

**Sudan University of Science and Technology**

**College of Graduate Studies**

**Development of New Vapor Pressure Correlation for  
Organic Compounds**

**تطوير علاقة إرتباط جديدة للضغط البخاري للمركبات العضوية**

**A Thesis Submitted to Postgraduate Studies at Sudan University  
of Science and Technology in Fulfillment for the Requirement of  
Doctor of Philosophy in Chemical Engineering**

**By**

**Nassereldein Musa Abakar Ali**

**Supervisor:**

**Prof. Ali A. Rabah**

**November 2020**

## **Dedication**

To the pillars of my life: Allah, then my parents. Without them, my life would fall apart.

I might not know where life's road will take me, but walking with you, Allah, through this journey has given me strength.

My mother, you have given me so much, thanks for your faith in me, and for helping and teaching me, and giving me support to continue and I should never surrender.

My father, you are everything for me, without your love and understanding I would not be able to make it.

My colleagues Dr. Mohammed and teacher Adam and Dr. Aljalb, you always give me support and telling me to "reach the stars" I think I got my first one. Thanks for inspiring my love for success.  
We made it...

## **Acknowledgments**

I wish to acknowledge the following people and organizations for their contribution to the success of this thesis and the completion of my Ph.D. degree.

First, I would like to thank my supervisor, Prof. Ali A. Rabah, for tireless support, ideas, and motivation during this work. Working with you has been a privilege and a great learning experience. Thanks for his help and supervision has been my mentor.

Second, I would like to thank the staff and personnel of the Sudan University of Science and Technology (SUST) (Leather Engineering Department) for their assistance, my time at the office is greatly appreciated. I would like to give a special thanks to:

Dr. Laila Sorkti from the University of Khartoum and Mr. Hamed from Peace University; your assistance helped me through the model solution and data insertion is greatly appreciated.

Last but not least I offer my special thanks to those involved directly or indirectly in this study.

## Table of Contents

Dedication .....	I
Acknowledgments.....	II
Table of Figures .....	V
List of Tables .....	VI
Abstract .....	VII
مستخلص.....	VIII
<b>CHAPTER ONE: INTRODUCTION</b>	
1.1 General Introduction: .....	1
1.2 General objectives:.....	3
<b>CHAPTER TWO: LITERATURE REVIEW</b>	
2.1 Vapor Pressure Models .....	4
2.2 Experimental Methods .....	4
2.3 Equations of state .....	4
2.4 Other correlations.....	5
2.4.1 Antoine Correlation .....	5
2.4.2 Wagner correlation.....	6
2.4.3 Extend Antoine Correlation: .....	6
2.4.4 Ambrose–Walton corresponding states method:.....	7
2.4.5 Riedel Corresponding States Method: .....	8
2.4.6 Lee–Kesler’s Method:.....	9
2.4.7 Velasco equation Method: .....	9
2.4.8 The Cox equation:.....	10
2.4.9 Generalized equation predicts the vapor pressure of hydrocarbons. Oil and gas: .....	11
2.4.10 Generalized correlation of normal Alkanes.....	12
<b>CHAPTER THREE: MODELING</b>	
3.0 Modeling .....	13
3.1 Model Equation.....	14
3.2 Model Validation .....	15

**CHAPTER FOUR: RESULTS AND DISCUSSIONS**

4.1 Results ..... 16  
4.2 Vapor pressure ..... 24

**CHAPTER FIVE: CONCLUSIONS AND RECOMMENDATIONS**

5.1 Conclusion: ..... 32  
5.2 Recommendations: ..... 33  
References: ..... 34  
Appendixes: ..... 39

## List of Figures

Figure 3.1: Model Vapor Pressure of 1.Dodecanol used Excel program .....	14
Figure 4.1: Dependency of Model coefficients on critical temperature.....	22
Figure 4.2: Dependency of Model coefficients on critical pressure.....	22
Figure 4.3: Dependency of Model coefficients on boiling point.....	23
Figure 4.4: Dependency of Model coefficients on accentric factor.....	23

## List of Tables

Table2. 1: Some cubic equations of state. ....	5
Table2.2: Wagner constants. ....	6
Table2. 3: Veter rules for Riedel constant k for acids and alcohols. ....	9
Table4.1: Model and Antoine correlation coefficients values. ....	17
Table4. 2: Experimental and model statistical data. ....	25
Table4.3: Antoine and model statistical data. ....	27

## Abstract

The vapor pressures of organic compounds are the most important thermodynamics property needed by engineers in different industries for instant petrochemical and chemical processes as it is a useful thermodynamic property related to many other properties.

The aim of this study is the development of new vapor pressure equation of organic compounds. The study covered the organic compounds (C1 to C12) namely n-alkanes, cycloalkanes, branched alkanes, alkenes, alkynes, haloalkanes, diene, aromatic hydrocarbons, halo benzene, alcohols, ethers, ketones, esters, amines, and xylene.

The original Antoine equation:

$$\ln P^s = A - \frac{B}{C + T} \quad 1.1$$

To generalize the equation the constants A, B and C has been determined using physical boundary conditions as critical condition, normal boiling point, and Accentric factor.

Series of tests for the validation of the model on two methods of experimental data and Antoine of each organic compound were conducted to determine the minimum Average Percent Deviation, maximum Average Percent Deviation and Average Absolute Percent Deviation (AAPD %) over the temperature range ( $T_{\min}$ ,  $T_{\max}$ ) for the different vapor pressure of organic compounds.

In the results, 25 pure substances (228 experimental data points) and 64 pure substances (666 Antoine data points) were used in the model validation. The model reproduces the vapor pressure with an overall (AAPD) of 5% and 10% respectively.

This research showed that the model has been successfully tested for a variety of compounds and can be used for organic compounds.

It is recommended to replace the Pitzer equation by other accentric factor equations in boundary conditions to determine the generalized model coefficients and estimate the vapor pressures.



## مستخلص

الضغط البخارى للمركبات العضوية من اكثر خصائص الديناميكا الحرارية أهمية ويحتاج اليها المهندسون فى مختلف الصناعات لحالات البتروكيميائيات والعمليات الكيميائية وهذا العنصر الديناميكي الحرارى يقود الى مجموعة من الخصائص الاخرى.

تهدف هذه الدراسة الى تطوير علاقة جديدة للضغط البخارى للمركبات العضوية. الدراسة أجريت فى المركبات العضوية من (C<sub>1</sub> الى C<sub>12</sub>) وتضمنت الالكانات, الالكانات الحلقية, الالكانات المتفرعة, الألكينات, الألكينات, هالوالكانات, دايبينات, الهيدروكربونات العطرية, الهالوبنزوين, الكحول الإيثرات, الكيتونات, الإسترات, الأمينات والزيلين. من معادلة أنتوني الاصلية:

$$1.1 \quad \ln P^s = A - \frac{B}{C+T}$$

تم تحديد الثوابت العامة A, B و C باستخدام الحدود الثلاثة الفاصلة وهى نقطة الغليان ودرجة الحرارة الحرجة وعنصر الاستريك.

تم إختبار التحقق من النموذج بطريقتين بإستخدام البيانات التجريبية ومعادلة أنتوني للمركبات العضوية المذكورة لتحديد اصغر متوسط نسبة إنحراف واكبر متوسط نسبة إنحراف ومتوسط نسبة الإنحراف المطلق لاعلى وادنى درجة حرارة (T<sub>min</sub>, T<sub>max</sub>) لمختلف الضغوط البخارية للمركبات العضوية. وقد اعطت نتيجة 25 مادة نقية (228 من البيانات التجريبية) و 64 مادة نقية (666 من بيانات أنتوني) تم إستخدامها للتحقق من صدق النموذج. وعند المقارنة النموذج أعطى متوسط نسبة انحراف مطلق قدرها 5% و 10% على التوالى.

من هذا البحث وجد ان النموذج قد نجح عند اختباره لمختلف المركبات وبالتالي يصلح لاستخدامه للمركبات العضوية.

كما وصت الدراسة الى إستبدال معادلة بيتزار بمعادلة اخرى فى الحد الفاصل لتحديد معاملات النموذج ومن ثم تقدير الضغط البخارى.

# CHAPTER ONE

## Introduction

### 1.1 General Introduction:

Thermodynamic properties of chemical compounds such as vapor pressure are very important in the design of different industries for instant petrochemical and chemical processes (Mehrdad, H., Ehsan, S. and Hamidreza, B.,2014). The vapor pressures of chemical compounds are the most important thermodynamics property needed by engineers and useful thermodynamic parameters that can be related to many other properties. The relationship of chemical compounds between the vapor pressure–temperature is of great importance in many areas of science and engineering. There have been many different representations of the vapor pressure–the temperature relationship for chemical compounds.

Numerous empirical vaporpressure models have beenpublishedto determine vapor pressure, This include the experimental methods such as static methods, dynamic method, effusion method, transpiration method and calorimetric method, equations of state(EOS) such as Maxwell criteria (Rabah, A. A., 2014), The (PSRK) equation of state(Lyle, F, A.,2009) and prediction correlation such as Antoine correlation, Wagner correlation, Extend Antoine correlation (Poling, E, Prausnitz, M and O’connel, P,2001),Ambrose–Walton corresponding states correlation(Sivanandam,S. N., Sumathi,S. and Deepa,S. N.,2006),Riedel Corresponding correlation(Riedel,L.,1954),Lee–Kesler’s correlation(Lee,B. I. and M. G. Kesler,1975),Velasco correlation(Sivanandam,S. N., Sumathi,S. and Deepa,S. N.,2006; Carey, F. A. and Sundberg, R. J.,2007),the Cox correlation(Ruzicka, K., Fulem M. and Ruzicka, V.),Generalized equation predicts vapor pressure of hydrocarbons. Oil and gas (Edalat, E., Bozar-Jomehri,R. B. and Mansoori, G. A.,1993), Generalized equation of vapor pressure of normal Alkanes (Rabah, A. A., 2014).

The most common prediction is Antoine modeling (Antoine, C., 1988), which has three-parameters but is valid only within a limited temperature range (Mehrdad, H., Ehsan, S. and Hamidreza, B., 2013). For this purpose, the most frequently used representation is the Antoine (Antoine, C., 1988) correlation (Eqn. 1.1) (Reid, R.C.; Prausnitz, J.M. and Poling, B.E., 1987) it has proved to be the best expression of the relationship of saturated vapor pressure and temperature and has been used recently for the calculation of the vapor pressure of chemical compounds (VDI, "VDI-GVC. VDI- Waermeatlas, 2007) and Wagner (Wagner, W., 1973) correlation, used an elaborate statistical method to develop an equation for representing the vapor pressure behavior of chemicals over the entire temperature range for which experimental data were available. (Mehrdad, H., Ehsan, S. and Hamidreza, B., 2013). (Eq. 1.2), where the relation between vapor pressure and temperature for chemical compounds is described in the following equations:

$$\ln P^s = A - \frac{B}{C + T} \quad 1.1$$

$$\ln P_r^s = (a + b\tau + c\tau^{1.5} + d\tau^3 + d\tau^8)(1 - \tau)^{-1} \quad 1.2$$

where

$$\tau = 1 - T_r \quad 1.3$$

Although Antoine correlation is widely used, Wagner correlation [Eqn. (1.2)] has a wide range of validity down to  $T_r = 0.5$  (Edalat, E., Bozar-Jomehri, R. B. and Mansoori, G. A., 1973).

These equations are widely used; however, they do have main shortcomings. First, the constants for Antoine (A, B, C) and Wagner (a, b, c, d, ...) are fluid specific. Hence a large data bank is needed for each fluid coefficient. On the other hand, by numerical computation, a large memory is needed to store and process the values of the coefficients. Second, both equations cannot predict the vapor pressure of newly developed fluids. With phasing out of CFCs new

refrigerants are developed or under development. These new fluids, their vapor pressure have to be determined experimentally. If a generalized model of vapor pressure correlation is available the task for developing a new correlation will be easy.

I have shown recently the use of the application of boundary conditions to determine the generalized modeling coefficients data in the calculation of the vapor pressure of organic compounds.

Furthermore, it is important to know the values of the vapor pressure of organic compounds under the boundary conditions such as boiling point ( $T_b$ ), critical temperature ( $T_c$ ) and critical pressure ( $P_c$ ) and acentric factor ( $\omega$ ). Such data also help predict the vapor pressure by estimating the generalized modeling coefficients of organic compounds.

In this study, I demonstrate the use of boundary conditions to estimating the generalized modeling coefficients of organic compounds and its vapor pressure, under any given conditions of pressure, as a function of temperature.

The vapor pressure as a function of temperature is calculated using generalized modeling to predict vapor pressure amounts without data bank constants needed for each fluid coefficient and also without large memory needed to store and process the values of the coefficients.

## **1.2 General objectives:**

1. Analysis of existing vapor pressure models.
2. Screening of existing model.
3. Develop generalized modeling for the vapor pressure correlation of organic compounds.

# CHAPTER TWO

## Literature Review

### 2.1 Vapor Pressure Models

The vapor pressure ( $P^\circ$ ) is the pressure of the vapor of a compound in equilibrium with its pure condensed phase (solid or liquid). Vapor pressures depend strongly on the temperature and vary widely with different compounds due to differences in the molecule – molecule interactions. The normal boiling point of a liquid is defined as the temperature at which the vapor pressure of the liquid is 1 atmosphere ( $P^\circ = 1 \text{ atm}$ ). The vapor pressure of a substance is an intrinsic physical property that plays a crucial role in determining its distribution to and from gaseous environmental phases (the atmosphere, marsh bubble gas). The vapor pressure is also crucial for the prediction of equilibrium distribution coefficients to and from natural waters, such as Henry's Law constant ( $K_H$ ). The vapor pressure is generally determined using experimental or theoretical or empirical methods.

### 2.2 Experimental Methods

Numerous experimental techniques exist for measuring vapor pressure; only five general methods have been widely applied to the study of organic compounds. These five generic techniques or methods are referred to as static, ebulliometric (dynamic), effusion (Knudsen and Langmuir), transpiration, and calorimetric (Weir, R. D. and De loos, Th. W., 2005).

### 2.3 Equations of state

The vapor pressure can be also predicted using Maxwell criteria (Rabah, A. A., 2014) equation (2.1)

$$P^s = \frac{1}{\Delta v} \int_1^2 P(T, v) dv \quad 2.1$$

The  $P(T, v)$  is pressure, can be obtained from the equation of state.

Table 2.1 shows some of most widely used cubic equations of state (EOS).

**Table2. 1** Some cubic equations of state (Rabah, A. A. and Mohamed, S.,2010)

EOS	Year	Correlation
VDI	1883	$\frac{a}{v^2}$
SRK	1972	$\frac{a(T)}{v(v+b)}$
PR	1976	$\frac{a(T)}{v(v+b)+b(v-b)}$
HK	1980	$\frac{a(T)}{v^2+c(\omega)bv-(c(\omega)-1)b^2}$
SW	1980	$\frac{a(T)}{v^2+(1+3\omega)bv-3\omega b^2}$
PT	1982	$\frac{a(T)}{v(v+b)+c(v-b)}$
ALS	1983	$\frac{a(T)}{(v-b_1(\omega))(v-b_2(\omega))}$
MNM	1988	$\frac{a(T)}{v^2+2bv-2b^2}$
LLS	1990	$\frac{a(T)}{v^2+\alpha bv-\beta(\omega)b^2}$

## 2.4 Other correlations

There are several vapor pressure correlations available in the literature.

A brief description is given to the most widely used correlations.

### 2.4.1 Antoine Correlation

The Antoine equation is a semi-empirical equation which expresses vapor pressure as a function of temperature, these simple correlation has been widely used over limited temperature ranges as

$$\ln P^s = A - \frac{B}{C+T} \quad 2.2$$

Where A, B, and C are constants that must be derived from experimental data and temperature is in C° and it depends on fluid specific (Rodgers, R. C. and Hill, G. E., 1978).

### 2.4.2 Wagner correlation

Wagner correlation used an elaborate statistical method to develop an equation for representing the vapor pressure behavior (Poling, E, Prausnitz, M and O'Connell, P, 2001), Wagner correlation (Eqn. 2.3) has a wide range of validity down to  $T_r = 0.5$  (Wagner, W., 1973).

$$\ln P_r^s = (a + b\tau + c\tau^{1.5} + d\tau^3 + e\tau^8)(1 - \tau)^{-1} \quad 2.3$$

Where

$$\tau = 1 - T_r, \quad T_r = \frac{T}{T_c}$$

Wagner constants (a, b, c, d, ...) are also dependent on fluid specific. Hence a large data bank is needed for each fluid coefficient. The values also (a, b, c, d, ...) are tabulated for a number of materials in Table 2.2.

**Table 2.2:** Wagner constants (Sencan, A. and Kalogirou, S. A., 2005).

Substance	T <sub>c</sub> , K	P <sub>c</sub> , bar	$\omega$	a	b	c	d
Propane	369.85	42.47	0.152	-6.76368	1.55481	-1.5872	-2.024
Octane	568.95	24.90	0.399	-8.04937	2.03865	-3.3120	-3.648
Benzene	562.16	48.98	0.21	-7.01433	1.55256	-1.8479	-3.713
Pentafluorotoluene	566.52	31.24	0.415	-8.08717	1.76131	-2.72838	-4.138

### 2.4.3 Extend Antoine Correlation

The Extend Antoine correlation reported by the thermodynamics Research Center at Texas A&M they have used the following (Eqn. 2.4) to extend the description of vapor pressure behavior to high temperatures:

$$\log_{10} P_{vp} = A - \frac{B}{C + T - 273.15} + 0.43429x^n + Ex^8 + Fx^{12} \quad 2.4$$

$$x = \frac{(T - t_o - 273.15)}{T_c}$$

Where  $P_{vp}$  in bar and  $T$  in kelvin, these equation is not meant to be extrapolated outside the range of  $T_{min}$  and  $T_{max}$  also the value of constants  $A, B, C, n, E, F$  and  $t_o$  as well as the value of  $T_c$  and  $T_{min}$  and  $T_{max}$  to be used with (Eqn.2.4) are listed in [ref.32].

#### 2.4.4 Ambrose–Walton corresponding states method

Ambrose and Walton (Eqn. 2.5) developed another representation of the Pitzer expansion with an additional term  $f^{(2)}(T_r)$  (Sivanandam, S. N., Sumathi, S. and Deepa, S. N., 2006).

$$\ln P_{vpr} = f^{(0)}(T_r) + \omega f^{(1)}(T_r) + \omega^2 f^{(2)}(T_r) \quad 2.5$$

$$f^{(0)} = \frac{-5.97616\tau + 1.29874\tau^{1.5} - 0.60394\tau^{2.5} - 1.06841\tau^5}{T_r} \quad 2.6$$

$$f^{(1)} = \frac{-5.03365\tau + 1.11505\tau^{1.5} - 5.41217\tau^{2.5} - 7.46628\tau^5}{T_r} \quad 2.7$$

$$f^{(2)} = \frac{-0.64771\tau + 2.41539\tau^{1.5} - 4.26979\tau^{2.5} - 3.2525\tau^5}{T_r} \quad 2.8$$

Where  $\omega$  is the acentric factor,  $P_c$  is the critical pressure (bars) of the fluid, and  $\tau = 1 - T_r$

This set of equations was fit to the vapor pressure behavior of the  $n$ -alkanes and more accurately describes this. The quantity,  $f^2$ , is important only for fluids with large acentric factors and at low reduced temperatures. In fact, it is zero at  $Tr = 0.7$  [Poling, E, Prausnitz, M and O'Connell, P, 2001].

#### 2.4.5 Riedel Corresponding States Method:

Riedel proposed a vapor pressure (Riedel, L., 1954) take the following form (eqn. 2.9):



$$\ln P_{vpr} = A + \frac{B}{T_r} + C \ln T_r + DT_r^6 \quad 2.9$$

The term  $T_r^6$  allows a description of the inflection point of the vapor pressure curve in the high-pressure region. The parameters A, B, C, and D are a function of T, T<sub>c</sub>, T<sub>b</sub>, and P<sub>C</sub>.

In the high-pressure region the values of constants in (Eqn.2.9), defined a parameter  $\alpha$ . (Poling, E, Prausnitz, M and O'Connell, P, 2001).

$$\alpha = \frac{d \ln P_{vp}}{d \ln T_r} \quad 2.10$$

From a study of experimental vapor pressure data, Plank and Riedel showed that

$$\frac{d\alpha}{dT_r} = 0 \text{ at } T_r = 0 \quad 2.11$$

Used (Eqn. 2.10) as a constraint on Riedel (Eqn. 2.9), found that

$$\ln P_{vpr} = A^+ + \frac{B^+}{T_r} + C^+ \ln T_r + D^+ T_r^6 \quad 2.12$$

Where  $A^+ = -35Q$ ,  $B^+ = -36Q$ ,  $C^+ = 42Q + \alpha_c$ ,  $D^+ = -Q$  and  $Q = k(3.758 - \alpha_c)$

The  $\alpha_c$  is  $\alpha$  at the critical point, and the Riedel originally chose K to be 0.0838, but

Vetere (1991) has found that for alcohols and acids, improved predictions result if the expressions shown in Table 2.3 are used. The correlating parameter in these expressions, h, is defined:

$$h = T_{br} \frac{\ln(P_c / 1.01325)}{1 - T_{br}} \quad 2.13$$

Since it is not easy (or desirable) to determine  $\alpha_c$  by its defining equation at the critical point,  $\alpha_c$  is usually found from (eqn.2.10) by inserting  $P = 1.01325$  bar at  $T = T_b$  and calculating  $\alpha_c$ .

$$\alpha_c = \frac{3.758K\Psi_b + \ln(P_c / 1.01325)}{K\Psi_b - \ln T_{br}} \quad 2.14$$

where

$$\Psi_b = -35 + \frac{36}{T_{br}} + 42 \ln T_{br} - T_{br}^6$$

**Table 2.3:** Vetere Rules for Riedel Constant K for Acids and Alcohols

Acids	$K = -0.120 + 0.025h$
Alcohol	$K = 0.373 - 0.030h$

#### 2.4.6 Lee–Kesler’s Method:

The vapor pressure can obtain by Lee–Kesler’s method (Lee, B. I. and M. G. Kesler, 1975) is one of the successful methods to predict the vapor pressure using the three-parameter formulations (Sivanandam, S. N., Sumathi, S. and Deepa, S. N., 2006) equation (2.15).

$$\ln P_{vpr} = f^{(0)}(T_r) + \omega f^{(1)}(T_r) \quad 2.15$$

where

$$f^{(0)} = 5.92714 - \frac{6.09648}{T_r} - 1.28862 \ln T_r + 0.169347 T_r^6$$

$$f^{(1)} = 15.2518 - \frac{15.6875}{T_r} - 13.4721 \ln T_r + 0.43577 T_r^6$$

$P_{vpr}$  is the reduced vapor pressure which equals to  $\frac{P}{P_c}$ ,  $P_c$  is the critical pressure (pascal),  $\omega$  is the acentric factor,  $T_r$  is the reduced temperature which equals  $\frac{T}{T_c}$ .

