STUDY OF VAPOR – LIQUID EQUILIBRIA OF PETROLEUM FRACTIONS

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in
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Abstract

The calculations of vapor – liquid equilibria for petroleum fractions are important in design and operation of petroleum processing equipment. The most important vapor – liquid calculation for petroleum fractions is well known as the equilibrium flash vaporization curve (*EFV*). The *EFV* curve can be predicted from the true boiling point curve (*TBP*) by using two methods: The graphical methods and the pseudo – components (computer) methods.

The purposes of the present work were divided into two parts: First part has two folds: First one graphical method and various pseudo – components methods were selected and tested to decide which method showed the greatest promise. Secondly, various attempts for improving the accuracy of existing methods were investigated. The selected flash method for part one were, the Raizi – Daubert graphical method (RD graph) and five pseudo – components flash methods including the Soave – Redlich, Kowng (SRK) and Peng – Robinson (PR) equations of state flash methods, activity coefficients flash methods in which the SRK and PR equations of state used for vapor phase and the van – Laar activity coefficients model used for liquid phase (SRK + Van and PR + Van) and finally the ideal solution *K* – values flash method (Ideal K) also used. To perform the purpose of part one, the data for 18 petroleum stocks were selected from literature including the *TBP, EFV* and the specific gravity data or curves.

As a results of part one investigations, it was concluded that the modified Ideal K flash method based on the present work of new suggested vapor pressure correlation was the most accurate and reliable flash method for estimation the *EFV* curves. The expression of the new suggested vapor pressure correlation is as follows:

$$ln\,P^{s} = ln\,P^{sA} + \left(Sp.gr - Sp.gr^{A}\right)F_1F_2 + \left(1 - \frac{0.85}{TBr}\right)$$

The average absolute deviation (*AAD%*) for the modified Ideal K is 15.62% as compared to 23.51%, 24.98%, 23.40%, 25.18%, 23.73% and 21.81% for unmodified SRK, SRK + Van, PR + Van, Ideal K and RD graph methods respectively. Using the modified Ideal K flash method had improved the values of *AAD%* for 10 petroleum stocks (out of 18 petroleum stocks used) by more than 30%. Improvement was limited by inaccurate in experimental data (*TBP* curve) and characterization parameters (*Tc, Pc, ω, …etc*).

For part two of the present work, the modified Ideal K flash method was used for predicting the *EFV* curves and the flash zone temperatures for Kirkuk, Basrah, Jambur and Bai – Hassan Iraqi crude oils. The *TBP* and the specific gravity curves for these crude oils were obtained experimentally at laboratory distillation unit in Daura refinery. The predicted flash zone temperatures were 318 °C, 327 °C, 335 °C and 290 °C for Kirkuk, Basrah, Jambur and Bai – Hassan crude oils respectively. These values of the flash zone temperatures must be considered as primary values and must be adjusted to the temperature, pressure and the amount of the stripping steam that usually used with crude oil tower.

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Notations

Symbols

Symbol	Meaning
a	Attractive term (parameter) of cubic equation of state
a, b, c	Parameters in equation (2.6)
a_i	Activity of species i Parameter in equations (3.84) and (3.97)
a_1, a_2, a_3	Constants in equation (3.1)
a_4, a_5, a_6	Constants in equation (3.2)
A	Mixture temperature dependent term defined in equations (3.80) and (3.93)
A', B', C'	Antonine's equation constants {equation (3.112)}
Ac, Bc	Adjustable parameters in equation (6.6)
A_i	Pure species combining parameters defined in equations (3.83) and (3.96)
A_{ij}	Interaction parameter for van – Laar equation {equation (3.145)}
A_0, A_1, A_2, A_4, A_5 A_6, A_7, A_8, A_9	Constants in equation (B.122)
$A_{10}, A_{11}, A_{12}, A_{14}$	Constants in equation (3.123)
A_1', B_1', C_1' D_1', E_1'	Constants of working *TBP* equation {equation (5.2)}
A_2', B_2'	Constants of working *Sp.gr* equation {equation (5.3)}
A_{12}', A_{21}'	Constants in van – Laar equation
ASTM D86 10%	*ASTM* temperature at 10% volume percent distilled, °R
ASTM D86 50%	*ASTM* temperature at 50% volume percent distilled , °R
b	Co volume term (parameter) of cubic equation of state
b_i	Pure species parameter defined in equations (3.84) and (3.97)
b_m	Mixing rule parameters defined in equations (3.82) and (3.95)
b_1, b_2	Constants in equation (3.3)

Symbol	Meaning
B	Mixture volume dependent term defined in equations (3.81) and (3.94)
B_i	Pure species combining parameters defined in equations (3.83) and (3.96)
c_1, c_2, c_3	Constants in equation (3.4)
C	Constant in equations (3.45) and (6.4)
CF	Correction factor
EFV 10%	*EFV* temperature at 10% volume percent distilled, °R
EFV 50%	*EFV* temperature at 50% volume percent distilled, °R
EFV 50%	Temperature at which 50% of petroleum stock vaporized
f_i^{id}	Ideal fugacity for pure species
$\overline{f}_i$	Partial fugacity coefficient
f_i^V , f_i^L	Fugacity for pure species in vapor and liquid phase
$\overline{f}_i^V$, $\overline{f}_i^L$	Partial fugacity of species *i* in mixture for vapor and liquid phase
F	Feed molar rate, mole/s
F_M	Parameter in equation (3.26)
F_P	Parameter in equation (3.28)
F_T	Parameter in equation (3.27)
F_L	Liquid molar rate, mole/s
F_V	Vapor molar rate, mole/s
$F_{(0)}, F_{(1)}$	Functions defined in equation (3.177)
F_1, F_2	Constants in equation (6.3)
G_i	Molar free energy for pure species
$\overline{G}_i$	Partial molar Gibbs free energy
$\overline{G}_i^E$	Partial molar Gibbs excess free energy
K_{ij}	Interaction parameters
K	Parameter in equation (3.90)
K_i	Equilibrium ratio or *K* – values

Symbol	Meaning
$K_{i(ideal)}$	Ideal K – values
K_{UOP}	Characterization factor defined as $\sqrt[3]{TB}/Sp.gr$
K_i^A	Initial value of K - values
$L^{(0)}$,$L^{(1)}$	Parameters in equations (3.104) and (3.105)
m	Parameter in equation (3.76)
M	Intensive real property,
$M^{(0)}$,$M^{(1)}$	Parameters in equations (3.104) and (3.105)
M^{id}	Intensive ideal property
M^E	Intensive excess property
$\overline{M}$	Intensive real partial property
$\overline{M}^{id}$	Intensive ideal partial property
$\overline{M}^{E}$	Intensive partial excess property
MW	Molecular weight
$N^{(0)}$, $N^{(1)}$	Parameter in equations (3.104) and (3.105)
N	Number of experimental points
Nc	Total number of species
N_i	Number of moles of cut or fraction
N_t	Total estimated moles
NP	Number of phases
P	Total pressure
P^{sA}	Vapor pressure for n – alkane species
Pc	Critical pressure, kPa, psia
P_i	Partial pressure of species i
Pr	Reduced pressure ($Pr=P/Pc$)
Pr^*	Reduced vapor pressure ($Pr^*=P^*/Pc$)
P_i^S	Vapor pressure of species i
R	Universal gas constant
$Sp.gr$	Specific gravity measured @ (15 °C/15 °C) (60 °F/60 °F)

Symbol	Meaning
$Sp.gr^A$	Specific gravity of n - alkane measured @ (15 °C/15 °C) (60 °F/60 °F)
t	*TBP* temperature at equation (2.6), R
T	Temperature
Tr	Reduced temperature ($Tr=T/Tc$)
Tc	Critical temperature, °C, R
TB	True boiling point temperature, °C, R
TBF	True boiling point temperature, °F
TBr	Reduced true boiling temperature ($TBr=TB/Tc$)
$TBP\ 50\%$	Temperature at which 50% of petroleum stock distilled
$TMEP$	Parameter in equation (3.102)
V	Volume, volume percent distilled in equations (5.2) and (5.3)
V^L	Molar volume, cm^3/gmol
Vc	Critical volume
V_i	Flash volume given in equations (5.14) and (5.15)
V_F	Molal volume in feed stream
V_V	Molal volume in vapor stream
V_1, V_2	Volume percent distilled in equation (2.5)
W_f	Feed total weight
W_i	Weight of cut or fraction
W_t	Total estimated weight
$\|x\|$	Parameter in equation (3.35)
x_i	Liquid phase mole fraction of species i, independent variable in equation (6.1)
X_m	Mid volume percent
y_i	Vapor phase mole fraction of species *i*
Z	Compressibility factor for cubic equation of state
Z^L	Liquid phase compressibility factor

Symbol	Meaning
Z^V	Vapor phase compressibility factor
Z_{RA}	Rackett equation constant
Z_i	Molar feed compositions

Greek litters

Symbol	Meaning
α	Alfa function term of cubic equation of state Parameter defined in equation (3.40)
α'	Original alfa function term of SRK equation of state defined in equation (3.76)
β	Vapor fraction in mole basis
β_V	Vapor fraction in volume basis
γ	Kinematic viscosity, c. stock
γ_i^L	liquid phase activity coefficient for species *i*
γ_i^V	Vapor phase activity coefficient for species *i*
δ_i	Solubility parameter of species *i* in mixture, J/cm^3
δ_j	Solubility parameter of species *j* in mixture, J/cm^3
ζ_i	Cavet equation constant
θ	Temperature in equation (2.6),and any physical property in equation (6.1)
θ^{ref}	Reference physical properties in equation (6.1)
θ_i	First partial deviation in equation (6.1)
θ_{ij}	Second partial deviation in equation (6.1)
θ_1, θ_2	First order deviation in equation (6.2)
λ_i	Heat of vaporization of species *i*
μ	Dynamic viscosity, Ns/m^2
μ_i	Chemical potential of species *i*
ρ	Density @ 15 °C (60 °F), g/cm^3

Σ	Summation

Symbol	Meaning
ϕ_i^L	Liquid phase fugacity coefficient of pure species *i*
ϕ_i^V	Vapor phase fugacity coefficient of pure species *i*
$\bar{\phi}_i^L$	Liquid phase partial fugacity coefficient of species *i* in mixture
$\bar{\phi}_i^V$	Vapor phase partial fugacity coefficient of species *i* in mixture
Φ_i	Volume fraction of species *i* in mixture
Φ_j	Volume fraction of species *j* in mixture
ω	Acentric factor
ω_A	Acentric factor of n – alkane
ϵ	Tolerance error

Super scripts

Symbol	Meaning
-	Partial properties
A	n – alkane, initial estimated values given in equation (5.11)
calcd	Calculated
exp	Experimental
L	liquid phase
LK	Lee – Kasler correlation
s	Saturation conditions
V	Vapor phase
0	Measured at $\omega = 0$
1	Measured at $\omega = 1$
1, 2	Number of phases in equilibrium
15	Measured at 15 °C (60 °F)
25	Measured at 25 °C (77 °F)

Sub scripts

Symbol	Meaning
f	Feed
i	Species *i* in mixture
j	Species *j* in mixture
M	Molecular weight in equations (3.29) and (3.32)
P	Critical pressure in equations (3.31) and (3.34)
r	Reduced conditions
t	Total
T	Critical temperature in equations (3.30) and (3.33)
V	Vapor phase and volume basis in equation (3.181)

Abbreviations

Symbol	Meaning
API	American petroleum institute
ASTM	American society for testing and materials
Cal	Calculation
C.S	Chao – Sender
EFV	Equilibrium vaporization curve
Eq.	Equation
Ideal K	Ideal solution *K* – values model
PR	Peng – Robinson equation of state
PR + Van	PR equation of state for vapor phase and van – Laar activity model for liquid phase
RD graph	Raizi – Daubert graphical method
RK	Redlich Kowng equation of state
SEFV	Slop of *EFV* curve
SRK	Soave Redlich Kowng equation of state
SRK + Van	SRK equation of state for vapor phase and van – Laar activity model for liquid phase

Symbol	Meaning
STBP	Slop of *TBP* curve
TBP	True boiling point curve
Van	van – Laar model
VLE	Vapor – liquid equilibrium

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Chapter One

Introduction

Since virtually all phase of petroleum refining involve the separation of petroleum fractions (or undefined mixtures) into liquid and vapor phases, a reliable vapor – liquid calculations are essential perquisite for efficient design and operation of petroleum processing equipment **[1]**. The most important vapor – liquid equilibrium calculations for petroleum fractions are the flash calculations, in which the flash vaporization curve (*EFV*) is estimated.

The flash vaporization curve (*EFV*) is defined as plot of temperature against percent by volume of liquid distilled, with the total vapor in equilibrium with the non vaporized liquid at constant pressure. Each point of the *EFV* curve represents a separate equilibrium experiment. Normally at least five such experiments are required to establish the *EFV* curve **[2, 3]**.

The costly of operations and tedious procedures necessary to obtain experimental *EFV* curves have given impetus to development of methods for predicting *EFV* curves from some other distillation curves such as true boiling point curves (*TBP*) **[4]**.

For complex mixtures such as the crude oil or petroleum fractions must have their compositions defined by empirical means because the identity of the hundreds or thousands of different hydrocarbons present are not known. A common method used for this is the true boiling point distillation curve (*TBP*). A *TBP* curve then is a plot of boiling point temperature of each small increment of volume and is obtained by measuring the volume percent distilled and the top temperature of high efficiency batch distillation column. *TBP* distillation is performed in column has the efficiency of 15 to 100 theoretical plates at relatively high reflux ratio (*i.e.* 5 to 1 or greater) **[5, 6]**.

Two important impacts of the accurate prediction of the *EFV* curve from the *TBP* curve can be obtained. The first impact; the designer needs to know how much vapor is going up to the feed zone of the crude tower, the later can be accomplished by knowing the flash zone temperature. The flash zone temperature is obtained from the *EFV* curve. Knowing the flash zone temperature and the amount of the vaporization have great rule in the design of the auxiliary crude oil tower (*e.g.* furnace, pre heater exchangers, …*etc*) **[6]**. The second impact; the accurate prediction of the *EFV* curve means that the accurate and reliable *K* – values predictions for each of petroleum fraction or cut are performed. The accurate predictions of the *K* – values have greater effect on the relative volatility of each cut, that used for estimation of the number of theoretical plates of crude oil tower. Error in the relative volatility can generate as much as 100% error in the number of theoretical plates. This means that for a column with 20 actual plates, the designer may design a column with 40 plates doubling the cost of investment **[7]**.

Two methods are used for predicting the *EFV* curve from available *TBP* curve, these are:

a) Graphical methods.

b) Pseudo – components (computer) methods.

The graphical methods are the oldest methods for predicting the *EFV* curves from the *TBP* curves. They are also known as empirical correlations because they relate the *TBP* curve with the *EFV* curve using a rather limited amount of data for both curves, consequently, the graphical methods are developed from published experimental data for both *TBP* and *EFV* curves **[4, 8]**. The most famous graphical methods that used for predicting the *EFV* curve from *TBP* curves are the Maxwell method **[9]** and the Raizi – Daubert method **[10]**, which is adopted by the *API* – technical data book **[11]**.

The pseudo – components methods (also known as computer methods) based on several types of thermodynamic models for predicting the *K* – values, have been proposed to replace the classical graphical methods for predicting the *EFV* curve from the available *TBP* curve. In the pseudo – components methods there are four main steps must be performed to obtain the EFV curve, these steps can be summarized as follows **[1, 6]**:

a) In the first step the *TBP* curve must be divided into a suitable number of cuts. Each cut has its average boiling point (*TB*) and specific gravity (*Sp.gr*).

b) In the second step, the (*TB*) and (*Sp.gr*) for each cut are used for estimation the basic characterization parameters using a suitable characterization correlations published in literatures **[12, 13]**. Basic characterization parameters including the molecular weight (*MW*), critical temperatures (*Tc*), critical pressures (*Pc*), acentric factors (ω), …*etc*. At this step the compositions of feed can be obtained.

c) In the third step, the *K* – values for each cut are estimated using available thermodynamic models such as equation of state models, activity coefficient models, …*etc*.

d) The final step including the estimation of the flash volumes or *EFV* curve by using the isothermal flash calculation.

