CHAPTER I

INTRODUCTION

Equations of state (EOS) have proven to be useful tools in the prediction of equilibrium phenomena from a relatively small amount of input data and can be applied very well to mixtures and pure component. Especially, the equations of state in the form of cubic equations of state have been favourably accepted because of their simplicity, low computational costs and reliablity.

Although most of the equations of state are able to reproduce with good accuracy pure compound properties, they loose much of their advantages when generalized or extended to mixtures. The predictive power of the mixtures of any equations of state is limited to the availablity of the parameters, called the binary interaction parameters (K_{ij}) used in combining pure component constants of the equations.

In this work, the optimum binary interaction parameters of some cubic equations of state were calculated from isothermal experimental vapor - liquid equilibrium data for systems containing methane, systems containing ethane, systems containing propane, system containing nitrogen and systems containing carbon dioxide at various temperature using five equations of states; Soave-Redlich-Kwong, Peng-Robinson, Patel-Teja, modified Soave-Redlich-Kwong, and modified Peng-Robinson. Furthermore, the applicability of the optimum K_{ij} values was tested with these five chosen EOS to predict the bubble point pressure of those mixtures and compared with the experimental data

<u>Purpose of the work</u>

1. To evaluate the binary interaction parameters of the equations of state for carbon dioxide-paraffin binary systems.
2. To predict the vapor-liquid equilibria of carbon dioxide-paraffin binary systems by the evaluated interaction parameters and compare with the experimental data.

Scope of the work

1. The work covers binary systems composed of hydrocarbons, C_1 -C_{10}, nitrogen and carbon dioxide.

2. The cubic equations of state are as follows:

1) Soave-Redlich-Kwong (SRK) Equation of State
2) Peng-Robinson (PR) Equation of State
3) Patel-Teja (PT) Equation of State
4) Modified Soave-Redlich-Kwong (MSRK) Equation of State
5) Modified Peng-Robinson (MPR) Equation of State

3. The criteria used for the evaluation of the binary interaction parameters are as follows:

1) Minimization of deviation in predicted bubble point pressures

2) Minimization of the deviation between calculated component vapor and liquid fugacities