The values of  $T_c$  and  $P_c$  can be found in the literature for many pure substances.

#### 2.4.7 Velasco equation Method

Velasco et al. [Carey, F. A. and Sundberg, R. J., 2007] developed a new simple equation for predicting the temperature dependence of the vapor pressure of a pure substance along with the entire (liquid + vapor) coexistence curve, from the triple point to the critical point. The formulation of this method is presented as follow:

$$\ln P_r = \frac{T_t}{T} \ln P_{tr} \frac{1-t}{(1+a_1t)[1+b_0t(t-t_b)]} \quad 2.16$$

where:

$$t = \frac{T_r - T_{tr}}{1 - T_{tr}} \quad 2.17$$

$$t_b = \frac{T_{br} - T_{tr}}{1 - T_{tr}} \quad 2.18$$

$a_1$  and  $b_0$  are constant substance-dependent parameters,  $T_t$  is triple point temperature, and  $T_b$  is normal boiling point temperature.

#### 2.4.8 The Cox equation:

Kvetoslav Ruzicka, Michal Fulem, Vlastimil Ruzicka, reported for the Cox (eqn. 2.19) showed below:

$$\ln\left(\frac{P_s}{P_0}\right) = \left(1 - \frac{T_0}{T}\right) \exp\left(\sum_{i=1}^n A_i T^i\right) \quad 2.19$$

It can be considered to be the most useful equations for extrapolations toward low pressures; the possibility of changing both the number of parameters and the reference condition  $T_0$  and  $P_0$  allows one to obtain different forms suitable for particular applications. The three-parameter form with the normal boiling point ( $T_0=T_b$  and  $P_0=101,325$  kPa) is very dependable in both simple and controlled extrapolation for all organic liquids exception for hydrogen-bonded compounds. In the latter case, the four-parameter equation gives very good results for extrapolation when vapor pressures and the thermal data are fitted simultaneously. For compounds decomposing below the normal boiling temperature, a vapor pressure corresponding to a lower temperature can always be used as a reference condition. On the other hand, the use of the critical point allows one to transform the Cox equations into a relationship suitable for the description of the complete vapor pressure line. The four-parameter form with

reference conditions  $T_c$  and  $P_c$  is comparable to the Wagner equation and behaves similarly in correlation and extrapolation toward low pressures.

The Wagner equations require the use of critical parameters that provide for the realistic prediction of the vapor-pressure saturation line up to the critical temperature. However, this constraint limits the flexibility of the relationship in low-pressure extrapolations and is both useless and inconvenient for high boiling chemicals that decompose below or near the normal boiling temperature (Ruzicka, K.; Fulem M.; Ruzicka, V.).

#### **2.4.9 Generalized equation predicts vapor pressure of hydrocarbons. Oil and gas:**

A new equation predicts vapor pressure of hydrocarbons [Edalat, E., Bozar-Jomehri, R. B. and Mansoori, G. A., 1993], this new equation (Eqn. 2.20) need in the critical industry and it is developed by Wagner's is a bit more generalized.

$a$ ,  $b$ ,  $c$  and  $d$  are characteristic constants for the fluid under study and  $P^s$  is vapor (saturation) pressure. If the parameters  $a$ ,  $b$ ,  $c$ ,  $d$  are available for pure hydrocarbons, the equation predicts vapor pressure within the acceptable accuracy down to a reduced temperature.

$$\ln P_r^s = [a(\omega)\tau + b(\omega)\tau^{1.5} + c(\omega)\tau^3 + d(\omega)\tau^6(1-\tau)^{-1}] \quad 2.20$$

where

$$\omega = (-\log P_r^s)_{T_r=0.7} - 1$$

$$a(\omega) = -6.1559 - 4.0855\omega$$

$$b(\omega) = 1.5737 - 1.0540\omega - 4.4365 \times 10^{-3} d(\omega)$$

$$c(\omega) = -0.8747 - 7.887\omega$$

$$d(\omega) = (-0.4893 - 0.9912\omega + 3.1551\omega^2)^{-1}$$

The equation has been successfully tested for a variety of fluids and can be readily used in the oil and gas industry.

This simple generalized equation (Eqn. 2.20) also presented here accurately estimates the vapor pressure of hydrocarbons, non hydrocarbons, and polar fluids.

The results predict vapor pressure of hydrocarbons, non hydrocarbons, and polar fluids, more accurately without the need for information about any additional parameters.

#### 2.4.10 Generalized correlation of normal Alkanes:

From Antoine correlation (eqn.2.2) developed generalized correlation of normal Alkanes (Rabah, A. A., 2014), it mentioned earlier Antoine coefficient is a function of the type of fluid as

$$y=(\text{fluid})$$

The y represents any of coefficients A, B and C and its dependency on physical parameters such as critical properties. Hence the equation becomes.

$$y = y(T, T_b, T_c, M, \omega)$$

Used the principles of the corresponding state to reduce to equation 2.21 as

$$\ln\left(\frac{P^s}{P_c}\right) = A' - \frac{B'}{C' + T_r} \quad 2.21$$

$$A' = A - \ln P_c, B' = \frac{B}{T_c}, C' = \frac{C}{T_c}, T_r = \frac{T}{T_c}$$

The acentric factor is a function of vapor pressure and the normal boiling point as

$$y' = y'(M)$$

The coefficient becomes A', B', C' within the range of  $T_{\min}$  and  $T_{\max}$  as well as physical parameters (M,  $T_c$ ,  $P_c$ ,  $\omega$ ) and A, B and C are Antoine coefficients are obtained from the literature.

# CHAPTER THREE

## Modeling

### 3.0 Modeling

The objective of this work is the develop of new vapor pressure correlation for the prediction of the vapor pressure of organic compounds namely n-alkanes, cycloalkanes, branched alkanes, alkenes, alkynes, haloalkanes, diene, aromatic hydrocarbons, halo benzene, alcohols, ethers, ketones, esters, amines, and xylene. The model is based on the original Antoine equation 3.1

$$\ln P^s = A - \frac{B}{C + T} \quad 3.1$$

To generalize the equation the constants A, B and C will be determined using physical boundary conditions as:

1. Critical condition  $T_c, P_c$ . The critical condition data is available for a wide range of fluid with high accuracy
2. Normal boiling point  $T_b$  at  $P=1$  atm. The  $T_b$  is available as well as for a wide range of fluid with high accuracy.
3. Acentric factor which is given by equation

$$\omega = -(\log P_r^s)_{T_r=0.7} - 1 \quad 3.2$$

Similarly the acentric is also available for many fluids with a high level of accuracy.

It means, the generalized coefficients or parameters  $A', B'$  and  $C'$  dependency on physical constant of organic compounds and it can be easy to find the physical constants of any organic compounds ( $T_{br}, P_C, \omega$ ) to predict the values of vapor pressure of organic compounds other than Antoine coefficients or parameters A, B, and C.

Apply the three boundary conditions to equation 3.1 the three constants are obtained with some algebraic manipulation as (for more details of derivation see appendix 7).

$$A' = \frac{\beta_1}{\beta_2} \quad 3.3$$

$$B' = \frac{\beta_1[\beta_2 + \beta_3]}{\beta_2^2} \quad 3.4$$

$$C' = \frac{\beta_3}{\beta_2} \quad 3.5$$

Where

$$\beta_1 = \ln P_c (1.6 - 2.3T_{br})(\omega + 1)$$

$$\beta_2 = 0.3 \ln P_c + 2.303(T_{br} - 1)(\omega + 1)$$

$$\beta_3 = -0.3T_{br} \ln P_c - 1.6(T_{br} - 1)(\omega + 1)$$

### 3.1 Model Equation:

The development of new vapor pressure equation(Eqn. 3.8):

$$\ln P - \ln P_c = A' - \frac{B'}{C' + T_{rb}} \quad 3.6$$

$$\ln P_s = A' - \frac{B'}{C' + T_{rb}} + \ln P_c \quad 3.7$$

$$P_s = \exp\left(A' - \frac{B'}{C' + T_{rb}} + \ln P_c\right) \quad 3.8$$

	A	B	C	D	E	F	G	H	I	J
	NO	Tcent	T	Pc	Tc	Tr	A'	B'	C'	P(mmHg)
2	1	264.64	537.79	20.8	720	0.75	10.814	12.51	0.157	793.4458
3	2	284.65	557.8	20.8	720	0.77	10.814	12.51	0.157	1068.448
4	3	314.7	587.85	20.8	720	0.82	10.814	12.51	0.157	2131.55
5	4	347.46	620.61	20.8	720	0.86	10.814	12.51	0.157	3527.073
6		365.4	638.55	20.8	720	0.89	10.814	12.51	0.157	5017.486
7		382	655.15	20.8	720	0.91	10.814	12.51	0.157	6276.999
8		405.7	678.85	20.8	720	0.94	10.814	12.51	0.157	8649.699
9		300	573.15	20.8	720	0.8	10.814	12.51	0.157	1631.097
10		290	563.15	20.8	720	0.78	10.814	12.51	0.157	1233.965
11		422.6	695.75	20.8	720	0.97	10.814	12.51	0.157	11717.54
12		435.7	708.85	20.8	720	0.98	10.814	12.51	0.157	12919.2
13		446.85	720	20.8	720	1	10.814	12.51	0.157	15625.55

Figure3.1: Model Vapor Pressure of 1.Dodecanol using Excel program.

### 3.2 Model Validation:

The model is validated using the following data

1. Experimental data obtained available from open sources compared with the model for a wide range of organic compounds.
2. The model compared with the original Antoine equation for a wide range of organic compounds namely n-alkanes, cycloalkanes, branched alkanes, alkenes, alkynes, haloalkanes, diene, aromatic hydrocarbons, halo benzene, alcohols, ethers, ketones, esters, amines, and xylene. The physical constants ( $T_c$ ,  $P_c$ ,  $T_b$ ,  $w$ , and  $M$ ) were collected from the literature as shown in Appendix 1.

For the comparison, the two statistical methods of Percent Deviation (PD) and Average Absolute Percent Deviation (AAPD) as given respectively and the all data computation and analysis by the Excel program.

$$PD = \frac{P_{Antoine} - P_{Dev.Generalized}}{P_{Antoine}} \times 100 \quad 3.9$$

$$AAPD = \frac{1}{N} \sum |PD| \quad 3.10$$

Where:

$P_{Antoine}$  = Vapor pressure of the Antoine equation.

$P_{Development}$  = Vapor pressure of development generalized modeling.

$N$  = Number of the data points.



# CHAPTER FOUR

## Results and Discussions

### 4.1 Results

#### 4.1.1 Values of model constants $A'$ , $B'$ , $C'$ :

The importance of this study that model coefficients depend on physical constants. The results based on the generalized modeling for the vapor pressure of organic compounds such as n-alkanes, cycloalkanes, branched alkanes, alkenes, alkynes, haloalkanes, diene, aromatic hydrocarbons, halo benzene, alcohols, ethers, ketones, esters, amines and xylene, Table 4.1 shows the values of the model constants  $A'$ ,  $B'$ ,  $C'$  its generated from using three physical boundary conditions as critical condition  $T_c$ ,  $P_c$ , normal boiling point  $T_b$  at  $P=1$  atm and Accentric factor which is given by Pitzer equation(Eqn.2.21) then applied on original Antoine equation 3.1. The new equations of  $A'$ ,  $B'$ ,  $C'$  [Eqns. 3.3, 3.4, 3.5] as function of  $T_c$ ,  $P_c$ ,  $T_b$ ,  $\omega$  with applied actual values of its parameters [reffer to appendix 1] I found the values of model constants  $A'$ ,  $B'$ ,  $C'$  and the Antoine constants generated from (Ref. 18) and the application temperature range for wide range of organic compounds.

The result of modeling more accuracy and it depends on physical constants other than the Antoine equation. The data shows a strong correlation between the physical boundary conditions. The trend in increasing or decreasing depends on its conditions.

**Table4.1:** Model and Antoine correlations coefficients values.

No	Compound	Model Constants (References: Model)			Antoine Constants (References: [65])			
		$A'$	$B'$	$C'$	$A$	$B$	$C$	Temperature range(°C) $T_{min}$ , $T_{max}$

<i>(1). n-Alkanes</i>								
1	Methane	4.850	4.489	-0.074	6.846	435.621	271.361	-182.48, -82.57
2	Ethane	6.124	6.279	0.025	6.953	699.106	260.264	-182.8, 32.27
3	Propane	6.290	6.358	0.011	7.019	889.864	257.084	-187.69, 96.67
4	Butane	5.826	5.407	-0.072	7.009	1022.48	248.145	-138.29, 152.03
5	Pentane	4.772	3.771	-0.210	7.009	1134.15	238.678	-129.73, 196.5
6	Hexane	7.501	7.736	0.031	6.990	1216.92	227.451	-95.31, 234.28
7	Heptane	1.822	0.826	-0.546	7.046	1341.89	223.733	-90.59, 267.11
8	Nonane	5.631	4.760	-0.155	7.188	1607.74	222.414	-53.52, 322.5
9	Decane	5.679	4.666	-0.178	7.217	1693.93	216.459	-29.66, 345.3
10	Undecane	5.943	4.905	-0.175	7.181	1706.26	200.897	-25.58, 365.61
11	Dodecane	6.367	5.368	-0.157	7.229	1807.47	199.381	-9.58, 385.05
<i>(2). Cycloalkanes</i>								
1	Cyclopentane	5.573	5.042	-0.095	7.043	1202.53	239.69	-93.87, 238.61
2	Cyclohexane	5.356	4.672	-0.128	7.009	1296.23	233.309	6.54, 280.39
3	Methylcyclohexane	6.701	6.695	-0.001	7.001	1375.13	232.819	-126.57, 299.04
<i>(3). Branched alkanes</i>								

1	3-Ethyl pentane	3.692	2.405	-0.349	7.109	1402.17	238.129	-118.6, 267.49
2	2-Methyloctane	17.492	35.156	1.001	7.137	1553.89	221.781	-80.37, 313.6
<i>(4). Alkenes</i>								
1	Ethene(Ethylene)	5.367	5.062	-0.057	6.966	649.806	262.73	-169.14, 9.21
2	Propene(Propylene)	5.080	4.463	-0.121	7.017	860.992	255.895	-184.15, 91.61
3	1-Butene	4.775	3.907	-0.182	7.034	1013.6	250.292	-185.35, 146.44
<i>(5). Alkynes</i>								
1	Ethyne(Acetylene)	5.591	5.102	-0.087	7.315	790.209	262.859	-80.75, 35.17
2	1-Pentyne	5.137	3.950	-0.231	7.212	1223.32	242.283	-105.7, 208.05
<i>(6). Haloalkanes</i>								
1	Difluoromethane	6.057	5.542	-0.085	7.290	863.592	247.503	-136.15, 78.45
2	Trichlorofluoro methane (R11)	5.628	5.127	-0.089	6.994	1081.98	239.265	-111.11, 198.05
3	Bromotrifluoromethane	6.265	6.213	-0.008	6.972	800.838	253.656	-168, 67
4	1,1-Difluoroethane (R152a)	7.303	7.592	0.040	7.120	928.549	244.854	-117, 113.45
5	1,1,1-Trifluoroethane (R143a)	6.338	6.014	-0.051	7.076	846.165	249.078	-111.3, 73.1
6	1,1,1,2-tetrafluoroethane (R134a)	5.549	4.646	-0.163	7.010	902.327	244.514	-101, 106.85
7	Pentafluoroethane (R125)	6.910	6.760	-0.022	6.995	811.133	245.168	-103, 68.85

8	1-Chloro-1,1,2,2-Tetrafluoroethane (R124)	6.621	6.468	-0.023	7.069	968.741	243.018	-15.41, 126.85
9	2-Chlorobutane	4.182	3.032	-0.275	7.253	1378.58	247.194	-131.3, 247.45
<i>(7). S-Alkyl</i>								
1	Methanethiol(Methyl mercaptan)	6.030	5.930	-0.0167	7.072	1008.88	234.729	-122.97, 196.8
2	3-Thiapentane(Diethyl sulfide)	6.414	6.045	-0.058	7.204	1423.41	237.112	-103.95, 284
<i>(8). Diene</i>								
1	1,3- Butadiene	6.061	5.805	-0.042	7.022	998.721	245.563	-108.9, 152.22
<i>(9). Aromatic hydrocarbons</i>								
1	Benzene	5.183	4.441	-0.143	7.064	1296.93	229.916	5.53, 289.01
2	Toluene	5.054	4.130	-0.183	7.136	1457.29	231.827	-94.97, 318.64
3	2-Methyl phenol(o-cresol)	4.029	2.652	-0.342	7.368	1727.17	193.918	31.04, 424.4
4	3-Methyl phenol(m-cresol)	7.706	7.498	-0.027	7.267	1670.93	178.653	12.24, 432.7
5	4-Methyl phenol(p-cresol)	10.065	11.513	0.144	7.458	1768.27	184.313	34.78, 431.5
6	Ethylbenzene	6.994	6.903	-0.013	7.166	1559.55	228.582	-95, 344.02
7	Butylbenzene	4.159	2.629	-0.368	7.185	1720.37	216.413	-87.85, 387.4
<i>(10). Halo benzene</i>								
1	Hexafluorobenzene	9.809	11.464	0.169	7.221	1329.93	226.134	5.1, 243.58

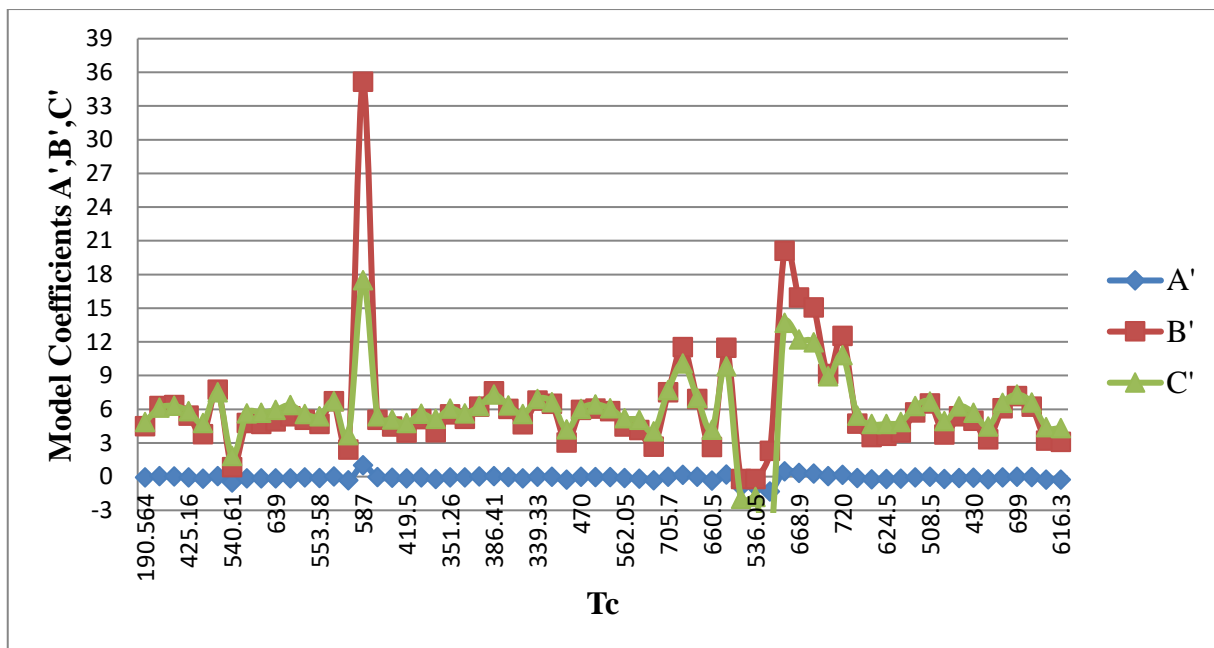
(11). Alcohols								
1	Isobutanol	-2.005	-0.214	-0.893	7.459	1386.1	195.079	-108, 274.58
2	Sec-butanol	-1.818	-0.224	-0.877	7.561	1448.35	209.886	-114.7, 262.86
3	1-Pentanol	-6.556	2.290	-1.349	7.458	1516.51	193.53	-77.59, 313
4	1-Octanol	13.698	20.106	0.468	7.160	1536.79	163.905	-15.5, 379.35
5	1-Nonanol	12.210	15.949	0.306	7.046	1520.83	152.06	-5, 399.85
6	1-Decanol	11.936	15.060	0.262	7.038	1579.82	149.864	6.9, 416.85
7	1-undecanol	8.922	9.121	0.022	6.911	1551.12	139.882	15.9, 430.85
8	1-dodecanol	10.814	12.510	0.157	6.889	1589.5	134.693	23.8, 447.85
(12). Ethers								
1	Methyl ethyl ether	5.417	4.700	-0.132	6.630	760.22	195.446	-113.15, 164.65
(13). Ketones								
1	Butanone(Methyl ethyl ketone)	4.668	3.520	-0.246	7.294	1400.37	237.655	-86.67, 262.35
2	Cyclopentanone	4.690	3.615	-0.229	7.566	1727.86	238.153	-51.3, 352.85
(14). Esters								
1	Methyl formate	4.853	3.897	-0.197	7.265	1178.19	236.959	-99, 214.05
2	Methyl acetate	6.273	5.709	-0.090	7.280	1276.29	233.155	-98, 233.65
3	Ethyl methanoate(Ethyl formate)	6.686	6.515	-0.026	7.218	1252.8	234.565	-79.6, 235.25
4	Ethyl acetate	4.925	3.746	-0.239	7.260	1338.46	228.608	-83.55,