The scope of the present work can be divided into two parts:

1. The first part has two folds, first the graphical methods, and the pseudo – components methods were tested to decide which method shows the greatest promise, secondly various attempts were tried to investigate the possibility for improving and increasing the accuracy of the existing flash method. To perform the purpose of part one of the present work, the data for 18 petroleum stocks were selected from literature including *TBP*, *EFV* and specific gravity data or curves.
2. Using the most accurate flash method suggested and developed in part one, the *EFV* curves for four Iraqi crude oils were predicted from their *TBP* curves. These crude oils are Kirkuk, Basrah, Jambour and Bai – Hassan. The *TBP* and specific gravity curves for these crude oils were obtained from the laboratory distillation unit in the Duara refinery laboratory.

Using the predicted *EFV* curves for the Kirkuk, Basrah, Jambour and Bai – Hassan crude oils, the flash zone temperatures were also predicted using the Nelson procedure **[3]**.

Chapter Two

Literature survey

2.1 Crude oil

Crude oil (also known as Petroleum), is the product of natural changes to organic debris over millennia. It is water white to black liquid which may vary from free flowing to having difficulty in being mobile at room temperature **[14]**. The crude oil consists almost entirely of compounds of carbon and hydrogen, with varying amount of organic and these elements can vary only between very narrow limits. The elementary analysis of crude oil shows that crude oils contain 83 – 86.9wt% carbon, 11.4 – 14.0wt% hydrogen, 0.04 – 8.0wt% of sulfur, 0.11 – 1.70wt% nitrogen, 0.5wt% oxygen and about 0.03wt% metals **[15]**.

Crudes contain high proportion of individual hydrocarbons so they vary from a thin (mobile), nearly colorless liquid to a thick (viscous), almost black oil. The specific gravity at 60°F (15.6°C) varies correspondingly from about 0.75 to 1.00 (57 – 10°*API*), with the specific gravity of most crude oils falling in range from 0.80 to 0.95 (45 - 17°*API*) thus, it is not surprising that crude oils vary in composition from one oil field to another, from one well to another in the same field. This variation can be in both molecular weight and types of molecules present in petroleum, thus crude oil may well be described as a mixture of organic molecules drawn from a wide distribution of molecular types that lie within a wide distribution of molecular weights, so that crude oil can be categorized based on the molecular weight distribution as light, medium and heavy crude oil **[14, 16]**.

2.1.2 Composition of crude oil

Crude oil is very complex mixture consisting of hydrocarbons and non – hydrocarbons compounds. There are many studies that have been applied as a mean of evaluating petroleum composition. In fact, these studies are so numerous as to be subject matter of several books and articles (**Rostler [17]**, **Altgeft and Gouw [18]** and **Speight [15]**). As a results of these studies, it was realized that the hydrocarbons in petroleum belong to several series of paraffins, naphthene (cyclo paraffin), branched paraffins and aromatics hydrocarbons. Non hydrocarbon such as nitrogen, oxygen, sulfur and traces of variety of metal – containing (vanadium and nickel) compounds are also present in crude oils. The amounts of these non hydrocarbon compounds increase with boiling point and also with increase of molecular weight **[14]**.

2.1.2.1 Hydrocarbon compounds

Hydrocarbons are the principal constituents of the petroleum. The hydrocarbon series are grouped into paraffins, naphthenes and aromatics **[3]**.

a- Paraffins

Normal paraffins are found in most petroleums and particularly in light types. The member of paraffins $C_1 - C_{35}$ group (molecular weight (16 – 492)) have been found in several crude oils **[16]**. Normal paraffins series (type formula C_nH_{2n+2}) is characterized by great stability, the name of each member ends in (ane), methane, ethane, hexane etc **[3]**. Branched – chain paraffins also have been found in light and middle point fractions **[14]**.

b- Naphthenes (cyclo paraffins)

Naphthenes (also known as cyclo paraffins) are widely found in crude oils and petroleum fractions. The characteristic of naphthenic hydrocarbons is the fact they contain saturated rings which have 5 or 6 carbon atoms **[20]**. Naphthenes has the formula of C_nH_{2n} and its presence in the petroleum all over the world varies from 30 to 60% with quantities increasing in the heavy fractions, and decreasing in the light fractions **[3]**.

c- Aromatics

Aromatics form the third main type of hydrocarbon compounds found in crude oils. Aromatic series have general type formula of C_nH_{2n-6}, and they differ chemically and physically from paraffin and naphthene compounds, *i.e.*, aromatics are unsaturated hydrocarbons and have relatively high specific gravity possessing good solvent properties **[3, 17, 20]**.

2.1.2.2 Non – hydrocarbon compounds

The non – hydrocarbon compounds can be summarized as follows:

a- Sulfur compounds

Sulfur compounds are among the most important of non hydrocarbon compounds of crude oils. Four types of sulfur compounds occur in crude oils and petroleum fractions, they are hydrogen sulfide, mercaptans, sulfide and thiocyclic compounds (containing sulfur ring) **[16, 21]**. Difficulties with oil that contains sulfur compounds arise in only three main ways: corrosion, color and poor explosion characteristic of gasoline fuels **[3]**.

b- Nitrogen compounds

The nitrogen compounds content of crude oils and petroleum fractions are much lower than the sulfur content. The typical nitrogen compounds found in crude oils are generally divided into two groups, basic and non basic compounds. The basic nitrogen compounds cause difficulty with many acid – catalyzed processes used in petroleum (*e.g.* reforming units) **[14, 20]**.

c- Oxygen compounds

The oxygen compounds found in crude oil and petroleum fractions are often products of exposure to air. The most common oxygen compounds are naphthenic acids which are organic acids found in some crudes, and phenol derivatives, which can appear in cracking units [14].

e- Metals compounds

The metal compounds (essentially nickel and vanadium) present in small quantities in crude oils and petroleum fractions. The metal content increases regularly with increasing the molecular weight of distillate fraction, and reaches maximum in residue. The crude oils also contain other non organic compounds such as water, sediments and mineral salts [20].

2.2 Physical properties of petroleum fractions

When dealing with the complex mixtures of hydrocarbons normally found in petroleum fractions, the average physical properties of the mixtures are often of greater importance than a knowledge of exact chemical compositions and of the physical properties of individual compounds [22].

A more important measurable physical properties will be discussed in the next sections.

2.2.1 Boiling point

The temperature at which a pure component boils at atmospheric pressure is an invariable property of the substance and is in fact a useful guide to the identity of the material. Mixtures (including petroleum fractions) do not have single boiling point, but they boil over a range of temperatures depending on pressure, composition and nature of the apparatus used to carry out the experiment [22].

Many physical properties (critical temperature, molecular weight, etc) of pure hydrocarbon can be correlated with normal boiling point as independent variables. However, for use in the petroleum industry, these correlations must also be applicable to petroleum fractions which are mixtures of a large number of compounds, usually having a wide variation in boiling points [19]. Thus, many physical properties of petroleum fractions can be correlated using several types of average boiling points. The several types of average boiling point with the proper physical properties can be shown in Table 2-1.

Table 2-1 Types of average boiling point with proper physical properties

Average boiling point	Physical properties
Volume average boiling point	Liquid viscosity Specific heat Specific gravity
Weight average boiling point	Critical temperature
Molal average boiling point	Critical temperature Thermal expansion of liquid
Mean average boiling point	Molecular weight Characterization factor Specific gravity, …etc
Mid. boiling point	Molecular weight Critical temperature Pressure Acentric factor, …etc

2.2.2 Specific gravity and *API* gravity

The specific gravity is the ratio of the weight of unit volume of oil to the weight of the same volume of water at standard temperature. Unless otherwise stated, both weights (oil and water) are measured at 15°C (60°F) [22].

Other ways of expressing densities are met in particular industries and in oil industry reference is often found to *API* gravities. This is derived from the specific gravity by using the following relationship [3]:

$$API = \left[\frac{141.5}{Sp.\ gr\ (60/60)} - 131.5 \right] \qquad \ldots(2.1)$$

The *API* scale allows representation of specific gravity of oils to vary only from less than 0 (heavy residual oils) to 340 (methane) **[5]**.

Density gives an indication of the crude oil quality. In fact under the same boiling point, paraffinic hydrocarbons have less densities (higher *API*), followed in order by naphthenic and aromatic hydrocarbons, with gradually greater density (lower *API*) **[23]**.

2.2.3 Viscosity

Viscosity is a measure of the ability of a fluid to resist shear. Dynamic viscosity is defined as the shear stress at a point divided by the velocity gradient at that point. The unit of dynamic viscosity in S.I. units is Ns/m^2 and in c.g.s. units is poise **[24]**.

The kinematic viscosity is defined as the ratio of the dynamic viscosity to the density, both at the same temperature. The unit of kinematic viscosity in S.I. units is m^2/s and c.g.s. units is stock **[25]**. The relation between the dynamic viscosity and kinematic viscosity is given by the following equation:

$$\gamma = \frac{\mu}{\rho} \qquad \ldots(2.2)$$

where: γ = kinematic viscosity

μ = dynamic viscosity

ρ = density at °C (60 °F)

2.2.4 Refractive index

Refractive index is defined as the ratio of the velocity of light in vacuum to the velocity of the same wave light in the substance. The value of refractive index varies with the wave length of light used, and also with temperature and both must be specified **[22]**.

2.3 Distillation and distillation curve

Distillation is a widely used method for separating liquid mixtures into their components and had been called the workhorse separation of petroleum, petrochemical, chemical and related industries. It is old in the art, having been practiced for crudes for many decades **[26]**.

Distillation is a separation process that differentiate between the component of a mixture through their volatility. The difference in volatility between the component of a mixture is often characterized by the difference between their boiling points or their vapor pressures **[20]**.

Distillation curve is a plot that relates the percentage distillate (volume or mass basis) of the component or fraction with the corresponding boiling temperature. The distillation curve gives information about initial boiling point temperature, final boiling point temperature and the temperature of any particulate cut or fraction, such as 10%, 20%, …etc **[27]**.

The most important types of distillations will be discussed in the next sections.

2.3.1 Types of distillation

2.3.1.1 True boiling point distillation (*TBP*)

It is also called "fractionating" distillation. This method of distillation is basically a batch distillation using 15 – 100 theoretical plates (or packed bed), with relatively high reflux ratio (5 to 1 or greater). The results are usually plotted as volume percentage distillate with the corresponding temperature, as shown in Fig. 2-1 **[3]**.

The high degree of fractionation in these distillations gives accurate component distributions for mixtures. The *TBP* distillation can be applied mainly for crude oils as well as for petroleum fractions, under atmospheric or vacuum pressure **[28]**.

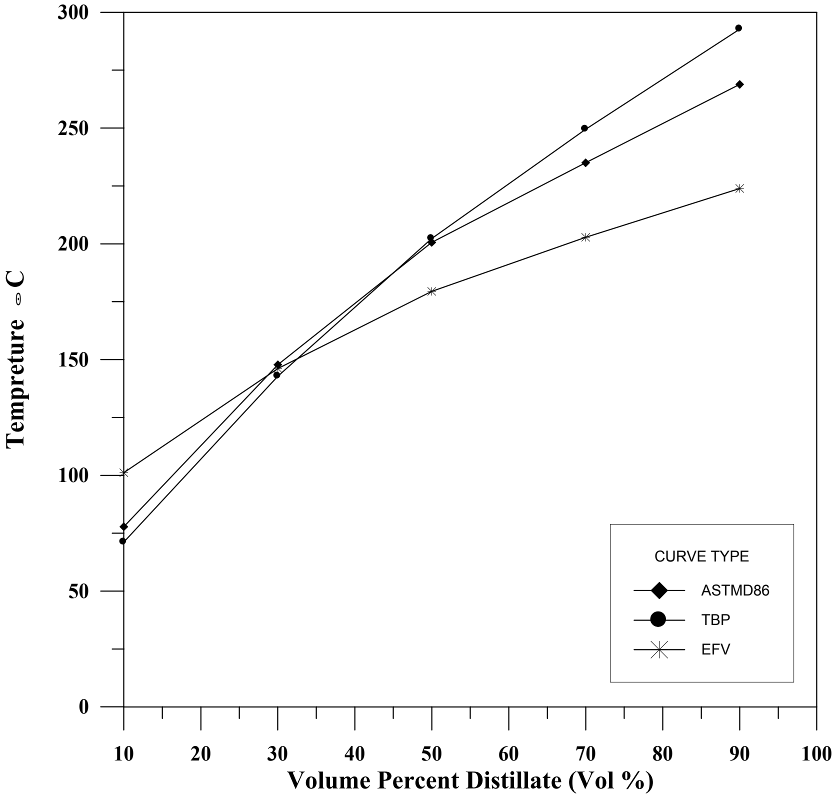

Figure 2-1 Types of distillation curves

2.3.1.2 Equilibrium flash vaporization distillation (*EFV*)

In this distillation, the mixture is heated in coil without allowing the vapor to separate from remaining liquid. As vapor is formed, it travels along in the tube with the remaining liquid until separation is permitted in a vapor separator or vaporizer. By contacting the operation at a series of outlet temperatures and pressures a curve of percentage vaporized versus temperature may by plotted as shown in Fig. 2-1 **[3]**.

Each point on the *EFV* curve represents a separate equilibrium experiment. The number of equilibrium experiments needed to define all portions of the *EFV* curve varies with the shape of the curve. The *EFV* curve can be applied under atmospheric pressure (or higher) and under vacuum pressure **[28]**.

2.3.1.3 Non – fractionating distillation (*ASTM* distillation)

It is best known as *ASTM* distillation or Engler distillation. *ASTM* distillations are run in Engler flask. No packing is employed and the reflux results only from heat loss through the neck of the flask. *ASTM* distillation are more widely used than *TBP* distillation because *ASTM* distillations are simpler, less expensive, require less sample and take only approximately one – tenth as much time **[28]**. *ASTM* distillation methods in use are:

i. *ASTM* method D 86.
ii. *ASTM* method D 216.
iii. *ASTM* method D 1160.

2.3.1.4 Semi – fractionating distillation

In this method of distillation, a mid degree of fractionating is attained by use of a section of packed column between the flask and the condenser. The best known method is the Hample distillation of the U.S. bureau of mines and *ASTM* D 285 for crude petroleum. The crude oil curves obtained by these methods are nearly the same form as *TBP* distillation curve **[3]**.

2.4 Characterization of petroleum fractions

Characterization of hydrocarbons and petroleum fractions (also known as undefined mixtures), involves with use of available bulk parameters such as boiling point, specific gravity, viscosity or refractive index to estimate the basic properties such as molecular weight (*MW*), acentric factor (ω) and critical constant (critical temperature (*Tc*), critical pressure (*Pc*) and critical volume (*Vc*)). The basic properties are used in equations of state or generalized correlations for calculation of physical and thermodynamic properties needed for process design and unit operation **[7, 29]**.

There are dozens of different characterization methods that have been developed for estimation of these basic properties of petroleum fractions. Early correlations in the 30's, 40's and 50's were mainly graphical, while from 60's the analytical correlations in the form of equations suitable for computer uses proposed. Some of these correlations are summarized in Table 2-2.

Table 2-2 Some of correlations that have been developed for estimation basic parameters for petroleum fractions

Correlation name	Type	Bulk properties used	Calculated basic properties
Watson & Wilson [30 – 32]	Graphical	*Sp.gr*, T_B, K_{UOP}	*MW*, *Tc*, *Pc*, ω, viscosity, …etc
Winn [33]	Nomograph	*Sp.gr*, T_B	*MW*, *Tc*, *Pc*, ω, K_{UOP}
Cavett [34]	Analytical	*API*, T_B	*Tc*, *Pc*
Hariu – Sage [6]	Analytical	*API*, T_B	*MW*
Mathur [35]	Analytical	*MW*	*Tc*, *Pc*
Kasler – Lee [12, 36]	Analytical	*Sp.gr*, T_B	*MW*, *Tc*, *Pc*, ω
Riazi – Daubert [13]	Analytical	*Sp.gr*, T_B	*MW*, *Tc*, *Pc*, ω, *Vc*, V_l, heat of vaporization, specific heat, …etc
Twu [37]	Analytical	*Sp.gr*, T_B	*MW*, *Tc*, *Pc*
Riazi – Daubert or API method **[2, 38]**	Analytical	*Sp.gr*, T_B, refractive index, viscosity, *MW*	*MW*, *Tc*, *Pc*, refractive index, viscosity, heat of vaporization
Sim – Daubert [1]	Analytical	*Sp.gr*, T_B	*MW*, *Tc*, *Pc*, ω
Edimister [4]	Analytical	*Tc*, *Pc*, T_B	ω
Riazi – Sahhaf [39]	Analytical	(Paraffinic – Naphthenic – Aromatic) composition, *MW*	*Tc*, *Pc*

2.5 Vapor – liquid equilibrium of petroleum fractions (undefined mixtures)

2.5.1 Definitions

Vapor – liquid equilibria (or phase equilibria) and fluid properties are required in the design of separation process, and analysis of petroleum operations. The separation of multi component mixtures into pure components (or fractions) of desired compositions is of great interest in the petroleum industry **[40]**.

