INVESTIGATION OF CORRELATION AND PREDICTION OF ENTHALPY OF PURE AND MIXTURE OF SATURATED VAPOR

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by

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ABSTRACT

The prediction of accurate values of saturated enthalpy of vapor is very important in process design calculations and other industrial applications. Experimental measurements of saturated enthalpy of vapor are not easy to perform. So in order to obtain accurate saturated enthalpy of vapor, attention has been turned to calculate them using equations of state. Some of these equations applied for both gas and liquid phases, and some of them applied for gas phase only, noting that those equations of state were developed primarily for calculating vapor-liquid equilibrium. To overcome these problems efforts were directed to modify or improve the equations of state. The accuracy of these equations are different depend on the selected type of systems. Five equations of state were used to calculate the residual enthalpy for pure compounds (polar and non polar). The AAD% for 25 pure compounds (polar and non polar) and 701 experimental data points are 2.5780, 6.7138, 1.8757, 2.2696, 3.4648, and 2.4914% when using Redlich-Kwong, Soave Redlich-Kwong, Peng-Robinson, Lee-Kesler, Virial equation truncated to second and to third terms respectively.

It is considered from the results obtained above that Peng-Robinson equation is the best equation that can be used to calculate the residual enthalpy of the saturated vapor compared with the other equations of state mentioned. Efforts were therefore directed toward possibility of modifying Peng-Robinson equation of state to increase its accuracy in predicting the residual enthalpy of saturated vapor.

For pure compounds, a new modified correlation was proposed to predict the enthalpy of saturated vapor. The modification was made by redefining the parameter *n* as a function of reduced temperature, pressure and acentric factor

by using statistical program. The correlation is given as in the following equations:

$$n = a_A + b_A \times \omega + c_A \times \omega^2$$

$a_A = 0.941018$

$b_A = \text{-}85.7291 \times \mathrm{T_r} + 105.6393 \times \mathrm{T_r}^2 + 4.303806 \times \mathrm{P_r} - 50.0757 \times \mathrm{T_r} \times \mathrm{P_r} + 22.98768 \times \mathrm{P_r}^2$

$c_A = 433.376 \times \mathrm{T_r} - 530.876 \times \mathrm{T_r}^2 - 35.3057 \times \mathrm{P_r} + 252.0676 \times \mathrm{T_r} \times \mathrm{P_r} - 108.396 \times \mathrm{P_r}^2$

For binary mixtures, the calculation of the saturated enthalpy of vapor was done by using two methods to calculate the residual enthalpy of saturated vapor, the first method was done by using Peng- Robinson equation with its mixing rules and the second method was done by using Teja equation with Peng-Robinson equation for pure compounds.

Again Peng-Robinson mixing rules were modified to increase its accuracy for mixtures. It can be considered that the modified Peng-Robinson equation with its mixing rules (this work) is relatively better equation for predicting the enthalpy of saturated vapor for binary mixture. The correlation is given as the following equations:

$$n = a_A + b_A\omega + c_A\omega^2$$

$a_A = 0.3704$

$b_A = 0.01267 - 0.20093 \times T_r + 0.1 \times P_r$

$c_A = -0.9048 + 0.945147 \times T_r - 0.17167 \times P_r$

These correlations can be further developed to be used directly for the design purpose of distillation operations, and other processes that involve vaporization and condensation phenomena.

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Nomenclatures

Symbol	**Meaning**	**Unit**
a, b	= Constant used in the cubic equation of state	-
a_f, b_f, c_f	= Coefficient of (Eq. 2-67)	-
a_A, b_A, c_A	= Coefficient of (Eq. 3-2, 3-6)	-
A, B, D	= Parameters used in the equations of state	-
B'	= Second Virial coefficient	-
C'	= Third Virial coefficient	-
C_v	= Heat Capacity at constant volume (Eq.2-17)	(J/mole. K)
C_P	= Heat Capacity at constant pressure (Eq.2-31)	(J/mole. K)
E	= Parameters of Lee-Kesler (Eq. 2-92)	-
H	= Enthalpy	(J/mole)
K_{ij}	= Cross coefficient for mixture	-
n	= Constant used in the cubic equation of state	-
n'	= Constant used in (Eq.2-28)	-
P	= Pressure	(kpa)
P_{vpr}	= Reduced vapor pressure	-
R	= Universal gas constant	(J/mole. K)
R11	= Trichlorofluoromethane (CCl_3F)	-
R12	= Dichlorodifluoromethane ($CCl_2 F_2$)	-
R13	= Chlorotrifluoromethane ($CClF_3$)	-
R21	= Dichloromonofluromethane ($CHCl_2F$)	-
R22	= Monochlorodifluoromethane (CHF_2C_6)	-
R32	= Difluoromethane (CH_2F_2)	-
R114	= 1, 1-Dichlorotetrafluoroethane ($C_2Cl_2F_4$)	-

R123	= 2, 2-Dichloro-1, 1, 1-Trifluoroethane	-
R134a	=1, 1, 1, 2-tetrafluoroethane ($C_2H_2F_4$)	-
T	= Temperature	(K)
U	= Internal energy	(J)
V	= Molar volume	(cm^3/mole)
x	= Mole fraction	-
Z	= Compressibility factor	-

Greek Symbols

α = Constant used in the cubic equation of state

ω = Acentric factor

Δ = Difference

γ = Parameter used in (Eq. 2-92)

β = Parameter used in (Eq. 2-92)

∂ = Derivative

Superscripts

ig = Ideal gas

R = Residual

$(R1)$ = Component 1 in Teja equation

$(R2)$ = Component 2 in Teja equation

$Sat.$ = Saturated

o = Simple fluid (Eq. 2-91)

r = Reference fluid (Eq. 2-91)

Subscripts

b = normal boiling point

br = Reduced normal boiling point

c = Critical point

i = Component i

ij = Components i and j

m = Mixture

o = Reference point

r = Redused

vap. = Vaporization

v = Vapor

vb = Vapor at normal boiling point

Abbreviations

AAD% =Average Absolute Deviation Percent

AD% = Absolute Deviation Percent

BWR = Benedict-Webb-Rubin

CSP = Corresponding State Principle

EOS = Equation of State

M.wt = Molecular weight

RK = Redlich -Kwong

RKS = Redlich -Kwong Soave

VLE = Vapor Liquid Equilibrium

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CHAPTER ONE

INTRODUCTION

The saturated vapor enthalpy of the substance represents a point on the saturated vapor curve and therefore depicts the limiting value of a gaseous isotherm just before condensation is initiated. Thus; the saturated vapor state becomes the point of intersection between a super heated gas isotherm and the corresponding vaporizing liquid isotherm.

Enthalpy is one of the most important thermodynamic properties of fluids which can be explicitly defined for any system by the mathematical expression:

$$H=U+PV \tag{1-1}$$

Where U= internal energy, P= absolute pressure, V= volume. The units of all terms of this equation must be the same. Though enthalpy is often required to a unit mass or to a mole, like volume and internal energy. Saturated enthalpy of vapor is useful as a thermodynamic property because the $U+PV$ group appears frequently, particularly in problems involving a flow process such as extraction, heat exchangers, evaporators, distillation columns, pumps, compressors, turbines, humidification, adsorption, petroleum refinery processes, refrigeration cycles, and power plants, etc..

Enthalpy departure (or residual enthalpy) is defined as a difference between enthalpy and what it would be in the ideal gas state at the same temperature and pressure, i.e.:

$$H^R = H - H^{ig} \tag{1-2}$$

The ideal gas is an imaginary gas at which $P = 0$ and $V = \infty$. For this gas all thermodynamic data are calculated accurately according to ideal gas law. Thus to know the enthalpy of the compound we need to know the value of the ideal gas enthalpy and the value of the enthalpy departure to be substituted into equation (1-2). The ideal gas enthalpy is available but there is no accurate method for the enthalpy departure of vapor.

For vapor or liquid and for gas phase, there are two sources for enthalpy data. First, the large quantity of experimental enthalpy data available in literature, and second from the accurate recommended methods, based on equation of state that predict enthalpy. But for saturated vapor, there is a shortage in experimental data, and there is no accurate recommended method for calculating enthalpy or enthalpy departure.

Redlich–Kwong, Soave, Peng-Robinson, Lee-Kesler and Virial equations of state are applicable for both liquid and vapor phases, and can be used for calculating the saturated enthalpy by calculating the compressibility factor and residual enthalpy.

The aim of this work is to evaluate each of the above equations can be applied in predicting the saturated vapor enthalpy for pure compounds. The work also involves evaluation of mixing rules for the best equation obtained that is the one with the lowest deviation from experimental values for predicting saturated vapor enthalpy for mixtures.

In addition to these aims mentioned efforts will be directed also toward the possibility of modifications of the equation with least deviation from experimental data for predicting saturated vapor enthalpy for pure compounds and mixtures using statistical methods.

CHAPTER TWO

THEORIES AND LITERATURE REVIEW

2.1 *P-V-T* Surface

Figure 2-1 can be regarded as representative of the *P-V–T* behavior for most pure substances. The coordinates of a point on the *P–V–T* surface represents the values that pressure, specific volume, and temperature would assume when the substance is at equilibrium.

There are regions on the *P–V–T* surface of Fig. 2-1 labeled solid, liquid, and vapor. In these single-phase regions, the state is fixed by any two of the properties: pressure, specific volume, and temperature, since all of these are independent when there is a single phase present.

Located between the single-phase regions are two-phase regions where two phases exist in equilibrium: liquid–vapor, solid–liquid, and solid–vapor. Two phases can coexist during changes in phase such as vaporization, melting, and sublimation. Within the two-phase regions, pressure and temperature are not independent; one cannot be changed without changing the other. In these regions the state cannot be fixed by temperature and pressure alone; however, the state can be fixed by specific volume and either pressure or temperature. Three phases can exist in equilibrium along the line labeled triple line.

A state at which a phase change begins or ends is called a saturation state. The dome shaped region composed of the two-phase liquid–vapor states is called the vapor dome. The lines bordering the vapor dome are called saturated liquid and saturated vapor lines. At the top of the dome, where the saturated liquid and saturated vapor lines meet, is the critical point. The critical temperature T_C of a pure substance is the maximum temperature at which liquid and vapor phases can coexist in equilibrium. The pressure at the critical point is called the critical pressure, P_C. The specific volume at this state is the critical specific volume.

If the *P–V–T* surface is projected onto the pressure–temperature plane, a property diagram known as a phase diagram results. As illustrated by Fig. 2-1b, when the surface is projected in this way, the two-phase regions reduce to lines. A point on any of these lines represents all two-phase mixtures at that particular temperature and pressure.

The term saturation temperature designates the temperature at which a phase change takes place at a given pressure, and this pressure is called the saturation pressure for the given temperature. It is apparent from the phase diagrams that for each saturation pressure there is a unique saturation temperature, and conversely.

The triple line of the three-dimensional *P–V–T* surface projects onto a point on the phase diagram. This is called the triple point [33].

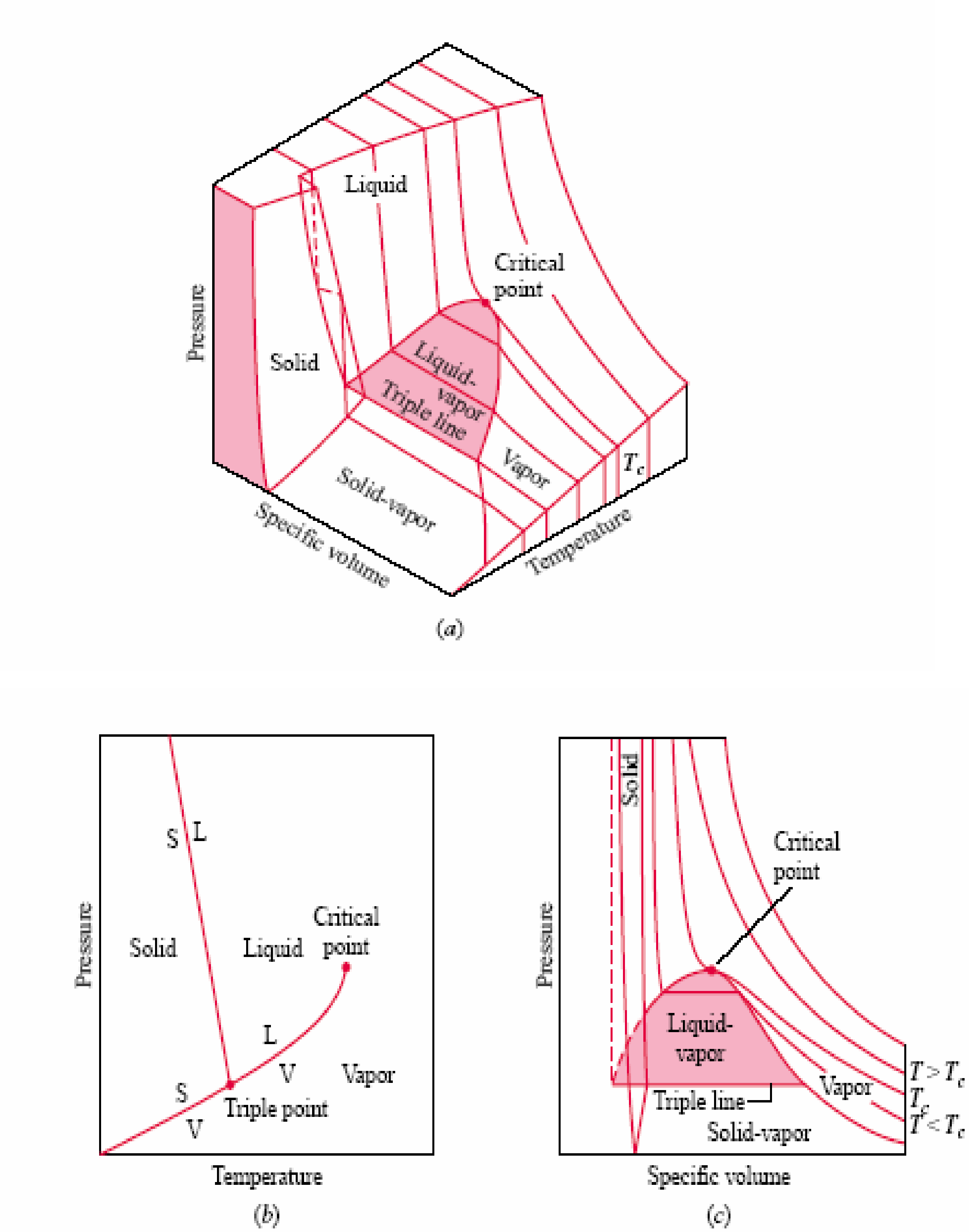

Figure 2-1 *P–V–T* surfaces of projections for water (not to scale).
(a) Three-dimensional view. (b) Phase diagram. (c) *P-V* diagram.

2.2 Enthalpy-Temperature (*H-T*) Diagram

Figure 2-2 is the *H-T* diagram for pure water. The region between the saturated liquid line and the saturated vapor line represents the area of two phases existing at the same time. The vertical distance between the two saturation lines represents the latent heat of vaporization. If pure water existed at (point A) on the saturated liquid line and an amount of heat was added equal to the latent heat of vaporization, then the water would change phase from a saturated liquid to a saturated vapor (point B), while maintaining a constant temperature. As shown in Fig. 2-2, operation outside the saturation lines results in a sub cooled liquid or superheated steam [24].

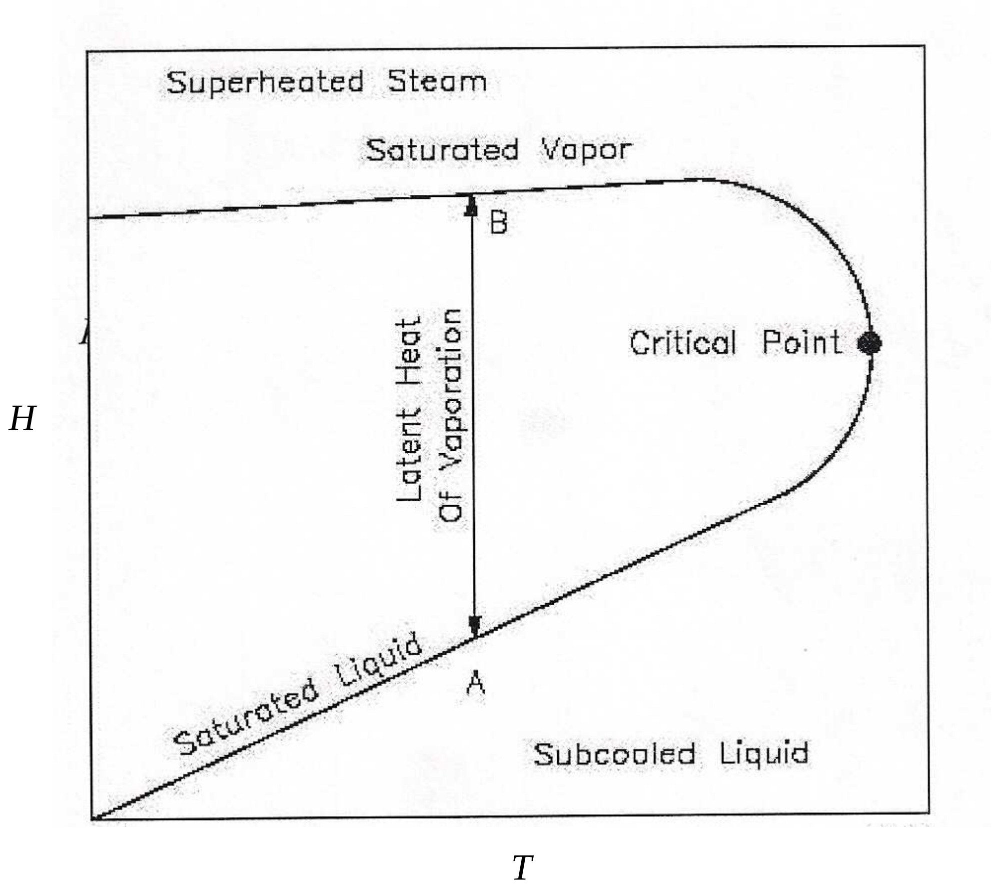

Figure 2-2 *H-T* diagram for water

2.3 Critical Properties

The critical temperature, T_C, of a material is the temperature above which distinct liquid and gas phases do not exist. As the critical temperature is approached, the properties of the gas and liquid phases become the same resulting in only one phase: the supercritical fluid. Above the critical temperature a liquid cannot be formed by an increase in pressure, but with enough pressure a solid may be formed for materials other than water. The critical pressure is the vapor pressure at the critical temperature. On the Fig. 2-3 showing the thermodynamic properties for a given substance, the point at critical temperature and critical pressure is called the critical point of the substance. The critical molar volume is the volume of one mole of material at the critical temperature and pressure.

Critical properties vary from material to material, just as is the case for the melting point and boiling point. Critical properties for many pure substances are readily available in the literature. Obtaining critical properties for mixtures is somewhat more problematic.

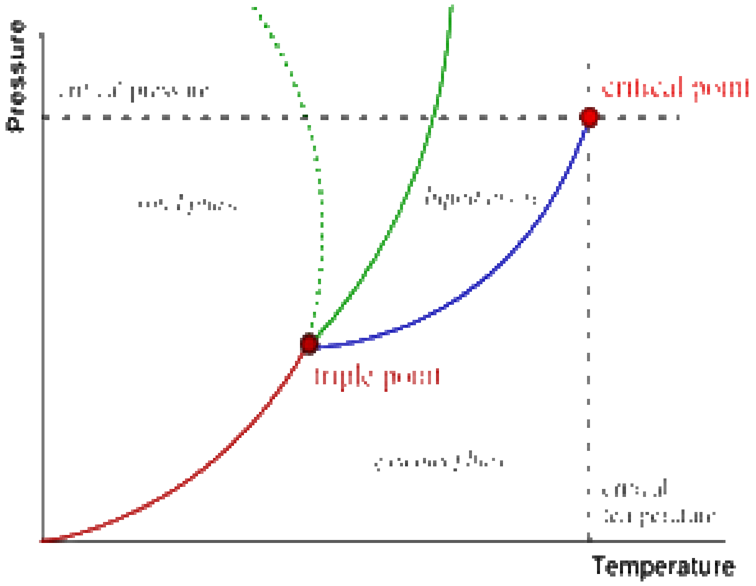

Figure 2-3 Pressure –temperature diagram

For pure substances, there is an inflection point in the critical isotherm on a *P*-*V* diagram Fig. 2-1c. This means that at the critical point:

$$\left(\frac{\partial P}{\partial V}\right)_T = \left(\frac{\partial^2 P}{\partial V^2}\right)_T = 0 \tag{2-1}$$

This relation can be used to evaluate two parameters for an equation of state in terms of the critical properties.

Sometimes a set of reduced properties are defined in terms of the critical properties [25], i.e.:

$$T_r = T / T\mathrm{c} \tag{2-2}$$

$$P_r = P / P_C \tag{2-3}$$

$$V_r = V / V_C \tag{2-4}$$

2.4 Equation of State

An equation of state is an analytic expression for the functional relationship,

$$f(\mathrm{P}, \mathrm{V}, \mathrm{T}) = 0 \tag{2-5}$$

The simplest such relation is the ideal gas law,

$$PV = RT \tag{2-6}$$

The purpose of such equations is to provide a *P*-*V*-*T* relation which is suitable in through the values assigned to constant included in the equation [31]. In functional mathematical form, the EOS can be written as $V = f\ (P, T)$. This form indicates that the volume is expressed as a function of pressure and temperature. However, The EOS can be equally well be written as $P\ (V,T)$ or even $T\ (P,V)$.Since pressure and temperature are usually specified in an experiment or in a process, the form $V(P,T)$ is most commonly employed [45]. In general, an equation of state is developed first for pure substances, and then extended to mixtures through the use of mixing rules for combining the pure component parameters. A good EOS is perhaps the best methods to handling a large amount of *P-V-T* data [12].

2.5 The Principle of Corresponding State [20, 21]

It has been found that, if different substances are compared at equal fractions of their critical temperatures and pressures, their properties are quite similar. The critical constants may be used to define a set of reduced variables P_r, V_r, and T_r.

$$P_r = \frac{P}{P_C} \qquad V_r = \frac{V}{V_C} \qquad T_r = \frac{T}{T_C} \tag{2-7}$$

The properties of a gas may be state in term of these reduced variables rather than $P, V,$ and T. According to the principle of corresponding states, all gases would obey the same equation of state if P_r ,V_r and T_r were used rather than P,V and T [39].

The assumption in applying corresponding states to mixture is that the *P-V-T* behavior of the mixture will be the same as that of pure component whose critical temperature and pressure are equal to the pseudo critical temperature and pressure of the mixture [40].

Both the van der Waals and Redlich-Kwong equation of state have been written in the form

$$Z = f(\mathrm{T_r}, P_r) \tag{2-8}$$

This functional relationship was first recognized by van der Waals. Thus the prediction of a unique relationship among Z, T_r, and P_r is known as the van der Waals two-parameter theorem of corresponding states. It states that any pure gas at the same reduced temperature and pressure should have the same compressibility factor. Expressions such as equation (2-8) are known as generalized equations, because of their general applicability to all substances.

An approach is to group fluids into several classes, where the critical compressibility is the third parameter. This method, first proposed by Lydersen, Greenkorn and Hougen [30] presents separate Z- T_r- P_r chart or tables for particular values of Z_c .That is, the charts represent the relation

$$Z = f(\mathrm{T_r}, P_r, Z_C) \tag{2-9}$$

This approach provided a significant improvement in accuracy [53].

2.6 The Third Parameter Acentric Factor

Pitzer [37] proposed another third parameter known as "acentric factor". Among the third parameters proposed, Pitzer's acentric factor has gained widest acceptance in both academic and industrial areas, because it is a simple extension of two parameter corresponding state principles and gives good accuracy for normal fluids including hydrocarbons [12].

Pitzer et al. attributed this difference in vapor-pressure variation to the degree of the sphericity of the molecular force field of a substance. They defined a third parameter ω, the acentric factor for a fluid, as the difference between the value of log $P_r^{\ sat.}$ for the fluid and that for simple fluid at fixed value of $T_r^{sat.}$.It was noted that log $P_r^{sat.}$= -1 at $T_r^{sat.} = 0.7$ for simple fluids. With the data point as a convenient reference, the definition of ω becomes

$$\omega = -1 - \log\,(P_r^{\ sat.})_{Tr=0.7} \tag{2-10}$$

The evaluation of ω only requires T_C, P_C, and the vapor pressure at $T_r = 0.7$. This choice for a definition of ω make $\omega = 0$ for a simple fluid and positive for nearly all other fluids. In a general sense, ω increases with polarity and with hydrocarbons it increases with molecular weight [53].

2.7 Enthalpy Departure or Residual Enthalpy

A residual thermodynamic property was defined as the difference between the actual value of the property and that in a hypothetical perfect gas at both the same temperature and density or at the same temperature and pressure [2]. For enthalpy calculations, it is more convenient first to calculate the enthalpy and entropy of a hypothetical ideal gas state and then to calculate the departure of these properties from that ideal gas reference state [43].

Enthalpy departure or residual enthalpy is a measure of deviation of actual enthalpy from ideal gas enthalpy, i.e,

$$H^R = H - H^{ig} \tag{2-11}$$

Where H^{ig} is the enthalpy of the ideal gas.

In order to obtain enthalpy departure by using an equation of state the following derivation was used [46]:

$$H = U + PV \quad \text{or} \quad \frac{H}{RT} = \frac{U}{RT} + \frac{PV}{RT} \tag{2-12}$$

But $\frac{PV}{RT} = 1$ for ideal gas, and $\frac{PV}{RT} = Z$ for real gas

$$\frac{H^{ig}}{RT} = \frac{U^{ig}}{RT} + 1 \tag{2-13}$$

$$\frac{H}{RT} = \frac{U}{RT} + Z \tag{2-14}$$

Subtracting equation (2-13) from equation (2.14)

$$\frac{H-H^{ig}}{RT}=\frac{U-U^{ig}}{RT}+Z-1 \tag{2-15}$$

But

$$dU=\left(\frac{\partial U}{\partial T}\right)_V dT+\left(\frac{\partial U}{\partial V}\right)_T dV \tag{2-16}$$

The first term is the heat capacity at constant volume, i.e.,

$$\left(\frac{\partial U}{\partial T}\right)_V=C_v \tag{2-17}$$

And the second term is to be found from Maxwell relation as:

$$\left(\frac{\partial U}{\partial V}\right)_T=\left[T\left(\frac{\partial P}{\partial T}\right)_V-P\right] \tag{2-18}$$

Combining equations (2-16), (2-17) and (2-18) gives:

$$dU=C_v dT+\left[T\left(\frac{\partial P}{\partial T}\right)_V-P\right]dV \tag{2-19}$$

At constant temperature, equation (2-19) becomes:

$$dU=\left\{\left[T\left(\frac{\partial P}{\partial T}\right)_V-P\right]dV\right\}_T \tag{2-20}$$

Integration of equation (2-20) between ideal gas and actual gas gives:

$$\frac{U-U^{ig}}{RT}=\frac{1}{RT}\int_{\infty}^{V}\left[T\left(\frac{dP}{dT}\right)_V-P\right]dV \tag{2-21}$$

Substituting equation (2-21) into equation (2-15) gives:

$$\frac{H-H^{ig}}{RT}=Z-1+\frac{1}{RT}\int_{\infty}^{V}\left[T\left(\frac{dP}{dT}\right)_V-P\right]dV \tag{2-22}$$

2.8 Enthalpy of Vaporization

The enthalpy of evaporation (ΔH_{vap}.) is a special form of latent heat of vaporization. It is the difference between the enthalpy of the saturated vapor and that of saturated liquid at the same temperature. The enthalpy change accompanying material transfer between phases is obtained by differencing the enthalpy of each state [43].

2.9 ΔH_v at the Normal Boiling Point

A pure component constant that is occasionally used in property correlation is the enthalpy of vaporization at the normal boiling point ΔH_{vb}, any one of the correlations can be used for this state where $T=T_b$, $P=1.01$ bar [43].

2.10 ΔH_{vb} from Vapor Pressure Relations [43]

1. Giacalone Method

Giacalone equation has been widely employed to make rapid estimates of ΔH_{vb} ; usually, in such cases, ΔZ_{vb} is set equal to unity.

$$\Delta H_{vb} = RT_C \Delta Z_{vb} \left(T_{br} \frac{\ln(P_C/1.01325)}{1-T_{br}} \right) \tag{2-23}$$

2. Riedel Method

Riedel [44] modified Giacalone equation slightly and proposed that

$$\Delta H_{vb} = 1.093 RT_C \left(T_{br} \frac{\ln P_C - 1.013}{0.930 - T_{br}} \right) \tag{2-24}$$

3. Chen Method

Chen [4] used Eq. (2-25) and a similar expression proposed by Pitzer, et al. to correlate vapor pressures so that the acentric factor is eliminated. He obtained a relation between ΔH_{vb} ,P_{vPr} and T_r. When applied to the normal boiling point:

$$\frac{\Delta \mathrm{H}_v}{RT_c} = \frac{T_r}{R}\left(\Delta S_v^{(o)} + \omega \Delta S_v^{(1)}\right) \tag{2-25}$$

$$\Delta H_{vb} = RT_C T_{br}\,\frac{3.978T_{br} - 3.958 + 1.555\ln P_C}{1.07 - T_{br}} \tag{2-26}$$

4. Vetere Methods

Vetere [52] proposed a relation similar to the one suggested by Chen. When applied to the normal boiling point:

$$\Delta H_{vb} = RT_C T_{br}\,\frac{0.4343\ln P_C - 0.69431 + 0.89584T_{br}}{0.37691 - 0.37306T_{br} + 0.15075P_C^{-1}T_{br}^{-2}} \tag{2-27}$$

2.11 Variation of ΔH_v with Temperature [43]

A widely used correlation between ΔH_v and T_r is the Watson relation [48]

$$\Delta \mathrm{H}_{v2} = \Delta \mathrm{H}_{v1}\left(\frac{1 - T_{r2}}{1 - T_{r1}}\right)^{n'} \tag{2-28}$$

Where subscripts 1 and 2 refer to reduced temperatures T_{r1} and T_{r2}. A common choice for n' is 0.375 or 0.38.

Viswanath and Kuloor [56] recommend that n' be obtaind by

$$n' = \left(0.00264\frac{\Delta \mathrm{H}_{vb}}{RT_b} + 0.8794\right)^{10} \tag{2-29}$$

2.12 Ideal Gas State Thermal Properties

The thermodynamic property calculation methods are used for calculating the isothermal departures of the properties from their ideal gas state values for pure fluids or mixtures. Therefore, it is imperative to know the ideal state properties of pure components for the calculation of thermodynamic properties of real fluids at given temperature and pressure. The most fundamental ideal gas state thermal property is the heat capacity [12]. Once this property is accurately known; all other ideal gas state thermal properties can be calculated from the thermodynamic relationships. The data compilation tabulates $C_p^{ig}, \left(H^{ig} - H_o^{ig}\right)$, as function of temperature over 298.15-1500 K for many hydrocarbons and associated gasses are available.

The molar or specific enthalpy of a substance may be therefore expressed as a function of two other state variables

$$H = f(\mathrm{T}, \mathrm{P}) \tag{2-30}$$

$$\Delta H = \int_{T1}^{T2} C_p dT \tag{2-31}$$

The ideal gas is a hypothetical state often used as a reference point for calculating thermodynamic properties such as enthalpy. It represents the enthalpy of pure species [47]

$$H^{ig} - H_o^{ig} = \int C_p^{ig} dT \tag{2-32}$$

Where

H^{ig} =ideal gas state enthalpy at T

H_o^{ig} =ideal gas state enthalpy at absolute zero temperature

Since ideal gas state properties are monatomic functions of temperature, many such equations have been proposed. The most notable ones are the polynomials with varying number of terms depending on the temperature range covered and the accuracy desired. For relatively short temperature range, the first or second order polynomials are sufficient, but for wide temperature range higher order of polynomials are needed [12].

2.13 Polar Compounds

Polar compounds expressed the effect of electrostatic forces between molecules. Polar compounds are alcohols, phenols, water, ketones, aldehydes, ether, and alknitriles. The first three are hydrogen bonding compounds (a bond forms between the hydrogen atom attached to oxygen in one molecule with the oxygen atom of another molecule), this makes their behavior in the vapor different and more complex than that of non-hydrogen bonding compounds (ketones, ect) [13].

2.14 Mixing Rules

The concept of a one-fluid mixture is that, for fixed composition, the mixture properties and their variations with T and P are the same as some pure component with appropriate parameter values. To describe all pure components as well as mixtures, the mixture parameters must vary with composition so that if the composition is actually for a pure component, the model describes that substance [42].

The equation of state are generally developed for pure fluids first, and then extended to mixture. The mixture extension requires the so-called mixing rules, which are simply means of calculating mixture parameters equivalent to those of pure substances. Except for those of virial coefficients, the mixing rules are more or less arbitrary rules that are to reflect the composition effect on the system properties. Most of the simple equations of state evolved from the van der Waal's equation use van der Waal's mixing rules with or without modifications [12].

2.15 van der Waals Equation

van der Waals [50] derived the first equation of state that was capable of expressing the continuity from gaseous to liquid states:

$$\left(P+\frac{a}{V^2}\right)(V-b)=RT \tag{2-33}$$

or

$$P=\frac{RT}{(V-b)}-\frac{a}{V^2} \tag{2-34}$$

Although not accurate, this equation deserves special mention because of its enormous contribution to the corresponding state principle and to the later development of similar equation of state. The parameter "*a*" is assumed to account for the attractive force between molecules, and the parameter "*b*" known as co-volume.