								250.15
5	Propyl ethanoate(Propyl acetate)	6.254	5.369	-0.141	7.223	1408.02	222.76	-95, 276.25
<i>(15). Amines</i>								
1	Methylamine	5.682	4.977	-0.124	7.364	1025.4	235.062	-93.46, 156.9
2	2-Propanamine(Methyl ethyl amine)	4.436	3.324	-0.251	6.870	943.96	200.649	-25.6, 201.85
3	1-Butanamine(Butyl amine)	6.549	6.074	-0.073	7.210	1316.41	226.655	-49.1, 258.75
4	Benzeneamine(Aniline)	7.301	7.168	-0.018	7.293	1668.15	193.636	-6.02, 425.85
<i>(16). Xylene</i>								
1	1,2-dimethylbenzene(O-Xylene)	6.585	6.214	-0.056	7.149	1566.59	222.596	-25.17, 357.22
2	1,3-dimethylbenzene (m-Xylene)	4.407	3.190	-0.276	7.181	1573.02	226.671	-47.85, 343.9
3	1,4-dimethylbenzene(P-Xylene)	4.311	3.088	-0.284	7.155	1553.95	225.23	13.26, 343.11

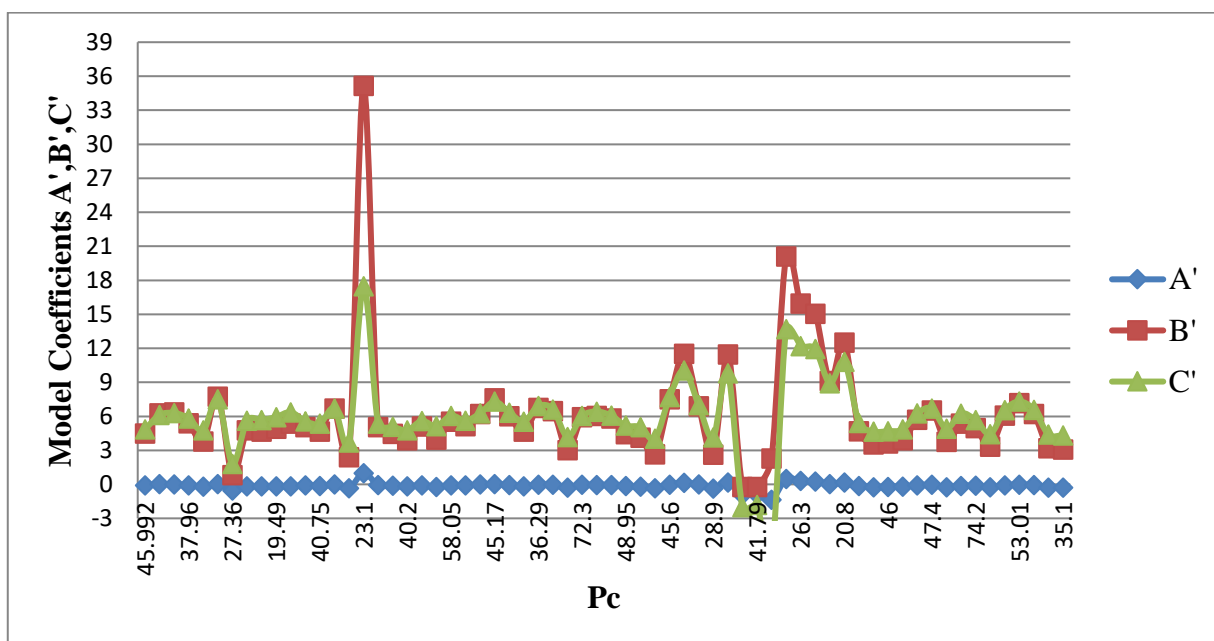
The figure 4.1 to 4.4 represents the dependency of the model coefficients with physical constants  $T_c$ ,  $P_c$ ,  $T_b$ , and  $\omega$ .

$$A', B', C' = f(T_c, P_c, T_b, \omega) \quad 1.4$$

The figure show strong and clear the variation of model coefficients with physical constants such as  $T_c$ ,  $P_c$ ,  $T_b$ , and  $\omega$ .



**Figure4.1:** Dependency of Model coefficients on critical temperature.



**Figure4.2:** Dependency of Model coefficients on critical pressure.

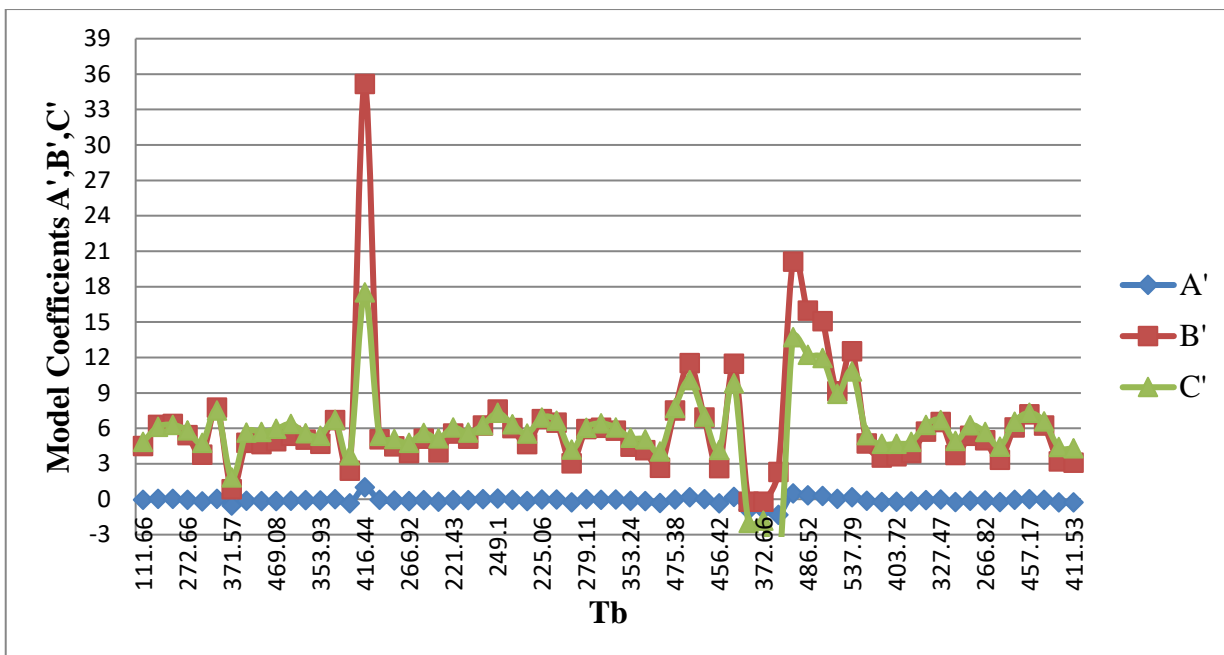


Figure 4.3: Dependency of Model coefficients on boiling point.

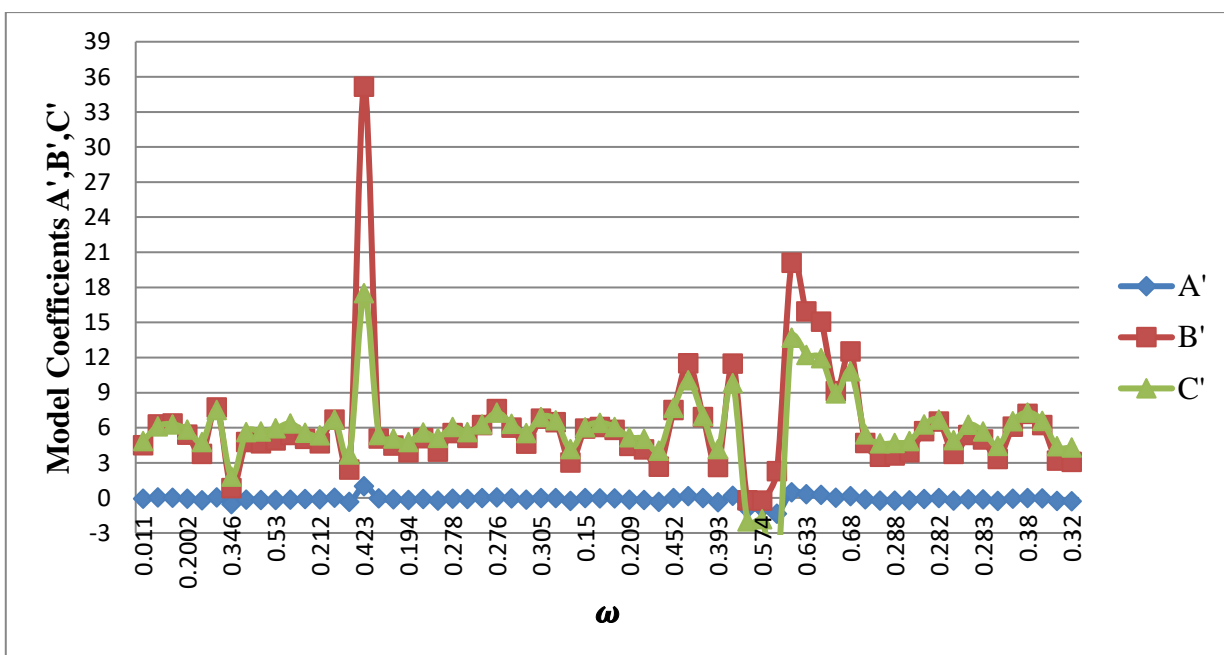


Figure 4.4: Dependency of Model coefficients on eccentric factor.



## 4.2 Vapor pressure

The modeling vapor pressure of organic compounds is carried out (see appendix 7), this model vapor pressure is validated using experimental data and Antoine equation respectively. The experimental data covered 25 of different available organic compounds of n-alkanes, cycloalkanes, branched alkanes, alkenes, alkynes, haloalkanes, diene, aromatic hydrocarbons, halo benzene, alcohols, ethers, ketones, esters, amines, and xylene. The data point is about 228. The experimental data are compared with the current model correlation and Statistical data were calculated. Table 4.2 shows the result of the comparison between the experimental data and model. Summary of PD, AAPD,  $T_{\min}$ ,  $T_{\max}$ , number of the data point. Most of the data fall within AAPD of 5% for each compound under study. The results show that the current equation is superior to the other correlation. This may be attributed to the fact that the current correlation is based on physical constants and is more accurate when compared with experimental data.

Also we shows that AAPD of some alkanes namely- heptanes, nonane, and decane are greater and the justify of this because the reduce boiling point of all above 0.69 just like alcohol and this model suitable according to limitation of Pitzer equation.

The few data that fall outside this range can be considered as random errors. On the other hand, it can be attributed to the Antoine equation and compared with model data. Table 4.3 shows Antoine and model Statistical data. The data covered 64 organic compounds of n-alkanes, cycloalkanes, branched alkanes, alkenes, alkynes, haloalkanes, diene, aromatic hydrocarbons, halo benzene, alcohols, ethers, ketones, esters, amines, and xylene. The data point is about 666. Statistical methods of PD and AAPD were calculated for 64 compounds. Table 4.3 shows a comparison with the Antoine correlation. Summary of PD, AAPD,  $T_{\min}$ ,  $T_{\max}$ , number of data points for each compound. Most of the data

fall within AAPD of 10%. (Table 4.3 indicated that the Antoine equation is associated with an error in the range of 10%).

**Table 4.2:** Experimental and Model Statistical data

No	Compound	T <sub>min</sub> °C	T <sub>max</sub> °C	APD <sub>min</sub> %	APD <sub>max</sub> %	AAPD %	Data points
<i>(1).n-Alkanes</i>							
1	Methane	-161.49	-82.586	0.29	6.94	3.18	10
2	Ethane	-88.6	32.18	0.65	6.99	3.10	7
3	Propane	-42.13	96.7	0.38	5.17	2.56	7
4	Butane	-0.49	152.01	0.04	7.57	3.49	7
5	Pentane	36.07	196.45	0.14	11.45	7.04	9
6	Hexane	68.73	234.45	0.07	12.90	4.02	10
7	Heptane	98.42	267.46	0.26	55.04	30.73	10
8	Nonane	150.82	321.48	0.21	29.83	13.47	10
9	Decane	174.15	344.45	0.93	17.08	9.96	10
Grand				0.33	17.00	8.62	80
<i>(2).Cycloalkanes</i>							
1	Cyclopentane	49.5	238.65	0.17	10.30	4.59	10
2	Cyclohexane	80.78	280.43	0.18	9.73	5.73	10
Grand				0.18	10.02	5.16	20
<i>(3).Alkenes</i>							
1	Ethene(Ethylene)	-103.73	9.19	1.92	5.28	4.09	7
2	Propene(Propylene)	-47.69	91.65	0.10	21.38	9.71	10
Grand				1.01	13.33	6.9	17
<i>(4).Alkynes</i>							
1	Ethyne(Acetylene)	-84.75	35.17	0.28	10.43	5.57	10
Grand				0.28	10.43	5.57	10
<i>(5).Haloalkanes</i>							

1	1,1-difluoroethane (R152a)	-24.05	113.26	0.26	6.22	3.57	7
2	1,1,1,2-tetrafluoroethane (R134a)	-26.11	101.03	1.03	9.18	4.75	7
3	Pentafluoroethane (R125)	-48.09	66.18	0.05	9.10	3.12	7
Grand				0.45	8.17	3.81	21
<i>(6).Diene</i>							
1	1,3- Butadiene	-4.53	152	0.15	5.47	2.90	10
Grand				0.15	5.47	2.90	10
<i>(7).Aromatic hydrocarbons</i>							
1	Toluene	110.64	318.65	0.22	8.34	2.64	10
2	Ethylbenzene	136.21	343.95	0.15	11.31	5.24	10
Grand				0.19	9.83	3.94	20
<i>(8).Esters</i>							
1	Methyl acetate	56.94	233.65	0.06	8.40	4.19	10
2	Ethyl acetate	77.06	250.1	0.25	12.49	6.56	10
Grand				0.16	10.45	5.38	20
<i>(9).Amines</i>							
1	Benzene amine(Aniline)	184.02	425.85	0.18	7.98	3.28	10
Grand				0.18	7.98	3.28	10
<i>(10).Xylene</i>							
1	1,2-dimethyl benzene (O-Xylene)	144.44	357.25	0.24	9.99	3.97	10
2	1,3-dimethyl benzene (m- Xylene)	139.19	343.85	0.09	12.61	7.09	10
Grand				0.17	11.3	5.53	20

<b>Total Grand</b>	<b>0.31</b>	<b>10.40</b>	<b>5.11</b>	<b>228</b>
--------------------	-------------	--------------	-------------	------------

Table 4.2 and table 4.3 shows clearly the comparison result between the model with experimental data and Antoine equation over the temperature range ( $T_{\min}$ ,  $T_{\max}$ ) of different organic compounds vapor pressures are summarized.

**Table 4.3:** Antoine and Model Statistical data

No	Compound	$T_{\min}$ °C	$T_{\max}$ °C	APD <sub>min</sub> %	APD <sub>max</sub> %	AAPD %	Data points
<i>(1).n-Alkanes</i>							
1	Methane	-161.49	-82.586	1.67	4.10	2.97	7
2	Ethane	-88.6	32.18	0.1	6.99	3.52	7
3	Propane	-42.13	96.7	0.01	4.55	1.96	11
4	Butane	-0.49	152.01	0.09	6.66	2.77	13
5	Pentane	36.07	196.45	0.13	9.92	3.28	13
6	Hexane	68.73	234.45	0.14	13.31	7.76	9
7	Heptane	98.42	267.46	0.17	48.55	25.20	14
8	Nonane	150.82	321.48	0.41	30.30	13.35	17
9	Decane	174.15	344.45	0.80	18.46	8.61	13
10	Undecane	195.93	365.85	1.26	17.75	6.65	15
11	Dodecane	216.33	384.85	0.09	12.50	7.56	8
Grand				0.44	15.74	7.60	127
<i>(2).Cycloalkanes</i>							
1	Cyclopentane	49.5	238.65	0.18	6.3	2.26	13
2	Cyclohexane	80.78	280.43	0.18	11.35	3.38	11
3	Methylcyclohexane	100.94	299.04	0.05	8.96	3.17	9
Grand				0.14	8.87	2.94	33
<i>(3).Branched alkanes</i>							
1	3-Ethyl pentane	93.48	267.35	0.02	19.97	10.22	9
2	2-Methyloctane	143.29	313.85	0.28	18.65	9.85	10

Grand				0.15	19.31	10.04	19
<i>(4).Alkenes</i>							
1	Ethene(Ethylene)	-103.73	9.19	0.14	6.73	3.17	8
2	Propene(Propylene)	-47.69	91.65	0.07	4.71	1.78	12
3	1-Butene	-6.23	146.35	0.05	7.64	3.08	10
Grand				0.09	6.36	2.68	30
<i>(5).Alkynes</i>							
1	Ethyne(Acetylene)	-84.75	35.17	0.2	5.78	3.11	6
2	1-Pentyne	40.23	196.85	1.35	17.65	11.65	8
Grand				11.72	17.65	7.38	14
<i>(6).Haloalkanes</i>							
1	Difluoromethane	-51.72	78.11	0.05	5.78	1.98	8
2	Trichlorofluoromethane (R11)	23.66	197.95	0.51	5.55	2.43	8
3	Bromotrifluoromethane	-58.01	67	0.01	8.78	4.09	8
4	1,1-difluoroethane (R152a)	-24.05	113.26	0.58	13.28	5.10	13
5	1,1,1-Trifluoroethane (R143a)	-47.29	73.15	0.99	8.06	2.54	7
6	1,1,1,2-tetrafluoroethane (R134a)	-26.11	101.03	5.71	22.07	14.35	12
7	Pentafluoroethane (R125)	-48.09	66.18	0.62	10.82	6.13	9
8	1-Chloro-1,1,2,2- Tetrafluoroethane (R124)	-11.77	126.85	0.17	8.26	4.70	6
9	2-Chlorobutane	68.09	247.45	0.96	12.32	4.01	8
Grand				1.07	10.55	5.04	79

<i>(7).S-Alkyl</i>							
1	Methanethiol(Methyl mercaptan)	5.96	196.85	0.01	7.81	3.84	10
2	3-Thiapentane(Diethyl sulfide)	92.1	283.85	0.07	5.42	2.31	8
Grand				0.04	6.62	3.08	18
<i>(8).Diene</i>							
1	1,3- Butadiene	-4.53	152	0.02	4.98	1.94	9
Grand				0.02	4.98	1.94	9
<i>(9).Aromatic hydrocarbons</i>							
1	Benzene	80.09	288.9	0.01	10.62	3.47	11
2	Toluene	110.64	318.65	0.01	8.34	3.50	15
3	2-Methyl phenol(o-cresol)	191.02	424.45	0.33	15.02	7.86	13
4	3-Methyl phenol(m-cresol)	202.23	432.55	0.20	13.62	8.40	11
5	4-Methyl phenol(p-cresol)	201.97	431.35	0.36	18.70	10.03	12
6	Ethylbenzene	136.21	343.95	1.09	12.94	6.06	17
7	Butylbenzene	183.27	387.35	0.01	48.03	10.62	10
Grand				0.29	18.18	7.13	89
<i>(10).Halo benzene</i>							
1	Hexafluorobenzene	80.25	243.58	0.39	19.90	10.51	10
Grand				0.39	19.90	10.51	10
<i>(11).Alcohols</i>							
1	Isobutanol	107.89	274.63	0.37	809.86	179.06	9
2	Sec-butanol	99.51	262.9	0.01	244.4	91.45	6
3	1-Pentanol	138.01	315	1.43	85.56	35.33	10
4	1-Octanol	195.18	379.35	0.26	13.23	7.41	8
5	1-Nonanol	213.37	395.75	0.82	9.01	6.62	8
6	1-Decanol	231.07	411.25	0.59	11.67	5.66	9

7	1-Undecanol	248.09	431.85	0.18	7.98	4.13	10
8	1-Dodecanol	264.64	446.85	2.07	14.85	6.28	12
Grand				0.72	149.57	41.99	72
<i>(12).Ethers</i>							
1	Methyl ethyl ether	7.35	164.65	0.16	9.96	4.63	9
Grand				0.16	9.96	4.63	9
<i>(13).Ketones</i>							
1	Butanone(Methyl ethyl ketone)	79.56	263.65	0.31	9.91	4.15	9
2	Cyclopentanone	130.57	351.35	0.62	19.93	7.65	10
Grand				0.47	14.92	5.90	19
<i>(14).Esters</i>							
1	Methyl formate	31.75	214.05	0.13	9.39	4.01	13
2	Methyl acetate	56.94	233.65	0.04	8.29	3.42	13
3	Ethyl methanoate(Ethyl formate)	54.32	235.35	0.14	8.78	4.56	11
4	Ethyl acetate	77.06	250.1	0.75	12.58	5.58	7
5	Propyl ethanoate(Propyl acetate)	101.5	276.25	0.42	19.3	6.90	10
Grand				0.30	11.67	4.89	54
<i>(15).Amines</i>							
1	Methylamine	-6.33	156.85	0.43	5.87	3.51	10
2	2-Propanamine(Methyl ethyl amine)	31.78	198.65	6.01	16.31	11.1	9
3	1-Butanamine(Butyl amine)	76.29	253.65	0.23	7.28	3.52	7
4	Benzeneamine(Aniline)	184.02	425.85	0.01	10.48	4.68	15
Grand				1.67	9.96	5.70	41
<i>(16).Xylene</i>							
1	1,2-dimethylbenzene	144.44	357.25	0.10	9.28	3.52	15

	(O-Xylene)						
2	1,3-dimethylbenzene (m- Xylene)	139.19	343.85	0.24	12.77	4.16	15
3	1,4-dimethyl benzene (P- Xylene)	138.38	343.15	0.08	13.51	4.76	13
Grand				0.14	11.85	4.15	43
<b>Total Grand</b>				<b>0.55</b>	<b>29.86</b>	<b>10.33</b>	<b>666</b>

The results of both model and experimental, model and Antoine produced results with Average absolute percent deviation AAPD of 5% and 10% respectively.