A number of important industrial processes, such as distillation bring two phases (vapor and liquid) into contact, when the phases are not in equilibrium, mass transfer occurs between the phases. The rate of mass transfer of each component depends on the departure of the system from equilibrium. Quantitative treatment of mass transfer rates requires knowledge of the equilibrium states (temperature T, pressure P and compositions) of the system **[41]**.

For the system of NP phases, the temperature, pressure, and partial molal fugacities $\overline{f}_i$ for each component are the same in all phases, and the equilibrium conditions can be stated as followed **[42]**:

$$T^{(1)} = T^{(2)} = T^{(NP)}$$

$$P^{(1)} = P^{(2)} = P^{(NP)}$$

$$\overline{f}_i^{(1)} = \overline{f}_i^{(2)} = \overline{f}_i^{(NP)} \qquad \text{where } i = 1, 2, 3, \ldots NP \qquad \ldots(2.3)$$

For vapor – liquid system of N components:

$$T^L = T^V$$

$$P^L = P^V$$

$$\bar{f}_i^{\,L} = \bar{f}_i^{\,V} \qquad \text{where } i = 1, 2, 3, \ldots N \qquad \ldots(2.4)$$

Since virtually all phases of petroleum refining involves the separation of petroleum fractions into liquid and vapor phases, a reliable estimate of equilibrium flash vaporization curve (*EFV*) (or data) is an essential prerequisite for efficient design and operation of petroleum processing equipment **[1]**.

The *EFV* curve (data) can be obtained experimentally by determining flash vaporization on the stock in question at desired temperature and pressure. Unfortunately this procedure generally so complex and requires a considerable amount of time and money. As a result several methods were developed to predict the (*EFV*) curve or data from simpler analytical true boiling point distillations (*TBP*) **[4]**.

The methods presented in the literatures for predicting the flash vaporization curve are of two general types:

- Graphical or empirical methods.
- Pseudo – component (computer) methods.

2.5.1.1 Graphical or empirical methods for predicting (*EFV*) curve

Graphical methods are the oldest methods that were used for predicting the equilibrium flash vaporization curve or data. They are also known as empirical correlations because they relate the true boiling point and equilibrium flash vaporization curves using a rather limited amount of data for both curves **[6, 8]**.

In 1929 Pirmoov and Beiwenger [43], developed the first such graphical method using experimental *EFV* distillation data on crude oils. In this method, the *EFV* curve is assumed to be straight line on the temperature versus percent volume vaporized scale. Also the relation between the slope of the *TBP* curve (*STBP*) and the slope of *EFV* curve (*SEFV*) are established using the temperature of 50% distillate of the *TBP* (*TBP* 50%) and the temperature of 50% distillate of the *EFV* (*EFV* 50%).

The slope of the *TBP* curve and *EFV* curve can be defined as follows:

$$STBP \;\; or \;\; SEFV = \frac{T_2 - T_1}{V_2 - V_1} \qquad \text{…(2.5)}$$

where T_2, T_1 and V_2, V_1 are the temperatures and their corresponding volume percent vaporized (or distillate), respectively.

Nelson and Souders [43], **Pakie [44]**, **Nelson – Harvey [45]**, **Edmister and Merien [46]** developed several correlations for relating the *STBP*, *SEFV*, *TBP* 50% and *EFV* 50%, based on the assumption of straight line *EFV* curve.

In their 1948 correlation, **Edmister and Pollock [47]**, avoided the assumption of straight line *EFV* curve and developed a new correlation for predicting the *EFV* curve using the experimental data on fractions of mid – continent crude oils, the workable scale charts of this correlation was published later by **Edmister [48]**.

Maxwell [9], proposed an empirical method for estimating the *EFV* curve from the *TBP* curve. The Maxwell method is a modification of the **Packi [44]** method that based on the assumption of the straight line *EFV*. The Maxwell method is a correction for the curvature effect of the *EFV* curve.

In 1966 House et al. [1] evaluated the above mentioned flash methods using the same data base as that used to develop the original correlations and methods. The evaluation indicated that the **Maxwell [9]** correlation gave the best results, with an average error of 14.9%, while the errors of the other methods all exceeded 20%. For this reason, only the Maxwell method was considered in *API* – technical data book (in their 1977 and 1982 editions) **[28, 49]**.

Arnold [50], computerized the Maxwell method through a set of n^{th} order polynomials equations.

Riazi – Daubert [10], proposed a new method for estimating the *EFV* curve from the *TBP* curve. The experimental data on *TBP* and *EFV* distillation of fractions were collected from **Edmister Pollock [47]**, **Chu and Staffel [11]** and **Edmister [4]**. Using this data set the following equation was found to be the best simple form for conversion of *TBP* curve to *EFV* curve:

$$t = a \; \theta^{b} \;\; Sp.gr^{c} \qquad \text{…(2.6)}$$

where t and θ are the *EFV* and *TBP* temperature at the same Vol.% vaporized, *Sp. gr*. Is the specific gravity, and a, b and c are constants. The graphical forms of equation (2.6) are also available for convenience and quick conversions.

Riazi – Daubert [10] evaluated and compared their method with the best method of *API* – technical data book (Maxwell method). The result of their evaluations was superior as compared to the Maxwell method. In addition their method is simpler, requires less time, and can be used on desk calculators as well as in large computers. For these reasons, their method was included in the *API* – technical data book (1988) **[12]**, and in various process simulators such as PRO/II and Hysys. plant **[51, 52]**.

2.5.1.2 Pseudo – component (computer) methods for predicting the *EFV* curve

The pseudo – component methods (also known as computer methods) have been proposed to replace the existing graphical method for predicting the *EFV* curves from the *TBP* curves. Graphical methods have several problems and limitations because of their empirical nature and they can not be yield by themselves the properties of the vapor and liquid phases such as molecular weight, specific gravity, …etc **[1, 6]**.

In pseudo – component method, the *TBP* curve of the crude oil or petroleum stock must first be divided into narrow fractions or cuts, with approximately (5 – 50 °C) boiling range (no sharp definition of narrow fractions or cuts boiling range). The narrow fractions then can be handled as pure components **[7, 53, 54]**.

Using the narrow fraction boiling range it is essential to ensure that pseudo – component can accurately be represented by an average boiling point (also known as mid – boiling point) and specific gravity. The average boiling point and the specific gravity of the pseudo – component can be used then to estimate the other characterization parameters or constants such as molecular weight, critical temperature, critical pressure, the acentric factor, …etc, by using the proper characterization correlations **[1]**.

The characterization constants can be used with the suitable thermodynamic models (such as equation of state models) to predict the flash volume, with vapor and liquid composition for the gas phase and liquid phase. The flash volume and the gas and liquid compositions can be obtained by performing the flash calculation based on the following material balance **[6, 42]**:

$$V = \frac{F(Z_i - x_i)}{x_i(K_i - 1)} \quad \ldots(2.7)$$

and, $\sum x_i = 1$ where ($i = 1, 2, \ldots N$) ...(2.8)

$$K_i = \frac{y_i}{x_i} \quad \ldots(2.9)$$

The K_i in equation (2.7) is well known as phase equilibrium constant or sometimes as K – value. It is the function of the system temperature, pressure and composition **[42, 55]**. Several thermodynamic models have been developed for predicting the K_i of the equation (2.7), and for performing the flash calculations for estimating the flash volume and the vapor and liquid composition, for the gas and liquid phases of the petroleum fractions **[1]**.

Chao – Sender (C. S.) [56] proposed a semi – empirical correlation for predicting the K – value and the flash volume. Their correlation was based on the using of the equation of state model for gas phase, and the activity model for liquid phase. They proposed the **Redlich Kwong [57]** equation of state (RK) for the gas phase, and the regular solution model of **Scatchard and Hilderband [58]**, for the liquid phase. The Chao – Seader model was widely used during the 60's in petroleum refining industry.

Grayson and Streed [59], extended the original constants of the Chao – Seader model for application to higher temperatures and pressures. Their improvement gave more accuracy for the prediction of the K – value at higher temperatures and pressures.

Hoffman [60] and **Hariu and Sage [6]**, had used the ideal solution model for predicting the K – value and flash volume for petroleum fractions. They suggested the ideal gas law for gas phase and the Raoult's law for the liquid phase. The K – value can be predicted using the following equation:

$$K_i = \frac{P_i^s}{P} \qquad \ldots(2.10)$$

equation (2.8) is well known as the Raoult's law K – value **[55]**. The **Hariu – Sage [6]** proposed the Esso chart **[64]** for calculation the vapor pressure (P_i^s) in equation (2.8).

Starling and Han [62], had proposed a generalized correlation for predicting the K – value. The proposed correlation was based on their equation of state. They suggested an iterative flash calculation procedure for estimation the flash volume by using equation (2.7). Their generalized correlation was applicable for virtually all mixture and conditions encountered in the hydrocarbons and petroleum industries.

Lee, Erbar and Edmister [63], developed their own equation of state. They suggested to use their equation of state for the gas phase, while they used the regular solution theory by Scatchard – Hilderbrand for the liquid phase.

Lion and Edmister [64], evaluated the Lee – Erbar and Ebmister method, and found it to be inferior to the Chao – Seader and Grayson Streed methods for calculating the flash volumes of petroleum fractions.

In 1978, Grabaski and Daubert [65, 66], indicated that the **Soave Redlich Kwong (SRK) [67]** equation of state worked well for the estimation of the vapor – liquid equilibrium behavior of a wide variety of technically important hydrocarbon mixtures. They presented the finished form of the (SRK) equation of state for treating mixtures of hydrocarbons of importance to the natural gas and petroleum refining industries. The complete correlation was generalized, requiring only the readily available characterization constants (Tc, Pc and ω) to make equilibrium calculations for petroleum fraction and pure hydrocarbon components.

Daubert et al. [68] tested the SRK, **Peng – Robinson (PR) [69]**, and Starling – Han methods on hydrocarbon mixtures and found that the (SRK) and (PR) equations of state gave nearly equivalent results, while the Starling – Han method is considerably less accurate for predicting flash volumes. As a result of their evaluation the SRK equation of state was adapted in the *API* – technical data book, as the best method for predicting the flash volume for the petroleum fractions and hydrocarbon mixtures **[70]**.

Sim and Daubert [1], evaluated the SRK, Chao – Seaders and Maxwell models for predicting the vapor – liquid equilibria of petroleum fractions. The flash data examined in their work come from the chemical engineering literature and industrial data. As a result of their investigation, it was concluded that the unmodified SRK model was the most accurate and reliable method for flash calculations. While the unmodified SRK model was satisfactory for simulating flash data in the 25 to 90 vol.% range, it predicts low flash volume less accurately. For that reason they proposed a modification on the SRK model to reduce the overall error in the low flash volume data (< 25 vol.%). Improvement was limited by inaccuracies in the experimental data (*TBP* curve), and characterizing constants (Tc, Pc and ω).

In its 1982, 1988, 1992 and 1997 editions **[71 – 74]**, the *API* – technical data book included the **Sim – Daubert [1]**, modified SRK model and procedure for predicting vapor – liquid equilibria calculations for petroleum fraction.

Numerous investigators **[75 – 77]**, had been tried to improve the Peng – Robinson (PR) equation of state for predicting the flash volume of petroleum fractions.

Recently **Twu, Wayne and Vince Tassone [78]**, developed a generalized method to improve the accuracy of PR equation of state in prediction the flash volume for hydrocarbon mixtures including the petroleum fractions. The suggested improvement allowed accurate prediction of the vapor pressure data from the triple point to the critical point.

Chapter Three

Correlations, theories and vapor-liquid equilibrium relations

Knowledge of vapor-liquid phase equilibria conditions of petroleum fractions is essential for the design of most petroleum equipment. This information can be obtained by determining an equilibrium flash vaporization curve(EFV)..

The methods currently available for estimation the *EFV* curves are mainly divided into two types:

i. Graphical methods

ii. Pseudo – component (or computer) methods

Both methods are based on the conversation of the available true boiling point curves (*TBP*) to the *EFV* curves.

3.1 Graphical methods

Graphical methods that relating *TBP* curves and *EFV* curves have been developed from laboratory distillations and flashes of a number of petroleum fractions **[4]**.

The graphical methods of **Maxwell [9]** and **Edmister [4]**, are the oldest methods for estimation the *EFV* curves from the *TBP* curves. These methods consist essentially of predicting the 50% temperature of *EFV* (*EFV* 50%) from the 50% temperature of *TBP* (*TBP* 50%), then predicting the differences in the *EFV* temperatures, in both direction from the 50% point, this is based on the equivalent temperature differences on the *TBP* curve. Maxwell method predicts the 760 mmHg *EFV* from 760 mmHg *TBP*. Edmister method predicts the 760 mmHg *EFV* and the super and sub – atmospheric *EFV*. The Maxwell method had been included in the *API* – technical data book **[28]**.

The **Raizi – Daubert [20]** graphical method is probably the most popular graphical method for estimation the *EFV* curve from *TBP* curve. Their method included in the *API* – technical data book **[2]**.

The Raizi – Daubert method will be considered only because it is simpler, requires less time and easily can be used on desk calculators as well as on large computers.

3.2 Raizi – Daubert graphical method

For cases in which one type of distillation data for a fraction is available, development of correlations for conversions to other distillation types is necessary. In most cases the *EFV* data should be predicted from any available *ASTM D86* or *TBP* data. This can be achieved by using the number of empirical correlations.

The success of any empirical correlation depends, to a large extent, upon the extent of data employed for its development. In Raizi – Daubert method **[10]**, the experimental data on *TBP*, *ASTM D86* and *EFV* distillation of fractions were collected from **Edmister and Pollock [47]**, **Chu and Staffel [79]** and **Lenoir and Hipkin [80]**. Using these data sets, Raizi – Daubert suggested the following general equation for inter conversion of distillation data:

$$t = a_1 \theta^{a_2} Sp.gr^{a_3} \qquad \ldots(3.1)$$

where t and θ are temperatures (in °R) at the same volume percent (vol. %) vaporized, *Sp.gr* is the specific gravity, and a_1, a_2 and a_3 are constants. For example, for conversion of *ASTM 10%* to *TBP 10%* boiling point, θ is the *ASTM 10%* and t is the corresponding *TBP* boiling temperature at 10% volume distilled.

The Raizi – Daubert method for converting *TBP* curve to *EFV* curve can be summarized in the following steps:

Step 1: The available *TBP* data must be converted to the corresponding *ASTM D86* data by using the following equation:

$$TBP = a_4 \left(ASTM \quad D86 \right)^{a_5} Sp.gr^{a_6} \qquad \ldots(3.2)$$

so that for obtaining the *ASTM D86* from *TBP* the equation (3.2) can be written as follows:

$$ASTM \quad D86 = b_1^{\left(-1/b_2\right)} \left(TBP \right)^{\left(1/b_2\right)} \qquad \ldots(3.3)$$

Values of b_1 and b_2 in equation (3.3) varying with percent of liquid sample distilled as given in Table 3-1.

Table 3-1 Equation (3.3) constants

Volume % distilled	b_1	b_2
0	0.9167	1.0019
10	0.5277	1.0900
30	0.7429	1.0425
50	0.8920	1.0176
70	0.8705	1.0226
90	0.9490	1.0110
95	0.8008	1.0355

Step 2: The *ASTM D86* temperature that obtained in step 1 must be then converted to the corresponding *EFV* temperature, using the following equation:

$$EFV = c_1 \left(ASTM \quad D86 \right)^{c_2} Sp.gr^{c_3} \qquad \ldots(3.4)$$

The values c_1, c_2 and c_3 of equation (3.4) vary with percent of liquid sample distilled as given in Table 3-2.