Determination of the parameters requires only two of the three critical properties (T_C ,P_C, and V_C). The critical Temperature and critical pressure are generally used to define the parameters, because the two properties are more readily available with reliable accuracy than the critical volume. Differentiating equation (2-34) at constant *T* with respect to *V* and setting it equal to zero at the critical point results in [12]:

$$\left(\frac{\partial P}{\partial V}\right)_{T_C}=\frac{RT_c}{(V_C-b)^2}+\frac{2a}{V_C^3}=0 \tag{2-35}$$

$$\left(\frac{\partial^2 P}{\partial V^2}\right)_{T_c}=\frac{RT_c}{(V_C-b)^3}-\frac{3a}{V_C^4}=0 \tag{2-36}$$

Solving equations (2-35) and (2-36) for *b* and *a* gives

$$b=V_C/3 \tag{2-37}$$

$$a=(9/8)RT_CV_C \tag{2-38}$$

Appling equation (2-34) to the critical point and combining with equation (2-37) and (2-38) gives

$$V_C = \left(\frac{3}{8}\right)\frac{RT_C}{P_C} \tag{2-39}$$

Then equation (2-37) and (2-38) become

$$b = \frac{RT_C}{8P_C} \tag{2-40}$$

$$a = \left(\frac{27}{64}\right)\frac{R^2T_C^2}{P_C} \tag{2-41}$$

Residual molar enthalpy

$$\frac{H^R}{RT} = \frac{b}{V-b} - \frac{2a}{RTV} \tag{2-42}$$

2.16 Redlich –Kwong Equation

Although the van der Waals equation was developed in 1873, no major improvement in cubic equation of state occurred until the publication of the Redlich –Kwong (RK) equation in 1949 [41]. It has proved to be one of the more useful and widely accepted cubic equation of state and is considerably more accurate than the van der Waals equation. The Two-parameter RK equation of state is given by [53]

$$p = \frac{RT}{V-b} - \frac{a}{\sqrt{T}V(V+b)} \tag{2-43}$$

The compressibility factor equation:

$$Z^3 - Z^2 + (A - B^2 - B)Z - AB = 0 \tag{2-44}$$

Where

$$A_i = 0.42748\frac{P_{r,i}}{T_{r.i}^{\;2.5}} \tag{2-45}$$

$$B_i = 0.08664\frac{P_{r,i}}{T_{r,i}} \tag{2-46}$$

$$a_i = 0.42748\frac{R^2 (T_{Ci})^{2.5}}{P_{C\,i}} \tag{2-47}$$

$$b_i = 0.08664\frac{RT_{ci}}{P_{ci}} \tag{2-48}$$

Mixing rules

$$a = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j (1-k_{ij})\sqrt{a_i a_j} \tag{2-49}$$

$$b = \sum_{i=1}^{n} x_i b_i \tag{2-50}$$

Residual molar enthalpy

$$\frac{H^R}{RT} = Z - 1 - \frac{1.5A}{B}\ln\left(1+\frac{B}{Z}\right) \tag{2-51}$$

This equation does not have strong theoretical background but proved to give good results for many gaseous systems, it should be also mentioned that, when Redlich and Kwong proposed their celebrated equation of state they were interested in developing a good equation for gases only [32].

2.17 Soave - Redlich -Kwong Equation

The Soave modification of the Redlich-kwong equation involved replacing the term ($a/T^{0.5}$) by a more complicated function of the temperature, $a\alpha(T)$, incorporating the acentric factor [2].

$$p = \frac{RT}{V-b} - \frac{a\alpha}{V(V+b)} \tag{2-52}$$

The compressibility factor equation:

$$Z^3 - (1-B)Z^2 + \left(A - B^2 - B\right)Z - AB = 0 \tag{2-53}$$

Where

$$A_i = 0.42747\alpha_i \frac{P_{r,i}}{T^2_{r,i}} \tag{2-54}$$

$$B_i = 0.08664\frac{P_{r,i}}{T_{r,i}} \tag{2-55}$$

$$a_i = 0.42747\frac{(RT_{Ci})^2}{P_{Ci}} \tag{2-56}$$

$$b_i = 0.08664\frac{RT_{Ci}}{P_{Ci}} \tag{2-57}$$

$$\alpha_i = \left[1 + n_i(1 - \sqrt{T_{r,i}})\right]^2 \tag{2-58}$$

$$n_i = 0.48508 + 1.55171\omega_i - 0.15613\omega_i^{\ 2} \tag{2-59}$$

$$D_i = \left\lfloor n_i(a_i\alpha_i)\sqrt{T_{r,i}/\alpha_i}\right\rfloor \tag{2-60}$$

Mixing rules

$$A = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j (1 - k_{ij})\sqrt{A_i A_j} \tag{2-61}$$

$$B = \sum_{i=1}^{n} x_i B_i \tag{2-62}$$

$$a\alpha = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j (1 - k_{ij})\sqrt{(a_i\alpha_i)(a_j\alpha_j)} \tag{2-63}$$

$$b = \sum_{i=1}^{n} x_i b_i \tag{2-64}$$

$$D = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j n_j (1 - k_{ij})\sqrt{(a_i\alpha_i)a_j T_{r,j}} \tag{2-65}$$

Residual molar enthalpy

$$\frac{H^R}{RT} = Z - 1 - \frac{A}{B}\left[1 + \frac{D}{a\alpha}\right]\ln\left(1 + \frac{B}{Z}\right) \tag{2-66}$$

The RKS equation was developed to predict reasonable vapor pressure for pure fluids. Thus, there is no reason to suspect it is more accurate than the RK equation in predicting *P-V-T* behavior in the superheat region. One use of the RKS equation or its modification has been the prediction of the thermodynamic properties of refrigerants [5].

2.17.1 Faiq Hussam Sirri

A modification on Soave- Redlich- Kowng [46] was made by introducing a new equation to calculate the n_i value in Soave equation. The new n equation becomes function of reduced temperature and pressure as well as acentric factor as follows:

$$n_i = a_f + b_f \times \omega_i + c_f \times \omega_i^2 \tag{2-67}$$

Where: $a_f = 0.4775746$ (2-68)

$$b_f = 2.509442 - 0.888598 \times T_r - 0.1387515 \times P_r \tag{2-69}$$

$$c_f = -3.278222 + 3.245485 \times T_r + 0.0930755 \times P_r \tag{2-70}$$

To extend the application of the proposed modified Soave equation to be applicable for mixtures, it was found that “the enthalpy departure of a mixture of compressed liquid is equal to the molar average of enthalpy departure of pure compounds at the same reduced temperature and pressure”, or mathematically as:

$$T_r = \frac{T}{T_{cm}} = \sum x_i \left(\frac{T_i}{T_{Ci}} \right) = \sum x_i T_{r,i} \tag{2-71}$$

$$P_r = \frac{P}{P_{cm}} = \sum x_i \left(\frac{P_i}{P_{Ci}} \right) = \sum x_i P_{r,i} \tag{2-72}$$

$$\left(H - H^{ig}\right)_{mixture} = \sum x_i \left(H - H^{ig}\right)_i \tag{2-73}$$

2.18 Peng-Robinson Equation

This equation of state was developed primarily for vapor-liquid equilibrium predictions and uses the same formula for α as appears in the RKS equation [35]. The equation of Peng-Robinson is structurally rather similar to the RKS equation, like the RKS, required only the critical constants and the acentric factor for its application to the pure fluid [2].

$$P = \frac{RT}{V - b} - \frac{a\alpha}{V(V + b) + b(V - b)} \qquad (2\text{-}74)$$

The compressibility factor equation:

$$Z^3 - (1 - B)Z^2 + \left(A - 3B^2 - 2B\right)Z - (AB - B^2 - B^3) = 0 \qquad (2\text{-}75)$$

Where

$$A_i = 0.45724\alpha_i \frac{P_{r,i}}{T_{r,i}^2} \qquad (2\text{-}76)$$

$$B_i = 0.07780 \frac{P_{r,i}}{T_{r,i}} \qquad (2\text{-}77)$$

$$a_i = 0.45724 \frac{(RT_{Ci})^2}{P_{Ci}} \qquad (2\text{-}78)$$

$$b_i = 0.07780 \frac{RT_{Ci}}{P_C} \qquad (2\text{-}79)$$

$$\alpha_i = \left[1 + n_i (1 - \sqrt{T_{r,i}})\right]^2 \qquad (2\text{-}80)$$

$$n_i = 0.37464 + 1.54226\omega_i - 0.26992\omega_i^{\ 2} \qquad (2\text{-}81)$$

$$D_i = \left[n_i (a_i \alpha_i)\sqrt{T_{r,i} / \alpha_i}\,\right] \qquad (2\text{-}82)$$

Mixing rules

$$A = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j (1 - k_{ij})\sqrt{A_i A_j} \qquad (2\text{-}83)$$

$$B = \sum_{i=1}^{n} x_i B_i \qquad (2\text{-}84)$$

$$a\alpha = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j (1 - k_{ij})\sqrt{(a_i\alpha_i)(a_j\alpha_j)} \qquad (2\text{-}85)$$

$$b = \sum_{i=1}^{n} x_i b_i \qquad (2\text{-}86)$$

$$D = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j n_j (1 - k_{ij})\sqrt{(a_i\alpha_i) a_j T_{r,j}} \qquad (2\text{-}87)$$

Residual molar enthalpy

$$\frac{H^R}{RT} = Z - 1 - \frac{A}{2.828B}\left[1 + \frac{D}{a\alpha}\right]\ln\left(\frac{Z + 2.414B}{Z - 0.414B}\right) \tag{2-88}$$

Soave equation together with that of Peng-Robinson are today probably the two most widely used equations of state. Because of the way in which the attractive term have been tailored to achieve a fit to vapor pressure data ,and the incorporation of the acentric factor, these equations usually permit VLE calculations to be made with acceptable accuracy [2].

2.19 Lee-Kesler Equation

Lee and Kesler developed a three-parameter corresponding-states correlation for pure nonpolar, nonhydrogen - bonding fluids - especially, hydrocarbons. Values are provided for acentric factor, vapor pressure, molar volume, residual enthalpy, residual entropy and fugacity coefficient.

The correlation is based on the Benedict-Webb-Rubin (BWR) equation of state. For the equation of state, the Lee - Kesler correlation expresses the compressibility factor Z as a linear function of the acentric factor ω:

$$Z = Z^o + \omega Z' \tag{2-89}$$

Where Z^o is the compressibility factor for simple fluids, ω is Pitzer's acentric factor, and Z' corrects Z for the effects of nonspherical intermolecular forces (primarily dispersion and overlap). Linear expressions are used for residual properties [22]:

$$\frac{H^R}{RT_C} = \left(\frac{H^R}{RT_C}\right)^o + \omega\left(\frac{H^R}{RT_C}\right)' \tag{2-90}$$

The compressibility factor of both simple fluid Z^o and the reference fluid Z^r have been represented by the following reduced form of a modified BWR equation of state.

$$Z = Z^o + \frac{\omega}{\omega^r}(Z^r - Z^o) = Z^o + \omega Z' \qquad (2\text{-}91)$$

ω^r is the acentric factor to n-octane = 0.3978

$$Z = \left(\frac{P_r V_r}{T_r}\right) = 1 + \frac{B}{V_r} + \frac{C}{V_r^2} + \frac{D}{V_r^5} + \frac{c_4}{T_r^3 V_r^2}\left(\beta + \frac{\gamma}{V_r^2}\right)\exp\left(-\frac{\gamma}{V_r^2}\right) \qquad (2\text{-}92)$$

$$B = b_1 - \frac{b_2}{T_r} - \frac{b_3}{T_r^2} - \frac{b_4}{T_r^3} \qquad (2\text{-}93)$$

$$C = c_1 - \frac{c_2}{T_r} + \frac{c_3}{T_r^3} \qquad (2\text{-}94)$$

$$D = d_1 + \frac{d_2}{T_r} \qquad (2\text{-}95)$$

Table 2-1 Constant for equation (2-92) [3]

Constants	**Simple fluids**	**Reference fluids**	**Constants**	**Simple fluids**	**Reference fluids**
b_1	0.1181193	0.2026579	c_3	0.0	0.016901
b_2	0.265728	0.331511	c_4	0.042724	0.041577
b_3	0.15479	0.027655	$d_1 \times 10^4$	0.155488	0.48736
b_4	0.030323	0.203488	$d_2 \times 10^4$	0.623689	0.04336
c_1	0.0236744	0.0313385	β	0.65392	1.226
c_2	0.0186984	0.0503618	γ	0.060167	0.03754

To calculate Z for the fluid of interest, given at T and P, first calculation of the appropriate value of $T_r = (T / T_C)$ and $P_r = (P / P_C)$ using critical properties of the fluid. From the simple fluid constants in table 2-1 and equation (2-92), solving for V_r. (This is not the correct reduced volume for the fluid of interest, but rather, it is defined as P_cV/RT_c with V a simple fluid volume). When V_r is employed in the first equality of equation (2-92), Z^o is calculated for the simple fluid. The next step is identical to the first except that the reference fluid constant of table 2-1 are used, but with the same T_r and p_r values of the fluid of interest that were determined in the first step. The result of the second step is Z^r. Finally, with the Z^o from the first step and Z^r from the second, compressibility factor Z for the fluid of the interest is determined from (2-91) [3].

The enthalpy departure is derived from equation (2-92)

$$\frac{H-H^{ig}}{RT_C}=T_r\left\{Z-1-\frac{b_2+\left({}^{2b_3}\!/\!{}_{T_r}\right)+\left({}^{3b_4}\!/\!{}_{T_r^2}\right)}{T_rV_r}-\frac{c_2-\left({}^{3c_3}\!/\!{}_{T_r^2}\right)}{2T_rV_r^2}+\frac{d_2}{5T_rV_r^5}+8E\right\} \tag{2-96}$$

Where

$$E=\frac{c_4}{2T_r^3\gamma}\left\{\beta+1-\left(\beta+1-\frac{\gamma}{V_r^2}\right)\exp\left(-\frac{\gamma}{V_r^2}\right)\right\} \tag{2-97}$$

Mixing rules

$$V_{Ci}=Z_{Ci}RT_{Ci}/P_{Ci} \tag{2-98}$$

$$Z_{Ci}=0.2905-0.085\omega_i \tag{2-99}$$

$$V_C=\frac{1}{8}\sum_{i=1}^{n}\sum_{j=1}^{n}x_ix_j\left(V_{Ci}^{1/3}+V_{Cj}^{1/3}\right)^3 \tag{2-100}$$

$$T_C=\frac{1}{8V_C}\sum_{i=1}^{n}\sum_{j=1}^{n}x_ix_i\left(V_{Ci}^{1/3}+V_{Cj}^{1/3}\right)^3(T_{Ci}T_{C_j})^{0.5} \tag{2-101}$$

$$\omega=\sum x_i\omega_i \tag{2-102}$$

$$P_C=\frac{Z_CRT_C}{V_C}=(0.2905-0.085\omega)\frac{RT_C}{V_C} \tag{2-103}$$

2.20 Teja Method

One method to extend CSP to substances more complex than normal fluids is to use more terms in equation (2-104) with new characteristic parameters to add in the effects of polarity and association on the properties.

$$Z = Z^{o}\left(\frac{T}{T_C},\frac{P}{P_C}\right) + \omega Z'\left(\frac{T}{T_C},\frac{P}{P_C}\right) \tag{2-104}$$

Most of these correlations are not very successful though the approach of Wilding [54, 55] showed reasonable accuracy. This lack of reliability may be due to the polar and associating forces affecting not only the volumetric behavior as the model tries to treat, but also the critical properties. The result is that to use them for dimensionless scaling is inconsistent with the molecular theory basis for CSP.

Alternative expansions to equation (2-104) have also appeared. Rather than use simple fluids as a single reference, multiple reference fluids can be used. For example, Lee and Kesler and Teja, et al. developed CSP treatments for normal fluids that give excellent accuracy. The concept is to write Z in two terms with two reference substances having acentric factors $\omega^{(R1)}$ and $\omega^{(R2)}$, $Z^{(R1)}(T_r, P_r, \omega^{(R1)})$ and $Z^{(R2)}(T_r, P_r, \omega^{(R2)})$ .The expression is

$$Z(T_r,P_r,\omega) = Z^{(R1)}(T_r,P_r,\omega^{(R1)}) + \frac{\omega-\omega^{(R1)}}{\omega^{(R2)}-\omega^{(R1)}}\left[Z^{(R2)}(T_r,P_r,\omega^{(R2)}) - Z^{(R1)}(T_r,P_r,\omega^{(R1)})\right] \tag{2-105}$$

Typical reference fluids to provide properties are simple fluids as $R1$ and a larger hydrocarbon such as n-octane for $R2$. It is also possible to use more reference fluids to extend CSP to more complex substances. For example, Golobic and Gaspersic [14] use three reference fluids (simple fluids, n-octane and water) with a modification of the second term in equation

(2-105) and an additional term, both of which include another characteristic parameter.

The Properties have been provided in tables rather than analytic equations. Golobic and Gaspersic [14] compared 20 different models for saturated vapor and liquid volumes with their method. Their comparisons with eight strongly polar alcohols and others were the most reliable, giving errors that were rarely more than any of the others and with maximum errors less than twice the average. Platzer and Maurer [38] also used a three-reference fluid approach but with an equation for the EOS. For the 24 normal and 18 polar and associating fluids for which they obtained T_C, P_C, ω, and a polar factor, the correlation was as good as other methods available. A typical formulation equivalent to equation (2-104) is

$$\frac{H^R}{RT_C} = \left(\frac{H^{ig} - H}{RT_C}\right) = \left(\frac{H^{ig} - H}{RT_C}\right)^o + \omega\left(\frac{H^{ig} - H}{RT_C}\right)' \qquad (2\text{-}106)$$

Where tables or graphs of the values of $\left(\left(H^{ig} - H/RT_C\right)\right)^o$ and $\left(\left(H^{ig} - H/RT_C\right)\right)'$ are given for specified values of $T_r = T / T_C$ and $P_r = P / P_C$. The equivalent of the two-reference approach of equation (2-105) is

$$\frac{H^R}{RT_C}\left(T_r, P_r, \omega\right) = \left(\frac{H^{ig} - H}{RT_C}\right)^{(R1)}\left(T_r, P_r, \omega^{(R1)}\right) + \frac{\omega - \omega^{(R1)}}{\omega^{(R2)} - \omega^{(R1)}}$$
$$\left[\left(\frac{H^{ig} - H}{RT_C}\right)^{(R2)}\left(T_r, P_r, \omega^{(R2)}\right) - \left(\frac{H^{ig} - H}{RT_C}\right)^{(R1)}\left(T_r, P_r, \omega^{(R1)}\right)\right] \qquad (2\text{-}107)$$

All of the opportunities and limitations of CSP for volumetric properties apply to obtaining departure functions. Also, all of the mixing rules for CSP apply to mixture departure functions [42].

2.21 Virial Expansion Equation

The virial expansion, also called the virial equation of state, is the most interesting and versatile of the equations of state for gases. The virial expansion is a power series in powers of the variable, *n/V*, and has the form,

$$\frac{PV}{nRT} = Z = 1 + B(T)\frac{n}{V} + C(T)\frac{n^2}{V^2} + \ldots.. \tag{2-108}$$

The coefficient, *B* (*T*), is a function of temperature and is called the "second virial coefficient" *C* (*T*) is called the third virial coefficient, and so on. The expansion is, in principle, an infinite series, and as such should be valid for all isotropic substances. In practice, however, terms above the third virial coefficient are rarely used in chemical thermodynamics.

The new virial coefficients, B', C'. . . can be calculated from the original virial coeffients, *B, C* . . . Equating the two virial expansions gives,

$$\frac{PV}{nRT} = Z = 1 + B(T)\frac{n}{V} + C(T)\frac{n^2}{V^2} + \ldots..\infty = 1 + B'(T)p + C'(T)p^2 + \ldots.. \tag{2-109}$$

Solving the original virial expansion for *p*,

$$p = \frac{nRT}{V}\left(1 + B(T)\frac{n}{V} + C(T)\frac{n^2}{V^2} + \ldots..\right) \tag{2-110}$$

and substitute this expression for *p* into the right-hand-side of equation (2-109),

$$1 + B\frac{n}{V} + C\frac{n^2}{V^2} + \ldots = 1 + B'\frac{nRT}{V}\left(1 + B\frac{n}{V} + C\frac{n^2}{V^2} + \ldots\right) + C'\left(\frac{nRT}{V}\right)^2\left(1 + B\frac{n}{V} + C\frac{n^2}{V^2} + \ldots\right)^2 + \ldots \tag{2-111a}$$

$$1 + B\frac{n}{V} + C\frac{n^2}{V^2} + \ldots = 1 + B'RT\frac{n}{V} + B'RTB\frac{n^2}{V^2} + \ldots + C'(RT)^2\frac{n^2}{V^2} + \ldots \tag{2-111b}$$

Both sides of Equation (2-111b) are power series in *n/V*. Since the two power series must be equal, the coefficients of each power of *n/V* must be the same on both sides. The coefficient of $(n/V)^0$ on each side is 1, which gives the reassuring but not very interesting result, 1 = 1. Equating the coefficient of $(n/V)^1$ on each side gives $B = B'RT$ and equating the coefficients of $(n/V)^2$ gives

$$C = B'RTB + C'(RT)^2 \tag{2-112}$$

These equations are easily solved to give B' and C' in terms of *B*, *C*, and *R* [23].

$$B' = \frac{B}{RT} \tag{2-113}$$

$$C' = \frac{C - B^2}{(RT)^2} \tag{2-114}$$

2.21.1 Second Virial Correlation

Second Virial coefficient can be determined from experimental data mostly complied by Dymond and Smith (1968) or calculated with a suitable correlation. It is well known that accurate procedures are required for the calculation of second Virial coefficient of gases .One of the correlations used to compute the second Virial coefficient is that based on semi empirical equations, this semi empirical estimation has the major advantage when theoretical approaches are tedious. Though it is possible to derive correlations from the original and modified Redlich-Kwong equations and molecular theory, such expressions are usually more complicated than those cited, even for simple substances, and so they have not been evaluated, an explanation was given for one of the practical techniques for estimating values for most types of pure substances (Tsonpoulos) [49].

Correlation of second Virial coefficient of both polar and nonpolar system is presented by [1]

$$Z = 1 + \frac{B}{V} = 1 + B'P = 1 + \frac{BP}{RT} \qquad (2\text{-}115)$$

Tsonpoulos correlation for B

$$B = \frac{RT_C}{P_C}(B^{(0)} + \omega B^{(1)}) \qquad (2\text{-}116)$$

$$B^{(0)} = 0.1445 - \frac{0.33}{T} - \frac{0.1385}{T_r^2} - \frac{0.0121}{T_r^3} - \frac{0.000607}{T_r^8} \qquad (2\text{-}117)$$

$$B^{(1)} = 0.0637 + \frac{0.331}{T_r^2} - \frac{0.423}{T_r^3} - \frac{0.008}{T_r^8} \qquad (2\text{-}118)$$

2.21.2 Third Virial Correlation

It is possible to derive the third Virial coefficient correlations from molecular theory, but these are not very successful.

The principle theoretical problem is that the trio intermolecular potential includes significant contributions that can not be determined from their pair potentials that describe second Virial coefficients .Thus, CSP is also used for calculating *C*, though the range of substances considered has been much more limited. This means that the users often must choose to use a complete equation of state [42].

For high pressure above 15 bar, equation (2-109) may be truncated after three terms. There are many correlations for third Virial coefficient such that Orbey Vera correlation C [34]

$$Z = 1 + \frac{B}{V} + \frac{C}{V^2} = 1 + B'P + C'P^2 = 1 + \frac{BP}{RT} + \left(\frac{C - B^2}{(RT)^2}\right)P^2 \qquad (2\text{-}119)$$

$$C = \left(\frac{RT_C}{P_C} \right)^2 \left(C^0 + \omega C' \right) \qquad (2\text{-}120)$$

$$C^0 = 0.01407 + \frac{0.04232}{T_r^{2.8}} - \frac{0.00313}{T_r^{10.5}} \qquad (2\text{-}121)$$

$$C' = -0.02676 + \frac{0.0177}{T_r^{2.8}} + \frac{0.04}{T_r^{3}} - \frac{0.003}{T_r^{6}} - \frac{0.00228}{T_r^{10.5}} \qquad (2\text{-}122)$$

By using the residual properties, the final expression of residual enthalpy after derivation can be expressed as [42]

$$\frac{H^R}{RT} = \frac{P}{RT}\left(B - T\frac{\partial B}{\partial T} \right) + \left(\frac{P}{RT} \right)^2 \left(C - B^2 - \frac{T}{2}\frac{\partial C}{\partial T} + BT\frac{\partial B}{\partial T} \right) \qquad (2\text{-}123)$$

CHAPTER THREE

INVESTIGATION AND DEVELOPMENT

3.1 Investigation of the Equations of State

The term equation of state is used to describe an empirically derived function, which provides a relation between pressure, volume, temperature and (for mixture) composition. Such relation provides mean of the calculation at all the configurationally and residual thermodynamic properties of the system within some domain of applicability. Sometimes, the term equation of state is attached to a more fundamental relation, which may be use to obtain both perfect–gas and residual properties. Many equations of state can represent adequately the properties of the gas phases, some are applied only to the liquids, but the most important category of equation of state models contain those that may be applied in the same form to both gaseous and liquid phases, There are no equation of state applicable simultaneously to solid , liquid and gas [2] .

Today the development of equations of state remains an active field of research, primarily in areas of:

1. Highly accurate equations often with many constants, for important pure substances such as water, ammonia, carbon dioxide, etc
2. Accurate equation of state models for specific mixtures such as those encountered in the natural gas and petroleum industries.
3. Simple equations of state that combine satisfactory predictive capabilities with the computational efficiency required for detailed simulations of chemical processing operations such as multistage separation processes for mixtures.

4. Models for complex system such as electrolytes, polymers, coal liquids and highly polar substances [2].

3.2 Experimental Data

It is a well known fact that the evaluation of any correlation or prediction method is done by comparison of the results with experimental dependable data. The deviation between the experimental results and the results of prediction or correlation determines the accuracy of the method. The experimental data of the enthalpy of saturated vapor, obtained from literature for the purpose of this investigation including 25 compounds with 701 data points (17 non-polar compounds with 439 data points and 8 polar compounds with 262 data points) for pure compounds and 5 mixtures with 95 data points as shown in tables 3-1 to 3-3.

Table 3-1 Saturated enthalpy data for pure non-polar compounds

	Compounds	**Temperature Range (K)**	**Pressure Range (kpa)**	**No. of Data Points**	**Data Ref.**
1	Benzene	280-535	5.3-3488	40	[51]
2	Cyclopropane	297.22-380.55	706.43-4154.29	15	[29]
3	Isobutene	270 - 407.5	140.84-3611.22	29	[6]
4	Isopentane	310 - 460	136.89-3360.64	27	[7]
5	Neopentane	347.22-433.33	644.04-3172.48	32	[10]
6	Propane	216.48-310.93	50.815-1289.33	18	[57]
7	n-butane	280 - 424.5	133.44-3753.07	31	[8]
8	n-pentane	310 - 469.5	104.263-3360.5	27	[9]
9	Ethylene	104 - 233.15	0.122-1421.975	13	[36]
10	Trichloroethylene	260.92-333.15	664.906-9846.82	14	[36]
11	N_2	65-120	17.4279-2512.86	9	[53]
12	SO_2	205.37-422.04	3.206-6805.167	40	[36]
13	R13	173.15-293.15	33.1-3170.8	24	[11]
14	R21	233.15-322.04	9.363-384.385	11	[36]
15	R114	213.15-413.15	3.7-2945.8	36	[11]
16	R123	233.15-453.15	1.8-3450.6	37	[58]
17	R134a	237.15-363.15	63.32-3243.5	36	[11]
	$\sum$			439	

Table 3-2 Saturated enthalpy data for pure polar compounds

	Compounds	**Temperature Range (K)**	**Pressure Range (kpa)**	**No. of Data Points**	**Data Ref.**
1	H_2O	278.15-643.15	0.8721-21028	74	[26]
2	NH_3	223.15-403.15	40.9-10892	36	[15]
3	R11	203.15-463.15	0.6-3932.4	27	[11]
4	R12	183.15-383.15	2.8-3978.5	36	[11]
5	R22	203.15-368.15	20.5-4883.5	34	[11]
6	R32	172.04-344.261	3.516-5003.3	15	[36]
7	Ethyl Chloride	243.15-328.15	15.169-395.486	17	[36]
8	Methyl Chloride	238.7-349.817	62.301-1957.433	23	[36]
	$\sum$			262	

Table 3-3 Saturated enthalpy data for mixture

	Compounds	**No. of Composition**	**No. of Data Points**	**Data Ref.**
1	Benzene- n-Pentane	4	22	[27]
2	Benzene -Cyclohexane	4	17	[28]
3	Benzene -Hexadecane	3	14	[17]
4	n-Pentane -Cyclohexane	4	18	[18]
5	n-Pentane - trans-Decalin	4	24	[19]
	$\sum$		95	

3.3 Application EOS for Pure Compounds

$$\underset{T_o,\,P_o}{\text{Saturated liquid}} \xrightarrow[(1)]{\Delta H_v} \underset{T_o,\,P_o}{\text{Saturated actual gas}} \xrightarrow[(2)]{-H^R} \underset{T_o,\,P_o}{\text{Ideal gas}} \xrightarrow[(3)]{\int_{To}^{T} cpdt}$$

$$\underset{T,\,P_o}{\text{Ideal gas}} \xrightarrow[(4)]{H=0} \underset{T,\,P}{\text{Ideal gas}} \xrightarrow[(5)]{H^R} \underset{T,\,P}{\text{Actual gas}}$$

First step Saturated enthalpy of vapor can be calculated by converting saturated liquid at reference temperature and pressure to saturated actual gas at the same temperature and pressure by using the enthalpy of vaporization at the normal boiling point ΔH_{vb}, and the best equation (more accurate) was Vetere equation and then using the correlation between ΔH_v and T_r (Watson's relation) to calculate ΔH_v at reference temperature.

Second step converting saturated actual gas at reference temperature and pressure to ideal gas at the same temperature and pressure by using a suitable enthalpy departure of an equation of state.

Third step converting ideal gas at reference temperature and pressure to ideal gas at the system temperature and reference pressure by using the molar or specific enthalpy equation of a substance.

Fourth step converting ideal gas at system temperature and reference pressure to ideal gas at the system temperature and pressure, the enthalpy change in this case is zero, because the pressure has no influence on enthalpy of ideal gas.

Fifth step converting ideal gas at system temperature and pressure to actual gas at the same temperature and pressure by using a suitable enthalpy departure of an equation of state.

All the above steps affected the calculation of saturated enthalpy of vapor.

There are several equations of state that were used to determine the residual enthalpy of vapor in steps 2 and 5, such as Redlich–Kwong, Soave, Peng-Robinson, Lee-Kesler and Virial equation truncated to second and to third terms. These equations are considered the most important and accurate equations that are used to determine the thermodynamic properties of the fluids (liquid and vapor phases).

The Average Absolute Deviation Percent AAD%, which is defined as follows:

$$AAD\% = \frac{\sum \left| \left(\mathrm{H}_{\mathrm{experimental}} - \mathrm{H}_{\mathrm{calculated}} \right) / \mathrm{H}_{\mathrm{experimental}} \right| \times 100}{\text{No. of experimental data points}} \qquad (3\text{-}1)$$

AAD% was considered as a factor for comparison between the different methods that were used for calculating actual enthalpy of saturated enthalpy of vapor of different compounds and experimental data.

Table 3-6 shows the AAD% results of saturated enthalpy calculations of vapor as compared with experimental data.

The followings are those equations that were employed in steps 2 and 5 for pure compounds.

1. Soave - Redlich- Kwong equation was used for calculating enthalpy departure. It was found that the AAD% for 25 pure compounds and 701 experimental data point was 6.7138% and it was found that this equation was not very accurate for this purpose. This accuracy is

further decreased when calculating saturated enthalpy for higher temperature and pressure. It was found that the overall average deviation of saturated enthalpy of vapor at T_r below 0.87 was better than the enthalpy of saturated vapor at T_r above 0.87 as shown in table 3-4 and 3-5.

Table 3-4 AAD% for pure compounds at T_r below 0.87 when applying RKS equation of state

	Compounds	**No. of Exp. Data Points**	**AAD%**
1	Benzene	30	1.8489
2	Cyclopropane	9	0.4628
3	Isobutene	9	0.4369
4	Isopentane	10	1.2371
5	Neopentane	11	1.1090
6	Propane	18	5.5271
7	n-butane	9	0.5179
8	n-pentane	10	3.3587
9	Ethylene	13	1.3143
10	Ethyl Chloride	17	2.8963
11	Methyl Chloride	23	0.8095
12	Trichloroethylene	14	3.5582
13	N_2	7	1.0966
14	SO_2	31	0.3015
15	H_2O	57	4.1293
16	NH_3	25	0.7231
17	R11	21	0.8785
18	R12	27	2.3685
19	R13	17	0.7082
20	R21	11	0.7836
21	R22	24	0.6372
22	R32	11	1.8171
23	R114	26	0.5236
24	R123	30	0.4940
25	R134a	31	2.1109

Table 3-5 AAD% for pure compounds at T_r above 0.87 when applying RKS equation of state

	Compounds	No. of Exp. Data Points	AAD%
1	Benzene	40	4.8699
2	cyclopropane	15	7.8719
3	Isobutene	29	15.0793
4	Isopentane	27	11.4724
5	Neopentane	32	13.0437
6	Propane	——	——
7	n-butane	31	16.3618
8	n-pentane	27	15.4969
9	Ethylene	——	——
10	Ethyl Chloride	——	——
11	Methyl Chloride	——	——
12	Trichloroethylene	——	——
13	N_2	9	5.5779
14	SO_2	40	3.8978
15	H_2O	74	6.4828
16	NH_3	36	6.2227
17	R11	27	3.7507
18	R12	36	4.9683
19	R13	24	7.7361
20	R21	——	——
21	R22	34	5.8136
22	R32	15	7.3900
23	R114	36	3.7195
24	R123	37	2.4144
25	R134a	36	4.314

2. Virial equation truncated to two terms was used for calculating enthalpy of saturated vapor to be compared with experimental data. It was found that the AAD% for 25 pure compounds and 701 experimental data point was 3.4648%.