From the predictive method, that is to say, the model has been successfully tested for a variety of compounds and can be readily used for organic compounds.



# CHAPTER FIVE

## Conclusions and Recommendations

### 5.1 Conclusions:

The vapor pressures of organic compounds are the most important thermodynamics property needed by engineers and useful thermodynamic properties that is related to many other properties.

The physical boundary conditions as critical condition, normal boiling point and accentric factor are used to predict the vapor pressure of organic compounds.

The generalized model is applied to predic the vapor pressure of organic compounds including n-alkanes, cycloalkanes, branched alkanes, alkenes, alkynes, haloalkanes, diene, aromatic hydrocarbons, halo benzene, alcohols, ethers, ketones, esters, amines and xylene over the temperature range ( $T_{\min}$ ,  $T_{\max}$ ) of specific compounds under the study.

The results of 25 pure substances with 228 data points of the generalized model and experimental, 64 pure substances with 666 data points of model and Antoine are compared and evaluated.

The validated produced results with Average absolute percent deviation AAPD of 5% of experimental and 10% of Antoine respectively are achieved.

In conclusion, it should be noted that the constants of organic compounds data such as boiling points, critical temperature, critical pressure, and acentric factor were used to calculate the generalized model coefficients to estimate the vapor pressure of organic compounds more easily and accurate other than commonly used models.

## **5.2 Recommendations:**

It is recommended to:

1. The Antoine constants data is few it should be available more sources of the data bank.
2. Collect all models constant from individual textbooks and papers in one easily available book to estimate the vapor pressure.
3. Developing new correlation methods to predict the vapor pressure of alcohol.
4. Apply inorganic compound boundary conditions to estimate the vapor pressure of inorganic compounds.
5. Replace the Pitzer equation by other accentric factor equation in boundary condition No.3 to estimate generalized model coefficients.

## References:

- [1] Antoine, C. and Compt. rend.,(1988), 107: 681-85.
- [2] Bettelheim, F. A., Brown, W. H., Campbell MK and Farrell, S. O., (2008), Introduction to general, organic and biochemistry. Cengage Learning, Belmont.
- [3] Bhushan, B.,(2007), Springer handbook of nanotechnology. Springer,Berlin
- [4] Brown, T. L., Lemay, H. E., Bursten, B. E., Murphy, C. J. and Woodward, P. M., (2009), Chemistry: the central science. PearsonEducation, Upper Saddle River.
- [5] Brown, W. H., Foote, C. S., Iverson, B. L. and Anslyn, E.V., (2011), Organic chemistry. Cengage Learning, Belmont.
- [6] Carey, F. A. and Sundberg, R. J.,(2007), Advanced organic chemistry: partA: structure andmechanisms. Springer,New York.
- [7] Chandler, J.P., (1975), Stillwater, Department of Computing and Information Sciences, Oklahoma State University, OK74074.
- [8] Cox, E. R., Pressure-Temperature Chart for Hydrocarbon Vapors, Ind. Eng. Chem., 15,1923, 592-593.
- [9] Diaz, O.C., (2012), Measurement and Modeling Methodology for Heavy Oil and Bitumen Vapor Pressure, Calgary-Alberta.
- [10] Danesh, A., (1998), PVT and Phase Behavior of Petroleum Reservoir Fluids, 2nd Edition, Elsevier Science, Amsterdam.
- [11] Daubert, T.E. and Danner, R.P., (1992), Physical and Thermodynamic Properties of Pure Chemicals, Data Compilation. Hemisphere Publishing Corp., London, UK.
- [12] Edalat, E., Bozar-Jomehri, R. B. and Mansoori, G. A., (1993), Generalized equation predicts vapor pressure of hydrocarbons. Oil and gas 1:39-40.
- [13] Friend, D. G., Ely, J.F. and Ingham, H., (1989), "Thermo physical Property of Methane", J. Phys. Chem. Ref. Data. 18(2): 583-638

- [14] Forziati, A. F., Norris, W. R. and Rossini, F. D., (1949), Vapor Pressures and Boiling Points of Sixty API-NBS Hydrocarbons. *Journal of Research of the National Bureau of Standards*. 43: 555-563
- [15] Ganguly, J., (2009), *Thermodynamics in the earth and planetary sciences*. Springer, Berlin
- [16] Greiner, W., Neise, L. and Stocker, H., (1995), *Thermodynamics and statistical mechanics*. Springer, Berlin.
- [17] Helmenstine, A. M., (2014), *Molecular weight definition*, Tennessee at Knoxville.
- [18] Irche, (2018), wireless. Antoine constants [available at: [http://www. Iranian chemical engineering website](http://www.Iranianchemicalengineeringwebsite.com) (Accessed 5 May 2018, time 11PM).
- [19] James, S, Ch. and Sarah, H, (1993), A group Additivity Approaches for the Estimation of Vapor Pressures of liquid hydrocarbons from 298 to 500K, *J. Org. Chem.* 58, 5345- 5350.
- [20] Klein, D. R., (2011), *Organic chemistry*. Wiley, Hoboken.
- [21] Lyle, F, A., (2009), *Albright Albright's chemical engineering handbook*, West Lafayette Indiana, USA.
- [22] Lide, D. R., (2008), *CRC handbook of chemistry and physics*. Taylor and Francis, Boca Raton.
- [23] Lide, D. R., (2005), *CRC Handbook of Chemistry and Physics*, CRC Press, Boca Raton, FL, USA.
- [24] Marsh, K. N., Abramson, A., Ambrose, D., Morton, D. W., Nikitin, E., Tsonopoulos, C. and Young, C. L., J. (2007) , *Chem. Eng. Data.* 52 1509–1538.
- [25] Michelsen, M. L., 1982, The Isothermal Flash Problem. Part II. Phase Split Calculation, *Fluid Phase Equilibria*, 9, b, 21-40.
- [26] Mathias, P.M. and Copeman, T.W. , (1983), *Fluid Phase Equilib.* 13 -91–108.

- [27] Mehrdad, H., Ehsan, S. and Hamidreza, B., (2014), Prediction of Saturated Vapor Pressures Using Non-Linear Equations and Artificial Neural Network Approach, *Journal of Mathematics and computer science*, 8-343 – 358(2013).
- [28] Michelsen, M. L., 1982a, The Isothermal Flash Problem. Part I. Stability, *Fluid Phase Equilibria*, 9, 1-19.
- [29] Nasrifar, Kh., Ayatollahi, Sh. and Moshfeghian, M., (1999), Generalized saturated liquid density prediction method for pure compounds and multi-component mixtures, Shiraz University, Iran.
- [30] Nemati Lay, E., Peyman, M. and Sanjari, E., (2012), *World Academy of Science, Engineering and Technology*. 67 -340-346.
- [31] Nannoolal, Y., 2006, Development and Critical Evaluation of Group Contribution Methods for the Estimation of Critical Properties, Liquid Vapour Pressure and Liquid Viscosity of Organic Compounds, Durban Campus.
- [32] Poling, E, Prausnitz, M and O'Connell, P, (2001), *the properties of gases and liquids*, 5<sup>th</sup> Edition, McGraw-Hill.
- [33] Ponce Espinosa, H, E, Ponce-Cruz, P and Molina, A. , (2014), *Artificial organic network*, Spring.
- [34] Quinkert, G., Egert, E. and Griesinger, C., (1996), *Aspects of organic chemistry: structure*. Wiley, New York.
- [35] Rabah, A. A., (2014), Generalized equation of vapor pressure of normal Alkanes, department of chemical engineering, University of Khartoum.
- [36] Rabah, A. A. and Mohamed, S. A., (2010), Prediction of Molar Volumes of the Sudanese Reservoir Fluids, *Journal of Thermodynamics*, 2010: 1-9- DOI:10.1155/2010/142475.
- [37] Rabah, A. A. and Mohamed, S., (2010), A new three parameters equation of state. *Scientia, Transactions C: Chemistry and Chemical Engineering*. 17( 2): 1-15
- [38] Riedel, L., (1954), *Chem. Ing. Tech.* 26 -679-683.

- [39] Rohani, A. A., Pazuki, G., Najafabadi, H. A., Seyfi, S. and Vossoughi, M., *Exp. Sys. Appl.* 38 (2011) 1738–1747.
- [40] Richard, F. D. and Sally, J. D., (2005), physical properties of organic compounds.
- [41] Ruzicka, K., Fulem M. and Ruzicka, V., *Vapor Pressure of Organic Compounds. Measurement and Correlation*, Department of Physical Chemistry, Institute of Chemical Technology.
- [42] Reid, R.C., Prausnitz, J.M. and Poling, B.E., (1987), *the Properties of Gases and Liquids*, 4<sup>th</sup> ed., McGraw-Hill.
- [43] Rodgers, R. C. and Hill, G. E., (1978), *Equations for Vapour Pressure Versus Temperature: Derivation and Use of the Antoine Equation on A hand held Programmable Calculator*, *British Journal of Anaesthesia*.
- [44] Sanjari, E., Nemati Lay, E. and Nat, J., (2012), *Gas. Sci. Eng.* 9 -220-226.
- [45] Setzmann, U. and Wagner, W., J., (1991), *Phys. Chem. Ref. Data* 20: 1061.
- [46] Sencan, A. and Kalogirou, S. A., (2005), *Energy. Conv. Man.* 46-2405–2418.
- [47] Sivanandam, S. N., Sumathi, S. and Deepa, S. N., (2006), *Introduction to Neural Networks Using Matlab 6.0*. McGraw-Hill Publishing, New Delhi.
- [48] Tewari, K.S., Vishoni, N. K. and Mehrotra, S.N., (2003), *A textbook of organic chemistry (second edition)*, christ church college (Kanpur).
- [49] Twu, C. H., Coon, J. E. and Cunningham, J. R., (1994), *A Generalized Vapor Pressure Equation for Heavy Hydrocarbons*, *Fluid Phase Equilibria*, 96, 19-31.
- [50] Yash, N., (2007), *Evaluation of Group Contribution Methods for the Estimation of Critical Properties, Liquid Vapour Pressure and Liquid Viscosity of Organic Compounds*, University of Kwazulu-Natal, Durban Campus.
- [51] Younglove, B. A. and Ely, J. F., (1987), *J. Phys. Chem. Ref. Data* 16: 577.
- [52] Vargaftik, N.B., (1975), *Tables on the thermophysical properties of liquids and gases, in normal and dissociated states*, 2nd ed. Hemisphere Publishing.

- [53] Velasco,S., Romaín,F. L., White,J. A. and Mulero,A., (2008), J. Chem. Thermodynamics. 40-789–797.
- [54] VDI, "VDI-GVC. VDI- ,(2007), Waermeatlas", 10. Aufl., Springer-Verlag, Berlin
- [55]Wagner, W., (1973),New vapor pressure measurement for Argon and Nitrogen and a new method for establishing a rational vapor pressure equation. Cryogenics. 13: 470-82
- [56] Wallas, S. M., 1985, Phase Equilibria in Chemical Engineering, Butterworth Publishers, U.S.A.
- [57]Weir,R. D. and De loos, Th. W.,(2005), Measurement of the Thermodynamic Properties of Multiple Phases, Experimental Thermodynamics-Volume II.

## Appendixes:

1. Physical constants of organic compounds (Poling, E, Prausnitz, M and O'Connell, P, 2001).

No	Compound	Formula	M	T <sub>b</sub> (K)	T <sub>c</sub> (K)	P <sub>c</sub> (bar)	T <sub>rb</sub>	ω
<b>(1). n-Alkanes</b>								
1	Methane	CH <sub>4</sub>	16.043	111.66	190.564	45.992	0.59	0.011
2	Ethane	C <sub>2</sub> H <sub>6</sub>	30.070	184.55	305.33	48.718	0.60	0.099
3	Propane	C <sub>3</sub> H <sub>8</sub>	44.097	231.02	369.85	42.477	0.62	0.149
4	n-Butane	C <sub>4</sub> H <sub>10</sub>	58.124	272.66	425.16	37.96	0.64	0.2002
5	n-Pentane	C <sub>5</sub> H <sub>12</sub>	72.151	309.22	469.6	33.69	0.66	0.251
6	n-Hexane	C <sub>6</sub> H <sub>14</sub>	86.177	341.88	507.60	30.25	0.67	0.300
7	n-Heptane	C <sub>7</sub> H <sub>16</sub>	100.204	371.57	540.61	27.36	0.69	0.346
8	n-Nonane	C <sub>9</sub> H <sub>20</sub>	128.259	423.97	594.63	22.89	0.71	0.446
9	n-Decane	C <sub>10</sub> H <sub>22</sub>	142.286	447.30	617.6	21.10	0.72	0.488
10	n-Undecane	C <sub>11</sub> H <sub>24</sub>	156.312	469.08	639	19.49	0.73	0.530
11	n-Dodecane	C <sub>12</sub> H <sub>26</sub>	170.338	489.48	658	18.20	0.74	0.576
<b>(2). Cycloalkanes</b>								
1	Cyclopentane	C <sub>5</sub> H <sub>10</sub>	70.134	322.38	511.8	45.08	0.63	0.196
2	Cyclohexane	C <sub>6</sub> H <sub>12</sub>	84.161	353.93	553.58	40.75	0.64	0.212
3	Methyl cyclo hexane	C <sub>7</sub> H <sub>14</sub>	98.188	374.09	572.19	34.71	0.65	0.235
<b>(3). Branched alkanes</b>								
1	3-Ethyl pentane	C <sub>7</sub> H <sub>16</sub>	100.204	366.63	540.50	28.90	0.68	0.311



2	2-Methyloctane	C <sub>9</sub> H <sub>20</sub>	128.258	416.44	587	23.10	0.71	0.423
<b>(4). Alkenes</b>								
1	Ethene(Ethylene)	C <sub>2</sub> H <sub>4</sub>	28.054	169.42	282.34	50.401	0.60	0.087
2	Propene(Propylene)	C <sub>3</sub> H <sub>6</sub>	42.081	225.46	364.8	46.1	0.62	0.142
3	1-Butene	C <sub>4</sub> H <sub>8</sub>	56.108	266.92	419.50	40.20	0.64	0.194
<b>(5). Alkynes</b>								
1	Ethyne(Acetylene)	C <sub>2</sub> H <sub>2</sub>	26.038	188.40	308.32	62.4	0.61	0.188
2	1-Pentyne	C <sub>5</sub> H <sub>8</sub>	68.119	313.38	470	41.70	0.67	0.394
<b>(6). Haloalkanes</b>								
1	Difluoromethane	CH <sub>2</sub> F <sub>2</sub>	52.024	221.43	351.26	58.05	0.63	0.278
2	Trichlorofluoromethane (R11)	CCl <sub>3</sub> F	137.368	296.81	471.10	44.72	0.63	0.195
3	Bromotrifluoromethane	CBrF <sub>3</sub>	148.910	215.14	340.15	39.72	0.63	0.174
4	1,1- Difluoroethane(R152a)	C <sub>2</sub> H <sub>4</sub> F <sub>2</sub>	66.052	249.10	386.41	45.17	0.64	0.276
5	1,1,1- Trifluoroethane (R143a)	C <sub>2</sub> H <sub>3</sub> F <sub>3</sub>	84.041	225.86	346.30	37.92	0.65	0.259
6	1,1,1,2- Tetrafluoroethane (R134a)	C <sub>2</sub> H <sub>2</sub> F <sub>4</sub>	102.036	247.04	374.18	40.56	0.66	0.326
7	Pentafluoroethane(R12 5)	C <sub>2</sub> HF <sub>5</sub>	120.028	225.06	339.33	36.29	0.66	0.305
8	1-Chloro-1,1,2,2- tetrafluoroethane(R124 )	C <sub>2</sub> HClF <sub>4</sub>	136.476	261.38	400.00	37.60	0.65	0.260
9	2-Chlorobutane	C <sub>4</sub> H <sub>9</sub> Cl	92.568	341.24	520.60	36.80	0.66	0.267
<b>(7). S-Alkyl</b>								
1	Methanethiol(Methyl mercaptan)	CH <sub>4</sub> S	48.109	279.11	470	72.30	0.59	0.15
2	3-Thiapentane(Diethyl sulfide)	C <sub>4</sub> H <sub>10</sub> S	90.189	365.25	557	39.60	0.66	0.295
<b>(8). Diene</b>								
1	1,3- Butadiene	C <sub>4</sub> H <sub>6</sub>	54.092	268.62	425.15	43.3	0.63	0.195

<b>(9). Aromatic hydrocarbons</b>								
1	Benzene	C <sub>6</sub> H <sub>6</sub>	78.114	353.24	562.05	48.95	0.63	0.209
2	Toluene	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	92.141	383.79	591.8	41.08	0.65	0.262
3	2-Methyl phenol(o-cresol)	C <sub>7</sub> H <sub>8</sub> O	108.140	464.17	697.60	50	0.67	0.436
4	3-Methyl phenol(m-cresol)	C <sub>7</sub> H <sub>8</sub> O	108.140	475.38	705.70	45.60	0.67	0.452
5	4-Methyl phenol(p-cresol)	C <sub>7</sub> H <sub>8</sub> O	108.140	475.12	704.50	51.50	0.67	0.510
6	Ethyl benzene	C <sub>8</sub> H <sub>10</sub>	106.167	409.36	617.1	36.1	0.66	0.304
7	Butylbenzene	C <sub>10</sub> H <sub>14</sub>	134.221	456.42	660.50	28.90	0.69	0.393
<b>(10). Halo benzene</b>								
1	Hexafluorobenzene	C <sub>6</sub> F <sub>6</sub>	186.056	353.40	516.73	32.75	0.68	0.396
<b>(11). Alcohols</b>								
1	Isobutanol	C <sub>4</sub> H <sub>10</sub> O	74.123	381.04	547.78	43	0.70	0.590
2	Sec-butanol	C <sub>4</sub> H <sub>10</sub> O	74.123	372.66	536.05	41.79	0.70	0.574
3	1-Pentanol	C <sub>5</sub> H <sub>12</sub> O	88.150	411.16	588.15	39.09	0.70	0.579
4	1-Octanol	C <sub>8</sub> H <sub>18</sub> O	130.230	468.33	652.50	28.60	0.72	0.594
5	1-Nonanol	C <sub>9</sub> H <sub>20</sub> O	144.257	486.52	668.90	26.30	0.73	0.633
6	1-Decanol	C <sub>10</sub> H <sub>22</sub> O	158.284	504.22	684.40	23.70	0.74	0.661
7	1-Undecanol	C <sub>11</sub> H <sub>24</sub> O	172.311	521.24	705	22.40	0.74	0.656
8	1-Dodecanol	C <sub>12</sub> H <sub>26</sub> O	186.338	537.79	720	20.80	0.75	0.68
<b>(12). Ethers</b>								
1	Methyl ethyl ether	C <sub>3</sub> H <sub>8</sub> O	60.096	280.50	437.80	44	0.64	0.236
<b>(13). Ketones</b>								
1	Butanone(Methyl ethyl ketone)	C <sub>4</sub> H <sub>8</sub> O	72.107	352.71	536.80	42.10	0.66	0.322
2	Cyclopentanone	C <sub>5</sub> H <sub>8</sub> O	84.118	403.72	624.50	46	0.65	0.288
<b>(14). Esters</b>								
1	Methyl formate	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	60.053	304.90	487.2	60.0	0.63	0.254
2	Methyl acetate	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	74.079	330.09	506.8	46.87	0.65	0.326
3	Ethyl methanoate(Ethyl formate)	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	74.079	327.47	508.50	47.40	0.64	0.282

4	Ethyl acetate	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	88.106	350.21	523.25	38.32	0.67	0.361
5	Propyl ethanoate (Propyl acetate)	C <sub>5</sub> H <sub>12</sub> O <sub>2</sub>	102.133	374.65	549.40	33.30	0.68	0.389
<b>(15). Amines</b>								
1	Methylamine	CH <sub>5</sub> N	31.057	266.82	430	74.20	0.62	0.283
2	2-Propanamine (Methyl ethyl amine)	C <sub>3</sub> H <sub>9</sub> N	59.111	304.93	471.80	45.40	0.65	0.277
3	1-Butanamine (Butyl amine)	C <sub>4</sub> H <sub>11</sub> N	73.138	349.44	526.80	40.40	0.66	0.338
4	Benzeneamine(Aniline)	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	93.128	457.17	699	53.01	0.65	0.380
<b>(16). Xylene</b>								
1	1,2-dimethylbenzene(O- Xylene)	C <sub>8</sub> H <sub>10</sub>	106.167	417.59	630.4	37.29	0.66	0.311
2	1,3-dimethylbenzene (m- Xylene)	C <sub>8</sub> H <sub>10</sub>	106.167	412.34	617	35.43	0.67	0.325
3	1,4-dimethyl benzene(P- Xylene)	C <sub>8</sub> H <sub>10</sub>	106.167	411.53	616.3	35.1	0.67	0.320

2.Optimized vapor pressure-dependent parameters of Mathias and Copeman's equation based on PSRK EOS(Nasrifar,Kh., Ayatollahi,Sh. and Moshfeghian,M.,1999).