Table 3-2 Equation (3.4) constants

Volume % distilled	c_1	c_2	c_3
0	3.2555	0.8466	0.4208
10	1.4881	0.9511	0.1287
30	0.8330	1.0315	0.0817
50	3.617	0.8274	0.6214
70	9.9607	0.6871	0.9340
90	13.0316	0.6529	1.1025
100	9.5654	0.6949	1.0737

If the values of specific gravity needed for equation (3.4) are unknown Raizi – Daubert developed two equations for predicting the specific gravity using the 10% and 50% *ASTM D86* temperature (*ASTM D86 10%* and *ASTM D 86 50%*) of the fraction or 10% and 50% *EFV* temperature (*EFV 10%* and *EFV 50%*). These equations are:

$$Sp.gr = 0.06711(ASTM\ \ D86\ \ 10\%)^{0.10731}(ASTM\ \ D86\ \ 50\%)^{0.3684} \quad \ldots(3.5)$$

$$Sp.gr = 0.074251(EFV\ \ 10\%)^{-0.01334}(EFV\ \ 50\%)^{0.3684} \quad \ldots(3.6)$$

Step 3: The *EFV* curve can be obtained by plotting the *EFV* temperature against the corresponding volume percent distilled (vol.%).

Example, A.1, in Appendix, illustrates the using of Raizi – Daubert method for predicting the *EFV* curve from the *TBP* curve.

For convenience and quick conversion of *TBP* curve to *EFV* curve, equations (3.3) and (3.4) are graphically represented by Figs. A-1 and A-2 in Appendix, A.

3.3 Pseudo – component (computer) methods

The pseudo – component methods, based on several thermodynamic models that have been proposed to replace the graphical methods for predicting the *EFV* curve from available *TBP* curve. The most important resource of the limitations of graphical methods are **[6]**:

- The empirical nature of these methods make them limited to the data set that were used to develop them.
- The graphical methods do not by themselves, yield properties of vapor and liquid phases such as, molecular weight, specific gravity, …etc.

The pseudo – component methods are also known as computer methods, because the electronic computers are used to do the tedious nature of trial and error multi component flash vaporization calculation to estimate the flash vaporization volume of petroleum cuts or fractions.

To obtain the *EFV* curve from the *TBP* curve using the pseudo – component methods, there are four main important steps that must be followed:

First, the *TBP* curve must be divided into suitable number of fractions or cuts. Each of these fractions have their average boiling point (*TB*), and specific gravity (*Sp.gr*).

In the second step, the average boiling point and the specific gravity for each fractions must be used for estimation the basic characterization parameters or constants such as critical temperature (*Tc*), critical pressure (*Pc*), the acentric factor (ω) and the molecular weight (*MW*), …etc. These constants can be estimated by using suitable characterization correlations (as mentioned in Chapter, 2). Steps one and two can be considered as characterization steps.

The third step includes the estimation of the vapor – liquid equilibrium constants (*K* – values) for each fractions using the available thermodynamic models.

Finally, in the fourth step, the flash volume, and thus, the *EFV* curve can be provided by performing the flash calculations.

The above steps will be discussed in details in the next sections.

3.4 Divided the *TBP* curve into fractions or cuts

The approach that, the pseudo – component methods have been taken in the dividing the crude oils *TBP* curves into fractions or cuts, where these fractions are well known as pseudo – components and then they can be handled as pure components.

In pseudo – component methods the crude oil divides into a number of fractions or cuts with a temperature boiling range of approximately 5°C – 25°C, or in volume percent range of 5vol.% – 10vol.%. These fractions are well known as narrow fractions **[1, 6]**. There is no sharp definition of the narrow fractions where these definitions vary from one source to another.

After the *TBP* is divided into suitable number of fractions, the average boiling point of each fractions can be determined. The latter can be performed by using the concept of the true boiling point mid point. The mid boiling point is simply the point at which 50 liquid volume percent of the fraction distilled **[3]**. To illustrate the mid boiling point concept, consider Fig. 3-1 in which the *TBP* curve with addition of steps, or horizontal lines showing the pseudo – component. Each of these horizontal lines must represent the average boiling point (also known as mid boiling point), if the triangular areas above and below the *TBP* curve are equal (as shown in the shaded area of Fig. 3-1). Trial and error procedure can be used to find the horizontal that satisfies the above condition. The intersection of these horizontal lines and the *TBP* curve represents the mid boiling conditions in which the 50 liquid volume percent (50 *LV%*) can be distilled. For example, refer to Fig. 3-1, the point C_2 for cut 2 represents the mid boiling point condition, and the points T_2 and V_2 are the average boiling point (T_B), and the mid volume percent (X_m), respectively.

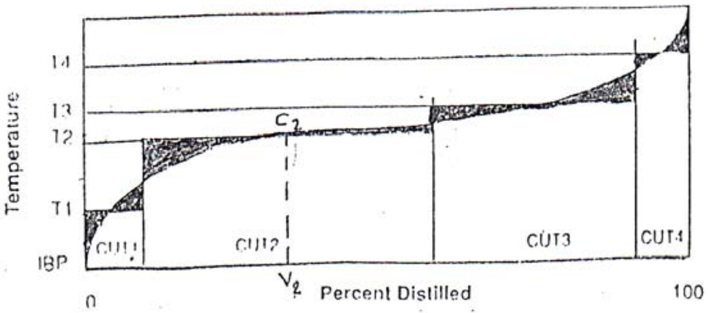

Figure 3-1 The mid boiling point concept

For straight line *TBP* curve the mid boiling point for each cuts can be determined by averaging the initial cut boiling point (*IBP*), and the final cut boiling point (*FBP*) {*i.e.* $TB=(IBP+FBP)/2$}. This is not true for curvature *TBP* curve **[81]**.

The mid boiling point concept, is also true with other physical properties curve such as specific gravity, viscosity …*etc*.

In some cases in which the specific gravity curve is not available, but just the bulk specific gravity is given, the specific gravity of each fractions can be determined by the Katz – Firoozabadi correlation **[82]**:

$$Sp.gr = 0.3067T_B^{0.1605} \qquad \ldots(3.7)$$

Where T_B is the mid boiling point temperature of fraction in °F.

It must be known here that for any available specific gravity input data {curves or using equation (3.7)}, the specific gravity of each cuts must be adjusted to satisfy the given petroleum stock specific gravity.

For most crude oils the *TBP* curve and the specific gravity curve are not available in full range of percent distilled (*i.e.* 0 – 100 *LV%*). In such cases these curves must be interpolated and extrapolated as necessary to complete the full range of the curves. The extrapolation and interpolation can be performed using a suitable numerical techniques **[83]**. These full range curves are known as the working curves which must be used in the mid boiling point concept for obtaining the pseudo – components or fractions of the *TBP* curve.

3.5 Estimation of the basic characterization parameters for the fractions or cuts

Characterization of petroleum fractions involves estimation of the basic parameters needed in thermodynamic models from readily measurable properties such as the specific gravity and average boiling point (mid boiling point). The basic characterization parameters include the critical properties (critical temperature (*Tc*) and critical pressure (*Pc*)), acentric factor (ω) and molecular weight (*MW*).

The critical properties with conjunction of the acentric factor are used in thermodynamic models for prediction the vapor – liquid equilibrium constant or *K* – values and other thermodynamic properties that needed for process design and unit operation.

The molecular weights have important rule in the pseudo – component methods. They are used with conjunction of the specific gravity to convert the liquid volume basis for the fractions to weight and mole basis, respectively. With the moles of each fractions, and suitable *K* – values, the flash calculation can be performed for obtaining the flash volume and, thus the *EFV* curve.

Since the 60's several analytical correlations (for estimation the characterization parameters), in form of equations suitable for computer uses have been proposed. The most important of these correlations, with their limitations can be summarized in the following table:

Table 3-3 Summary of characterization correlations

Correlation name	Estimated parameter	Equation	Function of	Limitations and comments
1. **Cavett [34]**	Tc, Pc	$Tc=768.071+1.7134TB-0.10834\times10^{-2}TB^2$ $+0.3889\times10^{-6}TB^3-0.89213\times10^{-2}TBAPI$ $+0.53095\times10^{-6}TB^2API+0.32712\times10^{-7}TB^2API^2$ (3.7) $\log Pc=2.829+0.9412\times10^{-3}TB$ $-0.30475\times10^{-5}TB^2+0.15141\times10^{-8}TB^3$ $-0.20876\times10^{-4}TBAPI$ $+0.11048\times10^{-7}TB^2API+0.32712\times10^{-7}TB^2API^2$ (3.8)	TB, API	TB, Tc (°F), Pc (psia) Limitations: not mentioned
2. **Lee – Kasler [36]**	Tc, Pc, ω, MW	$Tc=341.7+811Sp.gr+(0.4244+0.1174Sp.gr)T_B$ $+(0.4669-3.2623Sp.gr)\times10^5/T_B$ (3.9) $\ln Pc=8.3634-0.0566/Sp.gr$ $-(0.24244+2.2898/Sp.gr+0.11857/Sp.gr^2)\times10^{-3}T_B$ $+(1.4685+3.648/Sp.gr+0.47277/Sp.gr^2)\times10^{-7}T_B^{\,2}$ $-(0.42019+1.6977/Sp.gr^2)\times10^{-10}T_B^{\,3}$ (3.10) $MW=-12272.6+9486.4Sp.gr+(4.6523-3.3287Sp.gr)T_B$ $+(1-0.77084Sp.gr-0.020585Sp.gr^2)\times(1.3437$ $-720.79/T_B)\times10^7/T_B+(1-0.80882Sp.gr+0.02226Sp.gr^2)$ $\times(1.8828-181.96/T_B)\times10^{12}/T_B^{\,3}$ (3.11)	$Sp.gr$, Tc, Pc, TB, K_{UOP}	Tc (R), Pc (psia) Limitations: $60\leq MW\leq650$ TB<677°C (1250°F)

Continue, **Table 3-3** Summary of characterization correlations

Correlation name	Estimated parameter	Equation	Function of	Limitations and comments
2. **Lee – Kasler [36]**	Tc, Pc, ω, MW	$\omega=(\ln P_Br-5.92714+6.09648/TBr+1.28862\ln TBr-0.169347TBr^6)/(15.2518-15.6875/TBr-13.4721\ln TBr+0.43577TBr^6)$ $TBr<0.8$ (3.12) $\omega=7.904+0.1352K_{UOP}-0.007465K_{UOP}^2+8.359TBr+(1.408-0.01063)/TBr$ $TBr>0.8$ (3.13) $TBr=TB/Tc;\ P_Br=P_B/Pc$	$Sp.gr, Tc, Pc, TB, K_{UOP}$	Tc (R), Pc (psia) Limitations: $60\leq MW\leq 650$ $TB<677$°C (1250°F)
3. **Mathur et al. [35]**	Tc, Pc	$Tc=87.5(MW)^{0.4495}$ (3.14) $Pc=4532(MW)^{-0.979}$ (3.15)	TB, API	Tc (K), Pc (atm) Limitations: not mentioned
4. **Admister [4]**	ω	$\omega=3/7[\log Pc/(Tc/TB-1)]$ (3.16)	Tc, Pc, TB	Tc, TB (K), Pc (atm) Limitations: $TB<343°C\ (650°F)$
5. **Pen – State [84]**	MW, Tc, Pc	$MW=1.435\times10^{-5}(TB^{2.3776}/Sp.gr)^{0.9371}$ (3.17) $Tc=Exp(3.9935TB^{0.8615}Sp.gr^{0.04614})$ (3.18) $Pc=3.4824\times10^9Sp.gr^{2.4853}/TB^{2.3177}$ (3.19)	$TB, Sp.gr$	TB, Tc (R), Pc (psia) Limitations: $40°C\leq TB\leq 457°C$ $(100°F\leq TB\leq 850°F)$

Continue, **Table 3-3** Summary of characterization correlations

Correlation name	Estimated parameter	Equation	Function of	Limitations and comments
6. **Raizi – Daubert 1980 [13]**	MW, Tc, Pc	$MW=4.5673\times10^{-5}TB^{2.1962}Sp.gr^{-1.0164}$ (3.20) $Tc=24.2787TB^{0.5885}Sp.gr^{0.3596}$ (3.21) $Pc=3.1181\times10^{9}TB^{-2.3125}Sp.gr^{2.301}$ (3.22)	$TB, Sp.gr$	TB, Tc (K), Pc (Pa) Limitations: $80\leq MW\leq650$
7. **Sim – Winn [1]**	MW, Tc, Pc	$MW=5.805\times10^{-5}[TB^{2.3776}/Sp.gr^{0.9371}]$ (3.23) $Tc=[Exp(4.2009TB^{0.08615}/Sp.gr^{0.04614})]/1.8$ (3.24) $Pc=6.1483\times10^{12}TB^{-2.3177}Sp.gr^{2.4853}$ (3.25)	$TB, Sp.gr$	TB, Tc (K), Pc (Pa) Limitations: $80\leq MW\leq650$
8. **Twu [37]**	MW, Tc, Pc	$lnMW=lnMW_A[(1+2F_M)/(1-2F_M)]^2$ (3.26) $Tc=Tc_A[(1+2F_T)/(1-2F_T)]^2$ (3.27) $Pc=Pc_A[(1+2F_P)/(1-2F_P)]^2$ (3.28) $F_M=\Delta Sp.gr_M[\lvert x\rvert+(-0.01756+0.193168/TB^{0.5})\Delta Sp.gr$ (3.29) $F_T=\Delta Sp.gr_T[-0.36245/TB^{0.5}$ $+(0.03982-0.94812/TB^{0.5})]\Delta Sp.gr_T$ (3.30)	$TB, Sp.gr$ $Sp.gr_A$ TB_A	Pc, Pc_A (psia), TB (R), TB_F (°F) Limitations: $Sp.gr\leq1.436$ $TB\leq704°C$ $(TB\leq1300°F)$ Expansion from n - alkane

Continue, **Table 3-3** Summary of characterization correlations

Correlation name	Estimated parameter	Equation	Function of	Limitations and comments
8. **Twu [37]**	*MW, Tc, Pc*	$F_P=\Delta Sp.gr_P[2.5326-46.19/TB^{0.5}-0.00127+TB)$ $+(11.42+252.14/TB^{0.5}+0.0023TB)]\Delta Sp.gr_P$ (3.31) $\Delta Sp.gr_M=Exp[5(Sp.gr^A-Sp.gr)]-1$ (3.32) $\Delta Sp.gr_T=Exp[5(Sp.gr^A-Sp.gr)]-1$ (3.33) $\Delta Sp.gr_P=Exp[0.5(Sp.gr^A-Sp.gr)]-1$ (3.34) $\lvert x\rvert=\lvert 0.01234\;0-0.3280/TB^{0.5}\rvert$ (3.35) $MW_A=3.395\times10^{-15}TB_F^{\ 6}-1.2416\times10^{-11}TB_F^{\ 5}$ $+1.8256\times10^{-8}TB_F^{\ 4}-1.323\times10^{-5}TB_F^{\ 3}+0.00522TB_F^{\ 2}$ $-0.7416TB_F+116.19$ (3.36) $Tc_A=TB(0.5332+0.19101\times10^{-3}TB+0.7796\times10^{-7}TB^2$ $-0.2843\times10^{-10}TB^3+0.9596\times10^{23}/TB^{13})-1$ (3.37) $Pc_A=(3.8335+1.1962\alpha^{0.5}+34.888\alpha+36.1952\alpha^2$ $+104.193\alpha^4)^2$ (3.38) $Sp.gr^A=0.8435-0.1862\alpha-3.3615\alpha^3-13749.70\alpha^{12}$ (3.39) $\alpha=1-(TB/Tc_A)$ (3.40)	*TB, Sp.gr* $Sp.gr^A$	Pc, Pc_A *(psia)*, *TB (R)*, TB_F *(°F)* Limitations: $Sp.gr\leq1.436$ $TB\leq704°C$ $(TB\leq1300°F)$ Expansion from n -alkane

Continue, **Table 3-3** Summary of characterization correlations

Correlation name	Estimated parameter	Equation	Function of	Limitations and comments
9. **Raizi – Daubert 1987 [38]**, *API* method	MW, Tc, Pc	$MW=20.486[Exp(1.165\times10^{-4}TB-0.78712Sp.gr+1.158\times10^{-3}TBSp.gr)]TB^{1.20067}Sp.gr^{0.9830}$ (3.41) $Tc=10.6443[Exp(-5.1747\times10^{-4}TB-0.54444Sp.gr+3.5995\times10^{-4}$ (3.42) $Pc=6.162\times10^{6}[Exp(-4.725\times10^{-3}TB-4.801Sp.gr+3.1939\times10^{-3}TBSp.gr)]TB^{-0.4844}Sp.gr^{4.0846}$ (3.43)	$TB, Sp.gr$	TB, Tc (°R), Pc (psia), Limitations: For MW $32°C\leq TB\leq 582°C$ $(90°F\leq TB\leq 1050°F)$ For Tc and Pc $28°C\leq TB\leq 343°C$ $(80°F\leq TB\leq 650°F)$

The *API* – technical data book **[2, 11]** recommended the following correlations for estimation the basic characterization parameters:

- The Raizi – Dauber 1987, for estimation the critical temperature, critical pressure and molecular weight.
- The Lee – Kasler correlations for estimation the acentric factor.