3. Redlich-Kwong equation was also used for calculating enthalpy departure to be compared with experimental data. It was found that the AAD% was 2.5780%.

4. Virial equation truncated to three terms was used for calculating enthalpy of saturated vapor to be compared with experimental data. It was found that the AAD% was 2.4914 %.

5. Lee-Kesler equation also was employed for the same purpose. It was found that the AAD% was 2.2696 %.

6. Peng-Robinson equation was used for calculating enthalpy departure of vapor for experimental data. It is found that the AAD% was reduced to 1.8757 %.

7. Using Peng- Robinson equation with modified *n* parameter where it was found that the AAD% was reduced to 1.2725 %. This modification will be discussed soon.

Table 3.6 Comparison of the calculated saturated enthalpy of vapor obtained using different EOS for polar and non polar compound and experimental data

Compounds	No. of Exp. Data Points	Soave AAD%	Virial /B AAD%	Redlich-Kwong AAD%	Virial /C AAD%	Lee-Kesler AAD%	Peng-Robinson AAD%	This Work AAD%
Benzene	40	5.4833	1.8905	2.7291	2.0622	2.9383	2.9825	2.8269
Cyclopropane	15	7.8719	3.0300	1.1009	1.6200	0.6565	0.2729	0.2706
Isobutene	29	15.0793	8.0652	3.4952	6.0119	4.2776	1.4209	0.6369
Isopentane	27	11.4724	7.2177	3.7892	4.2134	3.4591	1.7483	0.6764
Neopentane	32	13.0437	4.2032	1.5020	2.4782	1.4753	0.4612	0.7015
Propane	18	5.5271	1.0177	1.3380	1.1218	1.2202	1.3368	1.3290
n-butane	31	15.9986	7.5796	3.4417	5.0582	3.1809	1.2848	0.3862
n-pentane	27	15.5069	3.7729	3.1863	3.1838	9.3157	4.6455	3.2392
Ethylene	13	1.3143	1.4188	1.2008	1.4759	1.5591	1.1969	1.1915
Ethyl Chloride	17	2.8963	2.9241	2.8339	2.8757	2.9956	2.8776	2.9387
Methyl Chloride	23	0.8095	0.9796	1.1771	0.7575	0.4605	0.9632	0.8778
Trichloroethylene	14	3.5582	3.5809	3.5537	3.6574	3.5763	3.5569	3.5694
N_2	9	5.5779	2.7544	1.5497	1.1800	0.8552	1.4829	0.9030
SO_2	40	3.8978	1.4603	1.1021	0.8637	0.9253	0.3700	1.2102
H_2O	74	6.4828	6.0854	6.1938	5.1479	4.0998	5.1903	2.1884
NH_3	36	6.2227	3.2046	2.4881	1.6377	1.4644	1.1886	0.5654
R11	27	3.7507	1.8906	1.6037	1.0314	0.6218	1.0750	0.7453
R12	36	4.9683	2.5000	1.6765	1.5659	1.1903	0.7828	0.3891
R13	24	7.7361	3.2038	2.0408	1.6049	0.5658	0.9587	0.4453
R21	11	0.7999	0.9842	0.7132	1.0548	1.0118	0.7757	0.9339
R22	34	5.8136	3.4482	2.3545	1.8007	1.1226	1.2173	0.6524
R32	15	7.3900	4.8936	4.0159	4.0173	2.1537	2.9959	2.0983
R114	36	3.7195	0.8314	0.4799	0.6533	1.3005	0.5958	1.6387
R123	37	2.4144	1.2416	0.8940	0.8686	1.0189	0.7134	0.5101
R134a	36	3.8742	2.8990	3.2030	2.1125	1.5244	2.3507	0.8693
$\sum$	**701**	**6.7138**	**3.4648**	**2.5780**	**2.4914**	**2.2696**	**1.8757**	**1.2725**

3.4 Modified Peng-Robinson Equation of State for Pure Compounds

Peng-Robinson equation of state proved to be better than Redlich-Kwong, Soave, Lee and Kesler and Virial truncated to B and C equations for perdiction of saturated enthalpy of vapor. There is still room for improving it for predicting actual enthalpy of saturated vapor. A Soave-Redlich- Kwong and Peng-Robinson equation of state were derived mainly to calculate vapor liquid equilibrium; so all the attentions were concentrated for that purpose in the derivation.

A new equation was improved for *n* parameter of Peng-Robinson equation to be used to calculate residual enthalpy of saturated vapor for pure compounds. Different equations for *n* parameter had been tried to calculate residual enthalpy of saturated vapor. It was found that the following equation gave the least deviation for enthalpy calculation as compared with the experimental enthalpy data for saturated vapor.

$$n = a_A + b_A \times \omega + c_A \times \omega^2 \qquad (3\text{-}2)$$

$a_A =$ Constant (3-3)

$$b_A = b_1 T_r + b_2 T_r^2 + b_3 P_r + b_4 T_r P_r + b_5 P_r^2 \qquad (3\text{-}4)$$

$$c_A = c_1 T_r + c_2 T_r^2 + c_3 P_r + c_4 T_r P_r + c_5 P_r^2 \qquad (3\text{-}5)$$

The coefficients of the *n* equation were obtained by using the statistical analysis as shown in table 3-7.

Table 3-7 Coefficients of equations (3-4 and 3-5)

Coefficients	Value	Coefficients	Value
a_A	0.941018	c_1	433.376
b_1	-85.7291	c_2	-530.876
b_2	105.6393	c_3	-35.3057
b_3	4.303806	c_4	252.0676
b_4	-50.0757	c_5	-108.396
b_5	22.98768		

The overall average deviation of saturated enthalpy of vapor using the equations above gave higher accuracy where AAD% 1.2725. Table 3-8 summarizes the comparison of AAD% for saturated enthalpy of vapor using different methods employed and the present work for 701 experimental data points of 25 pure compounds.

Table 3-8 Comparison of the deviation results for pure compounds

Equation Used	AAD%
Soave - Redlich-Kwong	6.7138
Virial Truncated to B	3.4648
Redlich - Kwong	2.5780
Virial Truncated to C	2.4914
Lee - Kesler	2.2696
Peng - Robinson	1.8757
This Work	1.2725

So the proposed Peng-Robinson modification can be recommended for the calculation of enthalpy of saturated vapor of pure polar and non polar compounds.

3.5 Example for Calculation of Saturated Enthalpy of Vapor for Pure n-Butane:

Calculation of the enthalpy of saturated vapor for n-Butane at 350 K and 947.8953 kpa on the basis H_o = 0 at 272.67 K and 101.325 kpa for saturated liquid [8] using modified Peng-Robinson equation.

Data required:

T_C (K)	425.2
P_C (kpa)	3800
ω	0.199

Saturated liquid $\xrightarrow{\Delta Hv}$ Saturated actual gas $\xrightarrow{-H^R}$ Ideal gas $\xrightarrow{\int_{To}^{T} cpdt}$

272.67 K, 101.325 kpa (1) 272.67 K, 101.325 kpa (2) 272.67 K, 101.325 kpa (3)

Ideal gas $\xrightarrow{H=0}$ Ideal gas $\xrightarrow{H^R}$ Actual gas

350 K., 101.325 kpa (4) 350 K , 947.8953 kpa (5) 350 K , 947.8953 kpa

Step (1) Calculation of the enthalpy of evaporation using Vetere method:

$$T_r = \frac{T_o}{T_C} = 0.64127$$

$$P_r = \frac{p_o}{p_c} = 0.0266$$

$$\Delta H_v = RT_C T_r \frac{0.4343 \ln P_C - 0.69431 + 0.89584 T_r}{0.37691 - 0.37306 T_r + 0.15075 P_C^{-1} T_r^{-2}} = 22466.29 \text{ J/mole}$$

Step (2) Calculation of the residual enthalpy at reference temperature and pressure:

$$a = 0.45724 \frac{(RT_c)^2}{P_c} = 1.50372$$

$$a_A = 0.941018$$

$$b_A = -85.7291\times \mathrm{T_r} + 105.6393\times \mathrm{T_r}^2 + 4.303806\times \mathrm{P_r} - 50.0757\times \mathrm{T_r}\times \mathrm{P_r} + 22.98768\times \mathrm{P_r}^2$$

$$= -12.25877$$

$$c_A = 433.376\times \mathrm{T_r} - 530.876\times \mathrm{T_r}^2 - 35.3057\times \mathrm{P_r} + 252.0676\times \mathrm{T_r}\times \mathrm{P_r} - 108.396\times \mathrm{P_r}^2$$

$$= 62.89149$$

$$n = a_A + b_A \times \omega + c_A \times \omega^2 \quad = 0.99208$$

$$\alpha = \left[1 + n(1-\sqrt{T_r})\right]^2 = 1.43432$$

$$A = 0.45724\alpha \frac{P_r}{T_r^2} = 0.04252$$

$$B = 0.07780\frac{P_r}{T_r} = 0.003235$$

$$D = \left[n(a\alpha)\sqrt{T_r/\alpha}\right] = 1.43074$$

$$Z^3 - (1-B)Z^2 + \left(A - 3B^2 - 2B\right)Z - (AB - B^2 - B^3) = 0$$

By Newton – Raphson Method find the value of Z starting with $Z_o = 1$ for vapor.

Z = 0.95935

$$\frac{H_1^R}{RT} = Z - 1 - \frac{A}{2.828B}\left[1 + \frac{D}{a\alpha}\right]\ln\left(\frac{Z + 2.414B}{Z - 0.414B}\right)$$

H_1^R = -258.7248 J/mole

Step (3)

$C_{p,o}$ = 9.487

$C_{p,1}$ = 0.3313

$C_{p,2} = -1.108\times10^{-4}$

$C_{p,3} = -2.822\times10^{-9}$

$$\Delta H^{ig} = \int_{To}^{T} C_p dt = C_{p,o}(T - T_o) + \frac{C_{p,1}}{2}\left(T^2 - T_o^2\right) + \frac{C_{p,2}}{3}\left(T^3 - T_o^3\right) + \frac{C_{p,3}}{4}\left(T^4 - T_o^4\right)$$

=7868.389 J/mole

Step (4) $\mathrm{H}^{\mathrm{R}} = 0$ because pressure has no effect on enthalpy of ideal gas.

Step (5) Calculation of the residual enthalpy at system temperature and pressure:

$$T_r = \frac{T}{T_C} = 0.82314$$

$$P_r = \frac{p}{p_c} = 0.24944$$

$$a = 0.45724\frac{(RT_C)^2}{P_C} = 1.50372$$

$$a_A = 0.941018$$

$$b_A = -85.7291 \times \mathrm{T_r} + 105.6393 \times \mathrm{T_r}^2 + 4.303806 \times \mathrm{P_r} - 50.0757 \times \mathrm{T_r} \times \mathrm{P_r} + 22.98768 \times \mathrm{P_r}^2$$

$$= -6.76822$$

$$c_A = 433.376 \times \mathrm{T_r} - 530.876 \times \mathrm{T_r}^2 - 35.3057 \times \mathrm{P_r} + 252.0676 \times \mathrm{T_r} \times \mathrm{P_r} - 108.396 \times \mathrm{P_r}^2$$

$$= 33.23351$$

$$n = a_A + b_A \times \omega + c_A \times \omega^2 \quad = 0.91025$$

$$\alpha = \left[1 + n(1 - \sqrt{T_r})\right]^2 = 1.17593$$

$$A = 0.45724\alpha\frac{P_r}{T_r^2} = 0.19795$$

$$B = 0.07780\frac{P_r}{T_r} = 0.02357$$

$$D = \left[n(a\alpha)\sqrt{T_r/\alpha}\right] = 1.34666$$

$$Z^3 - (1-B)Z^2 + \left(A - 3B^2 - 2B\right)Z - (AB - B^2 - B^3) = 0$$

By Newton – Raphson Method find the value of Z starting with $Z_o = 1$ for vapor.

$Z = 0.79541$

$$\frac{H_2^R}{RT} = Z - 1 - \frac{A}{2.828B}\left[1 + \frac{D}{a\alpha}\right]\ln\left(\frac{Z + 2.414B}{Z - 0.414B}\right)$$

$\mathrm{H}_2^{\mathrm{R}} = -1834.958$ J/mole

$H_{calculated} = \Delta H_v - H_1^R + \Delta H^{ig} + H_2^R$

=22466.29 +258.7248 +7868.389 -1834.958

=28758.4458 J/mole

The actual value of enthalpy is 28844.5 J/mole [8]

$$AD\% = \left| \frac{H_{actual} - H_{calculated}}{H_{actual}} \right| \times 100\%$$

$$AD\% = \left| \frac{28844.5 - 28758.45}{28844.5} \right| \times 100\%$$

= 0.2983 %

3.6 Applying EOS for Mixture Components

Since Peng-Robinson equation of state proved to be a better equation for predicting the saturated enthalpy of vapor for pure compounds, it was used for predicting saturated enthalpy of vapor for mixture components.

It is well known fact that the calculations of the thermodynamic properties of the mixtures are not as easy as the calculations for pure compounds. This is because of finding the critical constants that represents the mixture from critical constants of pure compounds and this is done by using what is called mixing rules. The mixing rules are not very accurate due to difference in chemical structures of the components .Usually adjustable parameter or parameters are needed to calculate any thermodynamic property of mixture very accurately.

To apply the corresponding state correlations to mixtures, the appropriate scaling factors must be determined. These scaling factors are called pseudo critical properties, which were derived from critical properties of pure compounds. To calculate the critical temperature, critical pressure and acentric factor for the mixture for the purpose of calculation of heat of vaporization ΔH_{vb} at normal boiling point equation (2-27) several sets of mixing rules have been studied.

The Lee-Kesler mixing rules have been found to give the best results which are given below [3]:

$$V_{ci} = Z_{ci} R T_{ci} / P_{ci} \tag{2-98}$$

$$Z_{ci} = 0.2905 - 0.085\omega_i \tag{2-99}$$

$$V_c = \frac{1}{8} \sum \sum x_i x_j \left(V_{Ci}^{1/3} + V_{Cj}^{1/3} \right)^3 \tag{2-100}$$

$$T_c = \frac{1}{8V_c}\sum\sum x_i x_j \left(V_{ci}^{1/3} + V_{cj}^{1/3}\right)^3 (T_{ci}T_{c_j})^{0.5} \qquad (2\text{-}101)$$

$$\omega = \sum x_i \omega_i \qquad (2\text{-}102)$$

$$P_c = \frac{Z_c R T_c}{V_c} = (0.2905 - 0.085\omega)\frac{RT_c}{V_c} \qquad (2\text{-}103)$$

In this work the prediction of the residual enthalpy of saturated vapors for binary mixtures were done by using two methods: The first method was Peng-Robinson equation of state with its mixing rules; the second method was Peng-Robinson with Teja equation. The results obtained from these two methods were listed in table 3-11.

3.7 Modified Peng-Robinson Equation of State for Mixture Components

Anew equation was derived for *n* parameter of Peng-Robinson equation to be used to calculate the residual enthalpy of saturated vapor for mixture components. Different equations for *n* parameter had been tried to calculate the residual enthalpy of saturated vapor for mixture components. It was found that the following equation gave the least deviation of the calculated enthalpy values as compared with those of experimental data for mixture for saturated vapor enthalpy.

$$n = a_A + b_A \times \omega + c_A \times \omega^2 \qquad (3\text{-}6)$$

$a_A =$ Constant (3-7)

$$b_A = b_o + b_1 T_r + b_2 P_r \qquad (3\text{-}8)$$

$$c_A = c_o + c_1 T_r + c_2 P_r \qquad (3\text{-}9)$$

The coefficients of the equation were predicted using the statistical analysis as shown in table 3-10.

Table 3-10 Coefficients in equations (3-8 and 3-9)

Coefficients	**Value**	**Coefficients**	**Value**
a_A	0.3704	c_o	-0.9048
b_o	0.01267	c_1	0.945147
b_1	-0.20093	c_2	-0.17167
b_2	0.1		

The overall average deviation of saturated enthalpy of vapor for mixture components using the equations above gave higher accuracy where AAD% 2.0362. Table 3-11 summarizes the comparison of AAD% for saturated enthalpy of vapor using different methods employed and present work for 96 data points of 5 binary mixture components.

Table 3-11 Comparison of the deviation values for mixture components

Components	**No. of Exp. Data Points**	**Peng Robinson with its mixing rules AAD%**	**Peng-Robinson with Teja AAD%**	**This work AAD%**
60.01 mole % Benzene & 39.999 mole % n-Pentane	6	1.4508	1.3064	0.7433
81.429 mole % Benzene & 18.571 mole % n-Pentane	7	2.3979	2.3012	0.9212
40.6706 mole % Benzene & 59.3294 mole % n-Pentane	5	1.9689	0.7855	0.7028
19.903 mole % Benzene & 80.0965 mole % n-Pentane	4	0.3895	0.1335	1.3094
81.1665 mole % Benzene & 18.8334 mole% Cyclohexane	4	3.4491	5.8555	1.3312
33.3362 mole % Benzene & 66.6638 mole% Cyclohexane	4	3.5768	3.6256	1.7896
61.2836 mole % Benzene & 38.7164 mole% Cyclohexane	5	5.6808	5.7374	1.4688
21.1154mole % Benzene & 78.8845 mole% Cyclohexane	4	2.9777	3.0204	2.4392
81.3663 mole % Benzene & 18.63365 mole % Hexadecane	2	6.9665	6.8697	6.4780
96.3087 mole % Benzene & 3.6912 mole % Hexadecane	6	3.1726	3.1223	2.1318
91.9694 mole % Benzene & 8.0305 mole % Hexadecane	6	4.4782	4.3824	3.7530
19.7mole % n-Pentane & 80.3 mole % Cyclohexane	6	1.0389	1.0145	0.6104
38.5 mole % n-Pentane & 61.5 mole % Cyclohexane	5	0.2880	0.2296	0.8120
61.2 mole % n-Pentane & 38.8 mole % Cyclohexane	4	0.5972	0.5046	0.4461
79.3 mole % Pentane & 20.7 mole % Cyclohexane	4	0.3737	0.2519	0.9131
32.2 mole % n-Pentane & 67.8 mole % trans-Decalin	6	5.4802	5.4363	5.1688
56.1 mole % n-Pentane & 43.9 mole % trans-Decalin	4	4.3878	4.3111	3.9614
72.2 mole % n- Pentane & 27.5 mole % trans-Decalin	7	3.9199	3.8055	3.3901
88.4 mole % n- Pentane & 11.6 mole % trans-Decalin	7	2.5581	2.4413	2.0308
$\sum$	**96**	**2.8384**	**2.8096**	**2.0362**

3.8 Example for Calculation of Saturated Enthalpy of Vapor for Benzene with n-Pentane Mixture:

Calculation of the enthalpy of saturated vapor for mixture of 60.01 mole % Benzene with 39.99 mole % n-Pentane at 509.5389 K and 3447.4 kpa on the basis H_o=0 at - 200 F (144.2611 K), saturated liquid [27]using modified Peng-Robinson equation.

Data required:

Compound	Benzene	n-Pentane
x	0.6001	0.3999
T_b (K)	353.2	309.2
T_C (K)	562.2	469.7
P_C (kpa)	4890	3370
ω	0.212	0.251
M.wt (kg/mole)	78.114	72.151
V_C (cm^3/mole)	259	304
Z_C	0.271	0.263

$$\text{Saturated liquid}\xrightarrow{\Delta Hv}\text{Saturated actual gas}\xrightarrow{-H^R}\text{Ideal gas}\xrightarrow{\int_{To}^{T} cpdt}$$

144.2611 K, 0 kpa (1) 144.2611 K, 0 kpa (2) 144.2611 K, 0 kpa (3)

$$\text{Ideal gas}\xrightarrow{H=0}\text{Ideal gas}\xrightarrow{H^R}\text{Actual gas}$$

509.5389 K., 0 kpa (4) 509.5389 K, 3447.4 kpa (5) 509.5389 K, 3447.4 kpa

Step 1 Calculation of the enthalpy of evaporation using Vetere method:

Applying the Lee and Kesler mixing rules

$$\omega = \sum x_i \omega_i = 0.2276$$

$$Z_C = 0.2905 - 0.085\omega = 0.27115$$

$$V_c = \frac{1}{8}\sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j \left(V_{Ci}^{1/3} + V_{Cj}^{1/3} \right)^3 = 2.76707 \times 10^{-4}\ \text{m}^3/\text{ mole}$$

$$T_C = \frac{1}{8V_C}\sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_i \left(V_{Ci}^{1/3} + V_{Cj}^{1/3} \right)^3 (T_{Ci} T_{C_j})^{0.5} = 522.4022\ \text{K}$$

$$P_C = \frac{Z_C R T_C}{V_C} = (0.2905 - 0.085\omega)\frac{RT_C}{V_C} = 4256.095\ \text{kpa}$$

$$T_r = \frac{T}{T_C} = 0.27615$$

$$\mathrm{T_b} = \sum T_{b,i} x_i = 335.6044\ \text{K}$$

$$T_{br} = \frac{T_b}{T_C} = 0.64242$$

$$\Delta H_{vb} = RT_C T_{br}\ \frac{0.4343 \ln P_C - 0.69431 + 0.89584 T_{br}}{0.37691 - 0.37306 T_{br} + 0.15075 P_C^{-1} T_{br}^{-2}} = 28896.59\ \text{J/mole}$$

$$n' = \left(0.00264 \frac{\Delta \mathrm{H}_{vb}}{RT_b} + 0.8794 \right)^{10} = 0.3757$$

$$\Delta \mathrm{H}_v = \Delta \mathrm{H}_{vb} \left(\frac{1 - T_r}{1 - T_{br}} \right)^{n'} = 37662.96\ \text{J/mole}$$

<u>Step (2)</u> $\mathrm{H}_1^{\mathrm{R}} = 0$

<u>Step (3)</u>

Compound	Benzene	n-Pentane
$Cp_{,o}$	-33.92	-3.626
$Cp_{,1}$	0.4739	0.4873
$Cp_{,2}$	-3.017×10^{-4}	-2.580×10^{-4}
$Cp_{,3}$	7.130×10^{-8}	5.305×10^{-8}

<u>For Benzene</u>

$$\Delta H_1^{ig} = \int_{To}^{T} C_p dt = C_{p,o}(T - T_o) + \frac{C_{p,1}}{2}\left(T^2 - T_o{}^2\right) + \frac{C_{p,2}}{3}\left(T^3 - T_o{}^3\right) + \frac{C_{p,3}}{4}\left(T^4 - T_o{}^4\right)$$

=32389.48 J/mole

For n-Pentane

$$\Delta H_2^{ig} = \int_{To}^{T} C_p dt = C_{p,o}\left(T - T_o\right) + \frac{C_{p,1}}{2}\left(T^2 - T_o^{\ 2}\right) + \frac{C_{p,2}}{3}\left(T^3 - T_o^{\ 3}\right) + \frac{C_{p,3}}{4}\left(T^4 - T_o^{\ 4}\right)$$

= 46633.03 J/mole

$\Delta H^{ig} = \sum \Delta H_i^{ig} x_i$ = 38085.42 J/mole

Step (4) $H^R = 0$ because pressure has no effect on enthalpy of ideal gas.

Step (5) Calculation of the residual enthalpy at system temperature and pressure:

For Benzene:

$$T_{r,i} = \frac{T}{T_{Ci}} = 0.9063$$

$$P_{r,i} = \frac{p}{p_{Ci}} = 0.70498$$

$$a_i = 0.45724 \frac{(RT_{Ci})^2}{P_{Ci}} = 2.0428$$

$$a_{A,i} = 0.3704$$

$$b_{A,i} = 0.01267 - 0.20093 \times T_{r,i} + 0.1 \times P_{r,i} = -0.09893$$

$$c_{A,i} = -0.9048 + 0.945147 \times T_{r,i} - 0.17167 \times P_{r,i} = -0.16923$$

$$n_i = a_{A,i} + b_{A,i}\omega_i + c_{A,i}\omega_i^2 = 0.34182$$

$$\alpha_i = \left[1 + n_i (1 - \sqrt{T_{r,i}})\right]^2 = 1.03307$$

$$A_i = 0.45724\alpha_i \frac{P_{r,i}}{T_{r,i}^2} = 0.4054$$

$$B_i = 0.07780 \frac{P_{r,i}}{T_{r,i}} = 0.0605$$

$$D_i = \left\lfloor n_i (a_i \alpha_i) \sqrt{T_{r,i} / \alpha_i} \right\rfloor = 0.67568$$

For n-Pentane

$T_{\mathrm{r,j}} = \dfrac{T}{T_{Cj}}$ = 1.0848

$P_{\mathrm{r,j}} = \dfrac{p}{p_{Cj}}$ = 1.0229

$a_j = 0.45724\dfrac{(RT_{Cj})^2}{P_{Cj}}$ =2.069

$a_{A,j} =$ 0.3704

$b_{A,j} = 0.01267 - 0.20093 \times T_{r,j} + 0.1 \times P_{r,j}$ = -0.103008

$c_{A,j} = -0.9048 + 0.945147 \times T_{r,j} - 0.17167 \times P_{r,j}$ = -0.0551057

$n_j = a_{A,j} + b_{A,j}\omega_j + c_{A,j}\omega_j^2$ = 0.341074

$\alpha_j = \left[1 + n_j(1 - \sqrt{T_{r,j}})\right]^2$ = 0.97186

$A_j = 0.45724\alpha_j \dfrac{P_{r,j}}{T_{r,j}^2}$ = 0.38627

$B_j = 0.07780\dfrac{P_{r,j}}{T_{r,j}}$ = 0.07336

$D_j = \left[n_j(a_j\alpha_j)\sqrt{T_{r,j}/\alpha_j}\right]$ = 0.7246

Mixing rules

K_{ij}= 0

$A = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j (1 - k_{ij})\sqrt{A_i A_j}$ = 0.3977

$B = \sum_{i=1}^{n} x_i B_i$ = 0.06565

$a\alpha = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j (1 - k_{ij})\sqrt{(a_i\alpha_i)(a_j\alpha_j)}$ = 2.0703

$D = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j n_j (1 - k_{ij})\sqrt{(a_i\alpha_i)a_j T_{r,j}}$ = 0.6956

$$Z^3-(1-B)Z^2+\left(A-3B^2-2B\right)Z-(AB-B^2-B^3)=0$$

By Newton – Raphson Method find the value of Z starting with Z_o = 1 for vapor.

Z = 0.53694

$$\frac{H_2^R}{RT}=Z-1-\frac{A}{2.828B}\left[1+\frac{D}{a\alpha}\right]\ln\left(\frac{Z+2.414B}{Z-0.414B}\right)$$

H_2^R= -5726.932 J/mole

$$H_{calculated}=\Delta \mathrm{H}_v - \mathrm{H}_1^{\mathrm{R}} + \Delta \mathrm{H}^{ig} + \mathrm{H}_2^{\mathrm{R}}$$

=37662.96 – 0 + 38085.42 - 5726.932

=70021.45 J/mole

The actual value of enthalpy is 69877.37 J/mole [27]

$$AD\% = abs\left|\frac{H_{actual}-\mathrm{H}_{calculated}}{H_{actual}}\right|\times 100\%$$

$$AD\% = abs\left|\frac{69877.37-70021.45}{69877.37}\right|\times 100\%$$

= 0.2062

CHAPTER FOUR

DISCUSSION OF RESULTS

4.1 Discussion

The saturated enthalpy of vapor for pure compounds and mixture are function of both temperature and pressure. The usual method available for predicting the residual enthalpy of saturated vapor for pure compounds is by using the equation of state.

In the present work the equations of state used were: Redlich–Kwong, Soave-Redlich-Kwong, Peng-Robinson, Lee-Kesler and Virial equations truncated to second and to third terms. Tables 4-1 and 4-2 indicate the AAD% of the calculated saturated enthalpy of vapor for polar and non polar compounds as compared with experimental values.

There are several equations used to calculate the enthalpy of vaporization, such as (Giacalone, Riedel, Chen and Vetere equation, …etc), and it was found that the best method (more accurate) is to calculate the enthalpy of vaporization at normal poiling point using Vetere equation and then using Watson equation to calculate the enthalpy of vaporization at the temperature of the system.

The AAD% for calculation of saturated enthalpy of vapor for 17 nonpolar compounds and 439 experimental data points are 2.1414, 7.6223, 1.5339, 2.3765, 3.324, and 2.3566 when using Redlich-Kwong, Soave Redlich–Kwong, Peng-Robinson, Lee - Kesler, Virial equation truncated to second and to third terms respectively. On the other hand the AAD% for 8 compounds and 262 experimental data points for polar compounds are

3.3096, 5.1917, 2.4484, 2.0906, 3.7008, and 2.7172 when using Redlich–Kwong, Soave Redlich–Kwong, Peng-Robinson, Lee-Kesler , Virial equation truncated to second and to third terms respectively, as shown in tables 4-1 and 4-2.

The AAD% for 25 nonpolar and polar compounds and 701 experimental data points are 2.57804, 6.7139, 1.8757, 2.2696, 3.4648, and 2.4914 when using Redlich–Kwong, Soave Redlich–Kwong, Peng-Robinson, Lee- Kesler , Virial equation truncated to second and to third terms respectively, as shown in table 3-6.

The AAD% for Methy Chloride, Nitrogen, NH_3 and Isobutene respectively as shown in tables 4-3 to 4-6, for other pure compounds see appendix C.

Figures 4-1 to 4-12 show the deviations from experimental data using the equations: Redlich-Kwong, Soave Redlich-Kwong, Peng-Robinson, Lee - Kesler and Virial equations truncated to second and to third terms, these figures are clearly indicated that Peng-Robinson equation is the best equation for the moderate conditions studied in this research, after these comparison one can conclude that the generalized Peng-Robinson equation is the most suitable equations to calculate the residual enthalpy of saturated vapor. Thus efforts were directed to modify this equation to increase its accuracy (decrease the deviation obtained from experimental data).