Compound	Parameters of Mathias & Copeman		
	C <sub>1</sub>	C <sub>2</sub>	C <sub>3</sub>
Halogenated paraffins			
Carbon Tetrachloride (R-10)	0.8587	-0.8465	2.1216
Dichlorofluoromethane (R-21)	0.8686	-0.8440	2.2961
Difluoromethane (R-32)	1.0054	-0.7979	1.2350
Methyl Chloride (R-40)	0.8352	-1.0274	2.1914
1,1,2,2-Tetrafluoroethane (R-134)	0.9483	0.1797	-2.0000
Pentafluoroethane (R-125)	1.0162	-0.6470	1.4038
1,1-Dichloro-1-fluoroethane (R-141b)	0.8833	-0.6832	1.7357
Monochlorodifluoroethane (R-142)	0.9453	-0.8263	1.6066

1,1,1-Trifluoroethane (R-143a)	0.7868	2.2324	-14.6918
1,3-Dichloro-1,1,2,2,3,3-hexafluoroethane (R-216)	1.0433	-1.0050	2.7623
1,1,1,2,2-Pentafluoropropane (R-245cb)	1.0279	-1.1929	3.6115
Octafluorocyclobutane (R-C318)	1.0521	-0.4022	1.1152
Chloroethane (R-160)	0.8327	-0.4152	0.6459
Azeotrope of R-12 and R-152a (R-500)	0.8566	-0.5110	0.8944
Azeotrope of R-12 and R-115 (R-502)	0.8630	-0.4620	1.0417
Azeotrope of R-23 and R-13 (R-503)	0.8456	-0.6568	1.7539
Azeotrope of R-12 and R-31 (R-505)	0.8277	-0.6855	1.4498
<i>Parraffins</i>			
<i>n</i> -Pentane	0.9820	-1.1695	2.7523
<i>i</i> -Pentane	0.8767	-0.6043	1.4025
<i>n</i> -Hexane	1.0430	-1.1553	2.9235
<i>n</i> -Heptane	1.1244	-1.1786	2.8656
<i>n</i> -Octane	1.2278	-1.5558	3.9361
<i>i</i> -Octane	1.0418	-1.0064	2.3894
<i>n</i> -Nonane	1.2798	-1.3822	3.3933
<i>n</i> -Decane	1.3432	-1.4550	3.7609
<i>n</i> -Dodecane	1.4001	-0.9851	2.7150
<i>n</i> -Tridecane	1.5250	-1.6367	4.3320
<i>n</i> -Tetradecane	1.6028	-2.1855	6.1629
<i>n</i> -Pentadecane	1.4718	0.1219	-0.8291
<i>n</i> -Hexadecane	1.6009	-1.2395	3.8971
<i>n</i> -Heptadecane	1.7894	-2.1890	5.6027
<i>n</i> -Octadecane	1.9229	-3.2251	8.7989
<i>n</i> -Nonadecane	1.9622	-3.0743	8.3779
<i>n</i> -Eichosane	1.8148	-2.2027	7.6877
<i>Cycloparaffins</i>			
Cyclopentane	0.8589	-0.8034	1.9739
Methyl Cyclopentane	0.9131	-0.7992	1.9094
Ethyl Cyclopentane	0.9630	-0.7185	1.7476

Cyclohexane	0.9004	-1.1193	3.0331
Methyl Cyclohexane	0.9144	-0.7259	1.7079
<i>Olefins, cyclic olefins, and diolefins</i>			
1-Butene	0.8623	-0.9746	2.5145
<i>cis</i> -2-Butene	1.1925	-2.8905	6.2451
<i>rans</i> -2-Butene	0.9561	-1.0857	1.9271
Isobutylene	0.8047	-0.1717	0.0777
1-Pentene	0.8852	-0.7889	1.7487
<i>cis</i> -2-Pentene	0.8821	-0.3450	0.7952
<i>trans</i> -2-Pentene	0.8901	-0.3991	0.9130
1-Hexene	0.9922	-0.7265	1.5313
1-Octene	1.1880	-1.2565	2.9551
Cyclopentene	0.8714	-0.7181	1.4110
Cyclohexene	0.8817	-0.8151	2.0567
1,3-Butadiene	0.9054	-1.2209	2.7928
Propadiene (Allene)	0.3028	2.9256	-5.5643
2-Methyl-1,3-Butadiene	0.6064	0.8848	-1.1175
<i>Aromatics</i>			
Benzene	0.8611	-0.6902	1.8617
Toluene	0.9247	-0.3793	0.7391
Ethylbenzene	1.0474	-1.0559	2.4376
Isopropylbenzene (Cumene)	0.8179	0.6686	-0.7808
Biphenyl	0.9418	0.6000	-1.7506
Chlorobenzene	0.9616	-0.9430	2.1995
<i>Alcohols</i>			
Methanol	1.4854	-1.3968	2.1661
1-Propanol	1.3797	-0.2084	1.7651
2-Propanol	1.6484	-1.4784	4.3961
<i>n</i> -Butanol	1.7026	-2.8376	7.8835
<i>Inorganic gases</i>			

Chlorine	0.6492	-0.5301	1.2918
Carbon Monoxide	0.6001	-0.4675	1.1440
Normal Deuterium	0.3100	-0.3833	0.1611
Fluorine	0.5583	0.0379	-0.2577
Hydrogen Sulfide	0.4548	2.6636	-10.8909
Krypton	0.5251	-0.4492	0.9010
Xenon	0.5354	-0.4842	0.9878
Sulfur Dioxide	0.9189	-0.5319	1.3446
<i>Ethers</i>			
Ethyl Ether (R-610)	0.9505	-0.5819	1.6169
Phenyl Ether	0.5755	2.5541	-4.5593
<i>Miscellaneous</i>			
Ethyl Acetate	1.1201	-0.9315	2.3427
Acetone	1.1165	-1.5473	3.6896
Acetic Acid	1.2821	-0.8636	0.4781
Benzoic Acid	1.6233	-3.2886	11.1387
Acetylene	0.9542	-2.0340	5.4165

3. Antoine equation parameters A, B, and C of organic compounds (Weir, R. D. and De loos, 2005).

No	Compound	A	B	C	Temperature range(°C) T <sub>min</sub> , T <sub>max</sub>
1	Methane	6.846	435.621	271.361	-182.48, -82.57
2	Methylamine	7.364	1025.4	235.062	-93.46, 156.9
3	Methanethiol(Methyl mercaptan)	7.072	1008.88	234.729	-122.97, 196.8
4	Difluoromethane	7.290	863.592	247.503	-136.15, 78.45
5	R11	6.994	1081.98	239.265	-111.11, 198.05
6	Bromotrifluoromethane	6.972	800.838	253.656	-168, 67
7	Ethane	6.953	699.106	260.264	-182.8, 32.27
8	Ethyne(Acetylene)	7.315	790.209	262.859	-80.75, 35.17

9	Ethene(Ethylene)	6.966	649.806	262.73	-169.14, 9.21
10	Methyl formate	7.265	1178.19	236.959	-99, 214.05
11	R152a	7.120	928.549	244.854	-117, 113.45
12	R143a(1,1,1-trifluoroethane)	7.076	846.165	249.078	-111.3, 73.1
13	R134a	7.010	902.327	244.514	-101, 106.85
14	R125	6.995	811.133	245.168	-103, 68.85
15	R124	7.069	968.741	243.018	-15.41, 126.85
16	Propane	7.019	889.864	257.084	-187.69, 96.67
17	Propene(Propylene)	7.017	860.992	255.895	-184.15, 91.61
18	Methyl ethyl ether	6.630	760.22	195.446	-113.15, 164.65
19	Methyl acetate	7.280	1276.29	233.155	-98, 233.65
20	Ethyl methanoate(Ethyl formate)	7.218	1252.8	234.565	-79.6, 235.25
21	2-Propanamine(Methyl ethyl amine)	6.870	943.96	200.649	-25.6, 201.85
22	n-Butane	7.009	1022.48	248.145	-138.29, 152.03
23	1-Butene	7.034	1013.6	250.292	-185.35, 146.44
24	1,3- Butadiene	7.022	998.721	245.563	-108.9, 152.22
25	Isobutanol	7.459	1386.1	195.079	-108, 274.58
26	Butanone(Methyl ethyl ketone)	7.294	1400.37	237.655	-86.67, 262.35
27	Ethyl acetate	7.260	1338.46	228.608	-83.55, 250.15
28	Sec-butanol	7.561	1448.35	209.886	-114.7, 262.86
29	2-Chlorobutane	7.253	1378.58	247.194	-131.3, 247.45
30	1-Butanamine(Butyl amine)	7.210	1316.41	226.655	-49.1, 258.75
31	3-Thiapentane(Diethyl sulfide)	7.204	1423.41	237.112	-103.95, 284
32	n-Pentane	7.009	1134.15	238.678	-129.73, 196.5
33	1-Pentyne	7.212	1223.32	242.283	-105.7, 208.05
34	Cyclopentane	7.043	1202.53	239.69	-93.87, 238.61
35	Cyclopentanone	7.566	1727.86	238.153	-51.3, 352.85
36	1-Pentanol	7.458	1516.51	193.53	-77.59, 313
37	Propyl ethanoate(Propyl acetate)	7.223	1408.02	222.76	-95, 276.25
38	n-Hexane	6.990	1216.92	227.451	-95.31, 234.28
39	Benzene	7.064	1296.93	229.916	5.53, 289.01
40	Cyclohexane	7.009	1296.23	233.309	6.54, 280.39

41	Benzeneamine(Aniline)	7.293	1668.15	193.636	-6.02, 425.85
42	Hexafluorobenzene	7.221	1329.93	226.134	5.1, 243.58
43	n-Heptane	7.046	1341.89	223.733	-90.59, 267.11
44	Toluene	7.136	1457.29	231.827	-94.97, 318.64
45	Methyl cyclo hexane	7.001	1375.13	232.819	-126.57, 299.04
46	3-Ethyl pentane	7.109	1402.17	238.129	-118.6, 267.49
47	2-Methyl phenol(o-cresol)	7.368	1727.17	193.918	31.04, 424.4
48	3-Methyl phenol(m-cresol)	7.267	1670.93	178.653	12.24, 432.7
49	4-Methyl phenol(p-cresol)	7.458	1768.27	184.313	34.78, 431.5
50	Ethyl benzene	7.166	1559.55	228.582	-95, 344.02
51	1,2-dimethylbenzene(O-Xylene)	7.149	1566.59	222.596	-25.17, 357.22
52	1,3-dimethylbenzene (m- Xylene)	7.181	1573.02	226.671	-47.85, 343.9
53	1,4-dimethylbenzene(P- Xylene)	7.155	1553.95	225.23	13.26, 343.11
54	1-Octanol	7.160	1536.79	163.905	-15.5, 379.35
55	n-Nonane	7.188	1607.74	222.414	-53.52, 322.5
56	2-methyloctane	7.137	1553.89	221.781	-80.37, 313.6
57	1-Nonanol	7.046	1520.83	152.06	-5, 399.85
58	n-Decane	7.217	1693.93	216.459	-29.66, 345.3
59	Butylbenzene	7.185	1720.37	216.413	-87.85, 387.4
60	1-Decanol	7.038	1579.82	149.864	6.9, 416.85
61	n-Undecane	7.181	1706.26	200.897	-25.58, 365.61
62	1-undecanol	6.911	1551.12	139.882	15.9, 430.85
63	n-Dodecane	7.229	1807.47	199.381	-9.58, 385.05
64	1-dodecanol	6.889	1589.5	134.693	23.8, 447.85



4. Comparison of vapor pressure equations (Edalat, E., Bozar-Jomehri, R. B. and Mansoori, G. A., 1993).

No. of data points	No. of compounds	Average error%		
		LK equation	AP equation	Equation 14
n-Alkanes and alkenes				
177	16	6.41	6.13	5.53
Aromatics				
85	7	2.66	8.47	2.40
Nonhydrocarbons				
96	7	9.82	11.97	8.63
Halogen				
49	3	2.98	13.69	2.49
Noble gases				
25	2	2.08	2.08	1.65
Alcohols				
140	11	6.19	20.37	14.73
<b>94 compounds 1106</b>	<b>94</b>	<b>6.87</b>	<b>11.63</b>	<b>6.06</b>

5. Antoine correlation coefficient of n-Alkanes (Rabah, A. A., 2014).

Comp.	Generalize Antoine			Antoine			Tr <sub>min</sub>	Tr <sub>max</sub>
	A'	B'	C'	A	B	C		
C1	4.754	4.712	-0.038	15.224	897.840	-7.160	0.49	0.63
C2	5.157	4.950	-0.056	15.664	1511.420	-17.160	0.44	0.65
C3	5.357	5.063	-0.068	15.726	1872.460	-25.160	0.46	0.67
nC4	5.421	5.069	-0.081	15.678	2154.900	-34.420	0.47	0.69
nC5	5.696	5.274	-0.085	15.833	2477.070	-39.940	0.49	0.70
nC6	5.807	5.314	-0.096	15.837	2697.550	-48.780	0.50	0.72
nC7	5.943	5.389	-0.105	15.874	2911.320	-56.510	0.51	0.73
nC8	6.108	5.487	-0.112	15.943	3120.290	-63.630	0.53	0.75
nC9	6.216	5.536	-0.120	15.967	3291.450	-71.330	0.54	0.76
nC10	6.342	5.596	-0.127	16.011	3456.800	-78.670	0.55	0.77
nC11	6.464	5.656	-0.134	16.054	3614.070	-85.450	0.56	0.78
nC12	6.592	5.736	-0.139	16.113	3774.560	-91.310	0.57	0.79
nC13	6.694	5.767	-0.147	16.136	3892.910	-98.930	0.58	0.80
nC14	6.774	5.784	-0.152	16.148	4008.520	-105.400	0.58	0.81
nC15	6.858	5.821	-0.158	16.172	4121.510	-111.800	0.59	0.81
nC16	6.925	5.830	-0.164	16.184	4214.910	-118.700	0.60	0.82
nC17	6.936	5.835	-0.168	16.151	4294.550	-124.000	0.59	0.78
nC18	6.961	5.839	-0.174	16.123	4361.790	-129.900	0.61	0.84

nC19	7.040	5.871	-0.179	16.153	4450.440	-135.600	0.62	0.85
nC20	7.397	6.094	-0.184	16.469	4680.460	-141.100	0.63	0.85

6. AAPD of Antoine and generalized Antoine correlation coefficients (Rabah, A. A., 2014).

Fluid	T <sub>max</sub>	T <sub>min</sub>	Antoine			Generalized Antoine			Data points
	K	K	AAPD%	APD <sub>max</sub> %	APD <sub>min</sub> %	AAPD%	APD <sub>max</sub> %	APD <sub>min</sub> %	
C1	180	153	2.28	5.16	0.20	5.11	6.65	4.35	5
C2	143	74	1.74	6.91	0.11	3.06	6.52	0.30	13
C3	199	24	1.72	5.58	0.20	4.00	6.58	0.07	6
C4	178	17	2.00	5.38	0.58	3.30	6.59	0.01	15
C5	153	57	1.15	5.81	0.35	2.87	6.56	0.32	21
C6	128	97	1.83	5.41	0.21	2.67	6.52	0.63	10
C7	400	270	1.68	5.83	0.71	2.00	6.05	0.06	29
C8	425	292	2.50	5.18	-0.23	2.08	3.66	0.31	9
C9	179	39	1.59	5.30	0.18	3.11	6.25	0.31	36
C10	203	57	2.50	6.57	0.04	2.15	6.41	0.27	10
C12	247	91	1.85	6.88	0.20	1.84	6.73	0.08	15
<b>Grand</b>			<b>1.90</b>	<b>5.82</b>	<b>0.23</b>	<b>2.93</b>	<b>6.23</b>	<b>0.61</b>	<b>169</b>

7. Apply the three boundary conditions to equation 3.1 and the three constants are obtained with some algebraic manipulation by the following steps:

$$\ln P^s = A - \frac{B}{C + T}$$

$$\ln\left(\frac{P}{P_c} \cdot P_c\right) = A - \frac{B}{C + \frac{T}{T_c} \cdot T_c}$$

$$\ln P_r + \ln P_c = A - \frac{\frac{B}{T_c}}{\frac{C}{T_c} + T_r}$$

$$\ln P_r = A - \ln P_c - \frac{\frac{B}{T_c}}{\frac{C}{T_c} + T_r}$$

Therefore:

$$A' = A - \ln P_c, B' = \frac{B}{T_c}, C' = \frac{C}{T_c}$$

Generalized Antoine equation:

$$\ln P_r = A' - \frac{B'}{C' + T_r}$$

**The boundary condition of normal of component:**

**Boundary condition (1):**

### 1. Normal boiling point

$$P = 1 \text{ atm} \quad T = T_b$$

$$\ln P_{rb} = A' - \frac{B'}{C' + T_{rb}}$$

$$\ln P - \ln P_c = A' - \frac{B'}{C' + T_{rb}}$$

$$A' - \frac{B'}{C' + T_r} = -\ln P_c$$

### Boundary condition (2):

#### 2. Critical point

$$P = P_c \quad T = T_c$$

$$\ln P_r = A' - \frac{B'}{C' + T_{rb}}$$

$$\ln \frac{P}{P_c} = A' - \frac{B'}{C' + \frac{T_b}{T_c}}$$

$$\ln 1 = A' - \frac{B'}{C' + 1}$$

$$A' - \frac{B'}{C' + 1} = 0$$

### Boundary condition (3):

#### 3. Accentric factor:

$$\omega = -(\log P_r^s)_{T_r=0.7} - 1$$

$$\omega + 1 = -(\log P_r^s)_{T_r=0.7} - \omega - 1 = \frac{(\ln P_r^s)_{T_r=0.7}}{\ln 10}$$

$$-2.303\omega - 2.303 = (\ln P_r^s)_{T_r=0.7}$$

$$A' - \frac{B'}{C' + 0.7} = -2.303\omega - 2.303$$

Use the three boundary condition equations to determine the model coefficients

$(A', B', C')$ .

$$A' - \frac{B'}{C' + T_r} = -\ln P_c$$

$$A' - \frac{B'}{C' + 1} = 0$$

$$A' - \frac{B'}{C' + 0.7} = -2.303\omega - 2.303$$

To determine the model coefficients  $(A', B', C')$  let:

$$A' = X \quad B' = Y \quad C' = Z$$

$$\ln P_c = C_1 T_r = C_2 \quad -2.303\omega - 2.303 = C_3$$

Replace:

$$A' = X \quad B' = Y \quad C' = Z$$

$$X - \frac{Y}{Z + 1} = 0$$

$$X(Z + 1) - Y = 0$$

$$Y = X(Z + 1)$$

and replace:

$$A' = X \quad B' = Y \quad C' = Z \quad T_r = C_2 \quad \ln P_c = C_1$$

$$X - \frac{Y}{Z + C_2} = -C_1$$

$$X(Z + C_2) - Y = -C_1(Z + C_2)$$

$$XZ + C_2X - Y = -C_1Z - C_1C_2$$

$$\cancel{XZ} + C_2X - \cancel{XZ} - X = -C_1Z - C_1C_2$$

$$C_2X - X + C_1Z = -C_1C_2$$

$$X(C_2 - 1) + C_1Z = -C_1C_2$$

also replace:

$$A' = X \quad B' = Y \quad C' = Z - 2.303\omega - 2.303 = C_3$$

$$X - \frac{Y}{Z + 0.7} = C_3$$

$$X(Z + 0.7) - Y = C_3(Z + 0.7)$$

$$X(Z + 0.7) - Y = C_3(Z + 0.7)$$

$$\cancel{XZ} + 0.7X - \cancel{XZ} - X = C_3Z + 0.7C_3$$

$$-0.3X - C_3Z = 0.7C_3$$

Replace the value of Z by the original factors:

$$C' = \frac{-0.3T_r \ln p_c - (1.6\omega + 1.6)T_r + 1.6\omega + 1.6}{0.3 \ln p_c + (2.303\omega + 2.303)T_r - 2.303\omega - 2.303}$$

$$C' = \frac{-0.3T_{rb} \ln p_c - 1.6(T_{rb} - 1)(\omega + 1)}{0.3 \ln p_c + 2.303(T_{rb} - 1)(\omega + 1)}$$

Replace also the value of X by the original factors:

$$A' = \frac{(1.6\omega + 1.6) \ln p_c - (2.3\omega + 2.3)T_r \ln p_c}{0.3 \ln p_c + (2.303\omega + 2.303)T_r - 2.303\omega - 2.303}$$

$$A' = \frac{\ln p_c (1.6 - 2.3T_{rb})(\omega + 1)}{0.3 \ln p_c + 2.303(T_{rb} - 1)(\omega + 1)}$$

Replace also the value of Y by the original factors:

$$B' = \left[ \frac{(1.6\omega + 1.6) \ln p_c - (2.3\omega + 2.3)T_r \ln p_c}{0.3 \ln p_c + (2.303\omega + 2.303)T_r - 2.303\omega - 2.303} \right] \times \left[ \frac{-0.3T_r \ln p_c - (1.6\omega + 1.6)T_r + 1.6\omega + 1.6}{0.3 \ln p_c + (2.303\omega + 2.303)T_r - 2.303\omega - 2.303} + 1 \right]$$

$$B' = \left[ \frac{\ln p_c (1.6 - 2.3T_{rb})(\omega + 1)}{0.3 \ln p_c + 2.303(T_{rb} - 1)(\omega + 1)} \right] \times \left[ \frac{-0.3T_{rb} \ln p_c - 1.6(T_{rb} - 1)(\omega + 1)}{0.3 \ln p_c + 2.303(T_{rb} - 1)(\omega + 1)} + 1 \right]$$