3.6 Prediction of vapor – liquid equilibrium constants (*K* – values) for fractions

The term "vapor – liquid equilibrium" (*VLE*), refers to systems in which a single liquid phase is in equilibrium with its vapor. In studies of phase equilibrium, however, the phase containing gradients is not considered. Whenever gradient exists there is a tendency for change with time, hence there is no equilibrium. On other hand, there can be two or more phases, each of which is homogenous throughout, with no tendency for any change in properties with time, even though the phases are in intimate physical contact with one another. The latter is the condition that is denoted by the term "phase equilibrium". In a condition of phase equilibrium there are some properties that are drastically different between the phases, and others that must be identical for all phases to prevent a change of properties within individual phases from change. The thermodynamic equilibrium determines how components in mixture are distributed between phases **[85, 86]**.

3.7 Thermodynamic of equilibrium

3.7.1 Fugacity and fugacity coefficient

The starting point for a phase equilibrium calculation is the thermodynamic requirement that the temperature, pressure, and chemical potential of each species be the same in all phases in which the species is present, that is:

$$\mu_i^{Ph_1} = \mu_i^{Ph_2} = \ldots \qquad (i = 1, 2, 3, \ldots Nc) \qquad ..(3.44)$$

where μ is the chemical potential of species i, Ph_1 and Ph_2 represent the phases in equilibrium.

Chemical potential can be expressed as an absolute quantity, and the numerical values of chemical potential are difficult to relate to more easily understood physical quantities. Furthermore, the chemical potential approaches an infinite negative value as pressure approaches zero. For these reasons, the chemical potential is not favored for phase equilibria calculations. Instead, fugacity invented by G. N. Lewis in 1901, is employed as a surrogate.

The partial fugacity of species i in the mixture is like a pseudo – pressure, defined in terms of the chemical potential by **[42]**:

$$\overline{f_i} = C\,exp\left[\frac{\mu_i}{RT}\right] \qquad ..(3.45)$$

where C is a temperature – dependent constant. Regardless of the value of C, it is shown by **Prausintz, Liehtenthaler and Azevedo [87]** that equation (3.40) can be replaced with:

$$\overline{f}_i^{Ph_1} = \overline{f}_i^{Ph_2} = \ldots \qquad (i = 1, 2, 3, \ldots Nc) \qquad ..(3.46)$$

thus, at equilibrium, a given species has the same partial molal fugacity in each existing phases. This equality together with equality of phase temperatures and pressures, thus:

$$T^{Ph_1} = T^{Ph_2} = \ldots T^{(NP)} \qquad ..(2.47)$$

and $$P^{Ph_1} = P^{Ph_2} = \ldots P^{(NP)} \qquad ..(2.48)$$

where NP is the number of phases. Equations (3.46) – (3.48) constitute the required conditions for phase equilibria.

For vapor – liquid equilibrium the above equations are reduced to:

$$\overline{f}_i^V = \overline{f}_i^L \quad ..(3.49)$$

$$T^V = T^L \quad ..(3.50)$$

$$P^V = P^L \quad ..(3.51)$$

Because of the close relationship between fugacity and pressure, it is convenient to define their ratio for pure species **[55]**:

$$\phi_i = \frac{f_i}{P} \quad ..(3.52)$$

where ϕ_i, is the pure species fugacity coefficient, and it represents the departure of fugacity due to pressure.

For a mixture, partial molal fugacity coefficient represents the departure of fugacity due to pressure and the partial molal fugacity coefficient can be defined for vapor and liquid phases as follows **[88]**:

$$\overline{\phi}_i^V = \frac{\overline{f}_i^V}{y_i P} \quad ..(3.53)$$

$$\overline{\phi}_i^L = \frac{\overline{f}_i^L}{x_i P} \quad ..(3.54)$$

For a pure ideal gas, fugacity is equal to the pressure ($f_i = P$) (*i.e.* $\phi_i = 1$), and for a species in the ideal gas mixture, the partial fugacity is equal to its partial pressure ($P_i = y_i P$), (*i.e.* $\phi_i^V = 1$).

3.7.2 Activity and activity coefficients

At a given temperature, the ratio of the partial molal fugacity of a component in mixture to its fugacity in some standard state is defined as activity. If the standard state is selected as the pure species at same pressure and temperature as the mixture, then the activity is equal **[89]**:

$$a_i = \frac{\overline{f}_i}{f_i} \qquad ..(3.55)$$

To represent the departure to partial fugacity due to composition, the activity coefficients based on concentration in mole fractions are defined by **[42]**:

$$\gamma_i^V = \frac{a_i^V}{y_i} \qquad ..(3.56)$$

$$\gamma_i^L = \frac{a_i^L}{x_i} \qquad ..(3.57)$$

substituting a_i in equations (3.56) and (3.57), gives:

$$\gamma_i^V = \frac{\overline{f}_i^V}{f_i^V y_i} \qquad ..(3.58)$$

$$\gamma_i^L = \frac{\overline{f}_i^L}{f_i^L x_i} \qquad ..(3.59)$$

3.7.3 *K* – values formulation

In the multi component system, the K – value of a given species is defined as the ratio of the mole fraction of the species in the vapor phase (y_i), to the mole fraction of the species in the liquid phase (x_i). Mathematically the relationship is expressed as **[89]**:

$$K_i = \frac{y_i}{x_i} \qquad ..(3.60)$$

To form the K – values, fugacities are replaced by equivalent expressions involving mole fractions. Two common pairs derived from equations (3.53), (3.54), (3.58) and (3.59), are:

Pair 1:

$$\overline{f}_i^V = \overline{\phi}_i^V y_i P \qquad ..(3.61)$$

and $$\overline{f}_i^L = \overline{\phi}_i^L x_i P \qquad ..(3.62)$$

Pair 2:

$$\overline{f}_i^V = \gamma_i^V f_i^V y_i \qquad ..(3.63)$$

and $$\overline{f}_i^L = \gamma_i^L f_i^L x_i \qquad ..(3.64)$$

If equations (3.61) and (3.62) are used with equation (3.49), a so called equation of state form of K – value (or $\phi - \phi$ K – value form) **[90]** is obtained:

$$K_i = \frac{\bar{\phi}_i^L}{\bar{\phi}_i^V} \quad ..(3.65)$$

If equations (3.61) and (3.64) are used with equation (3.49), a so called activity coefficient form of K – value (or $\phi - \gamma$ K – value form) **[89]**, is obtained:

$$K_i = \frac{\gamma_i^L f_i^L}{\bar{\phi}_i^V P} = \frac{\gamma_i^L \phi_i^L}{\bar{\phi}_i^V} \quad ..(3.66)$$

If equations (3.63) and (3.64) is used with equation (3.49) with conjunction of the ideal solution concept in which $\gamma_i^V = \gamma_i^L = 1$, a so called ideal solution K – value form **[73, 88]** is obtained:

$$K_i = \frac{f_i^L}{f_i^V} = \frac{\phi_i^L}{\phi_i^V} \quad ..(3.67)$$

The three forms of the K – value will be discussed in the next sections.

3.8 Equation of state forms for prediction the *K* – values ($\phi - \phi$ forms)

Equation of state are widely used in the prediction of thermodynamic properties of pure fluid and fluid mixtures (including petroleum fractions), in part because they provide a thermodynamically consistent route to the configurationally properties of both vapor and liquid phases. Consequently, equation of state model may be used to determine phase equilibrium conditions as well as other properties.

The term equation of state (also refers to $P - V - T$ relationship) is used to describe an empirically – derived function which provides a relation between, pressure, density, temperature and composition of the system. Of all types of equations of state, a most popular class is formed by the so called "cubic equation of state" (CEQS), so named because when usually written in pressure – explicit form, and the volume is given in cubic form **[86, 91]**, thus:

$$P = P(T, V, n_1 \ldots) \qquad ..(3.68)$$

An equation of state is always used to obtain the partial molal fugacity coefficient in the vapor and sometimes in the liquid phases ($\bar{\phi}_i^V, \bar{\phi}_i^L$) in terms of the pressure, temperature and composition of the system thus:

$$\bar{\phi}_i^V = F(T, P, y_i \ldots) \qquad ..(3.69)$$

$$\bar{\phi}_i^L = F(T, P, x_i \ldots) \qquad ..(3.70)$$

A rigorous relation exists between the partial molal fugacity coefficient of a component in a phase and the volumetric properties of that phase. This relation is conveniently expressed in the form of equation of state. In order to obtain the partial molal fugacity coefficient by using equation of state, the following expression is used **[88]**:

$$ln\bar{\phi}_i = \frac{1}{RT}\int_V^{\infty}\left[\left(\frac{\partial P}{\partial n_i}\right)_{T,V,n_{j\neq i}} - \frac{RT}{V}\right]dV - ln Z \qquad ..(3.71)$$

where n_i is the number of moles of component *i*.

Equation (3.71) is exact if the information needed to evaluate the integrals is at hand. These $P - V - T$ information can be obtained from suitable cubic equation of states.

The oldest, simplest and best known cubic equation of state is that proposed by van der Waals in 1873, his equation is:

$$P=\frac{RT}{V-b}-\frac{a}{V^2} \qquad ..(3.72)$$

where P, T, V are the pressure, temperature and molar volume, respectively. a and b are two constants and they can be obtained from the critical temperature and critical pressure. The first term of equation (3.72), ($\frac{RT}{V-b}$) expresses the effect of repulsion between molecules, assimilated to hard spheres, while the second term ($\frac{a}{V^2}$) expresses the attraction forces due to the van der Waals forces. The first term is also known as repulsive pressure term and the second term is also known as attractive pressure term. It should be mentioned that the van der Waals equation is not accurate for representation the $P-V-T$ behavior of species in the liquid and vapor states, but is historically important and useful for qualitative investigations **[89]**.

The modern development of cubic equation of state started in (1949), with publication of the Redlich – Kowng equation of state (RK) **[57]**:

$$P=\frac{RT}{V-b}-\frac{a}{T^{1/2}V(V+b)} \qquad ..(3.73)$$

Redlich – Kwong demonstrated that by a simple adjustment the van der Waals attractive pressure term ($\frac{a}{V^2}$) could considerably improve the prediction of the $P-V-T$ behavior and physical properties of the vapor phase. They replaced the attractive pressure term ($\frac{a}{V^2}$) with a generalized temperature dependence term ($\frac{a}{T^{1/2}}$) or alpha function (α). Their equation has the form:

$$P=\frac{RT}{V-b}-\frac{\alpha}{V(V+b)} \qquad ..(3.74)$$

a and *b* are also obtained from critical temperature and critical pressure. Redlich states that there was no particular theoretical basis for the equation, rather it is considered as an effective empirical modification of its predecessors.

More than 110 modification to the Ridlich – Kowng equation of state have been proposed to date to improve its representation of volumetric behavior and physical properties. These modifications including the widely used Soave (also known as Soave – Redlich – Kowng (SRK)) equation of state and Peng – Robinson (PR) equation of state. The SRK and PR equations of state today are the most important and popular equations of state, which are used for prediction the volumetric behavior and physical properties including the vapor – liquid equilibrium calculations for both polar and non polar mixtures including the petroleum fractions.

3.8.1 Soave – Relich – Kowng equation of state (SRK)

One of the most significant milestones in the development of cubic equation of state was the publication by **Soave [67]**, of a modification to the evaluation of parameter a in the attractive pressure term of the Redlich – Kowng (RK) equation of state {equation (3.73)}. Soave replaced the term $(\frac{a}{T^{1/2}})$ in equation (3.73) with a more generalized temperature dependent term, as denoted by ($a\alpha$) to give:

$$P = \frac{RT}{V-b} - \frac{a\alpha}{V(V+b)} \qquad ..(3.75)$$

where, α is a dimensionless factor that become unity at $T = Tc$ (α is also known as alpha function), α is a function of the reduced temperature and acentric factor ω (*i.e.* $\alpha = f(Tr, \omega)$) to overcome the difficulty of inability of equation of state to represent the entire fluid range which prevent their use for the vapor – liquid equilibria calculation. Soave back – calculated the α for various hydrocarbon species over a range of reduced temperature using vapor pressure data to obtain the following correlation for α:

$$\alpha = \left[1 + m\left(1 - T_r^{0.5}\right)\right]^2 \qquad ..(3.76)$$

where $m = 0.48 + 1.574\omega - 0.176\omega^2$ ..(3.77)

The ω in equation (3.77) is the acentric factor, which can be obtained by **Pitzer et al. [44]** as follows:

$$\omega = \left[-\log\left(P_r^*\right)_{T_r=0.7}\right] - 1 \qquad ..(3.78)$$

where P_r^* is the reduced vapor pressure (P^s/P).

All equations of state are generally developed for pure species first, and then extended to mixtures through the use of mixing rules. These mixing rules are simply means of calculating mixture parameters equivalent to those of pure species. The most conventional mixing rules is given by van der Waals.

Equation (3.75) of Soave – Redlich in polynomial form of Z will thus be:

$$Z^3 - (1 - B)Z^2 + \left(A - B^2 - B\right)Z - AB = 0 \qquad ..(3.79)$$

Where the mixing rules:

$$A = \sum_{i=1}^{N}\sum_{j=1}^{N} x_i x_j \left(1 - k_{ij}\right)\sqrt{A_i A_j} \qquad ..(3.80)$$

$$B = \sum_{i=1}^{N} x_i B_i \qquad ..(3.81)$$

$$b_m = \sum_{i=1}^{N} x_i b_i \qquad ..(3.82)$$

and, $A_i = 0.42747\alpha_i \dfrac{Pr_i}{Tr_i^2}$ $\qquad B_i = 0.08664 \dfrac{Pr_i}{Tr_i}$ ..(3.83)

$$a_i = 0.42747 \frac{(RTc_i)^2}{Pc_i} \qquad b_i = 0.08664 \frac{RTc_i}{Pc_i} \qquad ..(3.84)$$

x_i, is the mole fraction of species i.

The roots of equation (3.79) are obtained by numerical technique such as Newton – Raphson technique **[83]**. The latter is discussed in Appendix, B.

In two phases region, three real roots are exist. The liquid root is smallest of the three, and it represents the compressibility factor for liquid phase (Z^L), while the largest root is the compressibility factor for the vapor phase (Z^V). A non physical root exists between them. In solving equation (3.79) for the compressibility factor of the liquid phase (Z^L), the composition of the liquid x_i is used to calculate the coefficient A and B of equations (3.80) and (3.81), through the use of the mixing rules. For determining the compressibility factor for the vapor phase (Z^V), the above outlined procedure is used with composition of the vapor phase y_i replacing x_i.

