all mixtures are acceptable. Computing time are relatively short.

Benedict-Webb-Rubin-Starling(BWRS) equation has the greater deviations to calculate vapor-liquid equilibrium for mixtures with a broad boiling range.

Modification of Redlich-Kwong equation by Soave and Lu et al.: Both modifications give comparably good results for a large number of the test mixtures but greater deviations in the presence of nitrogen. Soave's modification fails for mixtures of hydrogen with the higher hydrocarbons when temperature-dependent critical constants for hydrogen are used.

Peng-Robinson(PR) equation provides vapor-liquid equilibria data with fair accuracy.

2.2 R. Eckermann (1983) purposed a physical property data bank for chemical engineering, DETHERM, which is developed such a computer assisted physical property information system for chemists and engineers. Configuration of the DETHERM data bank is as follows:



Physical property data retrieval system (SDR)

Retrieval system is used to store and search physical property data. This system is capable of retriving information of specific physical properties of many compounds.

Physical-property computing system (SDC)

SDC consists of programs for computing pure substance and mixture properties. It requires the pure substance base data (for example, boiling point, critical data etc.) which is stored in the memory, and calculates pure-substance and mixtures for any desired conditions.

Physical property data analysis system (SDA)

SDA consists of statistical analysis programs making possible the analysis and evaluation of correlation of physical data with any desirable models. The physical property analysis system is an aid for the evaluation of physical property data.

A comparison of approximated data from DETHERM and literature data shows a very small deviation.

2.3 E.H. Chimowitz and C.S. Lee (1985) purposed local thermodynamic model for high pressure process calculation. They present an algorithm of local model with Wang Henke distillation method. The results of local K-value model compared with those of Chao-Seader model on a ternary hydrocarbon system have the average deviation about 6.5%. The main benefit of the local model concept is the potential of enhancing the execution speed of algolithms for process design cal culations.

2.4 J.W. Ponton (1987) presented noniterative approximate methods for calculating vapor-liquid equilibria in three main variations: specified vapor fraction, specified enthapy, specified temperature. This methods are based on assumption of locally constant relative volatilities. The methods work best for resonably close boiling mixture, components with relative volatility ranges of less than a factor of about 50 but for wider boiling mixtures accuracy deteriorates. The results of the methods at a first estimation near ideal system are accurate around 1 %.

2.5 J.M. Le Lann, X. Joulia and B. Koehret (1988) purposed a computer program for calculation of thermodynamic properties and phase equilibria, which was developed with in the simulator PROSIM. Thermodynamic models designated for this program are used the method of equations of state and classical method. Work of Ried et al. (1977) has been used as the source of a database for the program.

2.6 M.de Valaminck (1990) presented prediction of thermodynamic properties of organic fluids with the help of computer software. Soave-Redlich-Kwong equation was used to predict compressibility factor and specific volume of saturated liquid. Vapor pressure was estimated by Lee-Kessler equation. Enthapy and entropy of superheated vapor were estimated by Redlich-Kwong-Soave equation with specific heat of an ideal gas. Latent heat of vaporization was predicted by Clapeyron equation. Six organic fluids with different structures such as three Freons (R11, R113, R114), an alkane (n-butane), a halogenated hydrocarbon (toluene) were chosen for testing the performance of the program. The mean relative error found in every case is less than 2%, with the exception of the vapor pressure of toluene which reaches 2.7%.