Development Generalized model coefficients(  $A'$ ,  $B'$ ,  $C'$  ) are:

$$A' = \frac{\beta_1}{\beta_2}$$

$$B' = \frac{\beta_1[\beta_2 + \beta_3]}{\beta_2^2}$$

$$C' = \frac{\beta_3}{\beta_2}$$

Vapor pressure of model equation:

$$\ln P_r = A' - \frac{B'}{C' + T_r}$$

$$\ln P_s = A' - \frac{B'}{C' + T_r} + \ln P_c$$

$$P_s = \exp\left(A' - \frac{B'}{C' + T_r} + \ln P_c\right)$$



8. Experimental data and model vapor pressure correlation:

No	Experimental Vapor Pressure, $P_{Exp}$ . And Model Vapor pressure, $P_{Mod}$ .			
	Temperature(°C)	Experimental Vapor pressure, $P_{Experimental}$ (mmHg)	Model Vapor Pressure, $P_{Model}$ (mmHg)	$ PD $
(1). <i>n</i> -Alkanes				
1. Methane ( $T_b = -161.49$ , $T_c = -82.586$ °C, $\omega = 0.011$ )				
1	-161.48	759.813	734.3682	3.35
2	-153.15	1435.618	1373.176	4.35
3	-143.15	2754.977	2673.202	2.97
4	-133.15	4809.396	4701.492	2.24
5	-123.15	7800.642	8342.097	6.94
6	-113.15	11941.73	12560.47	5.18
7	-103.15	17463.69	17986.87	3.00
8	-93.15	24641.03	24711.41	0.29
9	-88.15	28965.13	29394.95	1.48
10	-83.15	33892.29	34575.16	2.01
APD <sub>min</sub>				0.29
APD <sub>max</sub>				6.94
AAPD				3.18
2. Ethane ( $T_b = -88.6$ , $T_c = 32.18$ °C, $\omega = 0.099$ )				
1	-88.59	759.963	723.2855	4.83
2	-73.15	1629.734	1743.728	6.99
3	-53.15	3691.579	3648.298	1.17
4	-33.15	7253.246	7524.424	3.74
5	-13.15	12844.81	12761.7	0.65
6	6.85	21058.73	21715.02	3.12
7	26.85	32683.19	32287.74	1.21
APD <sub>min</sub>				0.65
APD <sub>max</sub>				6.99

AAPD				3.10
3. Propane ( $T_b = -42.13$ , $T_c = 96.7^\circ\text{C}$ , $\omega = 0.149$ )				
1	-42.07	759.963	722.7392	4.90
2	-18.15	1959.011	1976.767	0.91
3	6.85	4364.684	4503.837	3.19
4	26.85	7334.178	7442.067	1.47
5	46.85	11991.24	12610.93	5.17
6	66.85	18239.25	18581.14	1.87
7	89.3	27988.55	28095.83	0.38
APD <sub>min</sub>				0.38
APD <sub>max</sub>				5.17
AAPD				2.56
4. Butane ( $T_b = -0.49$ , $T_c = 152.01^\circ\text{C}$ , $\omega = 0.2002$ )				
1	-0.52	759.963	708.622	6.76
2	21.85	1656.136	1530.726	7.57
3	46.85	3432.207	3320.14	3.27
4	71.85	6347.097	6349.493	0.04
5	96.85	10768.64	11014.85	2.29
6	121.85	17127.66	17691.22	3.29
7	143.51	24724.28	25030.31	1.24
APD <sub>min</sub>				0.04
APD <sub>max</sub>				7.57
AAPD				3.49
5. Pentane ( $T_b = 36.07$ , $T_c = 196.45^\circ\text{C}$ , $\omega = 0.251$ )				
1	61.85	1702.64	1583.442	7.00
2	76.85	2557.71	2768.396	8.24
3	91.85	3690.303	3998.07	8.34
4	106.85	5160.424	5565.58	7.85
5	121.85	7013.077	7507.383	7.05
6	136.85	9368.27	9854.861	5.19

7	151.85	12256.01	13659.82	11.45
8	166.85	15773.8	17044.85	8.06
9	196.45	25269.58	25233.78	0.14
APD <sub>min</sub>				0.14
APD <sub>max</sub>				11.45
AAPD				7.04
6. Hexane ( $T_b = 68.73$ , $T_c = 234.45^\circ\text{C}$ , $\omega = 0.300$ )				
1	68.73	759.813	661.8165	12.90
2	96.85	1710.141	1579.842	7.62
3	111.85	2482.704	2323.027	6.43
4	126.85	3487.787	3320.917	4.78
5	141.85	4785.394	4629.341	3.26
6	156.85	6405.527	6308.927	1.51
7	171.85	8430.693	8424.373	0.07
8	186.85	10928.4	11043.64	1.05
9	201.85	13943.65	14237.11	2.10
10	234.29	22734.37	22635.1	0.44
APD <sub>min</sub>				0.07
APD <sub>max</sub>				12.90
AAPD				4.02
7. Heptane ( $T_b = 98.42$ , $T_c = 267.46^\circ\text{C}$ , $\omega = 0.346$ )				
1	98.45	759.813	409.5776	46.09
2	106.85	975.080	594.429	39.04
3	126.85	1642.635	1796.338	9.36
4	146.85	2617.715	3719.42	42.09
5	166.85	3967.826	5554.978	40.00
6	186.85	5407.945	8384.435	55.04
7	206.85	8205.675	11499.68	40.14
8	226.85	11348.43	13942.28	22.86

9	246.85	15346.26	17258.65	12.46
10	267.45	20521.69	20575.46	0.26
APD <sub>min</sub>				0.26
APD <sub>max</sub>				55.04
AAPD				30.73
8. Nonane ( $T_b = 150.82$ , $T_c = 321.48^\circ\text{C}$ , $\omega = 0.446$ )				
1	150.82	759.813	902.5996	18.79
2	161.85	1005.083	1216.332	21.02
3	181.85	1605.132	2083.945	29.83
4	201.85	2535.208	2986.958	17.82
5	221.85	3720.306	4146.433	11.45
6	241.85	5377.942	6151.88	14.39
7	261.85	7238.095	8043.293	11.12
8	281.85	9900.814	10300.22	4.03
9	301.85	13126.08	13923.94	6.08
10	321.48	17168.91	17132.28	0.21
APD <sub>min</sub>				0.21
APD <sub>max</sub>				29.83
AAPD				13.47
9. Decane ( $T_b = 174.15$ , $T_c = 344.45^\circ\text{C}$ , $\omega = 0.488$ )				
1	174.16	759.813	845.1993	11.24
2	186.85	1057.587	1148.185	8.57
3	206.85	1702.64	1993.402	17.08
4	226.85	2467.703	2879.918	16.70
5	246.85	3592.795	4024.235	12.01
6	266.85	5062.916	5462.457	7.89
7	286.85	6953.072	7896	13.56
8	306.85	9375.771	10148.38	8.24
9	326.85	12376.02	12797.62	3.41

10	344.45	15721.29	15867.52	0.93
APD <sub>min</sub>				0.93
APD <sub>max</sub>				17.08
AAPD				9.96
<i>(2).Cycloalkanes</i>				
1. Cyclopentane ( $T_b= 49.5$ , $T_c= 238.65^\circ\text{C}$ , $\omega= 0.196$ )				
1	49.25	759.813	718.593	5.43
2	76.85	1792.647	1608.071	10.30
3	96.85	3045.25	2791.667	8.33
4	116.85	4815.396	4535.267	5.82
5	136.85	7110.585	6973.141	1.93
6	156.85	9818.307	10237.46	4.27
7	176.85	13958.65	14453.1	3.54
8	196.85	20566.69	19733.62	4.05
9	216.85	26717.2	26178.47	2.02
10	238.65	33812.78	33871.3	0.17
APD <sub>min</sub>				0.17
APD <sub>max</sub>				10.30
AAPD				4.59
2. Cyclohexane ( $T_b= 80.78$ , $T_c= 280.43^\circ\text{C}$ , $\omega= 0.212$ )				
1	80.72	759.813	705.2916	7.18
2	86.85	930.077	840.015	9.68
3	111.85	1755.144	1836.798	4.65
4	136.85	3105.255	3132.618	0.88
5	161.85	5167.925	5575.903	7.89
6	186.85	8018.159	8336.016	3.96
7	211.85	11895.98	12975.85	9.08
8	236.85	17063.9	17758.53	4.07
9	261.85	27924.8	25208.03	9.73

10	281	30565.01	30510.1	0.18
APD <sub>min</sub>				0.18
APD <sub>max</sub>				9.73
AAPD				5.73
<i>(3).Alkenes</i>				
1. Ethene(Ethylene) ( $T_b = -103.73$ , $T_c = 9.19^\circ\text{C}$ , $\omega = 0.087$ )				
1	-103.75	758.312	724.0662	4.52
2	-88.15	1750.944	1830.736	4.56
3	-68.15	4171.693	4383.581	5.08
4	-48.15	8457.696	8903.911	5.28
5	-28.15	15282.51	16008.01	4.75
6	-13.15	22528.1	22961.66	1.92
7	2.85	32800.95	33619.99	2.50
APD <sub>min</sub>				1.92
APD <sub>max</sub>				5.28
AAPD				4.09
2. Propene (Propylene) ( $T_b = -47.69$ , $T_c = 91.65^\circ\text{C}$ , $\omega = 0.142$ )				
1	-47.7	759.813	922.2805	21.38
2	-33.15	1402.615	1674.509	19.38
3	-18.15	2497.705	2822.831	13.02
4	-3.15	3975.327	4476.283	12.60
5	11.85	6150.506	6745.192	9.67
6	26.85	9075.746	9736.435	7.28
7	41.85	12826.05	13549.54	5.64
8	56.85	18076.49	18273.8	1.09
9	71.85	23926.97	25576.66	6.89
10	91.65	34577.84	34544.16	0.10
APD <sub>min</sub>				0.10
APD <sub>max</sub>				21.38

AAPD				9.71
<i>(4).Alkynes</i>				
1. Ethyne(Acetylene) ( $T_b = -84.75$ , $T_c = 35.17^\circ\text{C}$ , $\omega = 0.188$ )				
1	-80.95	960.079	873.4825	9.02
2	-73.15	1417.617	1454.698	2.62
3	-63.15	2280.188	2300.797	0.90
4	-43.15	5167.925	5706.701	10.43
5	-33.15	7395.608	7962.732	7.67
6	-23.15	10275.85	10807.68	5.18
7	-3.15	18376.51	20149.3	9.65
8	6.85	23926.97	25474.92	6.47
9	16.85	30602.52	31681.18	3.52
10	35.55	46803.85	46936.45	0.28
APD <sub>min</sub>				0.28
APD <sub>max</sub>				10.43
AAPD				5.57
<i>(5).Haloalkanes</i>				
1. 1,1-difluoroethane (R152a) ( $T_b = -24.05$ , $T_c = 113.26^\circ\text{C}$ , $\omega = 0.276$ )				
1	-24.02	759.813	712.5733	6.22
2	-3.15	1766.47	1761.867	0.26
3	16.85	3491.012	3372.677	3.39
4	36.85	6270.216	5975.92	4.69
5	56.85	10453.61	9929.362	5.01
6	76.85	16444.35	17017.71	3.49
7	104.85	28884.13	29450.06	1.96
APD <sub>min</sub>				0.26
APD <sub>max</sub>				6.22
AAPD				3.57

2. 1,1,1,2-tetrafluoroethane (R134a) ( $T_b = -26.11$ , $T_c = 101.03^\circ\text{C}$ , $\omega = 0.326$ )				
1	-26.37	750.062	681.1955	9.18
2	-8.15	1617.658	1600.924	1.03
3	11.85	3306.497	3260.687	1.39
4	31.85	6090.276	6636.902	8.97
5	51.85	10353.1	10943.59	5.70
6	71.85	16545.61	16891.29	2.09
7	91.85	25270.33	26510.05	4.91
APD <sub>min</sub>				1.03
APD <sub>max</sub>				9.18
AAPD				4.75
3. Pentafluoroethane (R125) ( $T_b = -48.09$ , $T_c = 66.18^\circ\text{C}$ , $\omega = 0.305$ )				
1	-48.15	758.537	682.7211	9.10
2	-33.15	1501.248	1474.562	1.78
3	-13.15	3244.692	3243.034	0.05
4	6.85	6210.061	6344.611	2.17
5	26.85	10848.89	10331.06	4.77
6	46.85	17704.46	17289.65	2.34
7	56.85	22195.83	21826.85	1.66
APD <sub>min</sub>				0.05
APD <sub>max</sub>				9.10
AAPD				3.12
(6).Diene				
1. 1,3- Butadiene ( $T_b = -4.53$ , $T_c = 152^\circ\text{C}$ , $\omega = 0.195$ )				
1	-4.46	759.813	718.2798	5.47
2	11.85	1380.113	1347.057	2.40
3	26.85	2235.184	2343.002	4.82
4	41.85	3435.283	3403.941	0.91
5	56.85	5070.417	5342.529	5.37



6	76.85	8100.666	8005.375	1.18
7	96.85	12226.01	12562.09	2.75
8	116.85	17776.46	18726.42	5.34
9	136.85	25127.07	24978.7	0.59
10	152	32477.67	32526.46	0.15
APD <sub>min</sub>				0.15
APD <sub>max</sub>				5.47
AAPD				2.90
<i>(7).Aromatic hydrocarbons</i>				
1. Toluene ( $T_b = 110.64$ , $T_c = 318.65^\circ\text{C}$ , $\omega = 0.262$ )				
1	110.63	759.813	696.4484	8.34
2	126.85	1185.097	1187.752	0.22
3	151.85	2137.676	2205.703	3.18
4	176.85	3652.8	3759.212	2.91
5	201.85	5820.479	5978.935	2.72
6	226.85	9225.759	8986.94	2.59
7	251.85	13651.12	14017.93	2.69
8	276.85	19276.59	19166.04	0.57
9	301.85	25877.13	25384.66	1.90
10	320.85	30377.5	30779.29	1.32
APD <sub>min</sub>				0.22
APD <sub>max</sub>				8.34
AAPD				2.64
2. Ethyl benzene ( $T_b = 136.21$ , $T_c = 343.95^\circ\text{C}$ , $\omega = 0.304$ )				
1	136.15	759.813	686.2251	9.69
2	159.85	1417.617	1439.504	1.54
3	179.85	2227.683	2230.931	0.15
4	199.85	3352.776	3731.902	11.31
5	219.85	4837.898	5254.128	8.60

6	239.85	6773.057	7166.271	5.81
7	279.85	12301.01	13364.23	8.64
8	299.85	16126.33	16842.6	4.44
9	319.85	20776.71	20850.5	0.36
10	339.85	25877.13	25405.69	1.82
APD <sub>min</sub>				0.15
APD <sub>max</sub>				11.31
AAPD				5.24
<i>(8).Esters</i>				
1. Methyl acetate ( $T_b= 56.94$ , $T_c= 233.65^\circ\text{C}$ , $\omega= 0.326$ )				
1	57.85	759.813	696.3765	8.35
2	76.85	1500.123	1374.071	8.40
3	96.85	2692.721	2490.455	7.51
4	116.85	4027.831	4208.851	4.49
5	136.85	6405.527	6710.083	4.75
6	156.85	10080.83	10185.2	1.04
7	176.85	14476.19	14828.16	2.43
8	196.85	20161.66	20829.07	3.31
9	216.85	27924.8	28368.46	1.59
10	233.65	35155.39	35133.38	0.06
APD <sub>min</sub>				0.06
APD <sub>max</sub>				8.40
AAPD				4.19
2. Ethyl acetate ( $T_b= 77.06$ , $T_c= 250.1^\circ\text{C}$ , $\omega= 0.361$ )				
1	77.1	759.813	664.9502	12.49
2	96.85	1447.619	1391.081	3.91
3	116.85	2325.191	2592.566	11.50
4	136.85	3825.315	3892.913	1.77
5	156.85	5940.489	6270.574	5.56

6	176.85	8790.723	9498.805	8.05
7	196.85	12413.52	13683.64	10.23
8	216.85	17063.9	18907.86	10.81
9	236.85	23791.96	23544.33	1.04
10	250.05	28742.36	28815.16	0.25
APD <sub>min</sub>				0.25
APD <sub>max</sub>				12.49
AAPD				6.56
<i>(9).Amines</i>				
1. Benzeneamine(Aniline) ( $T_b= 184.02$ , $T_c= 425.85^\circ\text{C}$ , $\omega= 0.380$ )				
1	184.35	759.813	699.149	7.98
2	226.85	2070.17	2166.373	4.65
3	251.85	3420.281	3292.118	3.75
4	276.85	5370.442	5467.966	1.82
5	301.85	8100.666	7738.632	4.47
6	326.85	11700.96	11832.11	1.12
7	351.85	16501.36	15858.37	3.90
8	376.85	22576.86	22742.41	0.73
9	401.85	30377.5	31641.48	4.16
10	425.85	39753.27	39824.88	0.18
APD <sub>min</sub>				0.18
APD <sub>max</sub>				7.98
AAPD				3.28
<i>(10).Xylene</i>				
1. 1,2-dimethylbenzene(O-Xylene) ( $T_b= 144.44$ , $T_c= 357.25^\circ\text{C}$ , $\omega= 0.311$ )				
1	144.41	759.813	689.3859	9.27
2	156.85	1065.088	958.6704	9.99
3	181.85	1867.654	1746.636	6.48

4	206.85	3165.26	2972.552	6.09
5	231.85	4912.904	4777.774	2.75
6	256.85	7463.114	7316.302	1.97
7	281.85	10650.88	10749.54	0.93
8	306.85	15301.26	15241.1	0.39
9	331.85	20626.7	20951.95	1.58
10	357.25	27969.8	28036.25	0.24
APD <sub>min</sub>				0.24
APD <sub>max</sub>				9.99
AAPD				3.97
2. 1,3-dimethylbenzene (m- Xylene) ( $T_b = 139.19$ , $T_c = 343.85^\circ\text{C}$ , $\omega = 0.325$ )				
1	138.85	759.813	663.990	12.61
2	156.85	1215.1	1177.477	3.10
3	181.85	2107.673	2252.316	6.86
4	206.85	3540.291	3886.83	9.79
5	231.85	5557.957	6190.331	11.38
6	256.85	8408.191	9250.063	10.01
7	281.85	12008.49	13128.42	9.33
8	306.85	16981.4	17863.19	5.19
9	331.85	22891.88	23469.67	2.52
10	343.85	26574.69	26599.22	0.09
APD <sub>min</sub>				0.09
APD <sub>max</sub>				12.61
AAPD				7.09

9. Antoine and Model vapor pressure correlation:

No	Antoine Vapor Pressure, $P_{Antoine}$ And Model Vapor pressure, $P_{Model}$			
	Temperature(°C)	Antoine Vapor pressure,	Model Vapor Pressure,	$ PD $

		$P_{Antione}(\text{mmHg})$	$P_{Model}(\text{mmHg})$	
(1). <i>n</i> -Alkanes				
1. Methane ( $T_b = -161.49$ , $T_c = -82.586$ °C, $\omega = 0.011$ )				
1	-161.49	760.6054	734.3682	3.45
2	-151.5	1627.853	1583.713	3.45
3	-132.75	5049.412	5210.248	2.71
4	-110	14006.6	14580.31	3.19
5	-100.85	19552.53	19225.6	4.10
6	-90.75	27168.8	27778.89	1.67
7	-82.586	34544.57	34575.16	2.25
APD <sub>min</sub>				1.67
APD <sub>max</sub>				4.10
AAPD				2.97
2. Ethane ( $T_b = -88.6$ , $T_c = 32.18$ °C, $\omega = 0.099$ )				
1	-88.6	759.407	723.2855	4.76
2	-95.6	509.7395	518.8899	1.80
3	-75.75	1459.134	1522.306	4.33
4	-43	5435.357	5055.685	6.99
5	-15.5	12495.53	11745.72	6.00
6	22.3	30119.59	30322.68	0.67
7	32.18	36512.06	36473.83	0.10
APD <sub>min</sub>				0.1
APD <sub>max</sub>				6.99
AAPD				3.52
3. Propane ( $T_b = -42.13$ , $T_c = 96.7$ °C, $\omega = 0.149$ )				
1	-42.13	757.2023	722.7392	4.55
2	-25.78	1485.381	1514.511	1.96
3	-15	2203.697	2245.725	1.91
4	10.1	4880.578	5005.403	2.56
5	30.25	8356.66	8168.948	2.25
6	45.8	12051.2	11608.15	3.68

7	65.89	18356.14	18581.14	1.23
8	77	22667.65	22996.41	1.45
9	85.12	26218.61	26317.16	0.38
10	90.05	28545.68	28095.83	1.58
11	96.7	31895.19	31897.89	0.01
APD <sub>min</sub>				0.01
APD <sub>max</sub>				4.55
AAPD				1.96
<b>4. Butane (<math>T_b = -0.49</math>, <math>T_c = 152.01^\circ\text{C}</math>, <math>\omega = 0.2002</math>)</b>				
1	-0.49	759.1949	708.622	6.66
2	27.13	1970.631	2013.776	2.19
3	45.06	3324.659	3320.14	0.14
4	65	5543.747	5741.585	3.57
5	85.98	8888.488	8453.399	4.89
6	102.3	12340.65	11978.36	2.94
7	115	15609.01	15220.84	2.49
8	135.35	22018.38	21888.67	0.59
9	145	25599.37	25030.31	2.22
10	60	4907.066	4654.933	5.14
11	102	12269.82	11978.36	2.38
12	150.3	27721.96	28457.86	2.65
13	152.01	28430.87	28457.86	0.09
APD <sub>min</sub>				0.09
APD <sub>max</sub>				6.66
AAPD				2.77
<b>5. Pentane (<math>T_b = 36.07</math>, <math>T_c = 196.45^\circ\text{C}</math>, <math>\omega = 0.251</math>)</b>				
1	36.07	760.3884	684.9573	9.92
2	50.8	1233.348	1156.446	6.24
3	70.05	2164.601	2116.319	2.23