By combining the SRK equation of state equation (3.75) into the thermodynamic definition of the partial molal fugacity coefficient, equation (3.71), Soave proposed the following expression for the partial molal fugacity coefficient of the species in liquid mixture $\overline{\phi}_i^L$:

$$\begin{aligned}\ln\left(\overline{\phi}_i^L\right) &= \frac{B_i}{B}\left(Z^L - 1\right) - \ln\left(Z^L - B\right) \\ &+ \frac{A}{B}\left[\frac{B_i}{B} - \frac{2}{a\alpha}\sum_{j=1}^{Nc} x_j\left(1 - K_{ij}\right)\sqrt{(a_i\alpha_i)(a_j\alpha_j)}\right]\ln\left(1 + \frac{B}{Z^L}\right)\end{aligned} \qquad ..(3.85)$$

where $a\alpha = \displaystyle\sum_{i=1}^{N}\sum_{j=1}^{N} x_i x_j \left(1 - K_{ij}\right)\sqrt{(a_i\alpha_i)(a_j\alpha_j)}$ ..(3.86)

Equation (3.85) is also used to determine, the partial molal fugacity coefficient of species in the vapor mixture by using the composition of the vapor phase y_i in calculating A, B, Z^V and other composition dependent terms, thus:

$$\ln\left(\bar{\phi}_i^V\right) = \frac{B_i}{B}\left(Z^V - 1\right) - \ln\left(Z^V - B\right) + \frac{A}{B}\left[\frac{B_i}{B} - \frac{2}{a\alpha}\sum_{j=1}^{Nc} x_j\left(1 - K_{ij}\right)\sqrt{\left(a_i\alpha_i\right)\left(a_j\alpha_j\right)}\right]\ln\left(1 + \frac{B}{Z^V}\right) \quad ..(3.87)$$

where $a\alpha = \sum_{i=1}^{N}\sum_{j=1}^{N} y_i y_j \left(1 - K_{ij}\right)\sqrt{\left(a_i\alpha_i\right)\left(a_j\alpha_j\right)}$ ..(3.88)

The α_i and m_i are given by equations (3.76) and (3.77). The K_{ij} is the binary interaction parameters which is empirically determined from the VLE data. The K_{ij} have the following properties:

$$K_{ii} = 0$$

and $K_{ij} = K_{ji}$

3.8.2 Peng – Robinson equation of state (PR)

Peng and Robinson [69], conducted a comprehensive study to evaluate the use of SRK equation of state for predicting the behavior of naturally occurring hydrocarbon systems. They illustrated the need for an improvement in ability of equation of state to predict liquid densities and other fluid properties in the vicinity of the critical region. Peng – Robinson proposed the following equation of state:

$$P = \frac{RT}{V - b} - \frac{a\alpha}{V\left(V + b\right) + b\left(V - b\right)} \quad ..(3.89)$$

Peny – Robinson also adopted Soave's approach for calculating the α term of equation (3.89) thus,

$$\alpha = \left[1 + K\left(1 - Tr^{0.5}\right)\right]^2 \qquad ..(3.90)$$

where K has been correlated against the acentric factor. The resulting K equation is:

$$K = 0.37464 + 1.54226\omega - 0.26992\omega^2 \qquad ..(3.91)$$

Rearranging equation (3.89) into compressibility factor form gives:

$$Z^3 - (1 - B)Z^2 + \left(A - 3B^2 - 2B\right)Z - \left(AB - B^2 - B^3\right) = 0 \qquad ..(3.92)$$

where the mixing rules:

$$A = \sum_{i=1}^{N}\sum_{j=1}^{N} x_i x_j \left(1 - K_{ij}\right)\sqrt{A_i A_j} \qquad ..(3.93)$$

and, $B = \sum_{i=1}^{N} x_i B_i$ ..(3.94)

$$b_m = \sum_{i=1}^{N} x_i b_i \qquad ..(3.95)$$

and, $A_i = 0.45724\alpha_i \dfrac{Pr_i}{Tr_i^2} \qquad B_i = 0.07780\dfrac{Pr_i}{Tr_i}$ ..(3.96)

$$a_i = 0.45724\frac{\left(RTc_i\right)^2}{Pc_i} \qquad b_i = 0.07780\frac{RTc_i}{Pc_i} \qquad ..(3.97)$$

where x_i is the mole fraction of species i.

By combining PR equation of state equation (3.89) with equation (3.71), the partial molal fugacity coefficient of species i in liquid mixture $\overline{\phi}_i^L$ can be written as follows:

$$ln\left(\overline{\phi}_i^L\right) = \frac{B_i}{B}\left(Z^L - 1\right) - ln\left(Z^L - B\right) + \frac{A}{2.828B}\left[\frac{B_i}{B} - \frac{2}{a\alpha}\sum_{j=1}^{N} x_j\left(1 - K_{ij}\right)\sqrt{\left(a_i\alpha_i\right)\left(a_j\alpha_j\right)}\right] ln\left(\frac{Z^L + 2.414B}{Z^L - 0.414B}\right) \quad ..(3.98)$$

where $a\alpha = \sum_{i=1}^{N}\sum_{j=1}^{N} x_i x_j\left(1 - K_{ij}\right)\sqrt{\left(a_i\alpha_i\right)\left(a_j\alpha_j\right)}$ ..(3.99)

Equation (3.98) is also used to determine the partial molal fugacity coefficient of species i in the vapor mixture ($\overline{\phi}_i^V$), by replacing the composition of the liquid phase x_i with composition of vapor phase y_i in calculating A, B, Z^V and other composition dependent terms, thus:

$$ln\left(\overline{\phi}_i^V\right) = \frac{B_i}{B}\left(Z^V - 1\right) - ln\left(Z^V - B\right) + \frac{A}{2.828B}\left[\frac{B_i}{B} - \frac{2}{a\alpha}\sum_{j=1}^{N} x_j\left(1 - K_{ij}\right)\sqrt{\left(a_i\alpha_i\right)\left(a_j\alpha_j\right)}\right] ln\left(\frac{Z^V + 2.414B}{Z^V - 0.414B}\right) \quad (3.100)$$

where $a\alpha = \sum_{i=1}^{N}\sum_{j=1}^{N} y_i y_j\left(1 - K_{ij}\right)\sqrt{\left(a_i\alpha_i\right)\left(a_j\alpha_j\right)}$ (3.101)

The α_i and m_i are given by equations (3.90) and (3.91). The K_{ij} is the binary interaction parameter which is determined empirically from VLE data and have the same properties that are given in SRK equation of state K_{ij}.

The roots of equation (3.88) are calculated also by using Newton – Raphson technique. Here again the largest root is for the vapor phase compressibility factor Z^V, and the smallest one is for the liquid phase compressibility factor Z^L.

3.8.3 Improvement of SRK and PR equation of state for petroleum fraction

The accurate prediction of *K* – values from SRK and PR equations of state required an equally accurate prediction of pure component vapor pressure, which depends on the development of an appropriate alpha function α of the attractive pressure terms of cubic equation of state {*i.e.* equations (3.76) and (3.90)}. Alpha function is also known as temperature – dependency term **[78, 90]**.

Since the original alpha function (α) for both SRK equation of state and PR equation of state, are developed using the vapor pressure data of low molecular weight hydrocarbons, it is unlikely that those equations will be satisfactory for high molecular weight petroleum fractions **[65]**.

The most important modifications for alpha function (α) for petroleum fractions vapor – liquid equilibria calculations are:

i. **Sim – Daubert [1]**, modification for SRK equation of state.
ii. **Twu et al. [78]**, modification for PR equation of state.

3.8.3.1 Sim – Dauber modification for SRK equation of state

Sim – Dauber proposed a modification for original SRK alpha function. Their modification is based on the experimental *EFV* data that given by **Chu – Staffel [79]**. The modified α is:

$$\alpha = 0.0147 + 0.993\alpha' - 0.10(TMEP) \qquad (3.102)$$

where, α' is the original SRK equation of state α {equation (3.76)}, and *TMEP* is constant calculated as follows:

> *TMEP = 10 – The calculated flash volume when 20% TBP temperature is used as the flash temperature*

The modified α is only applicable if the (*TMEP*) is negative.

The Sim – Daubert modification for alpha function of SRK equation of state is recommended by the *API* – technical data book **[74]**.

3.8.3.2 Twu et al. modification for PR equation of state

For PR equation of state Twu et al., suggested the generalized alpha function (α) form, that replaced the original PR alpha function {*i.e.* equation (3.90)}. The generalized α has the following form:

$$\alpha = \alpha^{0} + \omega\left(\alpha^{(1)} - \alpha^{(0)}\right) \tag{3.103}$$

where $$\alpha^{(0)} = Tr^{N^{(0)}\left(M^{(0)}-1\right)} e^{L^{(0)}\left(1-Tr^{N^{(0)}M^{(0)}}\right)} \tag{3.104}$$

$$\alpha^{(1)} = Tr^{N^{(1)}\left(M^{(1)}-1\right)} e^{L^{(1)}\left(1-Tr^{N^{(1)}M^{(1)}}\right)} \tag{3.105}$$

The superscripts (*0*) and (*1*) in equations (3.103) – (3.105) are consistent with the definition of acentric factor at $\omega = 0$, and $\omega = 1$, respectively. In other words, these two alpha functions ($\alpha^{(0)}$ and $\alpha^{(1)}$) are forced to pass through the saturated pressure at $Tr = 0.7$ for $\omega = 0$, and $\omega = 1$, respectively.

The constants *L, M* and *N* for $\alpha^{(0)}$ and $\alpha^{(1)}$, are given in Table 3-4, for supercritical region ($Tr > 1$), and sub critical region ($Tr \leq 1$).

Table 3-4 The *L*, *M* and *N* data bank of the generalized alpha function for equations (3.104) and (3.105) with the PR equation of state

	$Tr \leq 1$		$Tr > 1$	
α parameter	$\alpha^{(0)}$	$\alpha^{(1)}$	$\alpha^{(0)}$	$\alpha^{(1)}$
L	0.2728	0.6257	0.3739	0.0239
M	0.92477	0.7920	4.7302	1.2461
N	1.1976	2.4602	–0.200	–8.00

The new generalized α alpha function for PR allows the accurate prediction of vapor pressure data from triple point to the critical point for light and heavy hydrocarbons.

3.9 Activity models for prediction *K* – values ($\gamma - \phi$ models)

An appropriate equation of state provides a thermodynamically consistent route to the partial molal fugacity of components in both vapor and liquid phases, and thus offers a very convenient basis for phase – equilibrium calculations. Alternatively, the combination of an equation of state for the vapor phase, and the activity coefficient model for the liquid phase offers a practical method for predicting *K* – values, and for phase equilibrium calculations **[91]**.

In the activity coefficient models, the *K* – values can be mathematically expressed by equation (3.62), or:

$$K_i = \frac{\gamma_i^L \phi_i^L}{\bar{\phi}_i^V} \quad ..(3.66)$$

To obtain the *K* – value using equation (3.66), three auxiliary function are required, those are:

i. The vapor phase partial molal fugacity coefficient $\bar{\phi}_i^V$.

ii. The pure liquid partial molal fugacity coefficient ϕ_i^L.

iii. The liquid phase activity coefficient γ_i^L.

The first auxiliary function, the vapor phase partial molal fugacity coefficient can be obtained using any of the suitable equation of state models, such as SRK and PR equation of state (as discussed in previous section). The other two auxiliary functions will be discussed hereafter.

3.9.1 The pure liquid fugacity coefficient (ϕ_i^L)

The second important auxiliary function of equation (3.66) is the pure liquid fugacity coefficient (ϕ_i^L). From the classical thermodynamic relation **[88]**, the pure species fugacity coefficient:

$$ln\phi_i = ln\left[\frac{1}{RT}\int_0^P\left(V - \frac{RT}{P}\right)dP\right] \tag{3.106}$$

By integrating equation (3.106) from *0* to P_i^s, and P_i^s to *P*,

$$ln\phi_i^L = ln\phi_i^{Vs} - ln\left(\frac{P}{P_i^s}\right) + \frac{1}{RT}\int_{P_i^s}^P V_i^L dP \tag{3.107}$$

where V_i^L is the liquid molar volume at system temperature and pressure. The last term of equation (3.107) is known as the Poynting factor (PF) **[55]**. If the liquid is incompressible, equation (3.107) reduces to:

$$\phi_i^L = \left(\frac{P_i^s}{P}\right)\phi_i^{Vs}\, exp\left[\frac{V_i^L\left(P - P_i^s\right)}{RT}\right] \tag{3.108}$$

where ϕ_i^{Vs} is the vapor phase pure species fugacity coefficient at saturated conditions.

The Poynting factor can not be negligible at high pressure or when the vapor pressure of species is higher than the system pressure.

For special case of ideal gas law, where the pressure is low so the Poynting factor is negligible and the equation (3.108) reduces to:

$$\phi_i^L = \left(\frac{P_i^s}{P} \right) \phi_i^{Vs} \tag{3.109}$$

The molar liquid volume V_i^L of species i can be calculated using modified Rackett equation of **Spencer – Danner [93]**, thus:

$$V_i^L = \left(\frac{RTc}{Pc} \right) Z_{RA}^{\left[1+(1-Tr)^{2/7}\right]} \tag{3.110}$$

where, Z_{RA} is the Rackett constant and must be back – calculated from measured molal volume at known temperature. For pure species, the values of the liquid molal volume can be found in many literatures measured usually at 25 °C (77 °F). For petroleum fraction, the specific gravity at 15.6 °C (60 °F) can be used to calculate the Z_{RA} for equation (3.110).

Equation (3.110) can be used for estimation the molar liquid volume up to the critical temperature of species. For the supercritical region, the **Cavett [88]** equation can be used. The mathematical form of Cavett equation is :

$$V_i^L = \zeta_i \left(5.7 + 3Tr_i \right) \tag{3.111}$$

where, ζ_i, is the Cavett constant, and can be back – calculated using the same way that described for obtaining Z_{RA} for equation (3.110).

The vapor pressure of species i (P_i^s), can be estimated from a widely used empirical correlations. By far the most well known empirical correlations for calculation of vapor pressure data for pure species is Antonine's equation:

$$ln\,P_i^s = A' - \frac{B'}{T + C'} \tag{3.112}$$

Values of the constants *A', B'* and *C'*, which appear in this equation are available for large number of pure species in the literatures **[94]**.

For petroleum fractions, the most convenient and recommended empirical correlation is given by **Lee – Kasler [12, 74, 89]**. Mathematically, the Lee – Kasler vapor pressure correlation has the following form:

$$ln\,Pr_i^s = ln\left(Pr_i^s\right)^0 + \omega_i\left(ln\,Pr_i^s\right)^1 \tag{3.113}$$

where $ln\left(Pr_i^s\right)^0 = 5.92714 - \frac{6.09648}{Tr_i} - 1.2886\,ln\,Tr_i + 0.1693Tr_i^6$ (3.114)

and, $ln\left(Pr_i^s\right)^1 = 15.2518 - \frac{15.6875}{Tr_i} - 13.4721\,ln\,Tr_i + 0.4357Tr_i^6$ (3.115)

and, $Pr_i^s = \frac{P_i^s}{Pc_i}$

It must be noticed here, that both Antonie's and Lee – Kasler correlations have a good accuracy for predicting the vapor pressure in the range from below normal boiling point temperature to the critical temperature **[91, 74]**.

The vapor phase fugacity coefficient of pure species at saturation conditions (ϕ_i^{Vs}), can be calculated using suitable equation of state models. The SRK and PR can be used for that purpose. From the classical thermodynamic relations, the pure species fugacity coefficient can be written **[88]**:

$$ln\phi_i = \int_0^P \left(\frac{Z - 1}{P}\right) dP \tag{3.116}$$

If SRK equation of state {equation (3.75)} is applied to above equation then the fugacity coefficient of pure species can be obtained as follows:

$$ln\phi_i = Z - 1 - ln(Z - B) - \frac{A}{B} ln\left(\frac{Z + B}{Z}\right) \tag{3.117}$$

For vapor phase equation (3.117), become:

$$ln\phi_i^V = Z^V - 1 - ln\left(Z^V - B\right) - \frac{A}{B} ln\left(\frac{Z^V + B}{Z^V}\right) \tag{3.118}$$

If PR equation of state (3.89) is used with equation (3.116), then:

$$ln\phi_i = Z - 1 - ln(Z - B) - \left[\frac{A}{2\sqrt{2}B}\right] ln\left(\frac{Z + \left(1 + \sqrt{2}\right)B}{Z + \left(1 - \sqrt{2}\right)B}\right) \tag{3.119}$$

For vapor phase equation (3.119) become:

$$ln\phi_i^V = Z^V - 1 - ln\left(Z^V - B\right) - \left[\frac{A}{2\sqrt{2}B}\right] ln\left(\frac{Z^V + \left(1 + \sqrt{2}\right)B}{Z^V + \left(1 - \sqrt{2}\right)B}\right) \tag{3.120}$$

The A and B parameters in equations (3.118) and (3.120) represent the pure species parameter given by equations (3.83) and (3.96) for SRK and PR equations of state, respectively.

The equations (3.79) of SRK equation of state and (3.92) for PR equation of state are still applicable for estimating the vapor and liquid phases compressibility factors (Z^V and Z^L) for each species. Here again, both equations give three roots, the largest one is the vapor phase compressibility factor (Z^V) and the smallest is the liquid phase compressibility factor (Z^L). Both of equations (3.79) and (3.92) must be solved for each species at system temperature and pressure (*i.e.* using Newton – Raphson method).

