CHAPTER I
INTRODUCTION

Acquisition of matter's properties is one of the main tasks for engineers and scientist in designing not only unit operations but also the whole plant. In many cases, it will be essential to fit physical characteristics from basic data to process conditions by suitable computations, especially when it is not possible to carry out measurements. Thus, it is desirable to have a material properties database which engineers to estimate any necessary properties.

Recently delvelopment of computer technology do not provide engineers only the speed of computations, but also the precision of computations. Application of a computer to collect and to help estimate properties of gases and liquids becomes feasible and useful for simulation and designing processes. Information of matter's properties regarded as a vital resources but it must be organized and utilized efficiently. Therefore, development of engineering database is one of the most important information activities of engineers. Relational database model is introduced to collect data in this work because of its simplicity. Data is collected in tables of records which consist of many fields. Key word, name of compounds, are used as indices to search the properties of the compounds in the database.

1.1 HISTORY OF STUDY ON THERMODYNAMIC CORRELATION TO PREDICT SUBSTANCE'S PROPERTIES

This begins with Boyle's experiments(1662), from which he deduced that at a given temperature the volume of gas is inversely proportional to its pressure. The effect of temperature on gas volume was investicated by Charles and Guy-Lussac (1802), who found the relation to be linear. These two laws were combined by Clapeyron (1834) into first statement of the ideal gas law as $PV = R(T+267)$. Investigations on mixed gases leads to Dalton's law of partial pressure (1801).

The law eplains that in an ideal mixture, each gas behaves as though it alone occupied the entire volume. Amagat's law (1880) states that the volume of a mixture is the summation of the volumes of the components at the temperature and pressure of the mixture. Above a certain pressure and temperature, the properties of the liquid and gas become indistinguishable. This condition, called the critical state, was discovered by Cagniard de la Tour (1822). Andrews (1863) comprehensively study the critical phenomena of pure substance and mixtures. Deviation from ideal gas law were described to be due to the finites volumes occupied by the molecules themselves and to forces of repulsion and attraction between the molecules. Both these factors were studied by Van der Waals (1973). He also proposes a modified equation of state, which can be used to predict substance's properties more correctly. Redlich and Kwong (1949), Soave (1972), and Peng and Robinson (1976) propose equations of state, which consist of two and three parameters. They can be used to predict substance's properties with high accuracy. These are also cubic equations whose parameters are expessed in terms of critical properties. Finally it is found that the simpler Peng-Robinson (1976) could be also used for predicting liquid densities.

The properties of gases and liquids are necessary to chemical engineer. In a situation which experimental data is not available, they must be estimated or predicted using correlations mentioned above. Estimation is based on theory, correlations of experimental data, or a combination of both. Prediction of thermodynamic properties can be made using basic data which is stored in data bank. In this research, many of basic equations of state are used to estimate the thermodynamic properties of gases and liquids and to predict its vapor-liquid equilibrium. The results of estimation will be shown on windows running on MS Windows platform.

1.2 OBJECTIVES

The objectives of this work are:

1.2.1 To develop a database system which can be used on microcomputers for searching and estimating properties of gases and liquids at various temperature and pressure.

1.2.2 To apply a concept of object-oriented programming for developing graphic user interfaces of the database system.

1.3 SCOPE OF WORK

The scope of this work is as follows:

1.3.1 Developing a database which is composed of

- Physical properties consisting of Molecular weight, normal boiling point, freezing point, liquid density, constants for calculating liquid viscosity.

- Thermodynamic properties consisting of critical temperature, critical pressure, critical volume, critical compressibility factor, constants for calculating vapor pressure, constants for calculating the isobaric heat capacity of the ideal gas, Pitzer's acetric factor, dipole moment, standard energy of formation, standard Gibbs' free energy of formation.

- Transport properties consisting of constants for calculating liquid viscosity.

1.3.2 Testing performance of the database system by comparing the value of gas and liquid's properties estimated by the program with the value estimated by other programs.

1.3.3 The database consists of 150 compounds which are hydrocarbon, inorganic compounds, alcohols, halogenated hydrocarbon, and other compounds.