4	90.08	3624.082	3552.575	1.97
5	110.15	5723.796	6169.6	7.79
6	135.13	9439.648	9854.861	4.40
7	160	14595.64	14736.59	0.97
8	170	17132.95	17044.85	0.51
9	180	19957.97	19562.24	1.98
10	190	23083.83	23735.83	2.82
11	90	3617.082	3552.575	1.78
12	75	2473.714	2426.638	1.90
13	196.45	25265.37	25233.78	0.13
APD <sub>min</sub>				0.13
APD <sub>max</sub>				9.92
AAPD				3.28
6. Hexane ( $T_b = 68.73$ , $T_c = 234.45^\circ\text{C}$ , $\omega = 0.300$ )				
1	68.73	760.845	661.8165	13.02
2	85.8	1274.066	1200.755	5.75
3	115.4	2757.95	2624.706	4.83
4	135	4290.674	3719.653	13.31
5	150.4	5879.839	5144.844	12.50
6	170.7	8581.667	7666.658	10.66
7	200	13902	13104.4	5.74
8	215.15	17399.06	16720.58	3.90
9	234.45	22667.81	22635.1	0.14
APD <sub>min</sub>				0.14
APD <sub>max</sub>				13.31
AAPD				7.76
7. Heptane ( $T_b = 98.42$ , $T_c = 267.46^\circ\text{C}$ , $\omega = 0.346$ )				
1	98.42	759.6595	409.5776	46.08
2	100	796.0647	409.5776	48.55

3	120.25	1396.253	1425.257	2.08
4	140	2273.96	2674.251	17.60
5	160.6	3585.276	4911.178	36.98
6	180	5275.863	7644.286	44.89
7	200	7571.308	10701.98	41.35
8	210	8957.446	11499.68	28.38
9	225.78	11502.48	13942.28	21.21
10	250	16346.05	18090.18	10.67
11	135	2020.053	2213.251	9.56
12	210.5	9031.224	11499.68	27.33
13	235	13206.59	15596.33	18.01
14	267.46	20611.06	20575.46	0.17
APD <sub>min</sub>				0.17
APD <sub>max</sub>				48.55
AAPD				25.20
8. Nonane ( $T_b = 150.82$ , $T_c = 321.48^\circ\text{C}$ , $\omega = 0.446$ )				
1	150.82	759.2896	902.5996	18.87
2	160	963.4139	1216.332	26.25
3	170	1232.961	1606.568	30.30
4	180	1558.695	1833.693	17.64
5	190	1948.21	2358.676	21.07
6	200	2409.481	2986.958	23.97
7	210	2950.82	3343.188	13.30
8	220	3580.824	4146.433	15.80
9	230	4308.321	5079.33	17.90
10	240	5142.318	5597.54	8.85
11	250	6091.949	6743.527	10.70
12	260	7166.422	8043.293	12.24
13	280	9726.795	10300.22	5.90



14	300	12896.72	12949.5	0.41
15	310	14732.7	14945.4	1.44
16	315	15717.27	16014.61	1.89
17	321.48	17061.59	17132.28	0.41
APD <sub>min</sub>				0.41
APD <sub>max</sub>				30.30
AAPD				13.35
9. Decane ( $T_b = 174.15$ , $T_c = 344.45^\circ\text{C}$ , $\omega = 0.488$ )				
1	174.15	759.2094	845.1993	11.33
2	190	1120.65	1327.544	18.46
3	210.16	1763.632	1993.402	13.03
4	230	2647.619	2879.918	8.77
5	250.45	3881.807	4469.251	15.13
6	270	5430.453	6013.155	10.73
7	290	7453.259	7896	5.94
8	310.34	10034.26	10148.38	1.14
9	320	11465.34	11868.9	3.52
10	235	2916.596	3230.899	10.78
11	230	2647.619	2879.918	8.77
12	320	11465.34	11868.9	3.52
13	344.45	15740.81	15867.52	0.80
APD <sub>min</sub>				0.80
APD <sub>max</sub>				18.46
AAPD				8.61
10. Undecane ( $T_b = 195.93$ , $T_c = 365.85^\circ\text{C}$ , $\omega = 0.530$ )				
1	195.93	760.7504	808.5311	6.28
2	200	841.1904	945.4311	12.39
3	220.4	1352.02	1464.632	8.33
4	250	2493.757	2774.999	11.28

5	270	3610.563	3890.879	7.76
6	290.05	5076.373	5300.785	4.42
7	310.15	6954.188	7041.578	1.26
8	260	3012.715	3116.629	3.45
9	320	8042.317	8403.203	4.49
10	235	1847.715	2175.594	17.75
11	280	4294.594	4795.835	11.67
12	350	12127.2	12580.32	3.74
13	360	13771.45	13556.92	1.56
14	344	11211.3	11652.15	3.93
15	365.85	14804.02	14582.86	1.49
APD <sub>min</sub>				1.26
APD <sub>max</sub>				17.75
AAPD				6.65
11. Dodecane ( $T_b = 216.33$ , $T_c = 384.85^\circ\text{C}$ , $\omega = 0.576$ )				
1	216.33	760.5008	797.1397	4.82
2	240.33	1313.451	1439.721	9.61
3	265.5	2192.667	2421.267	10.43
4	283.4	3055.826	3437.657	12.50
5	304	4348.506	4740.782	9.02
6	335.7	7096.804	7663.35	7.98
7	355.5	9366.964	9933.275	6.05
8	384.85	13653.4	13641.1	0.09
APD <sub>min</sub>				0.09
APD <sub>max</sub>				12.50
AAPD				7.56
(2). Cycloalkanes				
1. Cyclopentane ( $T_b = 49.5$ , $T_c = 238.65^\circ\text{C}$ , $\omega = 0.196$ )				
1	49.5	766.8852	718.593	6.30

2	69	1404.135	1384.229	1.42
3	99.05	3111.653	3169.841	1.87
4	130.4	6218.839	6291.268	1.16
5	145.3	8307.385	8493.967	2.25
6	165	11790.05	12218.96	3.64
7	185.96	16513.48	16953.68	2.67
8	200	20325.93	19733.62	2.91
9	225.25	28614.11	27981.77	2.21
10	230	30390.43	29864.3	1.73
11	90	2486.241	2448.474	1.52
12	235	32337.36	31827.14	1.58
13	238.65	33809.21	33871.3	0.18
APD <sub>min</sub>				0.18
APD <sub>max</sub>				6.3
AAPD				2.26
2. Cyclohexane ( $T_b = 80.78$ , $T_c = 280.43^\circ\text{C}$ , $\omega = 0.212$ )				
1	80.78	762.1645	705.2916	7.46
2	100	1318.336	1168.744	11.35
3	120.15	2196.488	2113.541	3.78
4	150.05	4243.819	3988.643	6.01
5	170	6237.531	6193.343	0.71
6	190	8848.372	9152.786	3.44
7	210.1	12180.69	11933.63	2.03
8	225.25	15214.36	15241.81	0.18
9	240.75	18822.53	19113.97	1.55
10	275	28768.5	28671.47	0.34
11	280.43	30610.51	30510.1	0.33
APD <sub>min</sub>				0.18
APD <sub>max</sub>				11.35

AAPD				3.38
3. Methyl cyclo hexane ( $T_b= 100.94$ , $T_c= 299.04$ °C, $\omega= 0.235$ )				
1	100.94	760.1012	700.8632	7.79
2	130.4	1640.768	1677.913	2.26
3	155.5	2882.451	2778.311	3.61
4	175.6	4305.673	3919.94	8.96
5	200	6665.796	6582.62	1.25
6	230	10710.14	10420.95	2.70
7	257.9	15802.44	15701.47	0.64
8	280	20868.37	21141.61	1.31
9	299.04	26030.58	26016.38	0.05
APD <sub>min</sub>				0.05
APD <sub>max</sub>				8.96
AAPD				3.17
<i>(3). Branched alkanes</i>				
1. 3-Ethyl pentane ( $T_b= 93.48$ , $T_c= 267.35$ °C, $\omega= 0.311$ )				
1	93.48	759.6553	607.9764	19.97
2	110	1205.782	1112.035	7.77
3	140.40	2539.449	2873.85	13.17
4	165.30	4299.024	4717.703	9.74
5	180	5695.885	6488.782	13.92
6	200	8102.913	9384.427	15.82
7	230	12993.79	13857.51	6.65
8	250	17236.94	18091.75	4.96
9	267.35	21630.02	21626.63	0.02
APD <sub>min</sub>				0.02
APD <sub>max</sub>				19.97
AAPD				10.22
2. 2-Methyl octane ( $T_b= 143.29$ , $T_c= 313.85$ °C, $\omega= 0.423$ )				

1	143.29	759.6177	816.4287	7.48
2	160	1166.519	1163.276	0.28
3	180	1859.923	1637.714	11.95
4	200	2837.163	2538.957	10.51
5	230	4983.378	4277.266	14.17
6	245	6427.636	5228.761	18.65
7	270	9490.313	8483.491	10.61
8	290	12611.3	11208.19	11.13
9	300	14419.49	13432	6.85
10	313.85	17216.87	16038.91	6.84
APD <sub>min</sub>				0.28
APD <sub>max</sub>				18.65
AAPD				9.85
(4). Alkenes				
1. Ethene(Ethylene) ( $T_b = -103.73$ , $T_c = 9.19^\circ\text{C}$ , $\omega = 0.087$ )				
1	-103.73	757.1289	724.0662	4.37
2	-93.71	1322.663	1372.639	3.78
3	-80.25	2541.142	2396.982	5.67
4	-70.14	3908.066	3913.448	0.14
5	-40.35	11064.9	10644.82	3.80
6	-10.75	24389.34	24557.44	0.69
7	-80	2569.809	2396.982	6.73
8	9.19	37696.8	37767.04	0.19
APD <sub>min</sub>				0.14
APD <sub>max</sub>				6.73
AAPD				3.17
2. Propene (Propylene) ( $T_b = -47.69$ , $T_c = 91.65^\circ\text{C}$ , $\omega = 0.142$ )				
1	-47.69	761.5371	725.6593	4.71
2	-25	1941.185	1895.179	2.37

3	-10	3277.464	3229.935	1.45
4	20	7875.471	7770.324	1.34
5	30.7	10298.84	10261.84	0.36
6	40.75	13018.71	13249.65	1.77
7	56.57	18260.68	18066.75	1.06
8	68.13	22899.31	23900.15	4.37
9	80	28426.46	28975.21	1.93
10	85	30996.96	30803.76	0.62
11	20	7875.471	7770.324	1.34
12	91.65	34645.43	34669.23	0.07
APD <sub>min</sub>				0.07
APD <sub>max</sub>				4.71
AAPD				1.78
3. 1-Butene( $T_b = -6.23$ , $T_c = 146.35^\circ\text{C}$ , $\omega = 0.194$ )				
1	-6.23	760.2509	705.1812	7.24
2	15.5	1661.467	1632.842	1.72
3	30.06	2621.472	2507.247	4.36
4	45.7	4069.894	4144.373	1.83
5	65	6594.81	7098.827	7.64
6	85.5	10362.5	10303.31	0.57
7	100	13817.01	14337.89	3.77
8	120.4	19936.76	20633.45	3.49
9	130.56	23582.98	23556.84	0.11
10	146.35	30098.65	30113.8	0.05
APD <sub>min</sub>				0.05
APD <sub>max</sub>				7.64
AAPD				3.08
(5). Alkynes				
1. Ethyne(Acetylene) ( $T_b = -84.75$ , $T_c = 35.17^\circ\text{C}$ , $\omega = 0.188$ )				

1	-84.75	755.6843	727.3899	3.74
2	-60.75	2542.05	2653.653	4.39
3	-40.75	5718.035	5706.701	0.20
4	-20.75	11249.77	11899.89	5.78
5	10.75	26724.17	27443.12	2.69
6	35.17	46083.98	46936.45	1.85
APD <sub>min</sub>				0.2
APD <sub>max</sub>				5.78
AAPD				3.11
2. 1- Pentyne ( $T_b= 40.23$ , $T_c= 196.85$ °C, $\omega= 0.394$ )				
1	40.23	761.8386	658.4802	13.57
2	60.23	1472.79	1395.921	5.22
3	80.90	2671.629	2635.601	1.35
4	100	4345.086	4543.564	4.57
5	120.5	6917.619	8116.172	17.33
6	140.05	10289.18	12104.95	17.65
7	160	14827.1	17235.22	16.24
8	196.85	26683.21	31291.93	17.27
APD <sub>min</sub>				1.35
APD <sub>max</sub>				17.65
AAPD				11.65
(6). <i>Haloalkanes</i>				
1. Difluoromethane ( $T_b= -51.72$ , $T_c= 78.11$ °C, $\omega= 0.278$ )				
1	-51.72	756.8935	713.1222	5.78
2	-31.01	1999.832	1954.969	2.24
3	-10	4506.808	4467.685	0.87
4	25.15	13262.75	13280.02	0.13
5	45.05	21781.29	22491.31	3.26
6	55	27238.22	26367.31	3.20

7	67.68	35483.78	35465.42	0.05
8	78.11	43430.65	43548.46	0.27
APD <sub>min</sub>				0.05
APD <sub>max</sub>				5.78
AAPD				1.98
2. Trichlorofluoromethane ( R11) ( $T_b= 23.66$ , $T_c= 197.95^\circ\text{C}$ , $\omega= 0.195$ )				
1	23.66	756.5438	714.5705	5.55
2	55.5	2105.461	2116.278	0.51
3	74.32	3496.581	3543.961	1.36
4	102.4	6717.595	6888.481	2.54
5	125.25	10610.29	11063.3	4.27
6	155.30	17856.25	18101.55	1.37
7	178.4	25319.49	25906.23	2.32
8	197.95	33059.08	33546.74	1.48
APD <sub>min</sub>				0.51
APD <sub>max</sub>				5.55
AAPD				2.43
3. Bromotrifluoromethane ( $T_b= -58.01$ , $T_c= 67^\circ\text{C}$ , $\omega= 0.174$ )				
1	-58.01	756.3082	719.2898	4.89
2	-30.01	2461.339	2245.274	8.78
3	-10.01	4842.932	4507.36	6.93
4	20.10	11133.42	10665.36	4.20
5	-58	756.6727	719.2898	4.94
6	42.08	18367.54	18553.22	1.01
7	15.7	9973.367	9780.545	1.93
8	67	29819.55	29848.97	0.01
APD <sub>min</sub>				0.01
APD <sub>max</sub>				8.78
AAPD				4.09
4. 1,1-difluoroethane(R152a) ( $T_b= -24.05$ , $T_c= 113.26^\circ\text{C}$ , $\omega= 0.276$ )				



1	-24.05	821.6582	712.5733	13.28
2	-12	1356.165	1324.969	2.30
3	6	2620.888	2307.95	11.94
4	17	3749.245	3372.677	10.04
5	30	5516.512	4793.672	13.10
6	40	7248.755	6646.355	8.31
7	55	10551.87	9929.362	5.90
8	75	16480.1	15630.71	5.15
9	85	20182.26	20066.05	0.58
10	90	22233.27	21734.36	2.24
11	100	26755.57	27357.8	2.25
12	110.75	32270.95	31657.01	1.90
13	113.26	33659.94	33982.08	0.96
APD <sub>min</sub>				0.58
APD <sub>max</sub>				13.28
AAPD				5.10
5. 1,1,1-trifluoroethane (R143a) ( $T_b = -47.29$ , $T_c = 73.15^\circ\text{C}$ , $\omega = 0.259$ )				
1	-47.29	763.2441	701.7431	8.06
2	-20.75	2344.668	2290.422	2.31
3	20	8537.231	8662.213	1.46
4	35.05	12528.18	12401.55	1.01
5	50	17650.41	17184.59	2.64
6	60.07	21822.92	21537.97	1.31
7	73.15	28184.98	28465.19	0.99
APD <sub>min</sub>				0.99
APD <sub>max</sub>				8.06
AAPD				2.54
6. 1,1,1,2-tetrafluoroethane (R134a) ( $T_b = -26.11$ , $T_c = 101.03^\circ\text{C}$ , $\omega = 0.326$ )				
1	-26.11	756.035	681.1955	9.90

2	-10	1453.294	1366.72	5.96
3	10.9	3000.533	3260.687	8.67
4	20	3969.505	4196.281	5.71
5	30	5284.475	5949.742	12.59
6	40	6894.967	8178.864	18.62
7	50	8835.212	9958.957	12.72
8	60	11138.56	13112.11	17.72
9	70	13837.05	16891.29	22.07
10	80	16960.99	19782.04	16.63
11	90	20538.72	24706.28	20.29
12	101.03	25042.46	30368.5	21.27
APD <sub>min</sub>				5.71
APD <sub>max</sub>				22.07
AAPD				14.35
7. Pentafluoroethane(R125) ( $T_b = -48.09$ , $T_c = 66.18^\circ\text{C}$ , $\omega = 0.305$ )				
1	-48.09	757.1871	682.7211	9.83
2	-30.05	1676.324	1697.453	1.26
3	-10.8	3420.287	3243.034	5.18
4	5.12	5678.079	5713.115	0.62
5	17.33	8034.262	8560.141	6.55
6	30.18	11198.33	11312.68	1.02
7	45	15834.67	17289.65	9.19
8	55.18	19695	21826.85	10.82
9	66.18	24534.12	27163.58	10.72
APD <sub>min</sub>				0.62
APD <sub>max</sub>				10.82
AAPD				6.13
8. 1-chloro-1,1,2,2-tetrafluoroethane(R124) ( $T_b = -11.77$ , $T_c = 126.85^\circ\text{C}$ , $\omega = 0.260$ )				
1	-11.77	758.2519	700.9034	7.56

2	20.3	2454.836	2252.159	8.26
3	31.6	3478.607	3268.349	6.04
4	72	9858.424	9325.995	5.40
5	102.56	18439.6	18301.25	0.75
6	126.85	28173.88	28223.02	0.17
APD <sub>min</sub>				0.17
APD <sub>max</sub>				8.26
AAPD				4.70
9. 2-Chlorobutane ( $T_b = 68.09$ , $T_c = 247.45$ °C, $\omega = 0.267$ )				
1	68.09	759.4475	686.9961	9.54
2	88.09	1384.591	1213.943	12.32
3	115.5	2831.75	3054.879	7.88
4	140.8	5010.762	5610.613	11.97
5	165.9	8237.463	8444.593	2.51
6	190	12582.14	13063.43	3.83
7	220	20055.54	20247.8	0.96
8	247.45	29240.55	27600.37	5.61
APD <sub>min</sub>				0.96
APD <sub>max</sub>				12.32
AAPD				4.01
(7). <i>S</i> -Alkyl				
1. Methanethiol (Methyl mercaptan)( $T_b = 5.96$ , $T_c = 196.85$ °C, $\omega = 0.15$ )				
1	5.96	759.2186	725.8584	4.39
2	20.75	1327.473	1425.069	7.35
3	45.54	2966.985	2953.753	0.45
4	65.8	5187.836	4911.332	5.33
5	88.9	9007.478	8595.12	4.58
6	100	11428.25	10535.92	7.81
7	130.07	20249.87	19912.06	1.67

8	155	30431.92	29515.54	3.01
9	180.07	43630.06	41962.78	3.82
10	196.85	54243.97	54190.81	0.01
APD <sub>min</sub>				0.01
APD <sub>max</sub>				7.81
AAPD				3.84
2. 3-Thiapentane(Diethyl sulfide) ( $T_b = 92.1$ , $T_c = 283.85^\circ\text{C}$ , $\omega = 0.295$ )				
1	92.1	759.1226	789.5446	4.01
2	120.3	1665.15	1705.327	2.41
3	150.50	3402.086	3300.646	2.98
4	180	6186.761	5851.309	5.42
5	210.1	10498.98	10597.82	0.94
6	240	16619.29	16321.26	1.79
7	260.6	22084.78	22274.79	0.86
8	283.85	29629.74	29607.62	0.07
APD <sub>min</sub>				0.07
APD <sub>max</sub>				5.42
AAPD				2.31
(8). Diene				
1. 1,3- Butadiene ( $T_b = -4.53$ , $T_c = 152^\circ\text{C}$ , $\omega = 0.195$ )				
1	-4.53	755.9565	718.2798	4.98
2	20.15	1833.81	1791.798	2.29
3	40.10	3356.209	3403.941	1.42
4	60.6	5753.651	5934.944	3.15
5	80	9001.74	8800.439	2.24
6	110	16336.39	16051.76	1.74
7	130	23053.48	23298.31	1.06
8	135	24984.75	24978.7	0.02

9	152	32351.36	32526.46	0.54
APD <sub>min</sub>				0.02
APD <sub>max</sub>				4.98
AAPD				1.94
<i>(9). Aromatic hydrocarbons</i>				
1. Benzene ( $T_b = 80.09$ , $T_c = 288.9^\circ\text{C}$ , $\omega = 0.209$ )				
1	80.09	759.3392	716.8441	5.60
2	100.09	1361.384	1216.84	10.62
3	120.5	2306.135	2254.954	2.22
4	140.5	3653.595	3847.173	5.30
5	160.5	5521.815	5491.849	0.54
6	180.5	8016.086	8398.294	4.77
7	200	11150.5	11185.37	0.31
8	230	17541.71	18534.26	5.66
9	250.55	23157.04	23179.11	0.01
10	275.75	31564.89	32470.93	2.87
11	288.9	36661.65	36751.14	0.24
APD <sub>min</sub>				0.01
APD <sub>max</sub>				10.62
AAPD				3.47
2. Toluene ( $T_b = 110.64$ , $T_c = 318.65^\circ\text{C}$ , $\omega = 0.262$ )				
1	110.64	759.8514	696.4484	8.34
2	130	1283.548	1187.752	7.46
3	150	2086.298	2205.703	5.72
4	177	3727.658	3759.212	0.85
5	182	4116.274	4246.718	3.17
6	135.75	1483.938	1399.29	5.70
7	155	2337.269	2205.703	5.63
8	166	2970.811	2907.227	2.14