For saturation conditions, each of equations (3.79) and (3.92) must be solved for system temperature and for pressure that equal to the vapor pressure for species *i* (*i.e.* $P = P_i^s$ and $Pr_i = P_i^s / Pc_i$).

A more serious problem for using equation (3.108) is posed by species whose critical temperatures are below the system temperature ($Tr_i > 1$) in which the vapor pressure curve is terminated. Attempts to overcome these difficulties via development of pure species fugacity correlations for that hypothetical state by extrapolation vapor pressure curve obtained at temperature below the critical region **[88, 94]**.

For petroleum industry and gas processing **Chao – Seader [56]** developed an empirical expression for pure species fugacity coefficient, that can be used for overcoming the problem of hypothetical state in supercritical region ($Tr_i > 1$). Choa – Seader correlation can be used up to $Tr_i \leq 1.3$. The correlations has the following formula:

$$log\phi_i^L = log\phi_i^{L(0)} + \omega_i \, log\phi_i^{L(1)} \tag{3.121}$$

where

$$\begin{aligned} log\phi_i^{L(0)} &= A_0 + \frac{A_1}{Tr_i} + A_2 Tr_i + A_3 Tr_i^2 + A_4 Tr_i^3 \\ &+ \left(A_3 + A_6 Tr_i + A_2 Tr_i^2\right) Pr_i + \left(A_8 + A_9 Tr_i\right) Pr_i^2 - log\,Pr_i \end{aligned} \tag{3.122}$$

$$log\phi_i^{L(1)} = A_{10} + A_{11} Tr_i + \frac{A_{12}}{Tr_i} + A_{13} Tr_i^3 + A_{14}\left(Pr_i - 0.6\right) \tag{3.123}$$

constants of equations (3.122) and (3.123) are shown in Table 3-5.

Table 3-5 Constants of equations (3.122) and (3.123)

Equation (3.118)		Equation (3.119)	
A_0	2.05135	A_{10}	-4.2389
A_1	-2.10899	A_{11}	8.65808
A_2	0	A_{12}	-1.2206
A_3	-0.19396	A_{13}	-3.1522
A_4	0.02282	A_{14}	-0.0250
A_5	0.08852		
A_6	0		
A_7	-0.00872		
A_8	-0.00351		
A_9	0.00203		

3.9.2 The liquid phase activity coefficient γ_i^L

The third auxiliary function of equation (3.66), is the liquid phase activity coefficient. The activity coefficient for liquid phase represents the departure from the ideal solution concept. The ideal solution occurs when molecular diameters are equal, chemical interaction are absent, and intermolecular forces between like and unlike molecules are equal **[55]**.

The starting point for calculating the activity coefficient for liquid phase γ_i^L, is the relation between the partial molar excess Gibbs free energy $\overline{G}_i^E$ and the activity coefficient γ_i^L.

The partial molar Gibbs free energy $\overline{G}_i$ can be defined as follows **[42]**:

$$d\overline{G}_i = RT\, ln\, \overline{f}_i \tag{3.124}$$

Equation (3.124) may be integrated at constant temperature and pressure for change of species *i* from state of pure *i*, where $\overline{G}_i = G_i$ and $\overline{f}_i = f_i$, to a state in real solution at arbitrary mole fraction x_i, thus:

$$\overline{G}_i - G_i = RT\,ln\frac{\overline{f}_i}{f_i} \tag{3.125}$$

For ideal solution, the partial fugacity for species *i* can be written as follows:

$$\overline{f}_i^{id} = x_i f_i \tag{3.126}$$

Equation (3.126) known as Lewis / Randall rule, *id* denotes to ideal solution.

Applying equation (3.125) for ideal solution:

$$\overline{G}_i^{id} - G_i = RT\,ln\frac{\overline{f}_i^{id}}{f_i} \tag{3.127}$$

Where, $\overline{f}_i^{id} = x_i f_i$, thus equation (3.127) becomes:

$$\overline{G}_i^{id} - G_i = RT\,ln\,x_i \tag{3.128}$$

If *M* represents the molar value of an extensive thermodynamic properties for example (*V, u, G, ...etc*), then an excess property M^E is defined as the difference between the actual property value of a solution and the value it would have if it is an ideal solution at the same temperature, pressure and composition **[39]**, thus:

$$M^E = M - M^{id} \tag{3.129}$$

or in partial molal term:

$$\overline{M}^E = \overline{M} - \overline{M}^{id} \tag{3.130}$$

If the above definition is applied to partial excess Gibbs energy, then:

$$\overline{G}_i^E = \overline{G}_i - \overline{G}_i^{id} \tag{3.131}$$

If equation (3.125) is subtracted from equation (3.128), the result is:

$$\overline{G}_i^E = RT\, ln\left(\frac{\overline{f}_i}{x_i f_i} \right) \tag{3.132}$$

Where the term $\left(\frac{\overline{f}_i}{x_i f_i} \right)$ is the definition of the activity coefficient given by equation (3.58), thus:

$$\overline{G}_i^E = RT\, ln\left(\gamma_i^L\right) \tag{3.133}$$

or: $$\frac{\overline{G}_i^E}{RT} = ln\left(\gamma_i^L\right) \tag{3.134}$$

It is clear from equation (3.134) that the (γ_i^L) is strongly depended upon the system temperature, pressure and composition or:

$$\gamma_i^L = F\left(T, P, x_1, x_2, \ldots x_N\right) \tag{3.135}$$

Several models have been proposed for predicting the activity coefficient (γ_i^L) from the excess Gibbs free energy, depending on the type of the liquid mixtures.

The liquid mixtures that contain dissimilar polar species, particularly those that can form or break hydrogen bonds, such mixtures can be classified as highly non ideal mixtures. Examples of those mixtures are the mixtures that contain water, alcohols, esters, …*etc* **[95]**. For such mixtures the most convenient activity models, that widely used are, the Wilson model **[96]**, the non – random two – liquid model (NRTL) **[97, 98]**, and the universal qusi – chemical model (UNIQUAC) **[99]**.

For non polar liquid mixtures, such as the hydrocarbons mixtures, the relatively simple activity models are recommended **[100]**. The latter is true for crude oils and petroleum fractions, because the bulk of them are consisting of hydrocarbon compounds (as discussed in Chapter 1 typically the hydrocarbon compounds representing more than 97% of crude oil or petroleum fractions). The other polar compounds such as sulfur, nitrogen, metals …etc. representing the miner constituents of crude oil or petroleum fractions.

The most relatively simple activity coefficient models that are widely used for predicting the activity coefficients for petroleum fractions and hydrocarbon mixtures are:

i. Regular solution models.
ii. van Laar models.

3.9.2.1 Regular solution models

Chao – Seader [56] and **Paul – Lachman [101]** proposed and extended the simple regular models that based on the regular solution theory of **Seatchard and Hilderbrand [58]** for predicting the (γ_i^L) for hydrocarbon mixtures and petroleum fractions. The regular solution theory is based on the premise that the non ideality in the liquid phase mixture is due to differences in van der Walls forces of attraction among the species present. Regular solutions have an endothermic heat of mixing and all activity coefficient are greater than unity (*i.e.* positive deviation from Raoult's law).

For a multi component regular solution, the partial molal excess free energy is:

$$\overline{G}_i^E = \sum_{i=1}^{N}\left(x_i V_i^L\right)\left[\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\Phi_i\Phi_j\left(\delta_i-\delta_j\right)^2\right] \tag{3.136}$$

where Φ is the volume fraction, assuming additive molar volumes (V^L), given as:

$$\Phi_j = \frac{x_j V_j^L}{\sum_{i=1}^{N} x_j V_j^L} = \frac{x_j V_j^L}{V^L} \tag{3.137}$$

and δ is the solubility parameter that can be evaluated by:

$$\delta_i = \frac{(\lambda_i - RT)^{1/2}}{V_i^L} \tag{3.138}$$

where λ is the heat of vaporization.

Relating equations (3.134) and (3.136) and with some arrangement an expression for the activity coefficient of regular solution theory can be obtained as:

$$ln\gamma_i^L = \frac{V_i^L \left(\delta_i - \sum_{i=1}^{N} \Phi_i \delta_i \right)^2}{RT} \tag{3.139}$$

The calculation of γ_i^L by regular solution model involves only pure species constants V_i^L and δ_i. Frequently, these constants are taken at some convenient reference temperature, such as 25 °C (77 °F). For petroleum fraction, the heat of vaporization (λ) can be calculated using the Raizi – Daubert correlation **[13]**:

$$\lambda = 8.4885 T_B^{1.1347} Sp.gr^{0.0214} \tag{3.140}$$

3.9.2.2 van Laar models

The excess Gibbs energy is a function of the temperature, pressure and composition of system (*P, T, x*), but for liquid at low to moderate pressures, it is a very weak function of *P*. Under these conditions, its pressure dependence or in other word, the pressure dependence of activity coefficients is usually neglected. Thus, a constant temperature is achieved **[55]**:

$$\frac{\overline{G}_i^E}{RT} = F(x_1, x_2, \ldots x_N) \tag{3.141}$$

In 1913 van Laar suggested a power series for representation equation (3.141). His proposed model for excess Gibbs energy for binary mixture:

$$\frac{\overline{G}_i^E}{RT} = \frac{x_1 x_2 A'_{12} A'_{21}}{A'_{12} x_1 + A'_{21} x_2} \tag{3.142}$$

The activity coefficients for binary mixtures are given by substituting equation (3.141) into equation (3.134), thus:

$$ln\gamma_1^L = \frac{A'_{12}}{\left[1 + \frac{x_1 A'_{12}}{x_2 A'_{21}}\right]^2} \tag{3.143}$$

and $$ln\gamma_2^L = \frac{A'_{21}}{\left[1 + \frac{x_2 A'_{21}}{x_1 A'_{12}}\right]^2} \tag{3.144}$$

where A'_{12} and A'_{21} are known as the binary interaction parameters and must be back – calculated from experimental data. These parameters are, in theory constants only for a particular binary pair at a given temperature. In practice, they are frequently computed from isobaric data covering a range of temperature.

Null [102], extended the van Laar model for a multi component mixture and the resulting expression for activity coefficient in this model depends only on composition and binary interaction parameters and is given by:

$$ln\gamma_i^L = \frac{\sum_{j=1}^{N}\left(x_j A_{ij}\right)}{1-x_i}\left[1-\frac{x_i\sum_{j=1}^{N}\left(x_j A_{ij}\right)}{x_i\sum_{j=1}^{N}\left(x_j A_{ij}\right)+\left(1-x_i\right)\sum_{j=1}^{N}\left(x_j A_{ji}\right)}\right]^2 \tag{3.145}$$

The interaction parameters A_{ij} and A_{ji} have the following properties:

1. $A_{ii} = A_{jj} = 0$.
2. $A_{ij} = A_{ji}$
3. For non polar hydrocarbon pairs A_{ij} and A_{ji} can be estimated as follows:

$$A_{ij} = \frac{V_i^L}{RT}\left(\delta_i - \delta_j\right)^2 \tag{3.146}$$

4. For polar pairs, the interaction parameters pairs A_{ij} and A_{ji} can be back calculated from experimental data.
5. If no useful data exist, a procedure based on estimation the binary activity coefficient at infinite dilution suggested by Null can be employed.

Because of the van Laar model, simplicity, flexibility and ability to fit many systems that have both positive (γ_i^L>1) and negative (γ_i^L<1) deviations from Raoult's law, it is widely used in practice **[39]**.

3.10 Working formula for activity coefficient model for predicting the *K* – values

The working formula for activity coefficient model for predicting the *K* – values can be obtained by combining equations (3.66) and (3.108), thus:

$$K_i = \left(\frac{P_i^s}{P}\right)\left(\frac{\phi_i^{Vs}}{\phi_i^V}\right)\gamma_i^L\left[Exp\frac{V_i^L\left(P - P_i^s\right)}{RT}\right] \tag{3.147}$$

3.11 Ideal solution models for prediction *K* – values

Separation operations are frequently conducted under or at vacuum pressure (*e.g.* crude oil tower). In such process, the ideal solution concept is more reliable, and applicable. The ideal solution concept has another important requirement that is the species in the mixture have essentially identical molecular size and intermolecular forces. Thus, a mixture of isomers, such as ortho, meta and para conforms very closely to ideal solution behavior. So do mixtures of adjacent members of a homologous series such the hydrocarbon mixtures **[55, 88]**.

If the ideal *K* – value equation (3.67) is recalled:

$$K_i = \frac{f_i^L}{f_i^V} \qquad ..(3.67)$$

or in fugacity coefficient term:

$$K_i = \frac{\phi_i^L}{\phi_i^V} \tag{3.148}$$

In equation (3.148), both the vapor and liquid phases obey the ideal solution behavior. Substituting equation (3.108) for ϕ_i^L, the following equation is obtained:

$$K_i = \left(\frac{P_i^s}{P}\right)\left(\frac{\phi_i^{Vs}}{\phi_i^V}\right) Exp\left[\frac{V_i^L\left(P - P_i^s\right)}{RT}\right] \qquad (3.149)$$

Equation (3.149), represents the working formula for ideal solution K – value. For special case at low pressure in which the vapor phase obeys the ideal gas law, and the species vapor pressures are close to system pressure, the ratio (ϕ_i^{Vs}/ϕ_i^V) will be unity and the Poynting factor (exponent term) may be neglected, thus equation (3.149) reduces to:

$$K_i = \frac{P_i^s}{P} \qquad (3.150)$$

Equation (3.150) is well known as Raoult's law K – value formula.

For the case in which the ideal gas law is valid and the ratio of (ϕ_i^{Vs}/ϕ_i^V) is not unity, and the species vapor pressures are widely differ from system pressure, so the Poynting factor can not be negligible. For such case, the ϕ_i^V and ϕ_i^{sV} must be obtained using a suitable equation of state models.

A more serious problem in using equation (3.140) is posed for species whose critical temperatures are below the system temperature (Tr > 1), where the hypothetical region occurs. For ideal solution mixture, only limited extrapolation of pure fugacity coefficients into hypothetical region are required. **Henly [88]**, suggested a simple procedure, that can be utilized for determining the pure species fugacity coefficient whether hypothetical region occurs or not.