Table 4-1 Comparison of the calculated saturated enthalpy of vapor obtained from different equations of state for non polar compounds as compared with experimental values

	Compounds	**No. of Experimental Data Points**	**Soave AAD%**	**Virial /B AAD%**	**Redlich-Kwong AAD%**	**Virial /C AAD%**	**Lee- Kesler AA%D**	**Peng Robinson AAD%**
1	Benzene	40	5.4833	1.8905	2.7291	2.0622	2.9383	2.9825
2	Cyclopropane	15	7.8719	3.0300	1.1009	1.6200	0.6565	0.2729
3	Isobutene	29	15.0793	8.0652	3.4952	6.0119	4.2776	1.4209
4	Isopentane	27	11.4724	7.2177	3.7892	4.2134	3.4591	1.7483
5	Neopentane	32	13.0437	4.2032	1.5020	2.4782	1.4753	0.4612
6	Propane	18	5.5271	1.0177	1.3380	1.1218	1.2202	1.3368
7	n-butane	31	15.9986	7.57964	3.4417	5.0582	3.1809	1.2848
8	n-pentane	27	15.5069	3.7729	3.1863	3.18380	9.3157	4.6455
9	Ethylene	13	1.3143	1.4188	1.2008	1.4759	1.5591	1.19695
10	Trichloroethylene	14	3.5582	3.5809	3.5537	3.6574	3.5763	3.5569
11	N_2	9	5.5779	2.7544	1.5497	1.1800	0.8552	1.4829
12	SO_2	40	3.8978	1.4603	1.1021	0.8637	0.9253	0.3700
13	R13	24	7.7361	3.2038	2.0408	1.6049	0.5658	0.9587
14	R21	11	0.7999	0.9842	0.7132	1.0548	1.0118	0.7757
15	R114	36	3.7195	0.8314	0.4799	0.6533	1.3005	0.5958
16	R123	37	2.4144	1.2416	0.8940	0.8686	1.0189	0.7134
17	R134a	36	3.8742	2.8990	3.2030	2.1125	1.5244	2.3507
	$\sum$	**439**	**7.6223**	**3.324**	**2.1414**	**2.3566**	**2.3765**	**1.5339**

Table 4-2 Comparison of the calculated saturated enthalpy of vapor obtained from different equations of state for polar compounds as compared with experimental values

	Compounds	No. of Experimental Data Points	Soave AAD%	Virial /B AAD%	Redlich - Kwong AAD%	Virial /C AAD%	Lee- Kesler AAD%	Peng Robinson AAD%
1	H_2O	74	6.4828	6.0854	6.1938	5.1479	4.0998	5.1903
2	NH_3	36	6.2227	3.2046	2.4881	1.6377	1.4644	1.1886
3	R11	27	3.7507	1.8906	1.6037	1.0314	0.6218	1.0750
4	R12	36	4.96835	2.5000	1.6765	1.5659	1.1903	0.7828
5	R22	34	5.8136	3.4482	2.3545	1.8007	1.1226	1.2173
6	R32	15	7.39	4.8936	4.0159	4.0173	2.1537	2.9959
7	Ethyl Chloride	17	2.8963	2.9241	2.8339	2.8757	2.9956	2.8776
8	Methyl Chloride	23	0.8095	0.9796	1.1771	0.7575	0.4605	0.9632
	$\sum$	**262**	**5.1917**	**3.7008**	**3.3096**	**2.7172**	**2.0906**	**2.4484**

Table 4-3 Comparison of the calculated saturated enthalpy of vapor obtained from different equations of state for Methyl Chloride compound as compared with experimental values

T (K)	**P (kpa)**	**Exp. Data (kj)**	**Soave AAD%**	**Virial /B AAD%**	**R-kwong AAD%**	**Virial/C AAD%**	**Lee-Kesler AAD%**	**Peng - Robinson AAD%**	**This work AAD%**
238.706	62.301	22.5569	0.1349	0.1682	0.1282	0.3351	0.1676	0.13172	0.1268
244.261	80.738	22.7225	0.0744	0.1401	0.0592	0.3214	0.1425	0.06739	0.0580
249.817	103.146	22.8846	0.0053	0.1013	0.0205	0.3072	0.1111	0.00620	0.0194
255.372	130.312	23.0443	0.0639	0.0599	0.1028	0.2816	0.0820	0.08081	0.0966
258.150	145.825	23.1253	0.0892	0.0470	0.1357	0.2533	0.0774	0.10922	0.1259
260.928	162.717	23.2028	0.1268	0.0208	0.1817	0.2467	0.0609	0.15012	0.1671
266.483	201.052	23.3508	0.2215	0.0551	0.2958	0.2266	0.0095	0.25242	0.2686
272.039	246.007	23.4905	0.3352	0.1561	0.4327	0.1625	0.0600	0.37507	0.3880
277.595	298.200	23.6244	0.4559	0.2717	0.5810	0.0724	0.1360	0.50619	0.5131
283.150	358.461	23.7548	0.5705	0.3904	0.7282	0.0334	0.2061	0.63316	0.6309
288.706	427.478	23.8781	0.6919	0.5269	0.8878	0.1436	0.2838	0.76908	0.7542
294.261	506.147	23.9967	0.8068	0.6697	1.0475	0.2730	0.3565	0.90115	0.8701
299.817	594.745	24.1059	0.9346	0.8406	1.2273	0.4103	0.4449	1.04913	0.9980
303.150	652.938	24.1681	1.0114	0.9515	1.3391	0.5779	0.4998	1.13967	1.0747
305.372	693.617	24.2069	1.0694	1.0360	1.4220	0.6880	0.5444	1.20758	1.1326
310.928	804.623	24.3020	1.1930	1.2403	1.6152	0.7726	0.6366	1.35939	1.2571
316.483	927.351	24.3913	1.3078	1.4587	1.8099	0.9784	0.7262	1.50747	1.3744
322.039	1063.178	24.4723	1.4169	1.6979	2.0113	1.2014	0.8171	1.65631	1.4896
327.595	1212.795	24.5463	1.5116	1.9532	2.2125	1.4484	0.9023	1.79868	1.5959
333.150	1376.202	24.6120	1.5958	2.2326	2.4193	1.7150	0.9881	1.93996	1.6992
338.706	1554.088	24.6731	1.6498	2.5211	2.6146	2.0096	1.0573	2.06283	1.7825
344.261	1747.832	24.7271	1.6738	2.8265	2.8030	2.3178	1.1128	2.17092	1.8503
349.817	1957.434	24.7706	1.6783	3.1659	2.9991	2.6473	1.1692	2.27854	1.9170
			0.8095	**0.9796**	**1.1771**	**0.7575**	**0.4605**	**0.96317**	**0.8778**

Table 4-4 Comparison of the calculated saturated enthalpy of vapor obtained from different equations of state for Nitrogen compound as compared with experimental values

T (K)	**P (kpa)**	**Exp. Data (kj)**	**Soave AAD%**	**Virial /B AAD%**	**R-kwong AAD%**	**Virial/C AAD%**	**Lee- Kesler AAD%**	**Peng-Robinson AAD%**	**This work AAD%**
65	17.4279	6.1012	0.8551	0.8277	0.8517	0.7804	0.8306	0.8578	0.8567
70	38.5035	6.2329	0.9266	0.8330	0.9147	0.8203	0.8248	0.9401	0.9294
77.36	101.325	6.4066	1.0597	0.9063	1.0452	0.7958	0.8197	1.1028	1.0415
80	136.6874	6.4598	1.1424	0.9905	1.1338	0.7864	0.8514	1.2021	1.1045
90	359.8051	6.6279	1.2774	1.3535	1.3644	0.8263	0.8353	1.4523	1.0746
100	777.7707	6.7035	1.2816	2.3206	1.7306	0.9181	0.9127	1.7647	0.7865
103.95	1013.25	6.7007	1.1330	2.9705	1.8978	1.3679	0.9487	1.8753	0.5410
110	1467.186	6.6475	0.4372	4.4776	2.1827	1.7144	0.9872	2.0134	0.0652
120	2512.86	6.3337	42.0878	10.1094	2.8262	2.6107	0.6864	2.1375	2.6302
			5.5779	**2.7544**	**1.5497**	**1.1800**	**0.8552**	**1.4829**	**0.9030**

Table 4-5 Comparison of the calculated saturated enthalpy of vapor obtained from different equations of state for NH_3 compound as compared with experimental values

T (K)	P (kpa)	Exp. Data (kj)	Soave AAD%	Virial /B AAD%	R-kwong AAD%	Virial/C AAD%	Lee-Kesler AAD%	Peng-Robinson AAD%	This work AAD%
223.15	40.9	23.3768	1.2098	1.2753	1.1940	1.2831	1.2615	1.2062	1.2875
228.15	54.5	23.5164	1.1344	1.1678	1.1257	1.1722	1.1616	1.1324	1.1760
238.15	93.2	23.9115	0.4746	0.4405	0.4853	0.5101	0.4439	0.4770	0.4275
243.15	119.5	24.0342	0.4515	0.3836	0.4751	0.4348	0.3876	0.4568	0.3523
248.15	151.6	24.1500	0.4454	0.3440	0.4846	0.3708	0.3453	0.4541	0.2883
253.15	190.2	24.2624	0.4406	0.3073	0.4984	0.3222	0.3018	0.4534	0.2208
258.15	236.3	24.3680	0.4493	0.2861	0.5291	0.2745	0.2691	0.4669	0.1618
263.15	290.9	24.4684	0.4622	0.2721	0.5679	0.2397	0.2383	0.4856	0.1026
268.15	354.9	24.5621	0.4847	0.2719	0.6208	0.2092	0.2152	0.5148	0.0493
273.15	429.6	24.6490	0.5141	0.2838	0.6854	0.1894	0.1969	0.5522	0.0006
278.15	515.9	24.7290	0.5489	0.3077	0.7609	0.1778	0.1828	0.5963	0.0473
283.15	615.2	24.8023	0.5860	0.3421	0.8451	0.1741	0.1699	0.6444	0.0934
288.15	728.6	24.8687	0.6234	0.3869	0.9367	0.1761	0.1570	0.6949	0.1399
293.15	857.5	24.9249	0.6720	0.4545	1.0474	0.1832	0.1551	0.7590	0.1752
298.15	1003.2	24.9726	0.7220	0.5378	1.1685	0.2074	0.1552	0.8273	0.2080
303.15	1167	25.0117	0.7706	0.6363	1.2984	0.2406	0.1551	0.8977	0.2402

308.15	1350.4	25.0390	0.8277	0.7630	1.4485	0.2819	0.1655	0.9810	0.2608
313.15	1554.9	25.0560	0.8824	0.9107	1.6097	0.3437	0.1764	1.0671	0.2798
318.15	1782	25.0611	0.9372	1.0859	1.7865	0.4177	0.1914	1.1598	0.2935
323.15	2033.1	25.0526	0.9941	1.2957	1.9835	0.5098	0.2139	1.2628	0.2983
328.15	2310.1	25.0526	0.9567	1.4496	2.1069	0.6263	0.1500	1.2817	0.3878
333.15	2614.4	25.0305	0.9419	1.6720	2.2785	0.6764	0.1178	1.3366	0.4442
338.15	2947.8	24.9930	0.9124	1.9354	2.4666	0.7827	0.0837	1.3942	0.5010
343.15	3312	24.9402	0.8566	2.2400	2.6666	0.9170	0.0404	1.4486	0.5647
348.15	3709	24.8670	0.7790	2.6071	2.8938	1.0784	0.0013	1.5127	0.6240
353.15	4140.5	24.7733	0.6588	3.0381	3.1424	1.2866	0.0519	1.5783	0.6872
358.15	4608.6	24.6575	0.4716	3.5411	3.4111	1.5418	0.1196	1.6411	0.7594
363.15	5115.3	24.5144	0.1904	4.1399	3.7115	1.8507	0.2022	1.7086	0.8330
368.15	5662.9	24.3407	0.2544	4.8521	4.0447	2.2348	0.3118	1.7769	0.9114
373.15	6253.7	24.1312	1.0141	5.7044	4.4150	2.7094	0.4629	1.8433	0.9950
378.15	6890.4	23.8775	2.5858	6.7414	4.8339	3.2985	0.6742	1.9093	1.0785
383.15	7575.7	23.5658	47.5558	8.0361	5.3239	4.0423	0.9714	1.9831	1.1472
388.15	8313.3	23.1792	44.4161	9.6866	5.8984	5.0087	1.4301	2.0542	1.2019
393.15	9107.2	22.6802	40.9023	11.9095	6.6130	6.2873	2.1809	2.1358	1.2164
398.15	9963.5	21.9938	36.7574	15.1626	7.5465	8.0803	3.6667	2.2108	1.2009
403.15	10892	20.8970	31.1343	20.8986	8.6662	10.8163	35.7103	1.8862	1.6988
			6.2227	**3.2046**	**2.4881**	**1.6377**	**1.4644**	**1.1886**	**0.5654**

Table 4-6 Comparison of the calculated saturated enthalpy of vapor obtained from different equations of state for Isobutane compound as compared with experimental values

T (K)	P (kpa)	Exp. Data (kj)	Soave AAD%	Virial /B AAD%	R-kwong AAD%	Virial/C AAD%	Lee-Kesler AAD%	Peng Robinson AAD%	This work AAD%
270	140.842	21.9827	0.6842	0.7144	0.6357	0.7592	0.7712	0.6689	0.7077
280	199.408	22.7735	0.6083	0.6425	0.4898	0.7512	0.7881	0.5708	0.6625
290	274.996	23.5308	0.3902	0.3885	0.1823	0.5776	0.6570	0.3237	0.4773
300	370.444	24.3049	0.2690	0.1796	0.0520	0.4677	0.6120	0.1640	0.3868
310	488.995	25.0956	0.2610	0.0180	0.2027	0.4262	0.6647	0.1042	0.4010
320	633.687	25.8822	0.3026	0.1788	0.3422	0.3729	0.7445	0.0746	0.4464
330	808.067	26.6353	0.3178	0.5135	0.5604	0.2085	0.7670	0.0114	0.4328
340	1015.277	27.3843	0.4622	0.8674	0.7215	0.0529	0.8716	0.0150	0.4937
350	1260.483	28.0788	0.6364	1.4093	0.9690	0.2559	0.9327	0.0718	0.4917
360	1545.206	28.7106	0.9197	2.1681	1.2995	0.7477	0.9650	0.1732	0.4354
370	1876.539	29.2043	1.3743	3.3837	1.8872	1.6488	0.8440	0.4746	0.1787
380	2257.521	29.5098	3.1963	5.2329	2.8030	3.1289	0.5711	1.0248	0.3029
385	2468.277	29.6060	36.0868	6.3466	3.2763	4.0353	0.5310	1.2748	0.4947
390	2694.232	29.4261	32.5339	8.4582	4.5363	5.9009	0.1258	2.2537	1.3764
395	2935.385	29.5809	29.7347	9.3434	4.3529	6.5531	0.8372	1.7648	0.7478
396	2985.034	29.5641	29.0635	9.6976	4.4473	6.8554	0.9435	1.7885	0.7338

397	3035.697	29.5223	28.3322	10.1443	4.6070	7.2463	1.0159	1.8703	0.7725
398	3087.373	29.5014	27.6522	10.5124	4.6656	7.5592	1.2198	1.8475	0.7020
399	3139.049	29.4470	26.8870	11.0095	4.8289	7.9981	1.3459	1.9256	0.7278
400	3192.751	29.3926	26.1246	11.5032	4.9394	8.4301	1.6105	1.9376	0.6768
401	3245.440	29.3173	25.3019	12.0849	5.1209	8.9502	1.8225	2.0240	0.6987
402	3300.155	29.2252	24.4377	12.7289	5.2931	9.5272	2.2171	2.0826	0.6772
403	3354.871	29.1039	23.4906	13.4936	5.5320	10.2218	2.7746	2.2019	0.7082
404	3410.600	28.9575	22.4714	14.3624	5.7831	11.0156	20.2742	2.3167	0.7172
405	3467.342	28.7525	21.2851	15.4735	6.1358	12.0427	18.8516	2.5055	0.7713
406	3524.083	28.5098	19.9760	16.7571	6.4956	13.2371	17.1722	2.6908	0.8004
406.5	3553.468	28.3424	19.1858	17.5950	6.7090	14.0222	16.1592	2.7742	0.7475
407	3581.838	28.1332	18.2609	18.6233	7.0414	14.9940	14.8435	3.0123	0.8849
407.5	3611.223	27.8320	17.0527	20.0597	7.4512	16.3588	13.1171	3.2574	0.8167
			15.0793	**8.0652**	**3.4952**	**6.0119**	**4.2776**	**1.4209**	**0.6369**

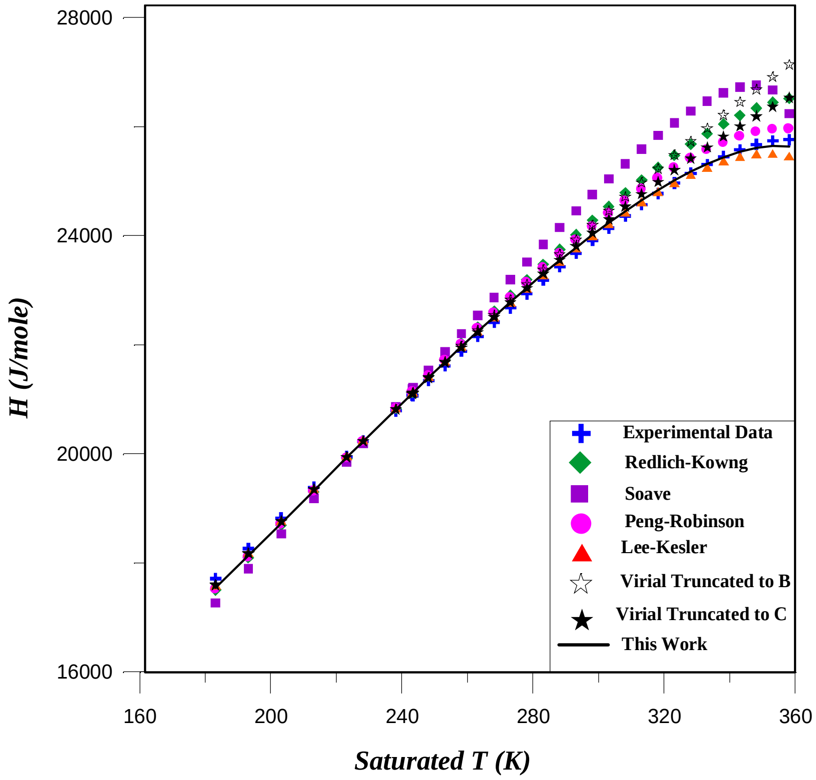

Figure 4-1 Saturated enthalpy of vapor vs. saturated temperature for R12 by using different equations of state

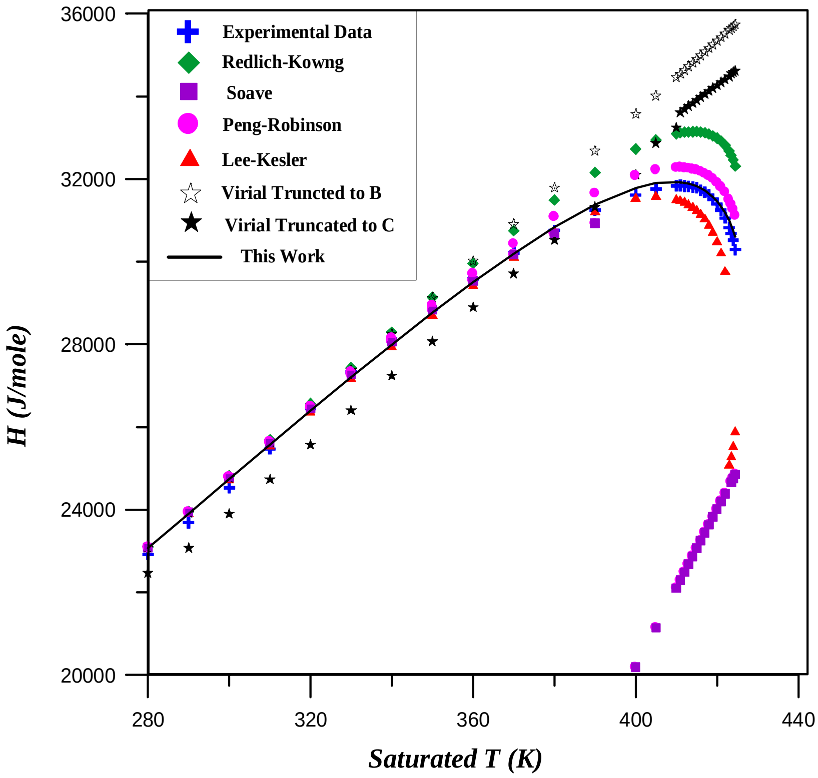

Figure 4-2 Saturated enthalpy of vapor vs. saturated temperature for n-Butane by using different equations of state

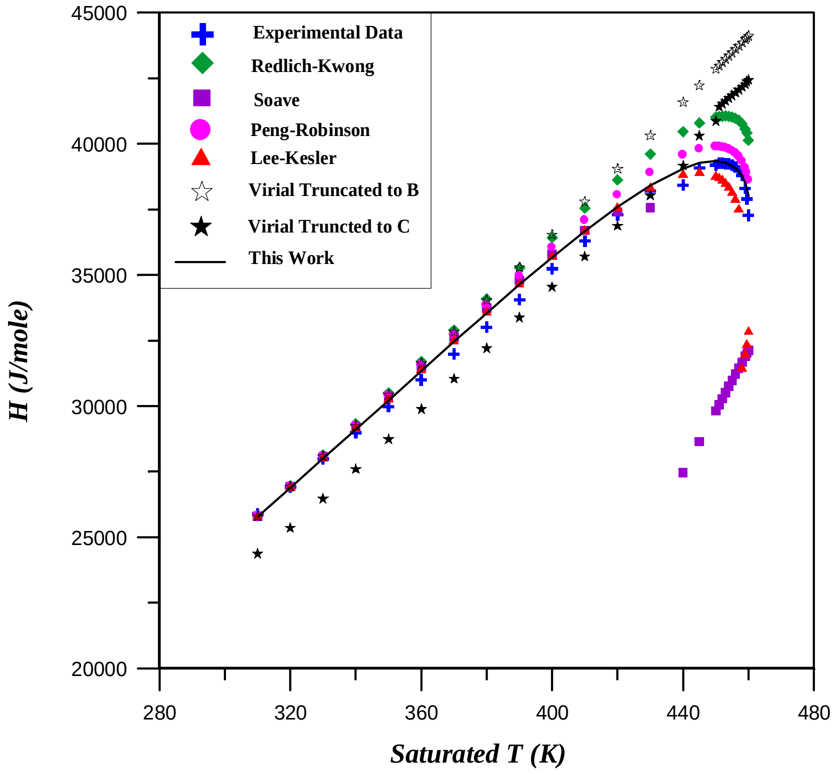

Figure 4-3 Saturated enthalpy of vapor vs. saturated temperature for Isopentane by using different equations of state

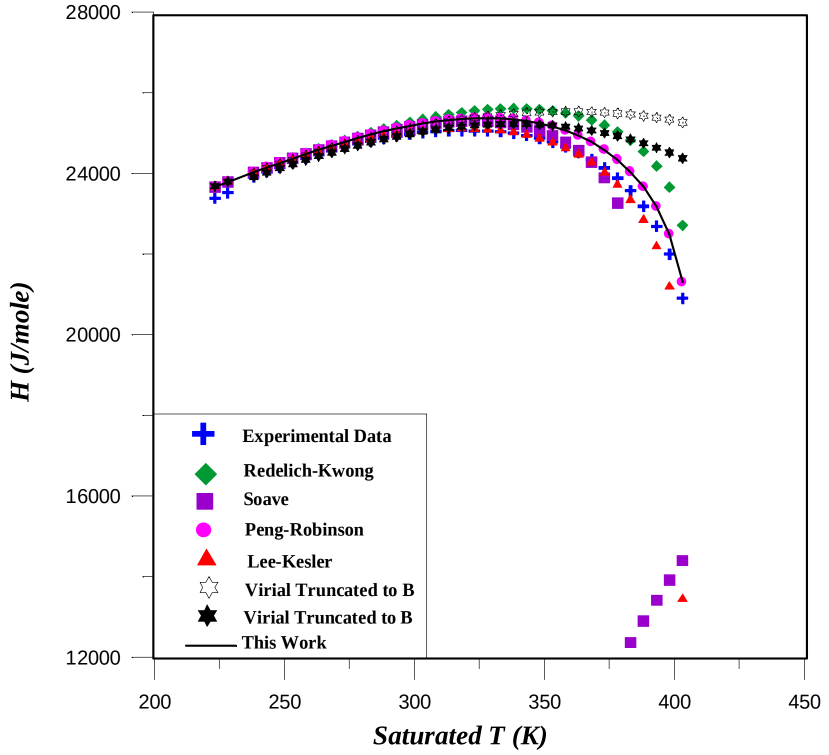

Figure 4-4 Saturated enthalpy of vapor vs. saturated temperature for NH_3 by using different equations of state

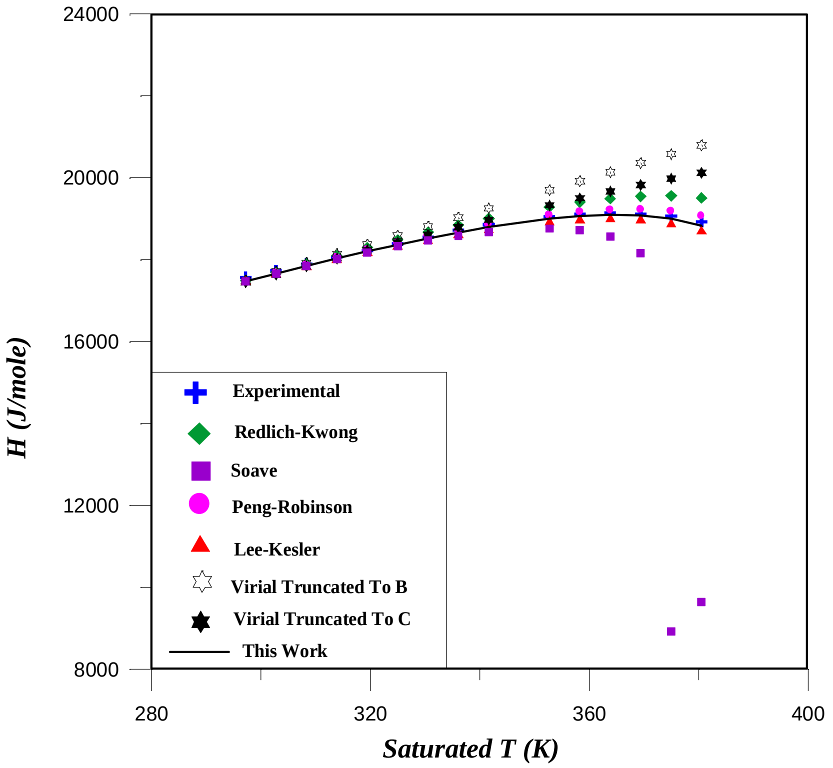

Figure 4-5 Saturated enthalpy of vapor vs. saturated temperature for Cyclopropane by using different equations of state

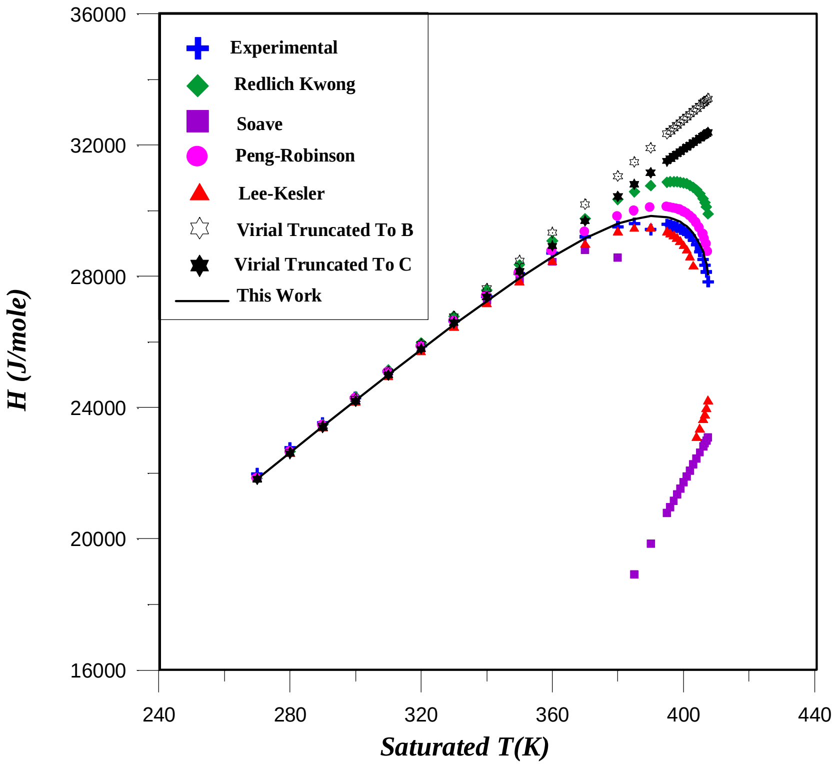

Figure 4-6 Saturated enthalpy of vapor vs. saturated temperature for Isobutane by using different equations of state

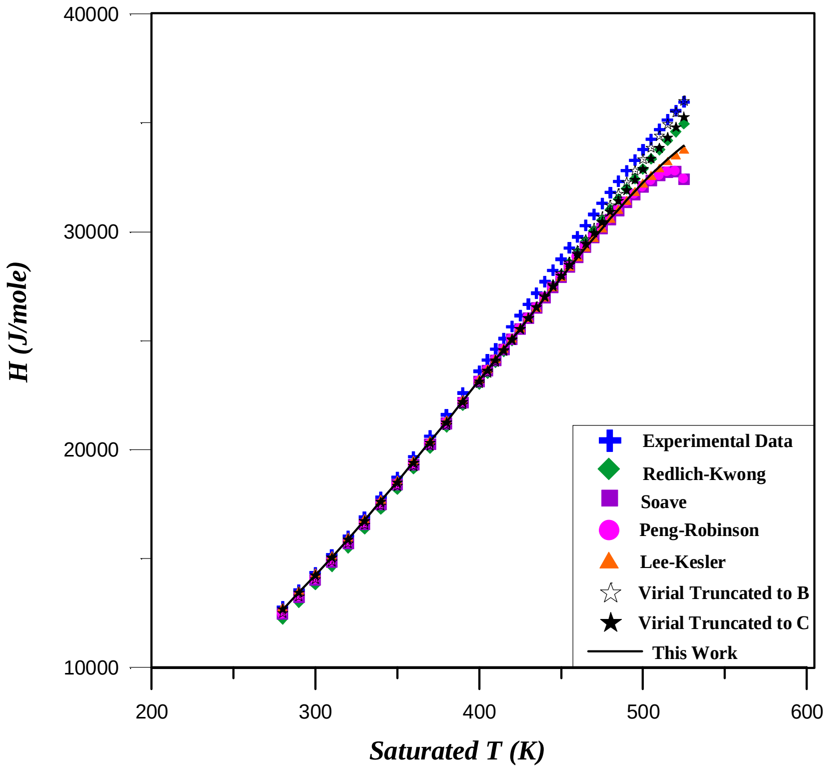

Figure 4-7 Saturated enthalpy of vapor vs. saturated temperature for Benzene by using different equations of state

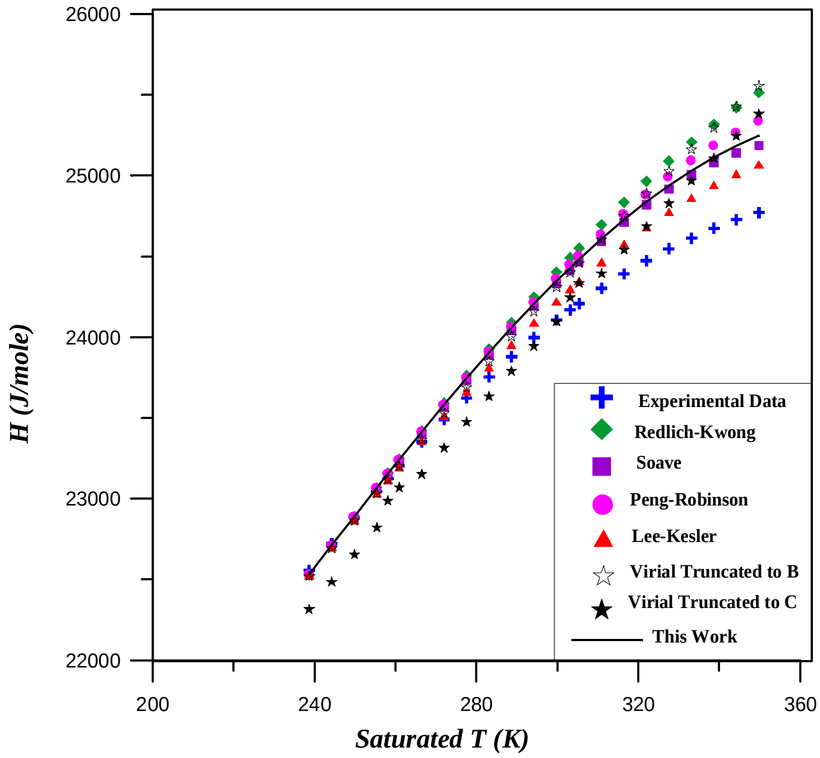

Figure 4-8 Saturated enthalpy of vapor vs. saturated temperature for Methyl Chloride by using different equations of state

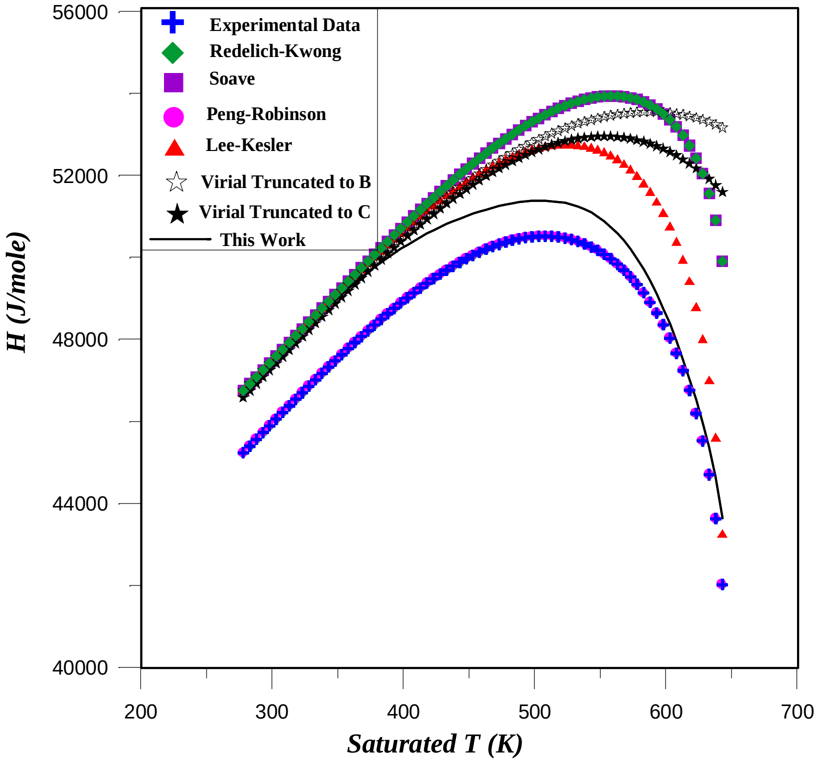

Figure 4-9 Saturated enthalpy of vapor vs. saturated temperature for water by using different equations of state

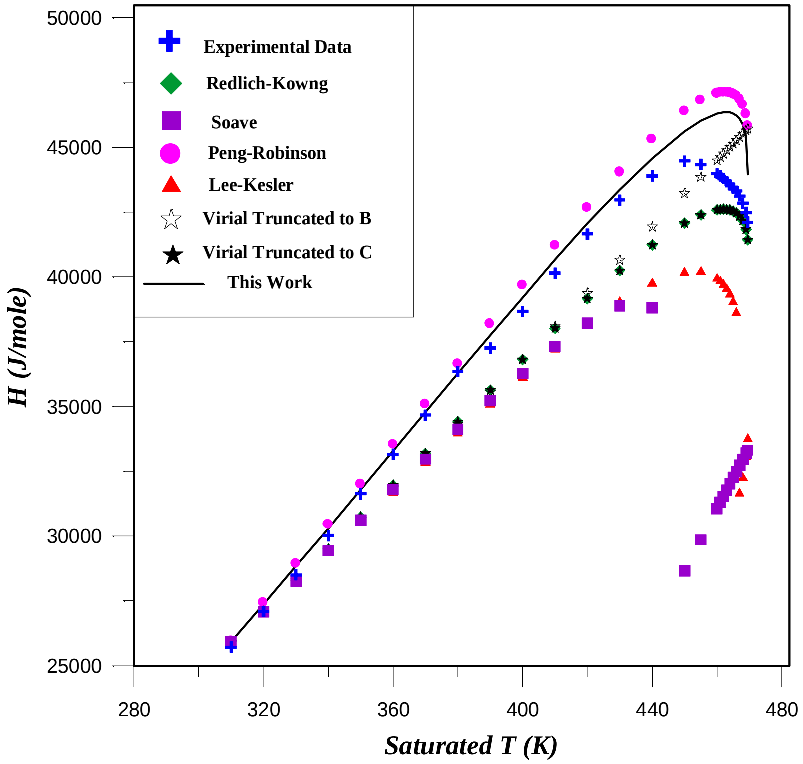

Figure 4-10 Saturated enthalpy of vapor vs. saturated temperature for n-Pentane by using different equations of state

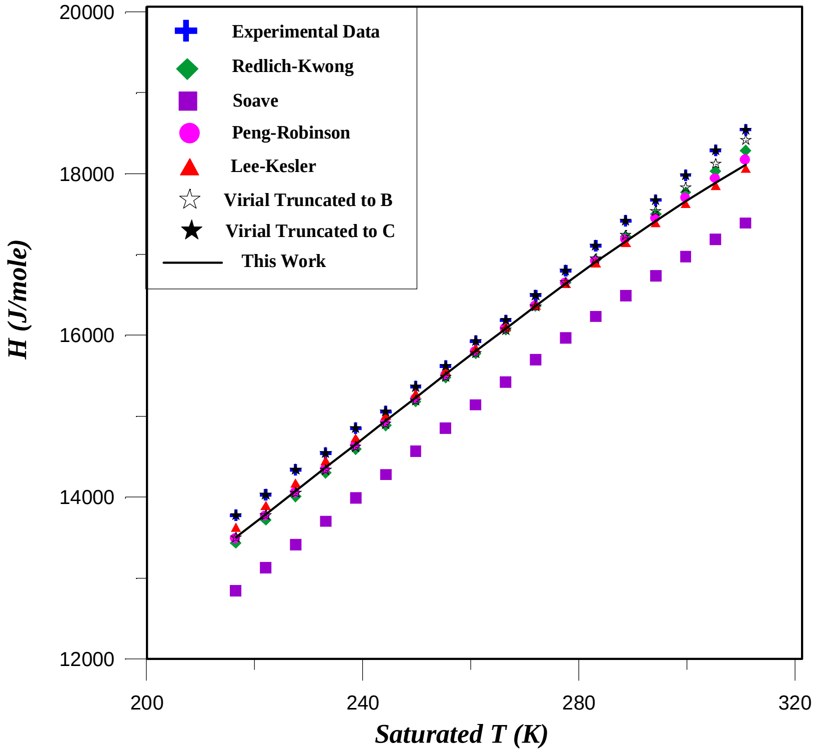

Figure 4-11 Saturated enthalpy of vapor vs. saturated temperature for Propane by using different equations of state

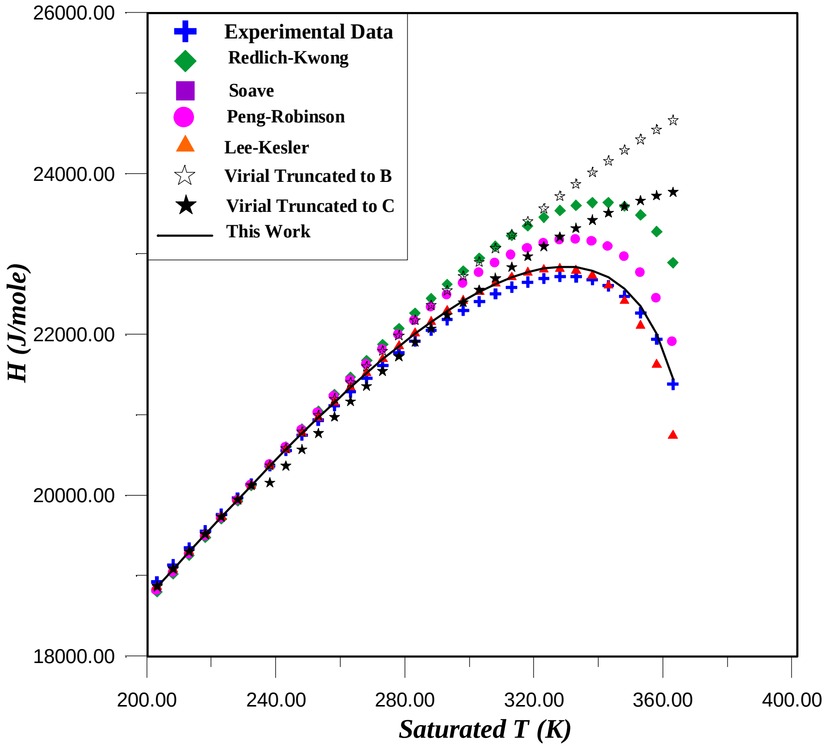

Figure 4-12 Saturated enthalpy of vapor vs. saturated temperature for R22 by using different equations of state

4.2 The Modified Correlation

After concluding that the best equation that calculates the residual enthalpy of vapor for saturation conditions (temperatures and pressures) was Peng-Robinson equation, efforts were tried to modify the Peng-Robinson equation to decrease the percent deviation as much as possible, this may done by using a statistical program and statistical methods that give the best form of the correlation.