9	157	2443.917	2538.688	3.88
10	188.5	4666.177	4777.888	2.39
11	225.13	8848.742	8986.94	1.56
12	265.5	16060.35	16461.78	2.50
13	290	22046.07	22138.23	0.42
14	305	26385.41	27112.35	2.76
15	318.65	30809.01	30779.29	0.01
APD <sub>min</sub>				0.01
APD <sub>max</sub>				8.34
AAPD				3.50
3. 2-Methyl phenol(o-cresol) ( $T_b = 191.02$ , $T_c = 424.45^\circ\text{C}$ , $\omega = 0.436$ )				
1	191.02	760.5392	649.2466	14.63
2	200	962.5145	824.7041	14.32
3	230	1966.518	1891.841	3.80
4	250	3000.951	3169.023	5.60
5	270	4415.632	4946.245	12.02
6	300	7432.313	8209.615	10.46
7	330	11785.78	12600.44	6.91
8	325	10954.53	12600.44	15.02
9	350	15580.32	16676.61	7.04
10	370	20192.8	21438.49	6.17
11	390.9	25980.88	26885.34	3.48
12	410.1	32250.19	33005.8	2.34
13	424.45	37574.2	37450.8	0.33
APD <sub>min</sub>				0.33
APD <sub>max</sub>				15.02
AAPD				7.86
4. 3-Methyl phenol(m-cresol) ( $T_b = 202.23$ , $T_c = 432.55^\circ\text{C}$ , $\omega = 0.452$ )				
1	202.23	758.5946	655.3038	13.62

2	225.4	1353.871	1297.28	4.18
3	250	2338.327	2058.914	11.95
4	278.9	4122.086	3599.535	12.68
5	300	5971.721	5271.517	11.73
6	325.25	8933.559	8395.844	6.02
7	350	12772.29	11566.99	9.44
8	375.7	17897.87	17148.17	4.19
9	330	9593.794	8395.844	12.47
10	400	23954.11	22528.87	5.95
11	432.55	34132.02	34200.63	0.20
APD <sub>min</sub>				0.20
APD <sub>max</sub>				13.62
AAPD				8.40
5. 4-Methyl phenol(p-cresol) ( $T_b= 201.97$ , $T_c= 431.35^\circ\text{C}$ , $\omega= 0.510$ )				
1	201.97	759.1818	653.9315	13.86
2	230.30	1560.024	1268.351	18.70
3	266.5	3432.398	3073.146	10.47
4	280	4463.158	4024.616	9.83
5	305.6	7057.402	5906.397	16.31
6	325.25	9723.676	8469.632	12.90
7	360	16194.7	14749.43	8.92
8	380.8	21327.72	20070.33	5.90
9	400	27024.79	26857.36	0.62
10	270.5	3716.16	3073.146	17.30
11	420.2	34110.26	32333.36	5.21
12	431.35	38535.46	38674.13	0.36
APD <sub>min</sub>				0.36
APD <sub>max</sub>				18.70
AAPD				10.03

6. Ethyl benzene ( $T_b= 136.21$ , $T_c= 343.95^\circ\text{C}$ , $\omega= 0.304$ )				
1	136.21	777.7213	686.2251	11.76
2	150	1113.138	1101.021	1.09
3	160	1420.893	1277.185	10.11
4	170	1791.655	1697.069	5.28
5	180	2233.667	1944.642	12.94
6	190	2755.54	2525.257	8.36
7	200	3366.199	3234.268	3.92
8	210	4074.821	3642.583	10.61
9	220	4890.78	4578.675	6.38
10	230	5823.587	5690.452	2.29
11	250	8078.129	7732.106	4.28
12	225	5341.979	5111.349	4.32
13	250.75	8173.529	7732.106	5.40
14	277	12059.72	11263.21	6.60
15	300	16427.03	15877.21	3.35
16	320	21043.85	20153.1	4.23
17	343.95	27672.44	27079.37	2.14
APD <sub>min</sub>				1.09
APD <sub>max</sub>				12.94
AAPD				6.06
7. Butyl benzene ( $T_b= 183.27$ , $T_c= 387.35^\circ\text{C}$ , $\omega= 0.393$ )				
1	183.27	759.7379	394.8085	48.03
2	200.27	1138.345	791.7511	30.45
3	235.7	2397.855	2004.592	16.40
4	265.4	4115.119	4132.449	0.42
5	285.8	5746.741	5935.106	3.28
6	300	7138.649	7375.694	3.32
7	335.9	11753.14	11852.76	0.85



8	350	14050.55	14000.43	0.36
9	365.5	16927.62	17604.11	3.10
10	387.35	21656.45	21659.23	0.01
APD <sub>min</sub>				0.01
APD <sub>max</sub>				48.03
AAPD				10.62
<i>(10). Halo benzene</i>				
1. Hexafluorobenzene( $T_b = 80.25$ , $T_c = 243.58$ °C, $\omega = 0.396$ )				
1	80.25	759.0506	611.0103	19.50
2	100.25	1400.425	1121.778	19.90
3	130.35	3092.528	2535.064	18.03
4	160.6	6055.147	5199.481	14.13
5	180	8838.756	8018.888	9.28
6	200	12591.58	11979.71	4.86
7	223	18192.88	17395.03	4.39
8	191	10783.11	9838.094	8.76
9	230	20199.64	19017.01	5.85
10	243.58	24526.68	24621.76	0.39
APD <sub>min</sub>				0.39
APD <sub>max</sub>				19.90
AAPD				10.51
<i>(11). Alcohols</i>				
1. Isobutanol ( $T_b = 107.89$ , $T_c = 274.63$ °C, $\omega = 0.590$ )				
1	107.89	765.4987	1433.031	87.20
2	127.8	1465.752	1168.495	20.28
3	157.69	3386.88	543.8566	83.94
4	175.7	5255.99	231.5623	95.59
5	200	8924.579	6.629352	99.93

6	245	20386.29	185487.3	809.86
7	150	2768.462	762.4357	72.46
8	255.05	23969.59	105914.3	341.87
9	274.63	32212.47	32091.79	0.37
APD <sub>min</sub>				0.37
APD <sub>max</sub>				809.86
AAPD				179.06
<b>2. Sec-butanol (<math>T_b = 99.51</math>, <math>T_c = 262.9^\circ\text{C}</math>, <math>\omega = 0.574</math>)</b>				
1	99.51	758.1976	1435.511	89.33
2	120.5	1503.794	1108.766	26.27
3	150	3439.784	387.6488	88.73
4	180.51	7096.58	1.269364	99.98
5	240	21959.82	75629.96	244.40
6	262.9	31445.84	31443.6	0.01
APD <sub>min</sub>				0.01
APD <sub>max</sub>				244.4
AAPD				91.45
<b>3. 1-Pentanol (<math>T_b = 138.01</math>, <math>T_c = 315^\circ\text{C}</math>, <math>\omega = 0.579</math>)</b>				
1	138.01	765.3518	1420.164	85.56
2	150.1	1108.649	1588.78	43.31
3	170.79	1974.345	1906.569	3.43
4	200.5	4067.082	2917.933	28.25
5	230	7539.74	4505.476	40.24
6	259	12788.48	6837.961	46.53
7	280	18006.79	11260.36	37.47
8	300	24278.3	17539.99	27.75
9	220	6176.879	3748.233	39.32
10	315	29912.68	29484.7	1.43
APD <sub>min</sub>				1.43
APD <sub>max</sub>				85.56

AAPD				35.33
4. 1-Octanol ( $T_b = 195.18$ , $T_c = 379.35^\circ\text{C}$ , $\omega = 0.594$ )				
1	195.18	759.034	851.7727	12.22
2	220.18	1441.546	1478.226	2.54
3	250.9	2852.008	2477.723	13.12
4	289	5845.424	5072.058	13.23
5	300	7035.166	6349.504	9.75
6	330.6	11278.88	10824.72	4.03
7	352.5	15277.79	14643.18	4.15
8	379.35	21436.03	21490.73	0.26
APD <sub>min</sub>				0.26
APD <sub>max</sub>				13.23
AAPD				7.41
5. 1-Nonanol ( $T_b = 213.37$ , $T_c = 395.75^\circ\text{C}$ , $\omega = 0.633$ )				
1	213.37	766.0293	816.4264	6.58
2	230.17	1167.254	1092.807	6.38
3	255.7	2071.484	1896.408	8.45
4	280.9	3414.806	3165.644	7.30
5	302	4972.752	4542.972	8.64
6	330.65	7859.447	7151.051	9.01
7	360.6	12007.51	12106.24	0.82
8	395.75	18612.31	19685.28	5.76
APD <sub>min</sub>				0.82
APD <sub>max</sub>				9.01
AAPD				6.62
6. 1-Decanol ( $T_b = 231.07$ , $T_c = 411.25^\circ\text{C}$ , $\omega = 0.661$ )				
1	231.07	777.6289	805.683	3.61
2	250.07	1224.047	1081.191	11.67
3	275.7	2116.912	1883.411	11.03

4	305.8	3723.298	3563.381	4.30
5	330.42	5606.019	5085.965	9.28
6	355	8105.893	7946.714	1.96
7	385.8	12266.65	12059.06	1.69
8	400.01	14619.81	14706.23	0.59
9	411.25	16691.44	17822.05	6.77
APD <sub>min</sub>				0.59
APD <sub>max</sub>				11.67
AAPD				5.66
7. 1-Undecanol ( $T_b = 248.09$ , $T_c = 431.85^\circ\text{C}$ , $\omega = 0.656$ )				
1	248.09	818.4262	797.4349	2.56
2	269.09	1313.019	1254.889	4.43
3	289.9	2004.077	1910.479	4.67
4	315.6	3202.968	3197.134	0.18
5	327.09	3884.586	3609.607	7.08
6	350	5555.031	5111.474	7.98
7	375.75	7994.809	7852.806	1.78
8	395.5	10322.36	10587.95	2.57
9	410.10	12322.24	12793.08	3.82
10	431.85	15775.41	16756.79	6.22
APD <sub>min</sub>				0.18
APD <sub>max</sub>				7.98
AAPD				4.13
8. 1-Dodecanol ( $T_b = 264.64$ , $T_c = 446.85^\circ\text{C}$ , $\omega = 0.68$ )				
1	264.64	810.2382	793.4458	2.07
2	284.65	1254.72	1068.448	14.85
3	314.7	2249.09	2131.55	5.23
4	347.46	3911.367	3527.073	9.83
5	365.4	5135.6	5017.486	2.30

6	382	6496.885	6276.999	3.38
7	405.7	8863.845	8649.699	2.42
8	300	1707.64	1631.097	4.48
9	290	1400.543	1233.965	11.89
10	422.6	10884.79	11717.54	7.65
11	435.7	12656.83	12919.2	2.07
12	446.85	14313.77	15625.55	9.16
APD <sub>min</sub>				2.07
APD <sub>max</sub>				14.85
AAPD				6.28
(12). <i>Ethers</i>				
1. Methyl ethyl ether ( $T_b = 7.35$ , $T_c = 164.65$ °C, $\omega = 0.236$ )				
1	7.35	760.8635	712.9253	6.30
2	25.35	1537.844	1400.666	8.92
3	56.6	4109.647	3700.292	9.96
4	77.8	7043.984	6538.199	7.18
5	90	9262.521	8846.885	4.49
6	110	13839.32	13876.09	0.27
7	130	19681.91	19089.2	3.01
8	150	26872.54	27248.49	1.40
9	164.65	33024.84	33077.17	0.16
APD <sub>min</sub>				0.16
APD <sub>max</sub>				9.96
AAPD				4.63
(13). <i>Ketones</i>				
1. Butanone(Methyl ethyl ketone) ( $T_b = 79.56$ , $T_c = 263.65$ °C, $\omega = 0.322$ )				
1	79.56	757.5706	682.5172	9.91
2	100	1401.717	1443.606	2.99

3	125.5	2740.804	2704.567	1.32
4	150	4803.822	5206.249	8.38
5	175	7951.312	8109.617	1.99
6	200	12424.76	13044.9	4.99
7	225	18500.67	19574.92	5.81
8	250	26445.95	26012.3	1.64
9	263.65	31662.92	31563.86	0.31
APD <sub>min</sub>				0.31
APD <sub>max</sub>				9.91
AAPD				4.15
2. Cyclopentanone ( $T_b = 130.57$ , $T_c = 351.35$ °C, $\omega = 0.288$ )				
1	130.57	758.4638	700.7131	7.61
2	150.3	1312.036	1240.507	5.45
3	180	2715.664	2760.668	1.66
4	200	4192.68	4150.098	1.02
5	230	7502.363	7455.937	0.62
6	250	10627.06	10119.98	4.77
7	280.90	17263.54	15832.35	8.29
8	300	22660.91	20075.36	11.41
9	320.20	29609.73	24957.44	15.71
10	351.35	43147.41	34547.17	19.93
APD <sub>min</sub>				0.62
APD <sub>max</sub>				19.93
AAPD				7.65
(14). Esters				
1. Methyl formate ( $T_b = 31.75$ , $T_c = 214.05$ °C, $\omega = 0.254$ )				
1	31.75	759.2212	711.5887	6.27
2	51.75	1527.949	1523.247	0.31
3	75.5	3121.025	3348.465	7.29

4	95	5197.526	5685.377	9.39
5	120.8	9370.214	9999.003	6.71
6	150.14	16647.92	17623.87	5.86
7	165.65	21807.83	22564.08	3.47
8	180.8	27844.38	28310.63	1.67
9	190.6	32313.23	32604.36	0.90
10	200	37039.07	37275.92	0.64
11	210.5	42848.14	42329.96	1.21
12	95	5197.526	5685.377	9.39
13	214.05	44942.52	45001.4	0.13
APD <sub>min</sub>				0.13
APD <sub>max</sub>				9.39
AAPD				4.01
2. Methyl acetate ( $T_b = 56.94$ , $T_c = 233.65^\circ\text{C}$ , $\omega = 0.326$ )				
1	56.94	759.3487	696.3765	8.29
2	76.94	1459.475	1374.071	5.85
3	100	2812.422	2856.797	1.58
4	125.05	5211.76	5349.824	2.65
5	150	8891.974	8313.77	6.50
6	165.65	12014.73	12348.66	2.78
7	185.02	16902.56	16193.82	4.19
8	190	18359.94	17647.3	3.88
9	200	21552.75	20829.07	3.36
10	220.2	29160.1	28368.46	2.71
11	100	2812.422	2856.797	1.58
12	227.75	32426.82	32767.75	1.05
13	233.65	35148.22	35133.38	0.04
APD <sub>min</sub>				0.04

APD <sub>max</sub>				8.29
AAPD				3.42
3. Ethyl methanoate(Ethyl formate) ( $T_b= 54.32$ , $T_c= 235.35^\circ\text{C}$ , $\omega= 0.282$ )				
1	54.32	760.8976	702.0668	7.73
2	74.78	1472.83	1343.46	8.78
3	94.01	2541.979	2385.513	6.16
4	114.8	4286.132	3978.881	7.17
5	135.35	6780.723	6294.711	7.17
6	170	13223.32	12652.16	4.32
7	188	17916.33	17941.44	0.14
8	195.95	20323.42	19483.16	4.13
9	200	21633.02	21118.81	2.38
10	215.15	27054.26	26619.6	1.61
11	235.35	35643.96	35449.56	0.55
APD <sub>min</sub>				0.14
APD <sub>max</sub>				8.78
AAPD				4.56
4. Ethyl acetate ( $T_b= 77.06$ , $T_c= 250.1^\circ\text{C}$ , $\omega= 0.361$ )				
1	77.06	760.671	664.9502	12.58
2	100.06	1540.363	1391.081	9.69
3	130.06	3374.8	3416.984	1.25
4	150.06	5313.087	5601.037	5.42
5	185.06	10578.16	11465.91	8.39
6	225.5	20537.68	20383.72	0.75
7	250.1	29108.23	28815.16	1.00
APD <sub>min</sub>				0.75
APD <sub>max</sub>				12.58
AAPD				5.58
5. Propyl ethanoate(Propyl acetate) ( $T_b= 101.5$ , $T_c= 276.25^\circ\text{C}$ , $\omega= 0.389$ )				
1	101.5	759.8779	613.1894	19.30



2	120.8	1332.529	1220.271	8.42
3	145	2479.487	2221.739	10.40
4	165.5	3949.232	3761.301	4.76
5	180	5334.232	4781.437	10.36
6	200	7806.527	7423.435	4.91
7	235	14031.65	13194.34	5.97
8	245	16325.5	15678.78	3.96
9	265	21691.69	21599.56	0.42
10	276.25	25198.41	25069.87	0.51
APD <sub>min</sub>				0.42
APD <sub>max</sub>				19.3
AAPD				6.90
(15). Amines				
1. Methylamine ( $T_b = -6.33$ , $T_c = 156.85$ °C, $\omega = 0.283$ )				
1	-6.3	761.3988	716.6915	5.87
2	15.5	1868.959	1796.391	3.88
3	35	3690.576	3859.328	4.57
4	50.75	5974.85	5758.547	3.62
5	70.3	10139.54	10368.15	2.25
6	90.3	16309.23	17215.2	5.55
7	120.75	30348.77	31457.95	3.65
8	135.82	39741.04	39477.88	0.66
9	35	3690.576	3859.328	4.57
10	156.85	55923.75	55682.03	0.43
APD <sub>min</sub>				0.43
APD <sub>max</sub>				5.87
AAPD				3.51
2. 2-Propanamine(Methyl ethyl amine) ( $T_b = 31.78$ , $T_c = 198.65$ °C, $\omega = 0.277$ )				

1	31.78	643.7493	692.8687	7.63
2	50.05	1272.588	1480.172	16.31
3	75.75	2849.655	3210.306	12.66
4	100	5373.521	6031.142	12.24
5	120	8435.204	9234.806	9.48
6	140	12558.46	14575.38	16.06
7	160	17889.88	19991.4	11.75
8	180	24554.44	26459.6	7.76
9	198.65	32059.52	33987.58	6.01
APD <sub>min</sub>				6.01
APD <sub>max</sub>				16.31
AAPD				11.1
<b>3. 1-Butanamine(Butyl amine) (<math>T_b= 76.29</math>, <math>T_c= 253.65^\circ\text{C}</math>, <math>\omega= 0.338</math>)</b>				
1	76.29	732.19	678.8875	7.28
2	100	1513.664	1529.45	1.04
3	140	4165.591	3931.415	5.62
4	180	9393.628	9415.091	0.23
5	200	13322.31	13675.57	2.65
6	225	19740.76	20787.38	5.30
7	253.65	29459.18	30202.08	2.52
APD <sub>min</sub>				0.23
APD <sub>max</sub>				7.28
AAPD				3.52
<b>4. Benzeneamine(Aniline) (<math>T_b= 184.02</math>, <math>T_c= 425.85^\circ\text{C}</math>, <math>\omega= 0.380</math>)</b>				
1	184.02	751.4238	699.149	6.96
2	200.02	1136.101	1168.927	2.89
3	240	2793.251	2500.436	10.48
4	260	4127.741	3756.559	8.99
5	280	5901.896	5467.966	7.35

6	300	8197.626	7738.632	5.60
7	320	11098.7	10681.32	3.76
8	349	16551.59	15858.37	4.19
9	360	19051.06	19067.9	0.09
10	380	24264.49	22742.41	6.27
11	400.25	30487.91	29210.81	4.19
12	410	33845.18	34217.5	1.10
13	370.8	21755.64	20844.62	4.19
14	415.15	35716.97	34217.5	4.20
15	425.85	39829.34	39824.88	0.01
APD <sub>min</sub>				0.01
APD <sub>max</sub>				10.48
AAPD				4.68
<i>(16). Xylene</i>				
1. 1,2-dimethylbenzene(O-Xylene) ( $T_b = 144.44$ , $T_c = 357.25^\circ\text{C}$ , $\omega = 0.311$ )				
1	144.44	759.9431	689.3859	9.28
2	160.5	1147.392	1121.72	2.24
3	180.75	1840.834	1746.636	5.12
4	205	3056.925	2972.552	2.76
5	220.25	4087.424	3793.361	7.19
6	250.3	6858.703	6604.172	3.71
7	270	9305.217	8910.85	4.24
8	295.5	13343.06	12852.86	3.67
9	310	16127.88	16548.34	2.61
10	330.45	20717.74	20951.95	1.13
11	340.5	23275.49	22588.44	2.95
12	200	2766.54	2617.54	5.39
13	350	25885.53	26128.34	0.94

14	343	23943.97	24313.15	1.54
15	357.25	28006.92	28036.25	0.10
APD <sub>min</sub>				0.10
APD <sub>max</sub>				9.28
AAPD				3.52
2. 1,3-dimethylbenzene (m- Xylene) ( $T_b = 139.19$ , $T_c = 343.85^\circ\text{C}$ , $\omega = 0.325$ )				
1	139.19	761.1991	663.9904	12.77
2	150.5	1024.295	981.8125	4.15
3	170	1642.278	1652.475	0.62
4	190	2545.606	2603.877	2.29
5	210	3790.529	3886.83	2.54
6	235	5939.754	6190.331	4.22
7	250	7603.053	8410.39	10.62
8	285	12785.56	13128.42	2.68
9	300.5	15743.83	16598.02	5.43
10	310.1	17802.32	19182.94	7.76
11	320	20116.26	20557.31	2.19
12	330.4	22764.94	23469.67	3.01
13	340	25415.79	25007.41	1.61
14	190	2545.606	2603.877	2.29
15	343.85	26536.03	26599.22	0.24
APD <sub>min</sub>				0.24
APD <sub>max</sub>				12.77
AAPD				4.16
3. 1,4-dimethylbenzene(P- Xylene) ( $T_b = 138.38$ , $T_c = 343.15^\circ\text{C}$ , $\omega = 0.320$ )				
1	138.38	760.9001	658.0998	13.51
2	150	1031.985	975.9831	5.43
3	170.25	1681.606	1647.127	2.05
4	195	2865.128	2986.811	4.25

5	205.5	3526.042	3879.844	10.03
6	240	6528.662	6861.483	5.01
7	270.45	10471.62	11027.51	5.31
8	300	15717.79	16467.94	4.77
9	310.23	17902.59	19009.99	6.19
10	330.3	22790.89	23215.49	1.86
11	315.15	19025.6	19009.99	0.08
12	340.15	25497.32	26278.53	3.06
13	343.15	26363.41	26278.53	0.32
APD <sub>min</sub>				0.08
APD <sub>max</sub>				13.51
AAPD				4.76