Many attempts were made to modify this equation in order to reduce the percent deviation as much as possible, this modification was applied for 25 pure compounds (701 Exp. data points) polar and nonpolar compounds and it is reduced the AAD% from 1.5339% to 1.2569% for non polar compounds and from 2.4484 to 1.2986% for polar compounds as shown in table 4-7 and 4-8. For examples, for Isobutane the AAD% by using Peng-Robinson equation was 1.4209%, while the AAD% by using the modified Peng-Robinson equation is 0.6369%, for n-Butane the AAD% by using Peng-Robinson equation is 1.2848% while the AAD% by using the modified equation is 0.3862% and for water the AAD% by using Peng-Robinson equation is 5.1903% where the AAD% by using the modified equation is 2.1884%. Thus this modification resulted in an equation which can be considered as more accurate equation to predict the saturated enthalpy of vapor for polar and nonpolar compounds.

Table 4-7 Comparison between Peng-Robinson and modified Peng-Robinson equations for calculating saturated enthalpy of vapor for non polar compounds as compared with experimental values

	Compounds	**No. of Exp. Data Points**	**Peng- Robinson AAD %**	**Modified Peng-Robinson AAD %**
1	Benzene	40	2.9825	2.8269
2	cyclopropane	15	0.2729	0.2706
3	Isobutene	29	1.4209	0.6369
4	Isopentane	27	1.7483	0.6764
5	Neopentane	32	0.4612	0.7015
6	Propane	18	1.3368	1.3290
7	n-butane	31	1.2848	0.3862
8	n-pentane	27	4.6455	3.2392
9	Ethylene	13	1.19695	1.19153
10	Trichloroethylene	14	3.5569	3.5694
11	N_2	9	1.4829	0.9030
12	SO_2	40	0.3700	1.2102
13	R13	24	0.9587	0.4453
14	R21	11	0.7757	0.9339
15	R114	36	0.5958	1.6387
16	R123	37	0.7134	0.5101
17	R134a	36	2.3507	0.8693
	$\sum$	**439**	**1.5339**	**1.2569**

Table 4-8 Comparison between Peng-Robinson and modified Peng-Robinson equations for calculating saturated enthalpy of vapor for polar compounds as compared with experimental values

	Compounds	**No. of Exp. Data Points**	**Peng- Robinson AAD %**	**Modified Peng-Robinson AAD %**
1	H_2O	74	5.1903	2.1884
2	NH_3	36	1.1886	0.5654
3	R11	27	1.0750	0.7453
4	R12	36	0.7828	0.3891
5	R22	34	1.2173	0.6524
6	R32	15	2.9959	2.0983
7	Ethyl Chloride	17	2.8776	2.9387
8	Methyl Chloride	23	0.96317	0.8778
	$\sum$	**262**	**2.4484**	**1.2986**

4.3 The Enthalpy of Saturated Vapor for Binary Mixtures

It is well known fact that the calculation of the thermodynamic properties of the mixtures is not as easy as the calculation for pure compounds. This is because of using the mixing rules to calculate the pseudo critical properties and acentric factor of mixture depending on critical properties and acentric factors of pure compounds. Many of the mixing rules are not quite accurate and need one or more adjustable parameters.

In this work the prediction of the saturated enthalpy of vapor for binary mixtures was performed by using two methods: The first method was done by using Peng- Robinson with its mixing rules which is given by the following equations [4]:

$$A = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j (1-k_{ij})\sqrt{A_i A_j} \tag{2-83}$$

$$B = \sum_{i=1}^{n} x_i B_i \tag{2-84}$$

$$a\alpha = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j (1-k_{ij})\sqrt{(a_i\alpha_i)(a_j\alpha_j)} \tag{2-85}$$

$$b = \sum_{i=1}^{n} x_i b_i \tag{2-86}$$

$$D = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j n_j (1-k_{ij})\sqrt{(a_i\alpha_i) a_j T_{r,j}} \tag{2-87}$$

The second method was accomplished by using Peng-Robinson equation to calculate the residual enthalpy of the mixture obtained at the same reduced conditions of T_r and P_r as the mixture. The reduced conditions of the mixture were obtained by using properties and acentric factor of the mixture.

This method is similar to Teja method for calculating the residual enthalpy of the mixture from the residual enthalpy of individual compound which is given by the following equations [42]:

$$\frac{H^R}{RT_C}(T_r,P_r,\omega)=\left(\frac{H^{ig}-H}{RT_C}\right)^{(R1)}\left(T_r,P_r,\omega^{(R1)}\right)+\frac{\omega-\omega^{(R1)}}{\omega^{(R2)}-\omega^{(R1)}}$$

$$\left[\left(\frac{H^{ig}-H}{RT_C}\right)^{(R2)}\left(T_r,P_r,\omega^{(R2)}\right)-\left(\frac{H^{ig}-H}{RT_c}\right)^{(R1)}\left(T_r,P_r,\omega^{(R1)}\right)\right] \quad (2\text{-}107)$$

Where the superscripts (R1) and (R2) refer to the two nonspherical reference fluids (the two pure compounds).

Table 3-11 shows the results of deviation of saturated enthalpy of vapor for binary mixtures from experimental data using the two methods mentioned above.

The AAD% for 5 mixtures and 95 experimental data point is 2.8384% when using Peng-Robinson method with its mixing rules. For the same 5 mixtures and 95 data point the AAD% is 2.8096 when using Peng- Robinson equation with Teja method. On the other hand the AAD% for the modified Peng- Robinson mixing rule is 2.0362%.

The AAD% for the binary mixture Benzene- n-Pentane as shown in tables 4-9 to 4-12, for other binary mixture components see appendix D.

Figures 4-13 to 4-20 show the deviation of the calculated enthalpy of saturated vapor for Benzene - n-Pentane system and Benzene - Cyclohexane system by using Peng - Robinson equation with its mixing rules, Teja equation with Peng - Robinson for pure compounds and modified Peng - Robinson with its mixing rules.

Table 4-9 Calculation of enthalpy deviations for mixture of 60.01 mole % Benzene & 39.999 mole % n-Pentane

T (K)	**P (kpa)**	**Exp. Data**	**Peng-Robinson mixing rules AAD%**	**Peng-Robinson with Teja AAD%**	**This work AAD%**
452.206	1378.960	65.6850	0.6998	1.5777	0.8684
479.872	2068.440	68.6619	0.4313	1.6451	0.7107
495.761	2757.920	69.6307	0.1174	1.6081	0.3647
509.539	3447.400	69.8773	1.1038	1.3686	0.2062
515.872	3861.088	68.9614	2.5947	0.9117	0.9617
517.483	3998.984	68.0806	3.7578	0.7271	1.3482
			1.4508	**1.3064**	**0.7433**

Table 4-10 Calculation of enthalpy deviations for mixture of 81.429 mole % Benzene & 18.571 mole % n- Pentane

T (K)	**P (kpa)**	**Exp. Data**	**Peng-Robinson mixing rules AAD%**	**Peng-Robinson with Teja AAD%**	**This work AAD%**
464.095	1378.960	66.4167	2.2960	2.2718	1.5975
491.650	2068.440	69.1034	2.1763	2.1394	1.2332
510.539	2757.920	70.6976	2.3083	2.2541	1.0970
525.039	3447.400	71.6111	2.6600	2.5784	1.1360
532.317	3861.088	71.3245	2.3265	2.2163	0.5626
536.483	4136.880	71.1633	2.6311	2.4863	0.6616
540.372	4412.672	70.0349	2.3870	2.1623	0.1602
			2.3979	**2.3012**	**0.9212**

Table 4-11 Calculation of enthalpy deviations for mixture of 40.6706 mole % Benzene & 59.3294 mole % n-Pentane

T (K)	P (kpa)	Exp. Data	Peng-Robinson mixing rules AAD%	Peng-Robinson with Teja AAD%	This work AAD%
440.650	1378.960	64.3899	0.6599	0.6016	0.1497
466.483	2068.440	67.2694	0.9979	0.9055	0.0971
483.150	2757.920	68.4836	1.1987	1.0473	0.2569
502.317	3861.088	66.6276	5.0193	0.5876	2.3074
			1.9689	0.7855	0.7028

Table 4-12 Calculation of enthalpy deviations for mixture of 19.903 mole % Benzene & 80.0965 mole % n-Pentane

T (K)	P (kpa)	Exp. Data	Peng-Robinson mixing rules AAD%	Peng-Robinson with Teja AAD%	This work AAD%
427.594	1378.960	62.7748	0.0887	0.1912	0.9956
452.428	2068.440	65.2995	0.0260	0.1996	1.2818
468.483	2757.920	66.2206	0.1888	0.1423	1.5621
481.983	3447.400	66.0159	1.2546	0.0011	1.3983
			0.3895	0.1335	1.3094

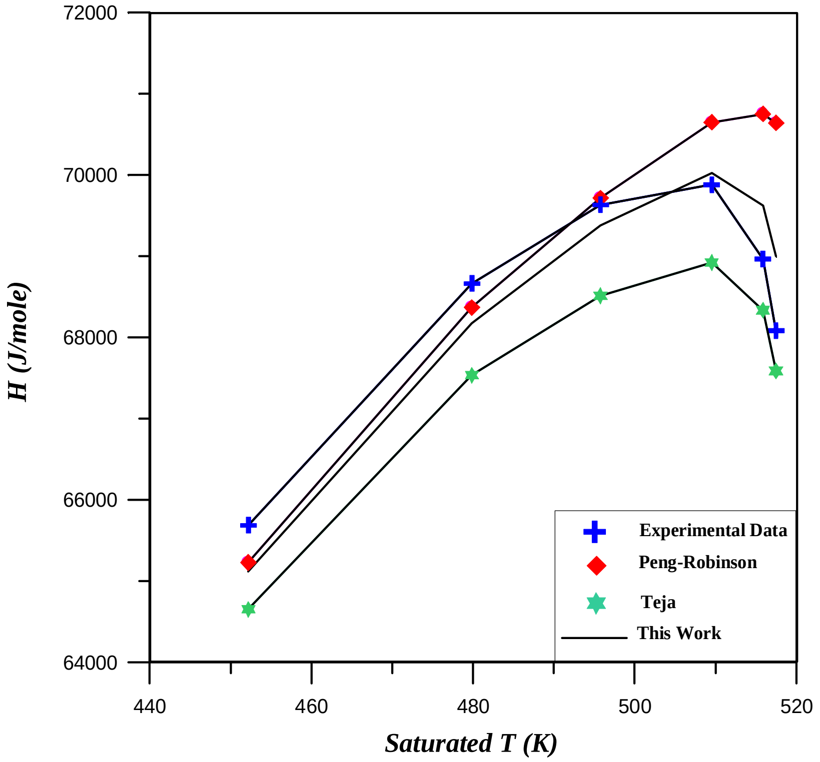

Figure 4-13 Saturated enthalpy of vapor vs. saturated temperature of mixture of 60.01 mole % Benzene and 39.999 mole % of n-Pentane

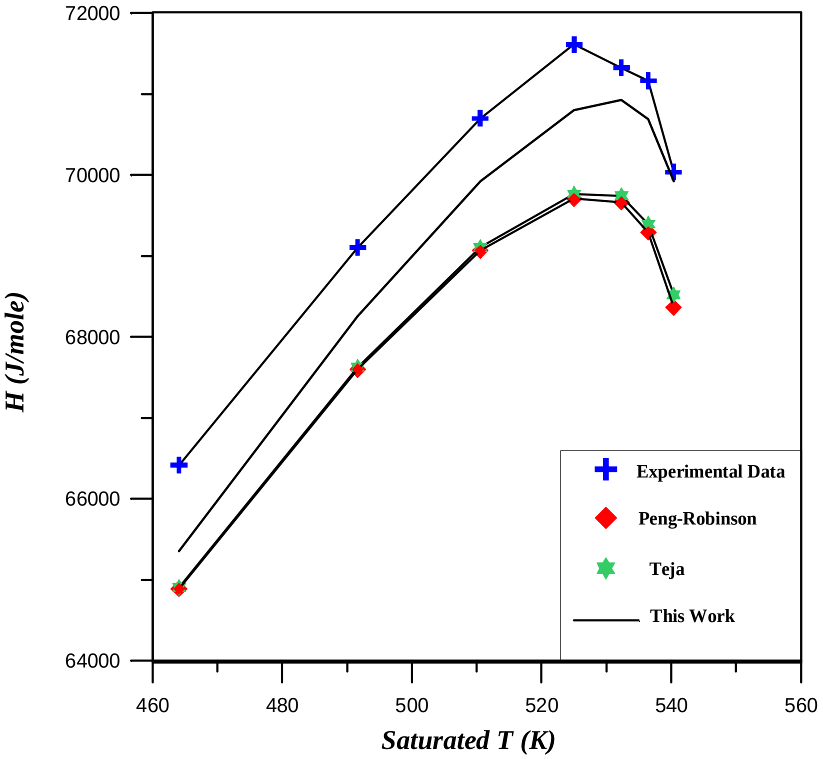

Figure 4-14 Saturated enthalpy of vapor vs. saturated temperature of mixture of 81.429 mole % Benzene and 18.571 mole % of n-Pentane

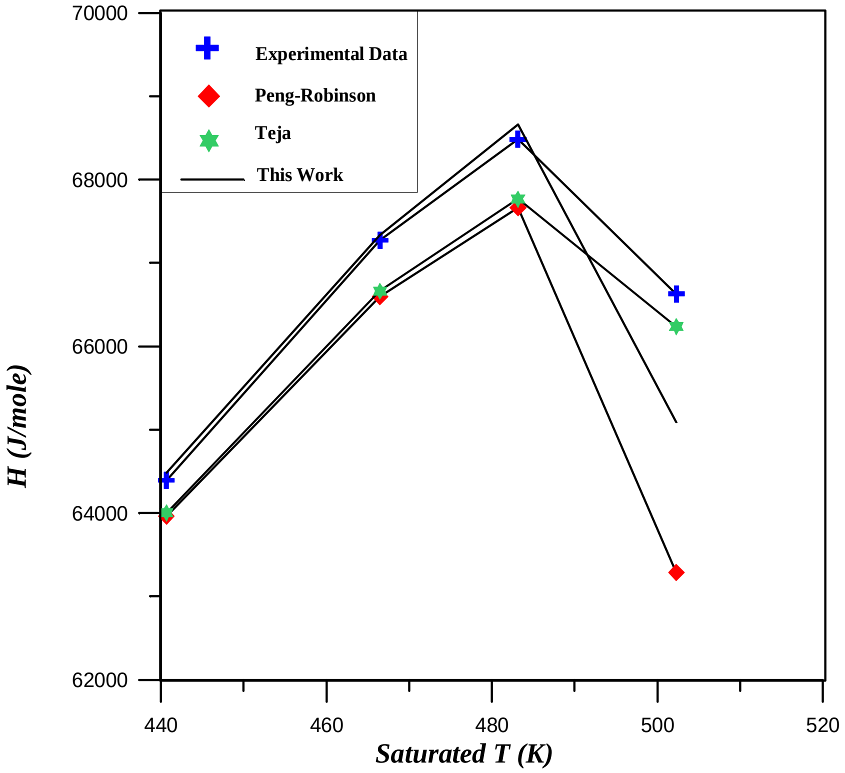

Figure 4-15 Saturated enthalpy of vapor vs. saturated temperature of mixture of 40.6706 mole % Benzene and 59.3294 mole % of n-Pentane

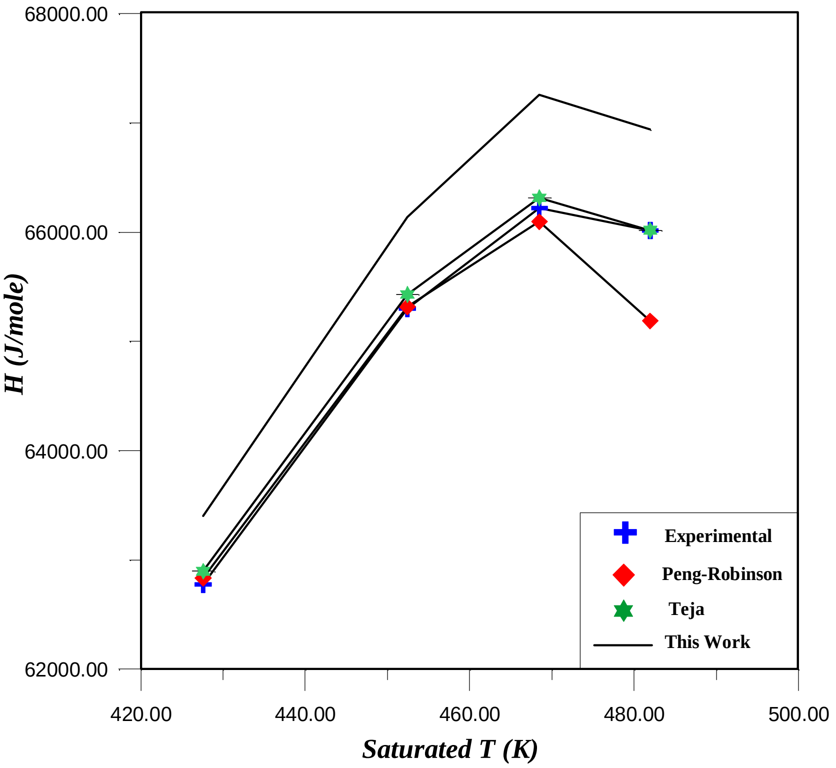

Figure 4-16 Saturated enthalpy of vapor vs. saturated temperature of mixture of 19.903 mole % Benzene and 80.0965 mole % of n-Pentane

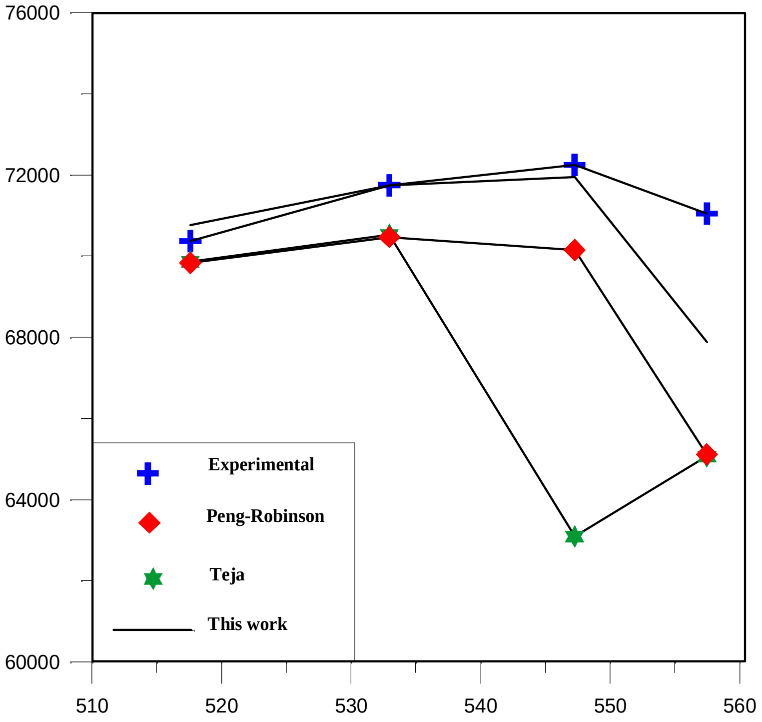

Figure 4-17 Saturated enthalpy of vapor vs. saturated temperature of mixture of 81.1668 mole % Benzene and 18.8336 mole % of Cyclohexane

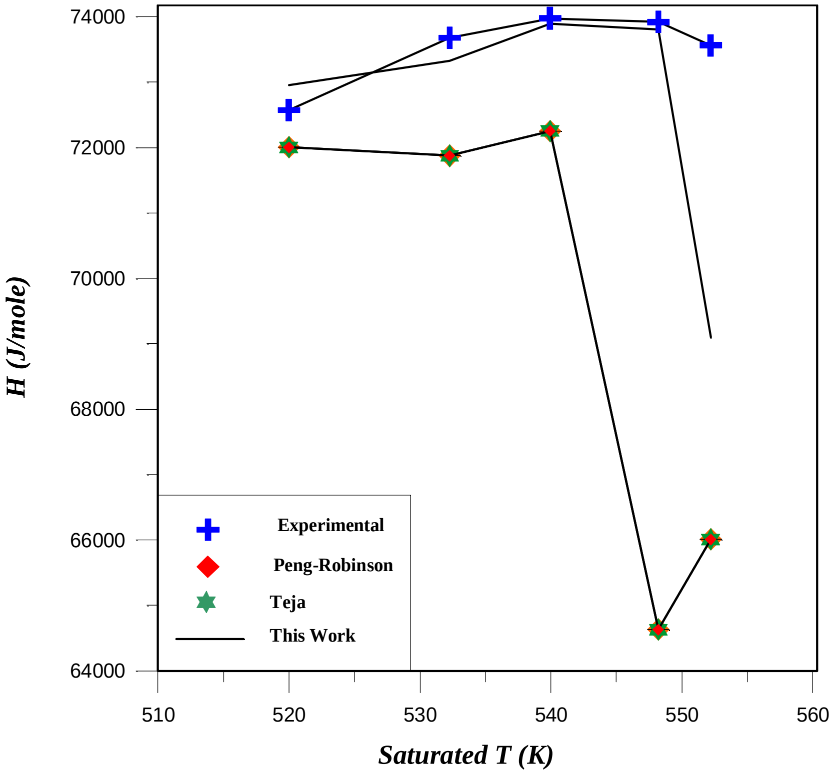

Figure 4-18 Saturated enthalpy of vapor vs. saturated temperature of mixture of 61.2833 mole % Benzene and 38.7167 mole % of Cyclohexane

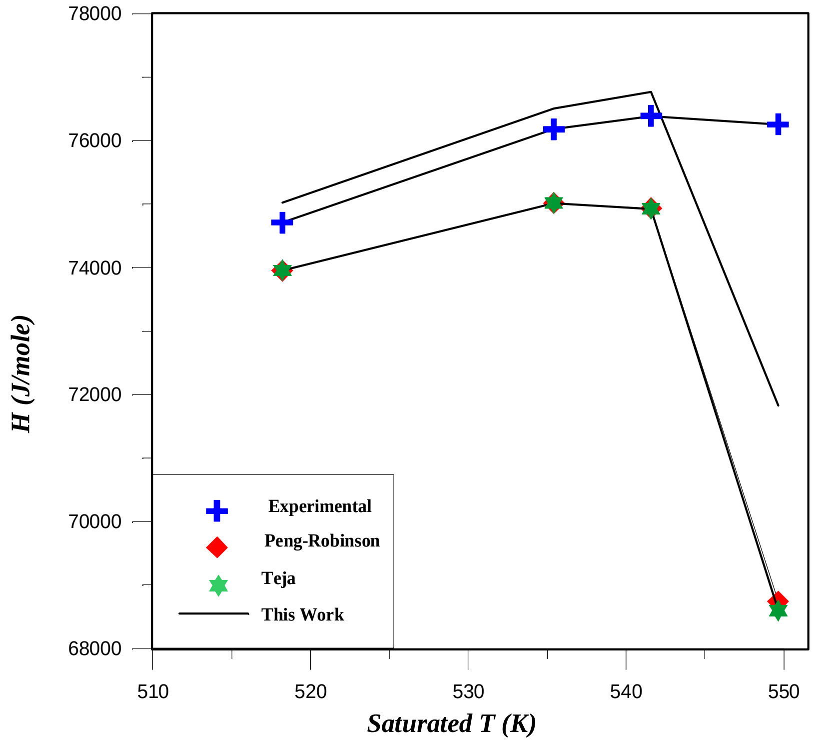

Figure 4-19 Saturated enthalpy of vapor vs. saturated temperature of mixture of 33.33592 mole % Benzene and 66.6641 mole % of Cyclohexane

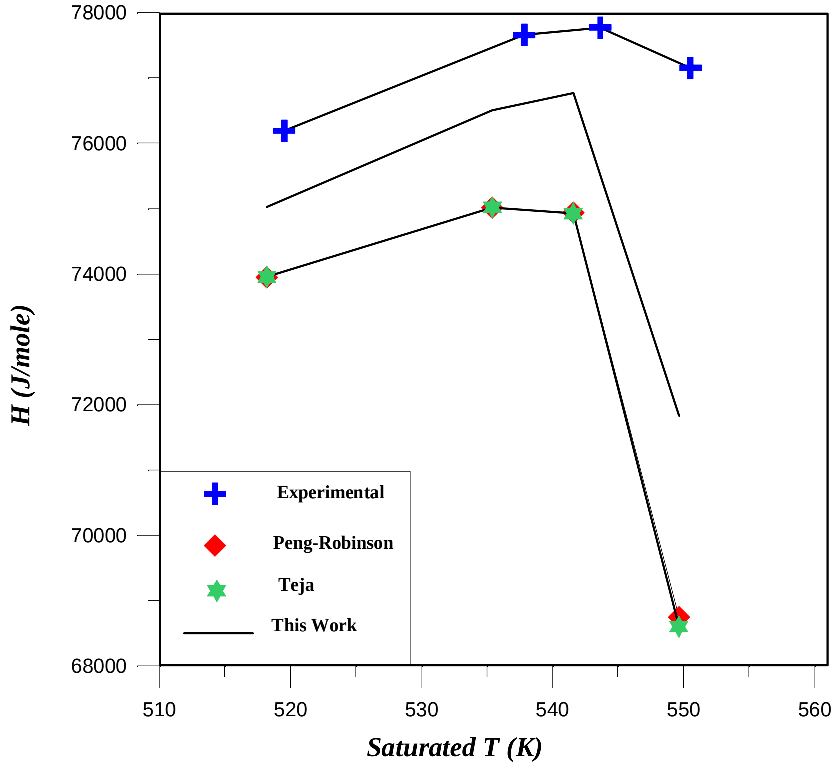

Figure 4-20 Saturated enthalpy of Vapor vs. saturated temperature of mixture of 21.11523 mole % Benzene and 78.8847 mole % of Cyclohexane

CHAPTER FIVE

CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

1. Five equations of state were used to calculate the residual enthalpy of saturated vapor for pure compounds (polar and non polar). The AAD% for 17 nonpolar compounds and 439 experimental data points are 2.1414, 7.6223, 1.5339, 2.3765, 3.324, and 2.3566% when using Redlich–Kwong, Soave Redlich–Kwong, Peng-Robinson, Lee - Kesler, Virial equation truncated to second and to third terms respectively.
2. The AAD% for 8 compounds and 262 experimental data points for polar compounds are 3.3096, 5.1917, 2.4484, 2.0906, 3.7008, and 2.7172% when using Redlich–Kwong, Soave Redlich–Kwong, Peng-Robinson, Lee - Kesler, Virial equation truncated to second and to third terms respectively.
3. The AAD% for 25 nonpolar and polar compounds and 701 experimental data points are 2.57804, 6.7139, 1.8757, 2.2696, 3.4648, and 2.4914% when using Redlich–Kwong, Soave Redlich–Kwong, Peng-Robinson, Lee - Kesler, Virial equation truncated to second and to third terms respectively.
4. Peng-Robinson equation is the most suitable equations to calculate the residual enthalpy of saturated vapor. For pure compounds, a new modified correlation was proposed to predict the enthalpy of saturated vapor. The modification was made by redefining the parameter n as function of reduced temperature, pressure and acentric factor by using statistical program. The correlation is given as the following equations:

$$n = a_A + b_A \times \omega + c_A \times \omega^2$$

$a_A = 0.941018$

$b_A = -85.7291 \times \mathrm{T_r} + 105.6393 \times \mathrm{T_r}^2 + 4.303806 \times \mathrm{P_r} - 50.0757 \times \mathrm{T_r} \times \mathrm{P_r} + 22.98768 \times \mathrm{P_r}^2$

$c_A = 433.376 \times \mathrm{T_r} - 530.876 \times \mathrm{T_r}^2 - 35.3057 \times \mathrm{P_r} + 252.0676 \times \mathrm{T_r} \times \mathrm{P_r} - 108.396 \times \mathrm{P_r}^2$

This new modification was compared with Peng-Robinson equation, the AAD% for 25 nonpolar and polar compounds and 701 experimental data points are 1.2725 while it is 1.8757 for Peng-Robinson equation without modification.

5. The effect on temperature appear clearly on Soave Redlich–Kwong equation, it was found that the AAD% of saturated enthalpy of vapor at T_r below 0.87 was better than the enthalpy of saturated vapor at T_r above 0.87.
6. For 95 experimental data points (5 mixtures) the AAD% of the Peng-Robinson with mixing rules is 2.8384%. While the AAD% of Peng-Robinson equation with Teja method based on Peng-Robinson for pure compounds is 2.8096%.
7. For 95 experimental data points (5 mixtures) the AAD% for the modified Peng- Robinson with its mixing rules is 2.0362%.
8. The modified Peng-Robinson equation with its mixing rules (this work) is the best equation for predicting the enthalpy of saturated vapor for binary mixture. The correlation is given as the following equations:

$$n = a_A + b_A\omega + c_A\omega^2$$

$a_A = 0.3704$

$b_A = 0.01267 - 0.20093 \times T_r + 0.1 \times P_r$

$c_A = -0.9048 + 0.945147 \times T_r - 0.17167 \times P_r$

5.2 Recommendations

For those who would carry future studies on related subject, the following recommendations may be considered:

1. Applying this method to saturated liquid enthalpy.
2. Appling these correlations to other thermodynamic properties like Gibbes free energy for saturated condition and entropy of pure and mixture of saturated vapor and liquid.
3. Investigating the possibility of applying this method to ternary vapor mixture and liquid mixture.
4. Investigating the possibility of applying this method to polar mixture.

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APPENDIX A

PHYSICAL PROPERTIES FOR PURE COMPOUNDS

Compound	**M.wt**	**T_b (k)**	**T_c (k)**	**P_c (bar)**	***?á***	**Z_c**	**V_c (cm^3/mole)**
Benzene	78.114	353.2	562.2	48.9	0.212	0.271	259.0
Cyclopropane	42.081	240.3	397.8	54.9	0.130	0.274	163.0
Isobutene	58.124	261.4	408.2	36.5	0.183	0.283	263.0
Isopentane	72.151	3010	460.4	33.9	0.227	0.271	306.0
Neopentane	72.151	282.6	433.8	32.0	0.197	0.269	303.0
Propane	44.094	231.1	369.8	42.5	0.153	0.281	203.0
n-butane	58.124	272.7	425.2	38.0	0.199	0.274	255.0
n-pentane	72.151	309.2	469.7	33.7	0.251	0.263	304.0
Ethylene	28.054	169.3	282.4	50.4	0.089	0.280	130.4
Ethyl Chloride	64.515	285.5	460.4	52.7	0.191	0.272	199.0
Methyl Chloride	50.488	249.1	416.3	67.0	0.153	0.269	138.9
Trichloroethylene	131.389	360.4	572.0	50.5	0.213	0.265	256.0
N_2	28.013	77.4	126.2	33.9	0.039	0.290	89.8
SO_2	64.063	263.2	430.8	78.8	0.256	0.269	122.2
H_2O	18.015	373.2	647.3	221.2	0.344	0.235	57.1
NH_3	17.031	239.8	405.5	113.5	0.250	0.244	72.5
trans-Decalin	138.254	460.5	687.1	31.4	0.303	0.272	480.0
Cyclohexane	84.162	353.8	553.5	40.7	0.212	0.273	308.0
R11	137.368	296.9	471.2	44.1	0.189	0.279	247.8
R12	120.914	245.2	385.0	41.4	0.204	0.280	216.7
R13	104.459	193.2	302.0	38.7	0.189	0.278	180.4
R21	102.923	282.1	451.6	51.8	0.210	0.271	196.4
R22	86.469	232.4	396.3	49.7	0.221	0.268	165.6
R32	52.023	221.5	351.6	58.3	0.271	0.241	120.8
R114	170.922	277.0	418.6	33.0	0.263	0.279	294.2
R123	152.931	301.0	456.94	3.674	0.282	0.243	278.1
R134a	102.031	247.0	374.21	4.056	0.326	0.251	198.1

APPENDIX B

COMPUTER PROGRAM FOR CALCULATING THE SATURATED ENTHALPY OF VAPOR FOR PURE COMPOUNDS

This program in QBASIC Language:

```
CLS
REM "*****************************************************"
REM "Computer Program for Calculation of the Saturated Enthalpy of Vapor for R12 Using Equation of State"
REM "****************************************************"

REM"******************************************************"
REM "Step (1): Calculation of the Enthalpy of Evaporation Using Vetere Method"
REM"******************************************************"
READ R, Tc, Pc, w, Tb, Pb, T, P
DATA 8.314, 385.15, 4116800, 0.204, 243.35, 101325,233.15,64200
Trb = Tb / Tc: Prb = Pb / Tc
Tr = T / Tc: Pr = P / Pc
Hvb= = R * Tc * Trb * (((0.4343 * LOG (Pc / 100000)) - 0.69431 + (0.89584 * Trb)) / (0.37691 - (0.37306 * Trb) + (0.1507 * (Pc / 100000) ^ -1 * Trb ^ -2)))
u = (0.00264 * (Hvb / (R   * Tb)) + 0.8794) ^ 10
Hv = Hvb * ((1 - Tr) / (1 - Trb)) ^ u
```

```
REM"*********************************************************"
REM "Step (2): Calculation of the Residual Enthalpy at Reference
Temperature and Pressure"
REM"*********************************************************"
af = 0.941018:b1 = -85.7291:b2 = 105.6393:b3 = 4.303806:b4 = -50.0757 :
b5 = 22.98768 :c1 = 433.376:c2 = -530.876:c3 = -35.3057:c4 = 252.0676
c5 = -108.396
n = af + (b1 * Tr * w) + (b2 * Tr ^ 2 * w) + (b3 * Pr * w) + (b4 * Tr * Pr
* w) + (b5 * Pr ^ 2 * w) + (c1 * Tr * w ^ 2) + (c2 * Tr ^ 2 * w ^ 2) + (c3
* Pr * w ^ 2) + (c4 * Tr * Pr * w ^ 2) + (c5 * Pr ^ 2 * w ^ 2)
g = 0.45724 * ((R * Tc) ^ 2) / Pc
m = (1 + (n * (1 - Tr ^ 0.5))) ^ 2
A = 0.45724 * m * (Pr / Tr ^ 2)
B = 0.0778 * (Pr / Tr)
D = n * g * m * (Tr / m) ^0.5

REM"*********************************************************"
REM "Calculation of Compressibility Factor"
REM"*********************************************************"
Z = 1
5 F1 = Z ^ 3 - (1 - B) * Z ^ 2 + (A - 3 * B ^ 2 - 2 * B) * Z - (A * B - B ^ 2- B^3)
dF1 = 3 * Z ^ 2 - 2 * (1 - B) * Z + (A - 3 * B ^ 2 - 2 * B)
Z1 = Z - (F1 / dF1)
IF ABS (Z1 - Z) >= 0.000000001 THEN Z = Z1: GOTO 5
Z = Z1
HR = R * T * (Z1 - 1 - ((A / (2.828 * B)) * (1 + (D / (g * m))) * LOG ((Z1 +
(2.414 * B)) / (Z1 - (0.414 * B)))))
```

```
REM"*******************************************************"
REM "Step (3): Calculation of the Heat Capacity at Constant Pressure"
REM"*******************************************************"
Cp (I) = ((31.6 * (T (I) - 233.15)) + ((0.1782 / 2) * (T (I) ^ 2 - 233.15 ^ 2))
+ ((-0.0001509 / 3) * (T (I) ^ 3 - 233.15 ^ 3)) + ((0.000000043 / 4) * (T (I) ^ 4
- 233.15^ 4)))

REM"*******************************************************"
REM "Step (4): HR=0 Because Pressure Has No Effect on Enthalpy of Ideal
Gas"
REM"*******************************************************"

REM"*******************************************************"
REM "Step (5): Calculation of the Residual Enthalpy at System Temperature
and Pressure"
REM"*******************************************************"
READ R, Tc, Pc, w
DATA 8.314, 385.15, 4116800, 0.204
FOR I = 1 TO 1
READ T (I), P (I), H (I)
DATA 183.15,2800, 17709.06444
Tr (I) = T(I) / Tc: Pr(I) = P(I) / Pc
g (I) = 0.45724 * ((R * Tc) ^ 2) / Pc
n (I) = af + (b1 * Tr(I) * w) + (b2 * Tr(I) ^ 2 * w) + (b3 * Pr(I) * w) + (b4
* Tr(I) * Pr(I) * w) + (b5 * Pr(I) ^ 2 * w) + (c1 * Tr(I) * w ^ 2) + (c2 * Tr
(I) ^ 2 * w ^ 2) + (c3 * Pr (I) * w ^ 2) + (c4 * Tr (I) * Pr (I) * w ^ 2) + (c5
* Pr (I) ^ 2 * w ^ 2)
m (I) = (1 + (n (I) * (1 - Tr(I) ^ 0.5))) ^ 2
A (I) = 0.45724 * m (I) * (Pr (I) / (Tr (I)) ^ 2)
```

```
B (I) = 0.0778 * (Pr (I) / Tr(I))
D (I) = n (I) * (g (I) * m (I)) * (Tr (I) / m (I)) ^0 .5

REM"*******************************************************"
REM "Calculation of Compressibility Factor"
REM"*******************************************************"
Z = 1
10 F (I) = Z ^ 3 - (1 - B (I)) * Z ^ 2 + (A (I) - 3 * B (I) ^ 2 - 2 * B (I)) * Z-
(A (I) * B (I) - B (I) ^ 2 - B (I) ^ 3)
DF (I) = 3 * Z ^ 2 - 2 * (1 - B (I)) * Z + (A (I) - 3 * B (I) ^ 2 - 2 * B (I))
Z1 = Z - (F(I) / DF (I))
IF ABS (Z1 - Z) >= 0. 000000001 THEN Z = Z1: GOTO 10
Z1 (I) = Z
HR(I) = R * T(I) * (Z1(I) - 1 - ((A(I) / (2.828 * B(I))) * (1 + (D(I) / (g(I)*
m(I)))) * LOG((Z1(I) + (2.414 * B(I))) / (Z1(I) - (0.414 * B(I))))))

REM"*******************************************************"
REM "Calculation of Actual Enthalpy of Saturated Vapor"
REM"*******************************************************"
Hact(I) = (Hv - HR + Cp(I) + HR(I))
AD% (I) = ABS ((H (I) - Hact(I)) / H(I)) * 100
NEXT I

REM"******************************************"
REM "Print of Computer Program Results"
REM "****************************************"
PRINT "T= "; T, "P="; P, "AD% (I) ="; AD% (I)
End
```

APPENDIX C

RESULTS FOR SATURATED ENTHALPY OF VAPOR FOR PURE COMPOUNDS

T = Temperature, Kelvin
P = Pressure, kpa
AAD% = Average Absolute Deviations Percent for Saturated Enthalpy of Vapor
Exp.Data= Experimental Data, kj/mole

Table C-1: Benzene [51]

T	P	Exp. Data	Soave AAD %	Virial /B AAD%	R-kwong AAD%	Virial /C AAD%	Lee-Kesler AAD%	Peng-Robinson AAD%	This Work AAD%
280	5.3	127.716	2.5391	2.2330	4.2856	0.8651	0.5493	3.0536	0.8942
290	8.8	135.449	2.3944	2.1892	4.0337	0.9035	0.5658	2.8770	0.8673
300	13.9	143.417	2.2312	2.1250	3.7688	0.9168	0.5609	2.6836	0.8194
310	21.5	151.697	2.1182	2.1133	3.5567	0.9806	0.6079	2.5413	0.8228
320	32.2	160.211	2.0097	2.1018	3.3514	1.0430	0.6583	2.4044	0.8310
330	46.7	168.960	1.9145	2.0946	3.1603	1.1090	0.7194	2.2813	0.8527
340	66.2	178.021	1.8888	2.1488	3.0371	1.2382	0.8495	2.2276	0.9460
350	91.7	187.239	1.8511	2.1786	2.9001	1.3451	0.9642	2.1617	1.0278
360	124.3	196.612	1.8135	2.1924	2.7599	1.4393	1.0742	2.0953	1.1093
370	165.4	206.221	1.8260	2.2378	2.6644	1.5703	1.2294	2.0776	1.2406
380	216.4	215.985	1.8583	2.2807	2.5819	1.7051	1.3977	2.0777	1.3895
390	278.6	225.905	1.9178	2.3242	2.5184	1.8477	1.5847	2.1025	1.5616
400	353.6	235.982	2.0140	2.3735	2.4812	2.0047	1.7985	2.1602	1.7644
405	396.3	241.059	2.0695	2.3926	2.4657	2.0809	1.9084	2.1948	1.8700
410	442.8	246.137	2.1221	2.3991	2.4437	2.1470	2.0122	2.2249	1.9702
415	493.2	250.902	2.0508	2.2718	2.2947	2.0815	1.9885	2.1297	1.9434
420	547.9	256.370	2.2546	2.4079	2.4158	2.2828	2.2368	2.3075	2.1890
425	606.9	261.525	2.3370	2.4109	2.4114	2.3535	2.3596	2.3618	2.3091
430	670.4	266.681	2.4218	2.4034	2.4045	2.4163	2.4803	2.4160	2.4273
435	738.8	271.836	2.5125	2.3877	2.3978	2.4742	2.6026	2.4730	2.5468
440	812.1	277.070	2.6368	2.3906	2.4186	2.5534	2.7532	2.5603	2.6942
445	890.6	282.225	2.7421	2.3578	2.4135	2.6001	2.8794	2.6245	2.8165
450	974.6	287.381	2.8593	2.3186	2.4122	2.6439	3.0116	2.6957	2.9437
455	1064	292.536	2.9883	2.2716	2.4143	2.6827	3.1484	2.7732	3.0745
460	1160	297.692	3.1395	2.2233	2.4269	2.7248	3.3009	2.8657	3.2189
465	1261	302.848	3.3012	2.1634	2.4405	2.7568	3.4539	2.9615	3.3625
470	1369	307.925	3.4668	2.0777	2.4426	2.7680	3.6016	3.0507	3.4981
475	1484	313.002	3.6639	1.9908	2.4590	2.7823	3.7694	3.1589	3.6507
480	1606	318.002	3.8720	1.8774	2.4660	2.7744	3.9340	3.2628	3.7968

485	1734	323.079	4.1343	1.7805	2.5065	2.7846	4.1347	3.4035	3.9755
490	1870	328.000	4.4040	1.6377	2.5223	2.7544	4.3212	3.5262	4.1349
495	2014	332.843	4.7146	1.4728	2.5395	2.7070	4.5201	3.6569	4.3008
500	2166	337.686	5.1019	1.3084	2.5830	2.6645	4.7569	3.8206	4.4976
505	2327	342.373	5.5530	1.1027	2.6165	2.5867	5.0012	3.9833	4.6929
510	2496	346.904	6.0930	0.8520	2.6382	2.4682	5.2502	4.1424	4.8827
515	2674	351.356	6.8185	0.5829	2.6812	2.3365	5.5430	4.3328	5.1032
520	2862	355.574	7.8551	0.2548	2.7153	2.1531	5.8597	4.5275	5.3294
525	3060	359.636	9.8799	0.1101	2.7715	1.9395	6.2380	4.7589	5.5937
530	3269	363.464	48.182	0.5302	2.8485	1.6791	6.6939	5.0300	5.9020
535	3488	366.901	45.778	1.0519	2.9155	1.3245	7.2110	5.3121	6.2255
			5.4833	**1.8905**	**2.7291**	**2.0622**	**2.9383**	**2.9825**	**2.8269**

Table C-2: Cyclopropane [29]

T	P	Exp. Data	Soave AAD%	Virial /B AAD%	R-kwong AAD%	Virial /C AAD%	Lee-Kesler AAD%	Peng-Robinson AAD%	This Work AAD%
297.22	706.43	17.570	0.5715	0.4475	0.4775	0.7384	0.6389	0.5281	0.5563
302.77	819.44	17.726	0.3894	0.1066	0.1864	0.5033	0.4887	0.2947	0.3559
308.33	944.99	17.893	0.3007	0.1814	0.0289	0.3320	0.4199	0.1444	0.2429
313.88	1083.99	18.059	0.2578	0.4706	0.2190	0.1712	0.3827	0.0274	0.1663
319.44	1237.26	18.225	0.2695	0.7601	0.3794	0.0222	0.3823	0.0510	0.1305
325.00	1405.70	18.382	0.2939	1.1030	0.5581	0.1665	0.3724	0.1379	0.0873
330.55	1590.13	18.548	0.4505	1.3908	0.6420	0.2871	0.4667	0.1196	0.1493
336.11	1791.67	18.715	0.7050	1.6761	0.6768	0.3907	0.6223	0.0405	0.2718
341.66	2011.20	18.852	0.9272	2.1173	0.8110	0.6329	0.6956	0.0468	0.3094
352.77	2508.86	19.048	1.5124	3.4047	1.2654	1.4639	0.7284	0.1947	0.2593
358.33	2789.41	19.106	2.0443	4.2491	1.5488	2.0472	0.7410	0.2936	0.2241
363.88	3092.71	19.136	2.9826	5.2465	1.8544	2.7582	0.7836	0.3886	0.2163
369.44	3420.28	19.116	5.0413	6.5075	2.2483	3.7018	0.8151	0.5384	0.1953
375.00	3773.63	19.067	53.2566	7.9298	2.5703	4.7750	1.0298	0.5763	0.3557
380.55	4154.29	18.930	49.0752	9.8596	3.0473	6.3093	1.2802	0.7114	0.5380
			7.8719	**3.0300**	**1.1009**	**1.6200**	**0.6565**	**0.2729**	**0.2706**

Table C-3: Isopentane [7]

T	P	Exp. Data	Soave AAD%	Virial /B AAD%	R-kwong AAD%	Virial/ C AAD%	Lee-Kesler AAD%	Peng-Robinson AAD%	This Work AAD%
310	136.89	25.8906	0.3639	0.3925	0.3076	2.4320	0.4484	0.3498	0.4556
320	187.25	26.9115	0.0658	0.0297	0.1978	2.0846	0.1067	0.0993	0.1282
330	250.68	27.9868	0.3000	0.2890	0.5231	1.6568	0.0452	0.3579	0.0082
340	329.00	28.9875	0.7919	0.8464	1.1255	1.4059	0.4628	0.8811	0.4102
350	424.45	29.9825	1.2674	1.4373	1.7347	0.8795	0.8751	1.3974	0.8083
360	538.95	30.9993	1.6215	1.9679	2.2502	0.3393	1.1819	1.8052	1.1040
370	674.93	31.9825	2.0153	2.6152	2.8420	0.1220	1.5486	2.2718	1.4643
380	834.72	33.0034	2.1956	3.1455	3.2665	0.6766	1.7307	2.5524	1.6470
390	1020.8	34.0536	2.1640	3.5904	3.5434	1.0943	1.7424	2.6641	1.6696
400	1236.1	35.2335	1.5853	3.6566	3.3642	1.4053	1.2725	2.2981	1.2261
410	1483.8	36.2878	1.1162	4.1032	3.4633	1.3219	1.0258	2.1760	1.0302
420	1767.0	37.2878	0.3179	4.6990	3.5716	1.5854	0.7107	2.0221	0.8089
430	2090.2	38.2041	1.6681	5.5084	3.6849	1.9675	0.2671	1.8157	0.5407
440	2458.55	38.4175	28.5201	8.2306	5.3209	2.5265	1.0243	3.0100	1.6598
445	2661.71	39.0786	26.7149	8.0243	4.3889	4.9042	0.4763	1.8407	0.4763
450	2878.95	39.1873	23.9209	9.3408	4.6637	4.5568	1.1097	1.7895	0.3921
451	2924.14	39.2501	23.4465	9.4883	4.5585	5.6708	1.4474	1.6131	0.2103
452	2970.04	39.2627	22.8766	9.7749	4.5623	5.7799	1.7156	1.5373	0.1264
453	3016.34	39.2459	22.2496	10.1439	4.6197	6.0227	1.9674	1.5098	0.0906
454	3063.56	39.2292	21.6246	10.5121	4.6382	6.3448	2.3173	1.4361	0.0058
455	3111.49	39.1957	20.9671	10.9274	4.6569	6.6648	2.7471	1.3537	0.0901
456	3159.82	39.1079	20.1987	11.4988	4.7706	7.0293	3.1923	1.3562	0.1031
457	3208.96	38.9781	19.3429	12.1923	4.9165	7.5442	3.8276	1.3758	0.1047
458	3259.02	38.7941	18.3699	13.0476	5.0846	8.1755	19.0163	1.3946	0.1182
459	3309.38	38.3003	16.7209	14.8327	5.9086	8.9612	16.5411	2.0324	0.4774
459	3334.61	37.8945	15.5275	16.2289	6.6364	10.6425	14.6820	2.6622	1.0978
460	3360.65	37.2669	13.8014	18.3531	7.7072	11.9680	11.9144	3.6011	2.0088
			11.4724	**7.2177**	**3.7892**	**4.2134**	**3.4591**	**1.7483**	**0.6764**

Table C-4: Neopentane [10]

T	P	Exp. Data	Soave AAD%	Virial /B AAD%	R-kwong AAD%	Virial /C AAD%	Lee-Kesler AAD%	Peng-Robinson AAD%	This Work AAD%
347.22	644.03	19.2677	1.2980	1.1641	1.2003	1.3658	1.4008	1.2585	1.2972
350.00	685.95	19.5480	1.1731	0.8945	0.9731	1.2343	1.2809	1.0910	1.1672
352.77	729.87	19.8501	1.1706	0.7362	0.8634	1.0365	1.2791	1.0426	1.1547
355.55	778.14	20.1404	1.1535	0.5415	0.7260	0.9515	1.2624	0.9722	1.1219
358.33	823.85	20.4173	1.0215	0.2367	0.4822	0.8392	1.1171	0.7892	0.9688
361.11	873.97	20.7177	1.0499	0.0698	0.3852	0.6041	1.1308	0.7584	0.9692
363.88	926.38	20.9963	0.9917	0.2009	0.1929	0.5151	1.0519	0.6348	0.8754
366.66	980.91	21.2984	1.0606	0.3599	0.1201	0.3249	1.0929	0.6320	0.9006
369.44	1037.79	21.5854	1.0789	0.5893	0.0138	0.2472	1.0755	0.5705	0.8655
372.22	1097.09	21.8522	1.0290	0.9101	0.2289	0.1012	0.9809	0.4308	0.7511
375	1158.87	22.1560	1.1720	1.0587	0.2626	0.1335	1.0687	0.4738	0.8173
377.77	1223.19	22.4346	1.2307	1.3211	0.3980	0.1954	1.0599	0.4186	0.7842
380.55	1290.00	22.7132	1.3210	1.5819	0.5202	0.3680	1.0678	0.3791	0.7653
383.33	1359.78	22.9867	1.4323	1.8606	0.6461	0.5374	1.0786	0.3398	0.7457
386.11	1432.04	23.2586	1.5774	2.1456	0.7650	0.7214	1.1007	0.3102	0.7347
388.88	1507.47	23.5221	1.7469	2.4619	0.8976	0.9104	1.1180	0.2715	0.7141
391.66	1585.31	23.7771	1.9392	2.8141	1.0502	1.1268	1.1209	0.2159	0.6758
394.44	1666.46	24.0289	2.2074	3.1743	1.1902	1.3778	1.1473	0.1781	0.6554
397.22	1750.23	24.2722	2.5420	3.5686	1.3443	1.6332	1.1679	0.1300	0.6245
400.00	1837.38	24.5072	3.0015	3.9921	1.5019	1.9209	1.1993	0.0844	0.5971
402.77	1927.70	24.7220	3.6224	4.4958	1.7107	2.2340	1.1955	0.0059	0.5267
405.55	2021.40	24.9586	4.8128	4.9011	1.7926	2.6232	1.3333	0.0352	0.5891
408.33	2118.48	25.1667	48.1103	5.4208	1.9500	2.9127	1.4190	0.0092	0.5876
411.11	2219.35	25.3480	45.9794	6.0448	2.1639	3.3114	1.4789	0.0632	0.5444
413.88	2323.80	25.5175	43.8435	6.7112	2.3681	3.8083	1.5809	0.1171	0.5249
416.66	2432.19	25.6702	41.6918	7.4397	2.5685	4.3432	1.7299	0.1561	0.5270
419.44	2544.71	25.7558	39.4059	8.4415	2.9489	4.9344	1.7639	0.3579	0.3763
422.22	2661.16	25.8682	37.2007	9.3246	3.1170	5.7875	2.0689	0.3406	0.4525
425.00	2782.10	25.9622	34.9747	10.2776	3.2143	6.5201	2.5355	0.2412	0.6210
427.77	2907.51	25.8699	32.2911	12.0241	3.8584	7.3150	2.6023	0.6654	0.2778
430.55	3038.03	25.7642	29.5695	13.8395	4.2489	8.8755	3.0373	0.8580	0.156
433.33	3172.48	25.6081	26.6978	15.9004	4.3599	10.4934	3.6614	0.9274	0.074
			13.0437	**4.2032**	**1.5020**	**2.4782**	**1.4753**	**0.4612**	**0.715**

Table C-5: Propane [57]

T	P	Exp. Data	Soave AAD%	Virial /B AAD%	R-kwong AAD%	Virial /C AAD%	Lee-Kesler AAD%	Peng-Robinson AAD%	This Work AAD%
216.48	50.815	13.774	6.7450	2.0071	2.4778	1.4335	1.2235	2.1347	1.9845
222.03	67.017	14.030	6.4305	1.8304	2.2237	1.2883	1.0733	1.8969	1.7430
227.59	86.874	14.338	6.4454	1.9885	2.3069	1.4836	1.2693	2.0000	1.8452
233.15	111.696	14.543	5.7962	1.4426	1.6879	0.9775	0.7654	1.4022	1.2476
238.70	139.964	14.851	5.7960	1.5559	1.7403	1.1358	0.9364	1.4805	1.3322
244.26	175.128	15.056	5.1675	1.0023	1.1260	0.6334	0.4483	0.8951	0.7552
249.81	216.497	15.363	5.1960	1.1155	1.1865	0.8070	0.6447	0.9905	0.8652
255.37	263.381	15.620	4.9060	0.8730	0.9058	0.6278	0.4966	0.7481	0.6430
260.92	317.161	15.928	4.9390	0.9436	0.9502	0.7687	0.6773	0.8363	0.7576
266.48	382.661	16.184	4.7229	0.7285	0.7153	0.6399	0.5968	0.6532	0.6043
272.03	457.125	16.492	4.8345	0.8210	0.8061	0.8280	0.8462	0.8026	0.7888
277.59	537.794	16.799	4.9385	0.8717	0.8779	0.9755	1.0676	0.9372	0.9649
283.15	632.943	17.107	5.1146	0.9516	0.9974	1.1714	1.3556	1.1302	1.2006
288.70	738.433	17.415	5.3216	1.0164	1.1279	1.3606	1.6561	1.3417	1.4575
294.26	854.955	17.671	5.2928	0.7809	0.9870	1.2598	1.6897	1.2906	1.4539
299.81	984.578	17.979	5.6034	0.8356	1.1681	1.4601	2.0514	1.5707	1.7806
305.37	1130.747	18.286	6.0118	0.9055	1.4051	1.6943	2.4861	1.9198	2.1722
310.92	1289.328	18.543	6.2261	0.6837	1.3937	1.6473	2.6794	2.0318	2.3264
			5.5271	**1.0177**	**1.3380**	**1.1218**	**1.2202**	**1.3368**	**1.3290**

Table C-6: n-butane [8]

T	P	Exp. Data	Soave AAD%	Virial /B AAD%	R-kwong AAD%	Virial /C AAD%	Lee-Kesler AAD%	Peng-Robinson AAD%	This Work AAD%
280	133.445	22.915	0.7268	0.69602	0.7679	0.3283	0.6531	0.7386	0.6882
290	188.059	23.681	1.0439	0.99812	1.1526	0.6612	0.8780	1.0753	0.9503
300	258.581	24.530	0.9979	0.97154	1.1915	0.9063	0.7443	1.0545	0.8481
310	347.545	25.468	0.5930	0.63021	0.8914	0.8081	0.2611	0.6823	0.3903
320	457.786	26.438	0.0571	0.21280	0.4845	0.3796	0.3397	0.1892	0.1902
330	592.549	27.329	0.2085	0.13598	0.3810	0.1424	0.6540	0.0182	0.4856
340	754.770	28.141	0.2590	0.36537	0.5359	0.3454	0.7300	0.0124	0.5411
350	947.895	28.844	0.0513	0.97590	1.0105	0.2661	0.5149	0.3372	0.2983
360	1175.370	29.576	0.1246	1.46883	1.2870	0.1661	0.5275	0.4372	0.2707
370	1440.842	30.212	0.1316	2.27206	1.7674	0.4535	0.3861	0.7050	0.0670
380	1747.856	30.756	0.2482	3.35879	2.3856	1.0173	0.1789	1.0659	0.2367
390	2102.494	31.246	1.0331	4.58686	2.9316	1.8276	0.1619	1.2947	0.4077
400	2507.794	31.614	36.1578	6.18387	3.5161	2.7367	0.3138	1.4778	0.5132
405	2730.709	31.756	33.4284	7.10957	3.7451	3.9663	0.5882	1.4627	0.4407
410	2969.836	31.836	30.5808	8.23280	3.9559	4.6888	1.0660	1.3805	0.2727
411	3018.472	31.840	29.9846	8.50005	4.0145	5.5886	1.1655	1.3771	0.2496
412	3069.134	31.827	29.3556	8.81933	4.0975	5.8104	1.2733	1.3891	0.2365
413	3119.797	31.823	28.7436	9.11230	4.1454	6.0796	1.4232	1.3663	0.1884
414	3171.472	31.798	28.0859	9.47589	4.2394	6.3238	1.5554	1.3832	0.1760

415	3223.148	31.785	27.4548	9.79880	4.2815	6.6354	1.7492	1.3492	0.1125
416	3275.837	31.731	26.7287	10.26576	4.4335	6.9080	1.8749	1.4160	0.1445
417	3329.540	31.681	26.0121	10.71837	4.5398	7.3194	2.0902	1.4314	0.1205
418	3384.255	31.610	25.2462	11.24464	4.6770	7.7153	2.3409	1.4680	0.1113
419	3438.970	31.509	24.4061	11.87934	4.8851	8.1814	2.5744	1.5719	0.1667
420	3494.699	31.392	23.5226	12.57680	5.0948	8.7534	2.9282	1.6669	0.2057
421	3550.428	31.246	22.5596	13.38785	5.3585	9.3847	3.3506	1.8142	0.2962
422	3607.170	31.053	21.4744	14.37449	5.6892	10.1268	4.1943	2.0163	0.4341
423	3664.925	30.819	20.2709	15.52884	6.0307	11.0375	18.6614	2.2208	0.5709
423	3694.310	30.685	19.6202	16.17502	6.1769	12.1091	17.6433	2.2964	0.6131
424	3723.694	30.522	18.8860	16.93957	6.3571	12.7108	16.3862	2.4196	0.7182
424.	3753.078	30.292	17.9630	17.97303	6.6687	13.4272	14.5785	2.7095	1.0262
			15.9986	**7.57964**	**3.4417**	**5.0582**	**3.1809**	**1.2848**	**0.3862**

Table C-7: n-Pentane [9]

T	P	Exp. Data	Soave AAD%	Virial /B AAD%	R-kwong AAD%	Virial /C AAD%	Lee-Kesler AAD %	Peng-Robinson AAD%	This Work AAD%
310	104.26	25.7107	0.8136	0.8095	0.8189	1.1753	0.8016	0.9123	0.8976
320	144.38	27.0914	0.0336	0.0675	0.0400	0.8059	0.1348	1.2384	1.0568
330	195.65	28.5014	0.8638	0.9015	0.7098	0.1168	1.0497	1.5052	1.1610
340	259.79	30.0244	1.9631	1.9730	1.7156	1.0064	2.2258	1.4264	0.9292
350	338.93	31.6269	3.1943	3.1392	2.8378	2.1435	3.5238	1.1462	0.5072
360	435.19	33.1457	4.0759	3.9107	3.5896	3.3866	4.4615	1.1781	0.4059
370	550.80	34.6644	4.9093	4.5792	4.2685	4.2486	5.3367	1.2218	0.3264
380	688.09	36.3464	6.1465	5.5861	5.3233	5.0220	6.5950	0.8053	0.2006
390	849.61	37.2502	5.4163	4.5233	4.3483	6.1467	5.8701	2.5022	1.3693
400	1048.1	38.6685	6.1906	4.8226	4.8024	5.2316	6.6150	2.6163	1.3341
410	1256.0	40.1413	7.0474	5.1100	5.3013	5.7073	7.3662	2.6512	1.3022
420	1506.8	41.6517	8.2808	5.4936	5.9955	6.1521	8.3936	2.4140	0.9608
430	1793.6	42.9613	9.5110	5.3972	6.3395	6.7303	9.1583	2.5074	0.9482
440	2120.4	43.8943	11.6126	4.4854	6.0710	6.8559	9.4699	3.2207	1.5584
450	2491.1	44.4634	35.5607	2.8177	5.3921	6.2047	9.6707	4.3278	2.5936
455	2694.5	44.3295	32.6471	1.0746	4.3899	4.8431	9.3633	5.5845	3.8299
460	2910.9	43.9822	29.3833	1.1658	3.1903	3.2874	9.2161	7.0318	5.2795
461	2955.8	43.8860	28.6830	1.6800	2.9400	1.2593	9.2526	7.3284	5.5799
462	3001.3	43.7981	27.9946	2.1767	2.7322	0.7909	9.3719	7.5756	5.8321
463	3047.3	43.6768	27.2487	2.7541	2.4774	0.3405	9.5015	7.8728	6.1346
464	3093.8	43.5513	26.4927	3.3447	2.2471	0.1881	9.7294	8.1408	6.4091
465	3141.0	43.4216	25.7270	3.9483	2.0561	0.7290	10.124	8.3613	6.6337
466	3188.7	43.3044	24.9798	4.5252	1.9551	1.2815	10.839	8.4793	6.7547
467	3237.1	43.1161	24.1053	5.2784	1.7872	1.8074	26.598	8.6672	6.9349
468	3286.0	42.8358	23.0600	6.2660	1.5679	2.5042	24.753	8.9075	7.1384
469	3335.5	42.4718	21.8488	7.4780	1.5179	3.4281	22.208	8.9676	6.9944
465	3360.5	42.1078	20.8961	8.5588	1.6144	4.5695	19.887	8.8381	4.3869
			15.5069	**3.7729**	**3.1863**	**3.1838**	**9.3157**	**4.6455**	**3.2392**

Table C-8: Ethylene [36]

T	P	Exp. Data	Soave AAD%	Virial /B AAD%	R-kwong AAD%	Virial /C AAD%	Lee-Kesler AAD%	Peng-Robinson AAD%	This Work AAD%
104.00	0.122	11.5172	4.7446	5.2094	4.7300	5.3142	5.1201	4.70406	4.55465
110.92	0.375	11.752	3.8080	4.2465	3.7933	4.3491	4.1721	3.76848	3.62318
122.03	1.793	12.1175	2.5800	2.9574	2.5645	3.0560	2.9174	2.54240	2.40670
133.15	6.140	12.4895	1.4767	1.7756	1.4598	1.8679	1.7718	1.44219	1.32301
144.26	17.124	12.8614	0.5094	0.7146	0.4915	0.7946	0.7399	0.48021	0.38805
155.37	40.73	13.2203	0.2757	0.1698	0.2914	0.1135	0.1346	0.29583	0.34994
166.48	84.80	13.5205	0.6049	0.5859	0.6101	0.5709	0.5737	0.61023	0.62130
177.59	159.84	13.7358	0.3782	0.4154	0.3567	0.4682	0.4723	0.35963	0.33355
188.70	277.38	13.9773	0.4694	0.5010	0.3942	0.6571	0.6908	0.41298	0.37260
199.81	452.07	14.1730	0.4353	0.3585	0.2631	0.6681	0.7723	0.31840	0.30186
210.92	696.07	14.3492	0.5280	0.1776	0.1926	0.7007	0.9410	0.31382	0.37239
222.03	1023.28	14.4797	0.6637	0.2141	0.0603	0.5975	1.0787	0.28738	0.47508
233.15	1421.97	14.538	0.6117	1.1188	0.4025	0.0289	0.8831	0.02478	0.36761
			1.3143	**1.4188**	**1.2008**	**1.4759**	**1.5591**	**1.19695**	**1.19153**

Table C-9: Ethyl Chloride [36]

T	P	Exp. Data	Soave AAD%	Virial /B AAD%	R-kwong AAD%	Virial /C AAD%	Lee-Kesler AAD%	Peng-Robinson AAD%	This Work AAD%
243.15	15.16	22.5569	0.5208	0.3433	0.5603	0.3114	0.3649	0.5340	0.4820
248.15	19.65	22.7225	1.0011	0.8531	1.0364	0.8244	0.8669	1.0128	0.9668
253.15	25.23	22.8845	1.3954	1.2776	1.4257	1.2528	1.2849	1.4053	1.3663
258.15	32.06	23.0442	1.7088	1.6213	1.7333	1.6012	1.6237	1.7168	1.6857
263.15	40.33	23.1253	2.0635	2.0061	2.0810	1.9916	2.0055	2.0691	2.0471
268.15	50.19	23.2028	2.4002	2.3718	2.4096	2.3639	2.3706	2.4032	2.3915
278.15	75.91	23.3507	2.8632	2.8902	2.8522	2.6653	2.8955	2.8598	2.8729
283.15	92.18	23.4905	3.1071	3.1591	3.0834	2.8995	3.1721	3.0998	3.1276
288.15	111.07	23.6244	3.3423	3.4168	3.3039	3.1792	3.4409	3.3305	3.3746
293.15	133.00	23.7547	3.4648	3.5593	3.4097	3.4493	3.5984	3.4480	3.5102
298.15	158.16	23.8780	3.5850	3.6960	3.5106	3.6063	3.7540	3.5624	3.6445
303.15	186.84	23.9966	3.7558	3.8790	3.6597	3.7596	3.9605	3.7267	3.8304
308.15	219.39	24.1059	3.8232	3.9539	3.7024	3.9614	4.0639	3.7867	3.9140
313.15	256.28	24.1681	3.9957	4.1285	3.8471	4.0578	4.2723	3.9508	4.1034
318.15	297.58	24.2068	4.0195	4.1479	3.8395	4.2565	4.3316	3.9651	4.1448
323.15	343.91	24.3020	4.1005	4.2173	3.8853	4.3031	4.4474	4.0351	4.2438
328.15	395.48	24.3912	4.0906	4.1878	3.8358	4.4030	4.4715	4.0127	4.2521
			2.8963	**2.9241**	**2.8339**	**2.8757**	**2.9956**	**2.8776**	**2.9387**

Table C-10: Trichloroethylene [36]

T	**P**	**Exp. Data**	**Soave AAD%**	**Virial /B AAD%**	**R-kwong AAD%**	**Virial /C AAD%**	**Lee-Kesler AAD%**	**Peng - Robinson AAD%**	**This Work AAD%**
260.92	664.90	34.894	6.5244	6.5195	6.5247	6.7986	6.5221	6.5245	6.5234
266.48	1336.28	35.450	6.0484	6.0376	6.0489	6.5194	6.0432	6.0486	6.0461
272.03	2013.56	36.037	5.5060	5.4841	5.5070	6.0375	5.4960	5.5064	5.5015
277.59	2696.89	36.621	4.9982	4.9628	5.0000	5.4837	4.9822	4.9989	4.9910
283.15	3386.37	37.330	4.1640	4.1147	4.1667	4.9622	4.1410	4.1650	4.1534
288.70	4081.91	38.027	3.4019	3.3381	3.4057	4.1136	3.3712	3.4033	3.3874
294.26	4783.17	38.818	2.4230	2.3432	2.4283	3.3364	2.3831	2.4249	2.4038
299.81	5490.51	39.613	1.4824	1.3873	1.4894	2.3407	1.4329	1.4849	1.4579
305.37	6204.05	40.505	0.3428	0.2341	0.3518	1.3839	0.2838	0.3459	0.3128
310.92	6924.09	41.382	0.7039	0.8238	0.6928	0.2296	0.7720	0.7002	0.7395
316.48	7647.55	42.241	1.6653	1.8042	1.6510	0.8294	1.7473	1.6606	1.7092
322.03	8376.47	43.207	2.8258	2.9824	2.8078	1.8118	2.9220	2.8201	2.8786
327.59	9109.18	44.283	4.1748	4.3515	4.1522	2.9924	4.2878	4.1678	4.2383
333.15	9846.82	45.404	5.5535	5.7490	5.5256	4.3648	5.6837	5.5450	5.6286
			3.5582	**3.5809**	**3.5537**	**3.6574**	**3.5763**	**3.5569**	**3.5694**

Table C-11: SO_2 [36]

T	**P**	**Exp. Data**	**Soave AAD%**	**Virial /B AAD%**	**R-kwong AAD%**	**Virial /C AAD%**	**Lee-Kesler AAD%**	**Peng-Robinson AAD%**	**This Work AAD%**
205.37	3.206	28.5206	0.6008	0.6147	0.6000	0.6109	0.6065	0.6006	0.6082
210.92	4.895	28.7143	0.5880	0.6176	0.5861	0.6149	0.6009	0.5875	0.6053
216.48	7.281	28.9080	0.5734	0.6207	0.5699	0.6181	0.5952	0.5725	0.6033
222.03	10.68	29.1017	0.5583	0.6265	0.5526	0.6216	0.5915	0.5568	0.6050
227.59	15.34	29.3103	0.5941	0.6854	0.5853	0.6282	0.6411	0.5919	0.6616
233.15	21.51	29.5040	0.5801	0.6962	0.5674	0.6882	0.6432	0.5770	0.6729
238.70	29.85	29.6829	0.5198	0.6639	0.5018	0.7006	0.6024	0.5154	0.6441
244.26	40.54	29.8617	0.4636	0.6366	0.4390	0.6706	0.5684	0.4578	0.6245
249.81	53.98	30.0554	0.4621	0.6641	0.4292	0.6465	0.5914	0.4545	0.6645
255.37	70.74	30.2193	0.3685	0.5998	0.3254	0.6781	0.5250	0.3587	0.6178
260.92	91.70	30.3981	0.3337	0.5947	0.2780	0.6190	0.5204	0.3211	0.6360
266.48	116.52	30.5918	0.3543	0.6418	0.2840	0.6208	0.5722	0.3387	0.7121
272.03	146.85	30.7557	0.2902	0.6037	0.2021	0.6761	0.5423	0.2707	0.7094
277.59	183.40	30.9494	0.3363	0.6735	0.2270	0.6485	0.6248	0.3123	0.8214
283.15	226.83	31.0985	0.2534	0.6116	0.1189	0.7312	0.5808	0.2240	0.8089
288.70	277.86	31.2624	0.2351	0.6094	0.0713	0.6850	0.6026	0.1993	0.8635
294.26	338.53	31.4114	0.1920	0.5781	0.0068	0.7016	0.6025	0.1483	0.8982
299.81	408.86	31.5455	0.1231	0.5138	0.1162	0.6935	0.5776	0.0702	0.9089
305.37	489.53	28.5206	0.0773	0.4634	0.2086	0.6567	0.5758	0.0134	0.9423
310.92	579.85	31.8137	0.0509	0.4209	0.2873	0.6381	0.5911	0.0256	0.9904
316.48	683.27	31.9627	0.1012	0.4429	0.2971	0.6311	0.6828	0.0095	1.1143

322.03	801.86	32.0670	0.0478	0.3474	0.4211	0.6946	0.6717	0.0624	1.1361
327.59	936.31	32.1564	0.0138	0.2258	0.5645	0.6479	0.6514	0.1466	1.1484
333.15	1087.31	32.2458	0.0352	0.1230	0.6797	0.5830	0.6685	0.1952	1.1970
338.70	1254.85	32.3650	0.0760	0.1278	0.6749	0.5448	0.8126	0.1168	1.3697
344.26	1441.01	32.4246	0.0508	0.0332	0.8236	0.6210	0.8163	0.1824	1.4015
349.81	1640.96	32.4992	0.1045	0.1458	0.9066	0.5413	0.8873	0.1766	1.4929
355.37	1875.38	32.5439	0.1739	0.2957	1.0095	0.5142	0.9734	0.1720	1.6117
360.92	2116.70	32.5737	0.2118	0.5123	1.1569	0.4713	1.0072	0.2090	1.6613
366.48	2392.49	32.6184	0.4153	0.6367	1.1835	0.3601	1.1944	0.1064	1.8726
372.03	2688.97	32.6184	0.5614	0.8904	1.3086	0.3610	1.2996	0.0894	1.9948
377.59	3013.02	32.6035	0.7833	1.1683	1.4188	0.2424	1.4470	0.0400	2.1550
383.15	3357.76	32.5886	1.1190	1.4424	1.4833	0.1139	1.6565	0.0676	2.3600
388.70	3743.87	32.4693	1.3933	1.9978	1.7621	0.0032	1.7207	0.0034	2.4183
394.26	4164.45	32.3203	1.9045	2.6251	2.0324	0.3718	1.8549	0.0347	2.5236
399.81	4612.62	32.0968	2.7156	3.4880	2.4448	0.7914	1.9138	0.1766	2.5041
405.37	5095.25	31.7839	39.7331	4.6351	3.0089	1.4287	1.9287	0.4247	2.3662
410.92	5626.15	31.3816	36.8730	6.0618	3.6360	2.3240	2.0817	0.6605	2.2441
416.48	6191.53	30.3683	32.6131	9.6735	6.1041	3.4580	0.7625	2.6038	0.4007
422.03	6805.16	29.9064	29.4323	11.4028	6.2123	6.6958	2.2255	2.1248	0.8390
			3.8978	**1.4603**	**1.1021**	**0.8637**	**0.9253**	**0.3700**	**1.2102**

Table C-12: water [26]

T	P	Exp. Data	Soave AAD%	Virial /B AAD%	R-kwong AAD%	Virial /C AAD%	Lee-Kesler AAD%	Peng-Robinson AAD%	This Work AAD%
278	0.8721	45.2274	3.3597	3.3568	3.3598	3.3691	3.3589	3.3597	3.3567
283	1.2276	45.3931	3.3509	3.3445	3.3511	3.3568	3.3491	3.3509	3.3439
288	1.705	45.5583	3.3435	3.3331	3.3439	3.3445	3.3405	3.3436	3.3314
293	2.339	45.7232	3.3371	3.3221	3.3377	3.3331	3.3325	3.3372	3.3186
298	3.169	45.8873	3.3323	3.3121	3.3333	3.3220	3.3260	3.3325	3.3059
303	4.246	46.0508	3.3288	3.3026	3.3302	3.3120	3.3202	3.3290	3.2926
308	5.628	46.2135	3.3271	3.2943	3.3291	3.3025	3.3159	3.3275	3.2790
313	7.384	46.3753	3.3273	3.2870	3.3298	3.2941	3.3130	3.3278	3.2648
318	9.593	46.5362	3.3291	3.2806	3.3324	3.2867	3.3112	3.3297	3.2495
323	12.35	46.6960	3.3328	3.2753	3.3371	3.2802	3.3106	3.3336	3.2330
328	15.758	46.8545	3.3387	3.2713	3.3442	3.2747	3.3116	3.3396	3.2153
333	19.941	47.0118	3.3465	3.2684	3.3534	3.2705	3.3139	3.3477	3.1958
338	25.03	47.1676	3.3565	3.2669	3.3651	3.2674	3.3177	3.3580	3.1745
343	31.19	47.3218	3.3689	3.2670	3.3796	3.2656	3.3230	3.3707	3.1511
348	38.58	47.4746	3.3831	3.2680	3.3961	3.2652	3.3292	3.3853	3.1249
353	47.39	47.6255	3.3996	3.2705	3.4154	3.2657	3.3369	3.4022	3.0962
358	57.83	47.7745	3.4185	3.2748	3.4377	3.2676	3.3461	3.4217	3.0649
363	70.14	47.9215	3.4397	3.2805	3.4626	3.2710	3.3566	3.4434	3.0305
368	84.55	48.0664	3.4632	3.2880	3.4905	3.2758	3.3684	3.4676	2.9930
373	101.3	48.2090	3.4888	3.2970	3.5211	3.2819	3.3813	3.4940	2.9525
378	120.8	48.3492	3.5167	3.3078	3.5549	3.2895	3.3954	3.5228	2.9084
383	143.3	48.4868	3.5469	3.3202	3.5916	3.2984	3.4107	3.5540	2.8611

388	169.1	48.6218	3.5793	3.3347	3.6314	3.3088	3.4273	3.5876	2.8109
393	198.5	48.7540	3.6138	3.3512	3.6743	3.3207	3.4448	3.6234	2.7581
398	232.1	48.8830	3.6508	3.3699	3.7207	3.3342	3.4637	3.6618	2.7022
403	270.1	49.0091	3.6895	3.3904	3.7699	3.3493	3.4833	3.7022	2.6438
408	313	49.1316	3.7310	3.4138	3.8231	3.3657	3.5046	3.7455	2.5839
413	361.3	49.2507	3.7743	3.4394	3.8795	3.3844	3.5268	3.7909	2.5219
418	415.4	49.3658	3.8205	3.4683	3.9402	3.4046	3.5507	3.8393	2.4593
423	475.9	49.4771	3.8684	3.4998	4.0042	3.4273	3.5754	3.8898	2.3954
428	543.1	49.5843	3.9188	3.5347	4.0722	3.4516	3.6017	3.9430	2.3321
433	617.8	49.6870	3.9716	3.5730	4.1445	3.4784	3.6295	3.9990	2.2690
438	700.5	49.7850	4.0269	3.6152	4.2212	3.5076	3.6588	4.0577	2.2069
443	791.7	49.8781	4.0846	3.6616	4.3024	3.5395	3.6899	4.1194	2.1467
448	892.8	49.9660	4.1440	3.7113	4.3878	3.5742	3.7215	4.1832	2.0858
453	1002.2	50.0486	4.2078	3.7683	4.4795	3.6108	3.7576	4.2518	2.0340
458	1122.7	50.1255	4.2732	3.8292	4.5755	3.6534	3.7943	4.3225	1.9825
463	1254.4	50.1965	4.3409	3.8955	4.6767	3.6982	3.8329	4.3963	1.9345
468	1397.8	50.2611	4.4115	3.9681	4.7838	3.7465	3.8739	4.4737	1.8912
473	1553.8	50.3191	4.4850	4.0473	4.8968	3.7993	3.9173	4.5546	1.8524
478	1723	50.3705	4.5606	4.1331	5.0156	3.8567	3.9628	4.6387	1.8182
483	1906.3	50.4146	4.6388	4.2264	5.1407	3.9184	4.0107	4.7263	1.7886
488	2104.2	50.4512	4.7199	4.3281	5.2727	3.9853	4.0616	4.8179	1.7647
493	2317.8	50.4802	4.8028	4.4377	5.4109	4.0581	4.1143	4.9126	1.7445
498	2547.7	50.5009	4.8883	4.5569	5.5565	4.1361	4.1700	5.0115	1.7293
503	2794.9	50.5132	4.9758	4.6858	5.7093	4.2209	4.2280	5.1140	1.7176
508	3060.1	50.5164	5.0656	4.8255	5.8700	4.3122	4.2890	5.2208	1.7099
513	3344.2	50.5106	5.1565	4.9760	6.0381	4.4112	4.3521	5.3309	1.7043
518	3648.2	50.4951	5.2487	5.1387	6.2145	4.5176	4.4176	5.4451	1.7003
523	3973	50.4694	5.3422	5.3147	6.3997	4.6324	4.4857	5.5635	1.6971
528	4319.5	50.4332	5.4357	5.5043	6.5935	4.7567	4.5558	5.6856	1.6929
533	4688.6	50.3860	5.5289	5.7089	6.7964	4.8906	4.6278	5.8117	1.6866
538	5081.3	50.3269	5.6216	5.9304	7.0095	5.0351	4.7021	5.9423	1.6775
543	5498.7	50.2555	5.7123	6.1694	7.2326	5.1918	4.7779	6.0769	1.6630
548	5941.8	50.1712	5.8001	6.4278	7.4665	5.3614	4.8550	6.2158	1.6417
553	6411.7	50.0732	5.8831	6.7073	7.7116	5.5452	4.9328	6.3588	1.6116
558	6909.4	49.9605	5.9602	7.0103	7.9693	5.7445	5.0115	6.5067	1.5720
563	7436	49.8318	6.0291	7.3396	8.2405	5.9617	5.0908	6.6598	1.5216
568	7992.8	49.6863	6.0863	7.6978	8.5261	6.1991	5.1696	6.8181	1.4584
573	8581	49.5222	6.1279	8.0888	8.8280	6.4589	5.2478	6.9824	1.3823
578	9201.8	49.3380	6.1473	8.5166	9.1473	6.7446	5.3241	7.1530	1.2929
583	9856.6	49.1318	6.1359	8.9865	9.4865	7.0597	5.3979	7.3309	1.1908
588	10547	48.9006	6.0798	9.5055	9.8486	7.4091	5.4679	7.5175	1.0778
593	11274	48.6419	5.9561	10.0812	10.2368	7.7989	5.5328	7.7142	0.9588
598	12040	48.3517	5.7209	10.7236	10.6549	8.2362	5.5892	7.9221	0.8365
603	12845	48.0253	5.2868	11.4471	11.1103	8.7301	5.6374	8.1464	0.7279
608	13694	47.6560	4.3670	12.2679	11.6076	9.2942	5.6668	8.3862	0.6314
613	14586	47.2355	33.8981	13.2121	12.1606	9.9426	5.6773	8.6515	0.5813
618	15525	46.7523	31.9019	14.3123	12.7811	10.7006	5.6537	8.9460	0.5950
623	16514	46.1890	29.7491	15.6207	13.4909	11.5983	5.5765	9.2802	0.7075
628	17554	45.5189	27.3869	17.2209	14.3275	12.6844	5.4190	9.6768	0.9866

633	18651	44.6952	24.7218	19.2586	15.3480	14.0388	5.1017	10.1620	1.4909
638	19807	43.6215	21.5458	22.0497	16.6897	15.7989	4.4646	10.8197	2.3649
643	21028	42.0131	17.2211	26.5495	18.7685	18.2671	2.8870	11.9190	3.8655
			6.4828	**6.0854**	**6.1938**	**5.1479**	**4.0998**	**5.1903**	**2.1884**

Table C-13: R11 [11]

T	**P**	**Exp. Data**	**Soave AAD%**	**Virial /B AAD%**	**R-kwong AAD%**	**Virial /C AAD%**	**Lee-Kesler AAD%**	**Peng-Robinson AAD%**	**This Work AAD%**
203	0.6	25.7923	0.2953	0.2079	0.2986	0.2057	0.2565	0.2970	0.2911
213	1.3	26.4896	0.1140	0.0495	0.1169	0.0476	0.0838	0.1155	0.1106
223	2.7	27.1963	0.0423	0.0762	0.0405	0.0774	0.0595	0.0415	0.0444
243	9.2	28.6342	0.3206	0.2805	0.3237	0.1874	0.2971	0.3219	0.3173
253	15.8	29.3619	0.4415	0.3569	0.4497	0.2782	0.3879	0.4448	0.4334
263	25.7	30.0936	0.5555	0.4256	0.5713	0.3506	0.4658	0.5615	0.5405
273	40.2	30.6193	0.6686	0.4931	0.6956	0.4132	0.5365	0.6784	0.6441
283	60.6	31.3116	0.7787	0.5604	0.8213	0.4714	0.5987	0.7935	0.7416
293	88.4	32.0012	0.8832	0.6277	0.9470	0.5252	0.6508	0.9045	0.8300
296	101.3	32.2622	0.9205	0.6530	0.9942	0.5741	0.6672	0.9448	0.8603
303	125.4	32.6839	0.9867	0.7028	1.0787	0.5907	0.6984	1.0165	0.9139
313	173.5	33.3598	1.0811	0.7814	1.2097	0.6244	0.7349	1.1220	0.9851
323	234.6	34.0260	1.1671	0.8692	1.3425	0.6705	0.7631	1.2223	1.0451
333	311.1	34.6785	1.2465	0.9728	1.4812	0.7170	0.7862	1.3203	1.0968
343	405.2	35.3186	1.3060	1.0857	1.6149	0.7687	0.7933	1.4040	1.1288
353	519.2	35.9409	1.3508	1.2212	1.7523	0.8177	0.7926	1.4806	1.1497
363	655.8	36.5440	1.3708	1.3789	1.8876	0.8756	0.7769	1.5428	1.1536
373	817.7	37.1237	1.3609	1.5672	2.0224	0.9403	0.7455	1.5903	1.1421
383	1007.6	37.6759	1.3121	1.7948	2.1566	1.0182	0.6957	1.6207	1.1153
393	1228.4	38.1951	1.2109	2.0734	2.2908	1.1161	0.6236	1.6320	1.0734
403	1483.4	38.6732	1.0357	2.4210	2.4279	1.2438	0.5243	1.6231	1.0168
413	1775.8	39.1004	0.7425	2.8599	2.5690	1.4165	0.3878	1.5902	0.9420
423	2109.1	39.4603	0.2394	3.4301	2.7225	1.6541	0.2033	1.5345	0.8474
433	2487	39.7282	0.7783	4.1938	2.9001	1.9934	0.0521	1.4562	0.7247
443	2913.8	39.8600	31.4060	5.2652	3.1245	2.4925	0.4278	1.3581	0.5567
453	3393.9	39.7694	27.3287	6.8818	3.4393	3.2590	1.0660	1.2433	0.3014
463	3932.4	39.1883	22.3243	9.8162	4.0207	4.5193	2.7125	1.1647	0.1179
			3.7507	**1.8906**	**1.6037**	**1.0314**	**0.6218**	**1.0750**	**0.7453**

Table C-14: R12 [11]

T	**P**	**Exp. Data**	**Soave AAD%**	**Virial /B AAD%**	**R-kwong AAD%**	**Virial /C AAD%**	**Lee-Kesler AAD%**	**Peng-Robinson AAD%**	**This Work AAD%**
183	2.8	17.709	2.52718	0.7050	1.1920	0.6404	0.7875	1.1355	0.9634
193	6.2	18.260	2.04335	0.5204	0.9253	0.4604	0.5693	0.8729	0.7184
203	12.3	18.819	1.54167	0.3564	0.6709	0.3034	0.3770	0.6248	0.4943
213	22.6	19.381	1.01955	0.2052	0.4210	0.1631	0.2058	0.3846	0.2865
223	39.1	19.944	0.48315	0.0668	0.1766	0.0415	0.0593	0.1549	0.0998
228	50.4	20.226	0.21303	0.0030	0.0582	0.0109	0.0025	0.0464	0.0172
238	80.7	20.785	0.34376	0.1324	0.1864	0.1160	0.1188	0.1724	0.1403
243	100.4	21.063	0.69197	0.2634	0.3677	0.2282	0.2301	0.3372	0.2703
243	101.3	21.074	0.55978	0.1318	0.2444	0.0943	0.1003	0.2132	0.1438
248	123.7	21.339	0.89902	0.2629	0.4220	0.2040	0.2058	0.3721	0.2662
253	150.9	21.612	1.17929	0.3330	0.5411	0.2475	0.2431	0.4688	0.3214
258	182.6	21.881	1.46245	0.4090	0.6633	0.2925	0.2780	0.5651	0.3730
263	219	22.150	1.73689	0.4816	0.7773	0.3298	0.3002	0.6497	0.4103
268	261	22.413	2.01310	0.5619	0.8949	0.3693	0.3195	0.7335	0.4437
273	308.6	22.675	2.28122	0.6430	1.0064	0.4045	0.3283	0.8070	0.4650
278	362.6	22.931	2.54679	0.7321	1.1187	0.4416	0.3318	0.8762	0.4799
283	423.3	23.184	2.80291	0.8247	1.2257	0.4761	0.3247	0.9350	0.4829
288	491.4	23.430	3.05549	0.9293	1.3345	0.5155	0.3130	0.9899	0.4807
293	567.3	23.672	3.29638	1.0409	1.4383	0.5548	0.2901	1.0336	0.4668
298	651.6	23.908	3.52619	1.1635	1.5395	0.5973	0.2574	1.0680	0.4434
303	744.9	24.136	3.74487	1.3014	1.6400	0.6467	0.2161	1.0942	0.4123
308	847.7	24.358	3.94714	1.4543	1.7370	0.7024	0.1627	1.1091	0.3706
313	960.7	24.569	4.13535	1.6308	1.8365	0.7721	0.1014	1.1174	0.3237
318	1084.3	24.771	4.30237	1.8314	1.9354	0.8562	0.0282	1.1155	0.2686
323	1219.3	24.9627	4.44074	2.0593	2.0327	0.9569	0.0605	1.1011	0.2031
328	1366.3	25.1404	4.54622	2.3237	2.1329	1.0830	0.1629	1.0775	0.1306
333	1525.9	25.3025	4.60907	2.6342	2.2394	1.2431	0.2792	1.0462	0.0528
338	1698.8	25.4476	4.60442	2.9947	2.3483	1.4406	0.4181	1.0018	0.0362
343	1885.8	25.5709	4.50373	3.4239	2.4681	1.6927	0.5787	0.9496	0.1319
348	2087.5	25.6688	4.23705	3.9367	2.6004	2.0135	0.7687	0.8882	0.2371
353	2304.6	25.7341	3.63788	4.5629	2.7567	2.4313	0.9911	0.8245	0.3474
358	2538	25.7595	1.86182	5.3327	2.9400	2.9741	1.2666	0.7549	0.4705
368	3056.9	25.6265	30.82553	7.5837	3.4763	4.7016	2.0803	0.6405	0.7433
373	3344.1	25.4065	26.99734	9.3488	3.9145	6.1570	2.7759	0.6360	0.8845
378	3650.9	24.9772	22.47845	12.0571	4.6366	8.5022	4.1246	0.7637	0.9853
383	3978.5	23.9398	15.76537	17.7576	6.4551	13.7061	23.1934	1.6208	0.6417
			4.96835	**2.5000**	**1.6765**	**1.5659**	**1.1903**	**0.7828**	**0.3891**

Table C-15: R13 [11]

T	P	Exp. Data	Soave AAD%	Virial /B AAD%	R-kwong AAD%	Virial /C AAD%	Lee-Kesler AAD%	Peng-Robinson AAD%	This Work AAD%
173	33.1	10.6903	2.1354	2.5328	3.3535	1.5011	1.0434	2.52871	1.4907
183	62.5	11.1248	1.6718	2.1941	2.7910	1.2470	0.7770	2.03432	1.1157
188	83.4	11.3390	1.4497	2.0235	2.5111	1.1264	0.6590	1.7946	0.9440
191	101.3	11.4884	1.3126	1.9178	2.3288	1.0605	0.5982	1.6439	0.8454
193	109.4	11.5489	1.2242	1.8384	2.2209	0.9978	0.5400	1.5496	0.7731
198	141.5	11.7558	1.0140	1.6550	1.9371	0.8791	0.4385	1.3174	0.6214
203	180.3	11.9574	0.8049	1.4538	1.6445	0.7513	0.3375	1.0834	0.4737
208	226.7	12.1538	0.6046	1.2383	1.3491	0.6193	0.2432	0.8545	0.3366
213	281.8	12.3439	0.4147	1.0053	1.0499	0.4817	0.1564	0.6309	0.2103
218	346.4	12.5277	0.2415	0.7549	0.7510	0.3394	0.0806	0.4181	0.0990
223	421.5	12.7043	0.0861	0.4811	0.4504	0.1881	0.0150	0.2150	0.0009
228	508	12.8724	0.0507	0.1766	0.1455	0.0215	0.0427	0.0205	0.0869
238	719.4	13.1806	0.2417	0.5407	0.4717	0.1641	0.1205	0.3306	0.2244
243	846.4	13.3185	0.2805	0.9666	0.7833	0.3673	0.1348	0.4826	0.2729
248	988.8	13.4428	0.2775	1.4587	1.1070	0.5994	0.1387	0.6260	0.3174
253	1147.9	13.5535	0.2009	2.0144	1.4286	0.8767	0.1118	0.7434	0.3415
258	1324.6	13.6486	0.0280	2.6507	1.7513	1.1940	0.0505	0.8347	0.3461
263	1520.2	13.7238	0.2745	3.3978	2.0862	1.5670	0.0457	0.9057	0.3367
268	1735.9	13.7760	0.7888	4.2802	2.4324	2.0232	0.1938	0.9491	0.3044
273	1972.9	13.8000	1.6842	5.3401	2.7964	2.5844	0.4115	0.9628	0.2430
278	2232.9	13.7885	3.5041	6.6363	3.1811	3.2894	0.7383	0.9359	0.1331
283	2517.6	13.7290	61.2040	8.2755	3.6031	4.1911	1.2320	0.8640	0.0450
288	2829.2	13.5995	55.9670	10.4523	4.0909	5.3880	2.0194	0.7378	0.3295
293	3170.8	13.3529	50.2061	13.6052	4.7145	7.0600	3.4503	0.5455	0.7952
			7.7361	**3.2038**	**2.0408**	**1.6049**	**0.5658**	**0.9587**	**0.4453**

Table C-16: R21 [36

T	P	Exp. Data	Soave AAD%	Virial /B AAD%	R-kwong AAD%	Virial /C AAD%	Lee-Kesler AAD%	Peng-Robinson AAD%	This Work AAD%
233.15	9.363	27.2803	1.2584	1.2584	1.2584	1.2584	1.2584	1.2584	1.2584
244.26	17.775	27.8518	1.1496	1.2030	1.1429	1.2071	1.1848	1.1474	1.1674
255.37	31.592	28.4257	1.0394	1.1505	1.0217	1.1619	1.1196	1.0339	1.0823
258.15	36.149	28.568	1.0096	1.1355	0.9883	1.1493	1.1026	1.0031	1.0600
266.48	53.083	28.7114	0.0634	0.1082	0.0982	0.1317	0.0730	0.0737	0.0136
277.59	84.944	29.5735	0.8357	1.0608	0.7768	1.1025	1.0346	0.8188	0.9542
288.70	130.312	30.1474	0.7663	1.0374	0.6727	1.1062	1.0362	0.7400	0.9356
299.81	192.779	30.7141	0.7120	1.0136	0.5711	1.1205	1.0584	0.6730	0.9400
303.15	215.325	30.8808	0.6940	1.0003	0.5360	1.1211	1.0637	0.6503	0.9407
310.92	276.068	31.2642	0.6559	0.9638	0.4517	1.1224	1.0809	0.5994	0.9481
322.03	384.385	31.7976	0.6145	0.8947	0.3269	1.1214	1.1171	0.5341	0.9731
			0.7999	**0.9842**	**0.7132**	**1.0548**	**1.0118**	**0.7757**	**0.9339**

Table C-17: R22 [11]

T	**P**	**Exp. Data**	**Soave AAD%**	**Virial /B AAD%**	**R-kwong AAD%**	**Virial /C AAD%**	**Lee-Kesler AAD%**	**Peng - Robinson AAD%**	**This Work AAD%**
203.15	20.5	18.921	0.5640	0.3222	0.6585	0.2579	0.3135	0.5886	0.3442
208.15	28.0	19.133	0.4942	0.2949	0.5794	0.2364	0.2778	0.5162	0.3014
213.15	37.5	19.343	0.4148	0.2577	0.4888	0.2064	0.2357	0.4338	0.2527
218.15	49.5	19.552	0.3338	0.2189	0.3941	0.1766	0.1954	0.3492	0.2063
223.15	64.4	19.759	0.2445	0.1704	0.2882	0.1395	0.1501	0.2556	0.1557
228.15	82.7	19.963	0.1499	0.1145	0.1736	0.0975	0.1023	0.1559	0.1036
232.35	101.3	20.134	7.8913	0.0746	0.0827	0.0719	0.0737	0.0799	0.0720
238.15	131.7	20.361	5.2181	0.0209	0.0804	0.0525	0.0020	0.0594	0.0020
243.15	163.5	20.556	0.1542	0.0981	0.2157	0.0001	0.0462	0.1698	0.0510
248.15	201	20.745	0.2626	0.1893	0.3629	0.0525	0.0995	0.2882	0.1038
253.15	244.8	20.930	0.3704	0.2895	0.5159	0.1141	0.1515	0.4078	0.1541
258.15	295.7	21.109	0.4817	0.4045	0.6798	0.1795	0.2067	0.5331	0.2065
263.15	354.3	21.283	0.5895	0.5300	0.8484	0.2538	0.2592	0.6576	0.2553
268.15	421.3	21.452	0.6904	0.6653	1.0194	0.3321	0.3064	0.7784	0.2981
273.15	497.6	21.612	0.7916	0.8203	1.2015	0.4130	0.3560	0.9034	0.3430
278.15	583.8	21.766	0.8856	0.9913	1.3886	0.5056	0.4020	1.0260	0.3843
283.15	680.7	21.913	0.9715	1.1813	1.5816	0.6056	0.4446	1.1464	0.4227
288.15	789.1	22.051	1.0436	1.3896	1.7773	0.7154	0.4797	1.2606	0.4545
293.15	909.9	22.180	1.1030	1.6232	1.9797	0.8335	0.5099	1.3716	0.4831
298.15	1043.9	22.298	1.1459	1.8854	2.1889	0.9658	0.5340	1.4785	0.5081
303.15	1191.9	22.405	1.1674	2.1802	2.4047	1.1151	0.5502	1.5798	0.5284
308.15	1354.8	22.501	1.1593	2.5108	2.6256	1.2844	0.5545	1.6729	0.5414
313.15	1533.5	22.581	1.1178	2.8889	2.8573	1.4762	0.5496	1.7617	0.5513
318.15	1729.0	22.646	1.0253	3.3178	3.0962	1.7008	0.5272	1.8402	0.5521
323.15	1942.3	22.692	0.8668	3.8133	3.3486	1.9608	0.4881	1.9125	0.5475
328.15	2174.4	22.716	0.6072	4.3877	3.6151	2.2703	0.4247	1.9757	0.5346
333.15	2426.6	22.713	0.1865	5.0650	3.9029	2.6404	0.3322	2.0326	0.5152
338.15	2699.9	22.679	0.5386	5.8717	4.2166	3.0927	0.1985	2.0819	0.4876
343.15	2995.9	22.603	2.0557	6.8545	4.5688	3.6518	0.0075	2.1271	0.4536
348.15	3316.1	22.472	44.1886	8.0816	4.9749	4.3604	0.2727	2.1704	0.4126
353.15	3662.3	22.264	40.6903	9.6744	5.4653	5.2819	0.7021	2.2197	0.3678
358.15	4036.8	21.936	36.7961	11.8807	6.1052	6.5299	1.4250	2.2967	0.3274
363.15	4442.5	21.378	32.1208	15.3410	7.0616	8.3378	2.9857	2.4585	0.3044
368.15	4883.5	19.998	24.3196	23.8308	9.3038	11.3125	24.0039	2.7977	10.955
			5.8136	**3.4482**	**2.3545**	**1.8007**	**1.1226**	**1.2173**	**0.6524**

Table C-18: R32 [36]

T	P	Exp. Data	Soave AAD%	Virial /B AAD%	R-kwong AAD%	Virial /C AAD%	Lee-Kesler AAD%	Peng-Robinson AAD%	This Work AAD%
172.03	3.516	17.3948	0.8202	1.3200	1.4327	0.6021	1.3002	0.7757	1.8637
177.59	5.709	17.5836	0.8415	1.3054	1.4160	0.6287	1.3010	0.7982	1.8454
188.70	13.679	17.9539	0.9181	1.2979	1.4028	0.7198	1.3240	0.8779	1.8149
199.81	29.351	18.3121	1.0368	1.3197	1.4147	0.8618	1.3700	1.0015	1.7812
210.92	57.489	18.6509	1.2134	1.3930	1.4706	1.0748	1.4531	1.1854	1.7545
222.03	104.34	18.9655	1.4449	1.5253	1.5733	1.3621	1.5712	1.4281	1.7344
244.26	286.36	19.5028	2.0432	2.0014	1.9273	2.1624	1.8967	2.0683	1.7326
255.37	440.94	19.7145	2.3906	2.3727	2.1895	2.6781	2.0973	2.4539	1.7690
266.48	652.82	19.8803	2.7504	2.8594	2.5213	3.2724	2.3156	2.8724	1.8371
277.59	934.72	19.9917	3.1037	3.4966	2.9451	3.9530	2.5464	3.3189	1.9350
288.70	1300.4	20.0364	3.4252	4.3424	3.5045	4.7377	2.7869	3.7949	2.0545
310.92	2347.0	19.8477	3.6790	7.0761	5.3668	6.7514	3.2431	4.8564	2.2738
322.03	3064.7	19.5355	3.0406	9.4289	7.0748	8.1529	3.4090	5.5092	2.3990
333.15	3941.1	18.9643	47.4569	13.1971	9.9852	10.0808	3.3641	6.3452	2.7209
344.26	5003.3	17.8607	36.6851	20.4680	16.0341	13.2008	2.3261	7.6519	3.9593
			7.3900	**4.8936**	**4.0173**	**4.0159**	**2.1537**	**2.9959**	**2.0983**

Table C-19: R114 [11]

T	P	Exp. Data	Soave AAD%	Virial /B AAD%	R-kwong AAD%	Virial /C AAD%	Lee-Kesler AAD%	Peng-Robinson AAD%	This Work AAD%
213.15	3.7	23.4641	0.9301	1.0440	0.9116	1.0513	1.0034	0.9259	1.0599
223.15	7.2	24.4555	0.8705	0.9295	0.8594	0.9341	0.9111	0.8680	0.9441
243.15	22.6	26.5014	0.6875	0.6257	0.7037	0.7881	0.6378	0.6910	0.5943
253.15	37	27.5457	0.5856	0.4643	0.6247	0.6181	0.4789	0.5938	0.3817
263.15	58	28.6020	0.4704	0.2953	0.5406	0.4449	0.3002	0.4851	0.1406
268.15	71.6	29.1336	0.4077	0.2092	0.4972	0.2583	0.2037	0.4264	0.0103
273.15	87.5	29.6652	0.3484	0.1303	0.4599	0.1607	0.1100	0.3718	0.1180
276.95	101.3	30.0668	0.3122	0.0819	0.4423	0.0683	0.0473	0.3394	0.2073
278.15	106.2	30.1985	0.2831	0.0487	0.4198	0.0082	0.0090	0.3117	0.2548
283.15	127.8	30.7317	0.2173	0.0280	0.3826	0.0292	0.0925	0.2522	0.3919
288.15	152.7	31.2650	0.1487	0.1020	0.3464	0.1244	0.1970	0.1907	0.5320
293.15	181.1	31.7966	0.0818	0.1676	0.3157	0.2198	0.2994	0.1319	0.6690
298.15	213.5	32.3281	0.0079	0.2327	0.2827	0.3097	0.4084	0.0675	0.8117
303.15	250	32.8580	0.0678	0.2905	0.2526	0.4025	0.5177	0.0028	0.9528
308.15	291.2	23.4641	0.1440	0.3391	0.2275	0.4915	0.6265	0.0607	1.0920
313.15	337.2	33.3844	0.2263	0.3822	0.2022	0.5752	0.7391	0.1281	1.2326
318.15	388.5	33.9092	0.3079	0.4119	0.1842	0.6574	0.8488	0.1923	1.3682
323.15	445.4	34.4288	0.3960	0.4335	0.1671	0.7304	0.9619	0.2600	1.5049
328.15	508.3	34.94	0.4886	0.4431	0.1538	0.7998	1.0759	0.3285	1.6403
333.15	577.5	35.4560	0.5835	0.4362	0.1476	0.8620	1.1879	0.3948	1.7714
338.15	653.4	35.9602	0.6892	0.4188	0.1414	0.9126	1.3052	0.4664	1.9057

343.15	736.4	36.4593	0.8005	0.3822	0.1423	0.9577	1.4216	0.5366	2.0372
348.15	827	36.9499	0.9229	0.3281	0.1472	0.9890	1.5413	0.6091	2.1702
353.15	925.4	37.4319	1.0562	0.2517	0.1588	1.0085	1.6619	0.6813	2.3017
358.15	1032.2	37.9036	1.2046	0.1505	0.1774	1.0113	1.7848	0.7538	2.4332
363.15	1147.9	38.3634	1.3738	0.0213	0.2035	0.9955	1.9116	0.8271	2.5655
368.15	1272.9	38.8095	1.5672	0.1436	0.2415	0.9584	2.0398	0.8973	2.6943
373.15	1407.8	39.2385	1.8000	0.3468	0.2899	0.8922	2.1740	0.9673	2.8222
378.15	1553.1	39.6487	2.0914	0.5959	0.3506	0.7950	2.3160	1.0363	2.9466
383.15	1709.7	40.0367	2.4763	0.9052	0.4304	0.6597	2.4655	1.0998	3.0619
388.15	1878.3	40.395	3.0398	1.2899	0.5344	0.4731	2.6255	1.1550	3.1614
393.15	2059.8	40.7187	4.0750	1.7735	0.6710	0.2208	2.7996	1.1967	3.2343
398.15	2255.5	40.9956	30.0913	2.3912	0.8517	0.1189	2.9968	1.2185	3.2661
403.15	2466.9	41.21	27.7694	3.2133	1.1071	0.5791	3.2211	1.1970	3.2204
408.15	2696	41.3357	25.2172	4.3731	1.4944	1.2262	3.4801	1.0855	3.0288
413.15	2945.8	41.3169	22.1610	6.2513	2.2144	2.1871	3.7166	0.6972	2.4644
			3.7195	**0.8314**	**0.4799**	**0.6533**	**1.3005**	**0.5958**	**1.6387**

Table C-20: R123 [58]

T	**P**	**Exp. Data**	**Soave AAD%**	**Virial /B AAD%**	**R-kwong AAD%**	**Virial /C AAD%**	**Lee-Kesler AAD%**	**Peng - Robinson AAD%**	**This Work AAD%**
223.15	1.8	29.1486	0.9548	0.9226	0.9580	0.9218	0.8695	0.9588	0.9628
243.15	6.7	30.9532	1.0364	1.0735	1.0313	1.0951	0.9926	1.0305	1.0250
253.15	12	31.8509	0.9759	1.0578	0.9626	1.0750	0.9633	0.9611	0.9483
263.15	20.2	32.7578	0.9015	1.0299	0.8763	1.0620	0.9262	0.8744	0.8532
273.15	32.6	33.6738	0.8245	1.0015	0.7822	1.0389	0.8939	0.7805	0.7505
278.15	40.8	34.1342	0.7846	0.9857	0.7316	1.0181	0.8791	0.7304	0.6961
283.15	50.6	34.5945	0.7414	0.9658	0.6756	1.0076	0.8624	0.6753	0.6370
288.15	62.1	35.0563	0.6995	0.9456	0.6192	0.9941	0.8481	0.6201	0.5786
293.15	75.6	35.5182	0.6566	0.9228	0.5596	0.9816	0.8342	0.5623	0.5184
298.15	91.4	35.9785	0.6103	0.8946	0.4942	0.9679	0.8182	0.4991	0.4539
300.95	101.3	36.2400	0.5952	0.8884	0.4672	0.9506	0.8203	0.4737	0.4283
303.15	109.6	36.4404	0.5694	0.8687	0.4315	0.9513	0.8081	0.4394	0.3942
308.15	130.5	36.9007	0.5270	0.8380	0.3646	0.9374	0.7973	0.3763	0.3327
313.15	154.5	37.3595	0.4855	0.8044	0.2955	0.9213	0.7881	0.3116	0.2715
318.15	181.7	37.8167	0.4452	0.7670	0.2241	0.9049	0.7802	0.2457	0.2112
323.15	212.5	38.2709	0.4042	0.7234	0.1483	0.8870	0.7716	0.1764	0.1497
328.15	247.1	38.7236	0.3673	0.6776	0.0727	0.8657	0.7669	0.1085	0.0920
333.15	285.9	39.1732	0.3329	0.6269	0.0050	0.8451	0.7640	0.0397	0.0360
338.15	329.2	39.6198	0.3023	0.5718	0.0838	0.8227	0.7642	0.0287	0.0170
343.15	377.2	40.0618	0.2728	0.5081	0.1667	0.7993	0.7641	0.0999	0.0702
348.15	430.4	40.4991	0.2473	0.4377	0.2517	0.7709	0.7665	0.1715	0.1214
353.15	489.1	40.9304	0.2238	0.3570	0.3414	0.7396	0.7689	0.2460	0.1732
358.15	553.6	41.3571	0.2081	0.2701	0.4308	0.7023	0.7766	0.3182	0.2205
363.15	624.2	41.7776	0.1985	0.1735	0.5224	0.6630	0.7872	0.3906	0.2662
368.15	701.4	42.1906	0.1951	0.0649	0.6175	0.6184	0.8003	0.4643	0.3117
373.15	785.5	42.5943	0.1972	0.0593	0.7184	0.5667	0.8142	0.5413	0.3593

378.15	876.9	42.9904	0.2122	0.1946	0.8193	0.5045	0.8353	0.6157	0.4036
383.15	976	43.3758	0.2379	0.3477	0.9253	0.4365	0.8597	0.6922	0.4495
388.15	1083.2	43.7489	0.2762	0.5216	1.0372	0.3562	0.8877	0.7716	0.4981
393.15	1199	44.1098	0.3351	0.7151	1.1520	0.2610	0.9240	0.8502	0.5460
398.15	1323.7	44.4539	0.4129	0.9388	1.2772	0.1523	0.9628	0.9356	0.6004
403.15	1457.8	44.7827	0.5262	1.1883	1.4052	0.0199	1.0142	1.0195	0.6528
413.15	1756.3	45.3731	0.9007	1.8094	1.6967	0.1316	1.1435	1.2078	0.7714
423.15	2098.7	45.8502	1.7795	2.6416	2.0387	0.5344	1.3445	1.4215	0.8901
433.15	2490.1	46.1499	28.5384	3.8240	2.4734	1.1151	1.6715	1.6928	0.9968
443.15	2937.2	46.1301	24.1404	5.6802	3.0913	2.0054	2.3026	2.0898	1.0578
453.15	3450.6	45.2018	18.2154	9.6430	4.3293	3.5137	4.3267	2.9737	1.1290
			2.4144	**1.2416**	**0.8940**	**0.8686**	**1.0189**	**0.7134**	**0.5101**

Table C-21: R134a [11]

T	**P**	**Exp. Data**	**Soave AAD%**	**Virial /B AAD %**	**R-kwong AAD %**	**Virial /C AAD%**	**Lee-Kesler AAD%**	**Peng-Robinson AAD%**	**This Work AAD%**
237.15	63.32	22.997	1.6040	1.5719	1.6246	1.5618	1.5669	1.6074	1.4519
241.15	77.04	23.252	1.6542	1.5916	1.6982	1.5630	1.5790	1.6614	1.3444
245.15	93.05	23.505	1.7105	1.6197	1.7812	1.5721	1.5956	1.7222	1.2388
247.15	101.99	23.632	1.7372	1.6333	1.8225	1.5876	1.6019	1.7514	1.1834
249.15	111.6	23.757	1.7671	1.6510	1.8679	1.5941	1.6110	1.7839	1.1307
251.15	121.92	23.883	1.7955	1.6680	1.9128	1.6040	1.6182	1.8152	1.0761
253.15	132.99	24.008	1.8222	1.6843	1.9570	1.6127	1.6235	1.8449	1.0196
255.15	144.83	24.133	1.8515	1.7044	2.0048	1.6200	1.6311	1.8774	0.9658
257.15	157.48	24.256	1.8831	1.7280	2.0560	1.6304	1.6408	1.9125	0.9145
261.15	185.4	24.502	1.9435	1.7764	2.1591	1.6436	1.6567	1.9807	0.8103
265.15	217.04	24.746	2.0020	1.8293	2.2652	1.6688	1.6702	2.0480	0.7070
269.15	252.74	24.987	2.0607	1.8898	2.3771	1.6950	1.6837	2.1169	0.6080
273.15	292.82	25.225	2.1181	1.9576	2.4936	1.7253	1.6958	2.1860	0.5125
277.15	337.65	25.459	2.1718	2.0317	2.6130	1.7586	1.7047	2.2533	0.4189
281.15	387.56	25.691	2.2201	2.1117	2.7342	1.7940	1.7091	2.3173	0.3261
285.15	442.94	25.918	2.2646	2.2011	2.8597	1.8306	1.7109	2.3801	0.2355
289.15	504.16	26.142	2.3029	2.2993	2.9878	1.8714	1.7083	2.4398	0.1445
293.15	571	26.360	2.3406	2.4138	3.1242	1.9156	1.7085	2.5023	0.0648
297.15	645.66	26.573	2.3619	2.5319	3.2576	1.9713	1.6930	2.5534	0.0396
299.15	685.3	26.679	2.3691	2.5957	3.3251	2.0226	1.6838	2.5774	0.0905
301.15	726.75	26.783	2.3722	2.6613	3.3916	2.0511	1.6714	2.5987	0.1448
303.15	770.06	26.885	2.3743	2.7325	3.4610	2.0796	1.6594	2.6207	0.1994
305.15	815.28	26.985	2.3751	2.8092	3.5329	2.1121	1.6472	2.6433	0.2549
307.15	862.47	27.084	2.3699	2.8875	3.6031	2.1483	1.6307	2.6620	0.3158
309.15	911.68	7.1810	2.3621	2.9713	3.6751	2.1843	1.6131	2.6805	0.3791
311.15	962.98	27.275	2.3508	3.0602	3.7487	2.2239	1.5940	2.6980	0.4457
313.15	1016.4	27.368	2.3354	3.1546	3.8235	2.2667	1.5728	2.7144	0.5162
315.15	1072	27.460	2.3112	3.2503	3.8953	2.3129	1.5453	2.7254	0.5950
317.15	1129.9	27.549	2.2843	3.3547	3.9712	2.3586	1.5179	2.7376	0.6767

321.15	1252.6	27.719	2.2123	3.5829	4.1268	2.4108	1.4548	2.7575	0.8556
325.15	1385.1	27.878	2.1112	3.8419	4.2894	2.5283	1.3797	2.7718	1.0588
329.15	1527.8	28.025	1.9710	4.1354	4.4589	2.6674	1.2894	2.7790	1.2885
333.15	1681.3	28.159	1.7741	4.4664	4.6330	2.8315	1.1771	2.7751	1.5499
343.15	2116.2	28.408	0.8715	5.5551	5.1389	3.0229	0.8030	2.7487	2.2977
353.15	2632.4	28.478	38.1847	7.2275	5.8001	3.7122	0.1859	2.6984	3.0616
363.15	3243.5	28.193	31.2299	10.182	6.8358	4.8980	1.0432	2.6822	3.3717
			3.8742	**2.8990**	**3.2030**	**2.1125**	**1.5244**	**2.3507**	**0.8693**

APPENDIX D

RESULTS FOR SATURATED ENTHALPY OF VAPOR FOR BINARY MIXTURE COMPONENTS

T = Temperature, Kelvin
P = Pressure, kpa
AAD% = Average Absolute Deviations Percent for Saturated Enthalpy of Vapor
Exp.Data= Experimental Data, kj/mole

Table D-1: Mixture of 81.16657 mole % Benzene & 18.8334 mole % Cyclohexane [28]

T	P	Exp. Data	Peng-Robinson mixing rule AAD%	Peng-Robinson with Teja AAD%	This Work AAD%
517.595	2757.920	70.3634	0.7608	0.7160	0.5708
532.983	3447.400	71.7459	1.7816	1.7035	0.0051
551.595	4343.724	72.1699	2.9117	12.5820	0.3021
557.483	4688.464	71.0454	8.3424	8.4207	4.4468
			3.4491	**5.8555**	**1.3312**

Table D-2: Mixture of 33.33621 mole % Benzene & 66.66379 mole % Cyclohexane [28]

T	P	Exp. Data	Peng-Robinson mixing rules AAD%	Peng-Robinson with Teja AAD%	This Work AAD%
518.206	2757.920	74.70825	1.0153	1.0084	0.4219
535.428	3447.400	76.17948	1.5324	1.5293	0.4312
541.595	3723.192	76.38966	1.9028	1.9187	0.4949
549.650	4136.880	76.25591	9.8568	10.0461	5.8105
			3.5768	**3.6256**	**1.7896**

Table D-3: Mixture of 61.2836 mole % Benzene & 38.71638 mole % Cyclohexane [28]

T	P	Exp. Data	Peng-Robinson mixing rules AAD%	Peng-Robinson with Teja AAD%	This Work AAD%
519.983	2757.920	72.5724	0.7821	0.7620	0.5249
532.261	3447.400	73.6765	2.4458	2.4036	0.4724
539.928	3743.876	73.9759	2.3327	2.2783	0.1165
548.206	4136.880	73.9198	12.5718	12.7623	0.1587
552.206	4343.724	73.5642	10.2714	10.4810	6.0717
			5.6808	**5.7374**	**1.4688**

Table D-4: Mixture of 21.1154 mole % Benzene & 78.8845 mole % Cyclohexane [28]

T	P	Exp. Data	Peng-Robinson mixing rules AAD%	Peng-Robinson with Teja AAD%	This Work AAD%
519.539	2757.920	76.1900	1.2007	1.1989	0.8884
537.872	3447.400	77.6552	1.1159	1.1204	0.6930
543.650	3709.402	77.7709	1.1782	1.1959	0.6616
550.539	4136.880	77.1539	8.4161	8.5663	7.5138
			2.9777	**3.0204**	**2.4392**

Table D-5: Mixture of 81.3663 mole % Benzene & 18.63365 mole % Hexadecane [17]

T	P	Exp. Data	Peng - Robinson mixing rules AAD%	Peng-Robinson with Teja AAD%	This Work AAD%
567.761	689.480	114.4074	6.9926	6.9124	6.5972
579.150	1034.220	116.4491	6.9404	6.8270	6.3589
			6.9665	**6.8697**	**6.4780**

Table D-6: Mixture of 96.3087 mole % Benzene & 3.6912 mole % Hexadecane [17]

T	P	Exp. Data	Peng - Robinson mixing rules AAD%	Peng-Robinson with Teja AAD%	This Work AAD%
497.039	689.480	75.1468	2.7314	2.6958	2.4042
510.761	1034.220	76.7412	2.7377	2.6871	2.2672
520.650	1378.960	77.8105	2.8294	2.7646	2.2114
539.261	2068.440	79.6576	2.8167	2.7289	1.9161
553.706	2757.920	81.0769	3.1554	3.0556	1.9551
562.595	3447.400	81.5047	3.7519	3.6710	2.1264
572.039	4136.880	81.6602	4.1857	4.2530	2.0421
			3.1726	**3.1223**	**2.1318**

Table D-7: Mixture of 91.9694 mole % Benzene & 8.0305 mole % Hexadecane [17]

T	P	Exp. Data	Peng-Robinson mixing rules AAD%	Peng-Robinson with Teja AAD%	This Work AAD%
530.372	689.480	88.0321	4.8368	4.7842	4.5066
544.372	1034.220	89.8120	4.5525	4.4786	4.0796
553.817	1378.960	91.0684	4.6224	4.5289	4.0026
570.261	2068.440	92.5342	4.1344	4.0105	3.2192
579.261	2757.920	92.9530	4.2448	4.1097	2.9570
			4.4782	**4.3824**	**3.7530**

Table D-8: Mixture of 19.7 mole % n-Pentane & 80.3 mole % Cyclohexane [18]

T	P	Exp. Data	Peng-Robinson mixing rules AAD%	Peng-Robinson with Teja AAD%	This Work AAD%
450.094	1034.220	68.0733	0.2758	0.2875	0.8728
467.039	1378.960	71.7262	1.6679	1.6529	0.9369
491.872	2068.440	74.0853	0.6812	0.6575	0.3645
511.706	2757.920	76.1401	0.5812	0.5470	0.7824
524.817	2757.920	77.0533	1.9886	1.9275	0.0955
			1.0389	**1.0145**	**0.6104**

Table D-9: Mixture of 38.5 mole % n-Pentane & 61.5 mole % Cyclohexane [18]

T	P	Exp. Data	Peng-Robinson mixing rules AAD%	Peng-Robinson with Teja AAD%	This Work AAD%
440.206	1034.220	66.5827	0.0082	0.0177	0.6103
457.206	1378.960	68.9692	0.2536	0.2194	0.5115
482.372	2068.440	72.0773	0.3362	0.2824	0.7218
500.150	2757.920	73.8533	0.5776	0.4933	0.8198
515.928	3447.400	74.5933	0.2645	0.1353	1.3965
			0.2880	**0.2296**	**0.8120**

Table D-10: Mixture of 61.2 mole % n-Pentane & 38.8 mole % Cyclohexane [18]

T	P	Exp. Data	Peng-Robinson mixing rules AAD%	Peng-Robinson with Teja AAD%	This Work AAD%
427.594	1034.220	64.4612	0.0233	0.0264	0.6334
443.039	1378.960	66.8375	0.8023	0.7352	0.0180
466.483	2068.440	69.3387	0.7277	0.6141	0.4359
484.428	2757.920	70.8752	0.8353	0.6427	0.6972
			0.5972	**0.5046**	**0.4461**

Table D-11: Mixture of 79.3 mole % n-Pentane & 20.7 mole % Cyclohexane [18]

T	P	Exp. Data	Peng-Robinson mixing rules AAD%	Peng-Robinson with Teja AAD%	This Work AAD %
415.650	1034.220	62.2203	0.3448	0.4215	1.0568
434.817	1378.960	64.9459	0.0794	0.0203	0.7660
454.928	2068.440	66.9076	0.3005	0.1193	0.9520
472.594	2757.920	68.5048	0.7699	0.4465	0.8776
			0.3737	**0.2519**	**0.9131**

Table D-12: Mixture of 32.2 mole % n-Pentane & 67.8 mole % trans-Decalin [19]

T	P	Exp. Data	Peng-Robinson mixing rules AAD%	Peng-Robinson with Teja AAD%	This Work AAD%
461.928	137.896	100.6113	6.4189	6.4070	6.3171
489.428	275.792	106.7057	5.6809	5.6594	5.5060
518.872	482.636	114.0787	5.4412	5.4073	5.1813
538.595	689.480	119.3841	5.5396	5.4939	5.2040
564.928	1034.220	125.7505	5.0205	4.9559	4.5772
582.483	1378.960	129.9404	4.7797	4.6943	4.2272
			5.4802	**5.4363**	**5.1688**

Table D-13: Mixture of 56.1 mole % n-Pentane & 43.9 mole % trans-Decalin [19]

T	P	Exp. Data	Peng-Robinson mixing rules AAD%	Peng-Robinson with Teja AAD%	This Work AAD%
497.428	482.636	97.6586	4.7635	4.7273	4.5288
515.150	689.480	101.212	4.3926	4.3438	4.0890
550.928	1378.960	108.6011	4.0827	3.9921	3.5771
575.261	2068.440	113.9193	4.3123	4.1810	3.6506
			4.3878	**4.3111**	**3.9614**

Table D-14: Mixture of 72.2 mole % n-Pentane & 27.5 mole % trans-Decalin [19]

T	P	Exp. Data	Peng - Robinson mixing rules AAD%	Peng-Robinson with Teja AAD%	This Work AAD%
454.817	275.792	81.9623	4.0655	4.0430	3.9176
487.872	482.636	85.1559	4.0720	4.0347	3.8375
487.872	689.480	88.0974	3.9852	3.9346	3.6807
520.372	1378.960	93.9384	3.8434	3.7489	3.3350
542.595	2068.440	97.6992	3.7296	3.5915	3.0625
554.817	2757.920	99.2961	3.9157	3.7237	3.0818
560.928	3447.400	98.7498	3.8278	3.5619	2.8158
			3.9199	**3.8055**	**3.3901**

Table D-15: Mixture of 88.4 mole % n-Pentane & 11.6 mole % trans-Decalin [19]

T	P	Exp. Data	Peng-Robinson mixing rules AAD%	Peng-Robinson with Teja AAD%	This Work AAD%
430.928	275.792	71.2930	2.4820	2.4604	2.3356
443.039	482.636	73.2424	2.6846	2.6477	2.4444
456.039	689.480	75.2661	2.6659	2.6150	2.3488
484.428	1378.960	79.3691	2.5098	2.4112	1.9687
506.872	2068.440	82.5253	2.3249	2.1802	1.6310
521.150	2757.920	84.3633	2.5183	2.3206	1.6963
529.261	3447.400	84.7532	2.7211	2.4539	1.7906
			2.5581	**2.4413**	**2.0308**

الخــــلاصة

التنبؤ بقيم دقيقة للمحتوى الحراري للبخار المشبع مهم جداً في الحسابات التصميمية وبعض التطبيقات الصناعية الأخرى. وبما أنه من الصعب الحصول على قيم المحتوى الحراري للبخار المشبع مختبرياً فقد حول الاهتمام الى حسابها من معادلات الحالة ، البعض من هذه المعادلات يطبق على كلا الطورين السائل والغاز، والبعض منها يطبق على الطور الغازي فقط، مع ملاحظة أن معادلات الحالة تلك تم تطويرها أساسا للتوازن بين حالتي البخار والسائل، وللتخلص من هذه المشكلة وجهت الاهتمامات لتعديل أو تصحيح معادلات الحالة. ان دقة هذه المعادلات مختلفة. خمسة من معادلات الحالة استخدمت لحساب المحتوى الحراري المتبقي للمركبات النقية (قطبية وغير قطبية). النسبة المئوية لمعدل الانحراف لـ ٢٥ مركب غير قطبي وقطبي و٧٠١ نقطة تجريبية هي ٢,٥٧٨٠، ٦,٧١٣٩، ١,٨٧٥٧، ٢,٢٦٩٦، ٣,٤٦٤٨، و٢,٤٩١٤ عند معادلة Redlich-Kowng، Soave Redlich-Kowng، Peng-Robinson، Lee-Kesler، ومعادلة Virial المقطوعة للحد الثاني والحد الثالث على التوالي.

من النتائج اعلاة يمكن بسهولة ان ندرك ان معادلة Peng-Robinson هي احسن معادلة يمكن استخدامها لحساب المحتوى الحراري المتبقي للبخارالمشبع بالمقارنة مع معادلات الحالة الاخرى التي ذكرت. لهذا الجهود وجهت نحو امكانية تعديل معادلة Peng-Robinson للحالة لزيادة دقة التنبؤ بالمحتوى الحراري المتبقي للبخار المشبع .

للمركبات النقية، اقترح ارتباط معدل جديد للتنبؤ بالمحتوى الحراري للبخارالمشبع. التعديل تم بإعادة تعريف قيمة n بدلالة درجة الحرارة و الضغط المنقوصين بالإضافة الى عامل اللامركزية باستعمال البرنامج الإحصائي. إن الارتباط هو كما في المعادلات التالية:

$$n = a_A + b_A \times \omega + c_A \times \omega^2$$

$$a_A = 0.941018$$

$$b_A = -85.7291 \times \mathrm{T_r} + 105.6393 \times \mathrm{T_r}^2 + 4.303806 \times \mathrm{P_r} - 50.0757 \times \mathrm{T_r} \times \mathrm{P_r} + 22.98768 \times \mathrm{P_r}^2$$

$$c_A = 433.376 \times \mathrm{T_r} - 530.876 \times \mathrm{T_r}^2 - 35.3057 \times \mathrm{P_r} + 252.0676 \times \mathrm{T_r} \times \mathrm{P_r} - 108.396 \times \mathrm{P_r}^2$$

أما الخلائط الثنائية، فحساب المحتوى الحراري للبخارالمشبع تم باستخدام طريقتان لحساب المحتوى الحراري المتبقي للبخارالمشبع، الطريقة الاولى تمت باستخدام معادلة Peng-Robinson للخلائط والطريقة الثانية تمت باستخدام معادلة Teja مع معادلةِ Peng-Robinson للمكونات النقية. لـ٩٥ نقطةِ تجريبية (٥ خلائط) النسبة المؤوية لمعدل الانحراف لمعادلة Peng-Robinson للخلائط هي ٢,٨٣٨٤ %. بينما النسبة المئوية لمعدل الانحراف لمعادلة Peng-Robinson بطريقة Teja مستندة على Peng-Robinson للخلائط هي ٢,٨٠٩٦ %.

مرة اخرى معادلة Peng-Robinson للخلائط طورت لزيادة الدقة للخلائط . ولهذا يمكن ان تعتبر ان معادلة Peng-Robinson للخلائط أفضل معادلة نسبياً للتنبؤ بالمحتوى الحراري للبخار المشبع للخليط الثنائي. إن هذا الارتباط هو كما في المعادلات التالية:

$$n = a_A + b_A\omega + c_A\omega^2$$

$$a_A = 0.3704$$

$$b_A = 0.01267 - 0.20093 \times T_r + 0.1 \times P_r$$

$$c_A = -0.9048 + 0.945147 \times T_r - 0.17167 \times P_r$$

هذه الإرتباطات يمكن أن تَطور بشكل أكبر لكي تستعمل مباشرة لغرض تصميم عمليات التقطير، وعمليات أخرى التي تَتضمن ظواهر التبخير و التكثيف.

شكر وتقدير

أبدأ بشكر الله عز وجل الذي وفقني لإكمال متطلبات هذا البحث، ولا يسعني إلا أن أتقدم بوافر الشكر وعظيم الامتنان إلى كل من الأستاذ الدكتور محمود عمر عبد الله المحترم والدكتور سرمد طالب العاني المحترم لإشرافهما على الرسالة ومتابعتهما العلمية المستمرة للبحث وماترتب على ذلك من توجيهات قيمة وأراء سديدة .

كما وأتقدم بالشكر الجزيل إلى السيد عميد كلية الهندسة المحترم والسيد رئيس قسم الهندسة الكيمياوية المحترم وجميع أساتذة قسم الهندسة الكيمياوية وأتقدم بجزيل شكري وإمتناني إلى رئاسة جامعة النهرين وأدعو من الله أن يوفقهم جميعاً لخدمة المسيرة العلمية.

ولا أنسى أن أتقدم بجزيل شكري وعظيم إمتناني إلى أغلى من في هذه الدنيا إلى أبي وأمي وإلى زوجي شريك الأفراح والأحزان وإلى جميع أفراد عائلتي لدعمهم المتواصل وتشجيعهم المستمر لي أثناء مسيرتي العلمية.

البحث في الإرتباط والتنبؤ للمحتوى الحراري للمركبات النقية والمخاليط للبخار المشبع

رسالة
مقدمة إلى كلية الهندسة في جامعة النهرين
وهي جزء من متطلبات نيل درجة ماجستير علوم
في الهندسة الكيماوية

من قبل

أغاريد أياد شاكر الوائلي
(بكالوريوس علوم في الهندسة الكيمياوية ٢٠٠٥)

محرم ١٤٣٠
كانون الثاني ٢٠٠٩