In Henly procedure, the pure species fugacity coefficient can be determined using equation (3.116) as:

$$ln\phi_i = \int_0^P \left(\frac{Z-1}{P}\right) dP \qquad (3.116)$$

At low to moderate pressures of the ideal solution mixture, the integration of equation (3.116) is approximately constant, for a given temperature. The integration is thus readily performed, with the following result in reduced form:

$$\phi_i^V = Exp\left[Pr_i \left(\frac{Z-1}{Pr_i} \right)_{Pr_i=0} \right] \tag{3.151}$$

The term ($Z - 1/Pr_i$) at $Pr_i = 0$ is determined from appropriate equation of state models. If the SRK equation of state is used, a reduced form is convenient. It is derived as follows, recalling SRK equation of state {equation (3.75)}.

$$P = \frac{RT}{V-b} - \frac{a\alpha}{V(V+b)} \tag{3.75}$$

Equation (3.175) can be written in Z term, as:

$$Z = \frac{1}{1+h} + \frac{a\alpha}{RTV}\left(\frac{1}{1+h} \right) \tag{3.152}$$

where $h = \frac{BP}{Z}$ and $B = \frac{b}{RT}$

Multiplying and dividing equation (3.152) by b, so the following equation is obtained:

$$Z = \frac{1}{1+h} + \frac{a\alpha}{RTb}\left(\frac{h}{1+h} \right) \tag{3.153}$$

The a and b can be obtained from equation (3.83), and h can be written as follows:

$$h = \frac{b}{RT} = \frac{0.08664\, Pr_i}{ZTr_i} \tag{3.154}$$

Substituting equations (3.83) and (3.154) into equation (3.153) to obtain the following equation:

$$Z = \frac{1}{1 + \frac{0.08664\, Pr_i}{ZTr_i}} - \frac{0.4274\alpha\, Pr_i}{Tr_i^2 Z}\left[\frac{1}{1 + \frac{0.08664\, Pr_i}{ZTr_i}}\right] \tag{3.155}$$

If equation (3.155) is rearranged in form of $(Z - 1)/Pr_i$ and in the limit of $Pr_i = 0$ where $Z \rightarrow 1$, then:

$$\left.\frac{Z - 1}{Pr_i}\right|_{\substack{Pr_i = 0 \\ Z \rightarrow 1}} = \frac{0.08664}{Tr_i} - \frac{0.4274\alpha}{Tr_i^2} \tag{3.156}$$

Substituting equation (3.156) into equation (3.151) gives:

$$\phi_i^V = Exp\left[\frac{0.08664\, Pr_i}{Tr_i} - \frac{0.4274\, Pr_i\, \alpha}{Tr_i^2}\right] \tag{3.157}$$

or in the saturation conditions:

$$\phi_i^{Vs} = Exp\left[\frac{0.08664\, Pr_i^s}{Tr_i} - \frac{0.4274\, Pr_i^s\, \alpha}{Tr_i^2}\right] \tag{3.158}$$

where: $Pr_i^s = P_i^s / Pc$

Substituting equations (3.157) and (3.158) into equation (3.149) gives:

$$K_i = \left(\frac{P_i^s}{P} \right) \frac{Exp\left[\frac{0.08664\, Pr_i^s}{Tr_i} - \frac{0.4274\, Pr_i^s\, \alpha}{Tr_i^2} \right]}{Exp\left[\frac{0.08664\, Pr_i}{Tr_i} - \frac{0.4274\, Pr_i\, \alpha}{Tr_i^2} \right]} \times Exp\left[\frac{V_i^L\, (P - P_i^s}{RT} \right] \qquad (3.159)$$

Rearranging equation (3.159), with $Pr_i = P/Pc_i$ and $Pr_i^s = P_i^s / Pc_i$, thus the following working formula is obtained for the ideal *K* – value as follows:

$$K_{i(ideal)} = \left(\frac{P_i^s}{P} \right) Exp\left[\left(\frac{0.08664}{Tr_i Pc_i} - \frac{0.4278 \alpha_i}{Tr_i^2 Pc_i} - \frac{V_i^L}{RT} \right) \left(P_i^s - P \right) \right] \qquad (3.160)$$

Equation (3.160) has the following properties:

1. It is applicable for ideal solution at low to moderate pressures.
2. The exponential term is the correlation for the simple Raoult's law *K* – value.
3. The ideal *K* – value is depending only on temperature and pressure of the system and it is independent of the composition of the system or,

$$K_{i(ideal)} = F(T,P) \qquad (3.161)$$

For the equation of state model and activity coefficient model where the solution is not ideal solution or the pressure is high, the *K* – value depends on temperature, pressure and composition of the system as:

$$K_i = F(T,P,x) \qquad (3.162)$$

3.12 Calculation of flash volume by flash calculations

One further vapor – liquid equilibrium is the flash calculation. The origin of the name comes when the change occurs when a liquid under pressure passes through a valve to a pressure low enough so that some of liquid vaporizes (flashes) producing a two phase stream of vapor and liquid in equilibrium **[55]**.

The same idea is used in crude oil tower, but instead of using the valve for reducing the pressure, the heated crude oil stream is flashed at the flash zone area in the tower. The pressure in flash zone area is approximately atmospheric pressure **[3]**. The other important factor in vaporization of crude oil in the flash zone is the flash zone temperature. The flash zone temperature must be fixed in such way to ensure all economically markable range of products from the complex mixtures of crude oil are vaporized **[22, 103]**.

Three types of flash vaporization process depending on the conditions of operation, that can be found in literatures **[91]**, those are:

1. Constant temperature and pressure (isothermal flash).
2. Constant enthalpy and pressure (isenthalpic flash).
3. Constant entropy and pressure (isentropic flash).

The constant temperature and pressure (isothermal flash) are considered here because it is widely used in petroleum refinery operations.

3.12.1 Constant temperature and pressure (isothermal flash)

It is also known as ($P – T$) flash process which refers to any flash calculation of system in equilibrium at known temperature and pressure (T, P) and overall feed composition **[55]**. Consider Fig. 3-2, that illustrates schematically the ($P – T$) flash process. The feed, at temperature T and pressure P, passes through at throttle and enters flash tower or vessel, where liquid and vapor phases may separate. The heat is supplied or removed at a rate of Q through a heat exchanger, so as to maintain isothermal conditions at temperature T. The molar rate of the feed to the unit is specified, together with the overall composition (mole fraction Z_i), and the temperature and pressure at which the unit operates. The objectives of the calculation are to determine the compositions (y_i and x_i), and the molar flow rate (F_V and F_L) of the vapor and liquid streams leaving the unit.

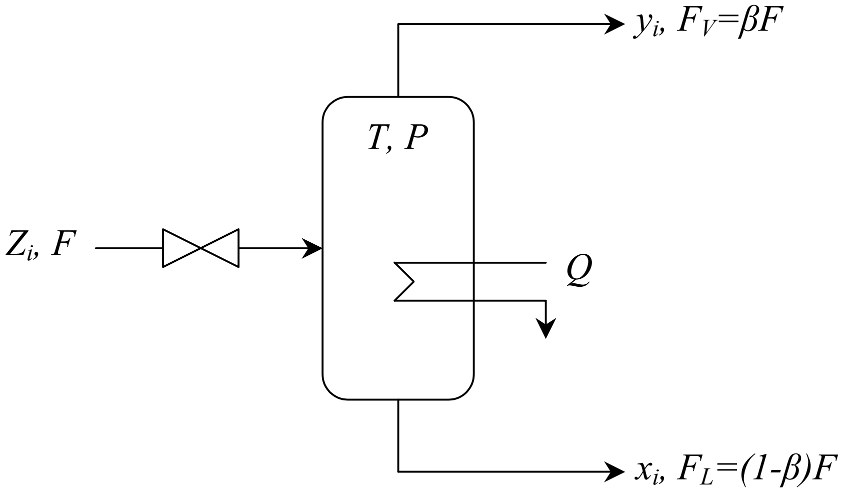

Figure 3-2 *P* – *T* flash unit

Since only the overall composition of mixture is known, a material balance for each species of *N*C species is required, thus:

$$FZ_i = F_V y_i + F_L x_i \tag{3.163}$$

The overall material balance is:

$$F = F_V + F_L \tag{3.164}$$

Substituting equation (3.164) into equation (3.162), to eliminate *L*, gives,

$$FZ_i = (F - F_V)x_i + F_V y_i \tag{3.165}$$

The phase equilibrium relation is:

$$y_i = K_i x_i \tag{3.166}$$

or $$x_i = \frac{y_i}{K_i} \tag{3.167}$$

Combining equation (3.166) with equation (3.165) to eliminate the y_i or,

$$FZ_i = (F - F_V)x_i = F_V K_i x_i \tag{3.168}$$

Or if equation (3.167) is used with equation (3.165) to eliminate x_i, yields:

$$FZ_i = (F - F_V)\left(\frac{y_i}{K_i}\right) + F_V y_i \tag{3.169}$$

Rearranging equations (3.168) and (3.169) to obtain the expression for y_i and x_i, as:

$$x_i = \frac{Z_i}{1 + \beta(K_i - 1)} \tag{3.170}$$

and $$y_i = \frac{Z_i K_i}{1 + \beta(K_i - 1)} \tag{3.171}$$

where $\beta = F_V/F$, and it is the vapor fraction for multi component system of NC species, since:

$$\sum_{i=1}^{N} z_i = 1 \tag{3.172}$$

$$\sum_{i=1}^{N} y_i = 1 \tag{3.173}$$

$$\sum_{i=1}^{N} x_i = 1 \tag{3.174}$$

And from overall material balance, is:

$$\sum_{i=1}^{N} y_i - \sum_{i=1}^{N} x_i = 0 \tag{3.175}$$

Substituting equations (3.170) and (3.171) into equation (3.175) gives:

$$\sum_{i=1}^{N} \frac{Z_i K_i - z_i}{1+\beta(K_i - 1)} = 0 \tag{3.176}$$

or, $$F(\beta) = \sum_{i=1}^{N} \frac{Z_i(1-K_i)}{1+\beta(K_i - 1)} = 0 \tag{3.177}$$

Equation (3.177) is nonlinear in β only, and it can be solved by trial and error by guessing values of β between 0 and 1, until the $F(\beta) = 0$. The most widely employed method for solving equation (3.177) is the Newton – Raphson method **[83]**. The latter is discussed in Appendix B.

It must be noted; that before proceeding in flash calculation, it is be sure that the input feed at a given temperature and pressure is in the two phase region. The latter can be accomplished using equation (3.177) with the following conditions **[42]**:

1. If $F(0) > 0$, the mixture is below its bubble point (sub cooled liquid).
2. If $F(1) < 0$, the mixture is above the dew point (super heated vapor).
3. If $F(0) < 0$ and $F(1) > 0$, the mixture in the two phase region, and the flash calculation can be proceeded (*i.e.* β between 0 and 1).

The *EFV* curve is usually obtained by plotting the volume percent vaporized against the temperature. As a result of that the vapor fraction β in mole percent must be converted to volume percent. The latter can be done by using the following equation **[29]**:

$$\beta_V = \left(\frac{V_V}{V_F}\right) \cdot \left(\frac{F_V}{F}\right) \times 100 \tag{3.178}$$

Where: V_F = Molal volume of the feed stream

V = Molal volume of the vapor stream

The molal volume of the vapor stream can be obtained by the following equation:

$$V_V = \sum_{i=1}^{N} \frac{y_i MW_i}{\rho_i} \tag{3.179}$$

Where: MW_i is the species i molecular weight

ρ_i is the species i liquid density at 15 °C (60 °F)

The molal volume of the feed stream can be obtained as follows:

$$V_F = \sum_{i=1}^{N} \frac{z_i MW_i}{\rho_i} \tag{3.180}$$

Because of (F_V / F) represents the vapor vaporized β, so that equation (3.178) can be written as follows:

$$\beta_V = \left(\frac{V_V}{V_F} \right) \beta \times 100 \tag{3.181}$$

Chapter Four

Experimental work

4.1 Aim of the experimental work

1. Kirkuk, Basrah, Jambour and Bai – Hassan crude oils fractionating into approximately 10 °C narrow fractions in the range of *IBP* – 370 °C (*IBP* – 698 °F).
2. Construction of *TBP* curve for each of crude oils by plotting total cumulative volume (or weight) percent distilled against measured boiling point temperature.
3. Specific gravities determination for all narrow fractions distillate from Kirkuk, Basrah, Jambour and Bai – Hassan crude oils.
4. Construction of specific gravity curve by plotting total cumulative volume (or weight) percent distilled against measured specific gravity.
5. The exponential work were performed in laboratory of Dura refinery.

4.2 Feed stocks

The feed stocks used in this experimental work were Kirkuk, Basrah, Jambour and Bai – Hassan crude oils. The properties of Kirkuk, Basrah, Jambour and Bai – Hassan crude oils are given in Table 4-1. All properties were made at the laboratory of Dura refinery.

Table 4-1 Properties of Kirkuk, Basrah, Jambour and Bai – Hassan crude oils

Item	Test	Kirkuk crude oil	Basrah crude oil	Jambour crude oil	Bai – Hassan crude oil
1	Specific gravity @ 15.6/15.6 °C	0.8428	0.8756	0.8363	0.8686
2	*API*	36.4	30.1	37.7	31.4
3	*R.V.P.* @ 37.8 °C, kg/cm^2	0.47	0.43	0.52	0.32
4	Salt content, wt.%	0.0009	0.0007	0.0009	0.0012
5	Pour point, °C	- 23.3	- 29	- 28	- 18.5
6	Bottom water & Sediment content, vol.%	0.05	0.05	0.05	0.1
7	Conradson carbon, wt.%	3.38	5.05	2.45	5.7
8	Viscosity @ 10 °C, sc	9.7	34	7.05	21.4
9	Viscosity @ 40 °C, sc	4.36	11.55	3.35	8.4
10	Asphaltene, wt.%	3.38	2.01	0.12	2.97
11	Ash content, wt.%	0.0045	0.0085	0.01	0.0095
12	H_2S content, ppm	22	6	150	7
13	Total sulfur content, wt.%	2.1	3.06	1.78	3.06
14	*ASTM* distillation, vol.%				
	Recovery @ *IBP*	41.0	40.0	43.0	47.0
	50 °C	1.50	1.50	1.00	0.50
	75 °C	6.00	4.50	4.00	4.20
	100 °C	10.5	8.50	9.00	8.50
	125 °C	17.5	13.0	14.0	13.0
	150 °C	24.5	17.0	20.0	18.0
	175 °C	29.0	20.5	26.0	23.0
	200 °C	35.0	25.0	33.0	28.0
	225 °C	39.5	29.5	40.0	32.0
	250 °C	44.0	33.5	45.0	36.0
	275 °C	48.0	37.0	49.0	40.0
	300 °C	53.0	41.0	53.0	46.0
	Total distillate, vol.%	55.0	43.0	55.0	48.0
	Total residue, vol.%	45.0	57.0	45.0	52.0

4.3 Distillation unit

Fractional distillation unit may be looked upon as a process in which vapors leaving the liquid in the distillation flask are allowed to pass upwards through a column at the top of which they are condensed. A portion of the condensate is returned as "reflex" downwards through the column where it is brought into more or less intimate contact with the ascending vapors. Here a heat interchange takes place between the relatively cooler liquid and warmer vapors so that more volatile part of the liquid is vaporized, while the more easily condensable part of the vapors is condensed. The net result is a concentration of more volatile material in the top of the column with increasing concentration of less volatile material as the bottom of the column is approached **[3, 104]**.

4.3.1 Laboratory distillation unit

Distillation process was achieved on laboratory distillation apparatus (according to *ASTM* D2892 – 87). The main parts of the laboratory distillation apparatus are; the distillation flask, heating mantle, distillation column, reflux condenser, timer, distillate condenser, vacuum system, instrumentations for measuring the temperature and pressure of the system, fraction receiver, variable resistance for heat input controlling and simple control panel. Fig. 4-1 shows a photographs picture for the laboratory distillation unit, and Fig. 4-2 shows the schematic diagram of the laboratory distillation unit.

Referring to Fig. 4-2, size of distillation flask (1), is 5 liters and provided with two side streams, first side stream used to change the crude oil, and the second side stream contains glass bulb for thermocouple type J, (2), for measurement of the bottom temperature. The specifications of thermocouple type J is given in Table C-1. The distillation flask mounted with 3kW heating mantels (3), connecting with variable resistance to control the heat input to the flask. The flask equipped with semi ball joint for connection with column. The semi ball joint was lubricated with a paste of silicone to insure a good sealing between the column and the flask.

Distillation column consisted of a packed bed (4), of 25mm inside diameter and 910mm length. The packed bed consists with Helipak type packing materials, the length of the packed bed was selected to satisfy the requirement of *ASTM D2892 – 87* (*i.e.* the length of packed bed ensures that fractionating column having an efficiency of 14 to 18 theoretical plate). The column was isolated by highly vacuum jacket containing multiple metallic reflectors (5), to minimize the heat loss. The specification of Helipak materials is given in Table C-2.

The top of the packed bed column was connected with a glass reflux condenser (6), of 290mm high and 50mm inside diameter and isolated by highly vacuum jacket containing multiple metallic reflectors. The glass reflux condenser was used to condense and cool the distillate. Ethylene glycol alcohol with temperature below –20°C introduced into the condenser by circulating pump of cooling machine. The use of low temperature cooling medium is essential for reducing the light hydrocarbons (mainly C_4). Two side streams (7), were used for introducing the cooling medium (*i.e.* ethylene glycol alcohol) into the reflux condenser. The cooling by ethylene glycol alcohol continued until the temperature of the vapor reached to 75 °C, after that the cooling medium was replaced or turned to ordinary tap water. The temperature of the vapor in the head of reflux condenser was recorded by a thermocouple type J (8).

The reflux ratio was controlled by using magnetic solenoid valve (a), connected with reflux timer (10). The reflux ratio of 5:1 was used for atmospheric distillation and 3:1 for vacuum distillation.

The bottom of the packed bed was connected to double expansion coil (11) of height 250mm, this expansion coil was used for introducing the vapor from distillation flask into the packed bed column. The expansion coil is also ensures the suitable velocity and good distillation of the vapor through the bed column.

For more details of the packed bed column, reflux condenser and the expansion coil are shown in Fig. C-2.

The vapor trap (12) was connected to the top of the reflux condenser and it was isolated by vacuum jacket. The vapor trap was maintained at the temperature below –58 °C by using a mixture of solid ice and NaCl salt as cooling medium or refrigerant (13). The using of vapor trap is useful for reducing the light hydrocarbons loss.

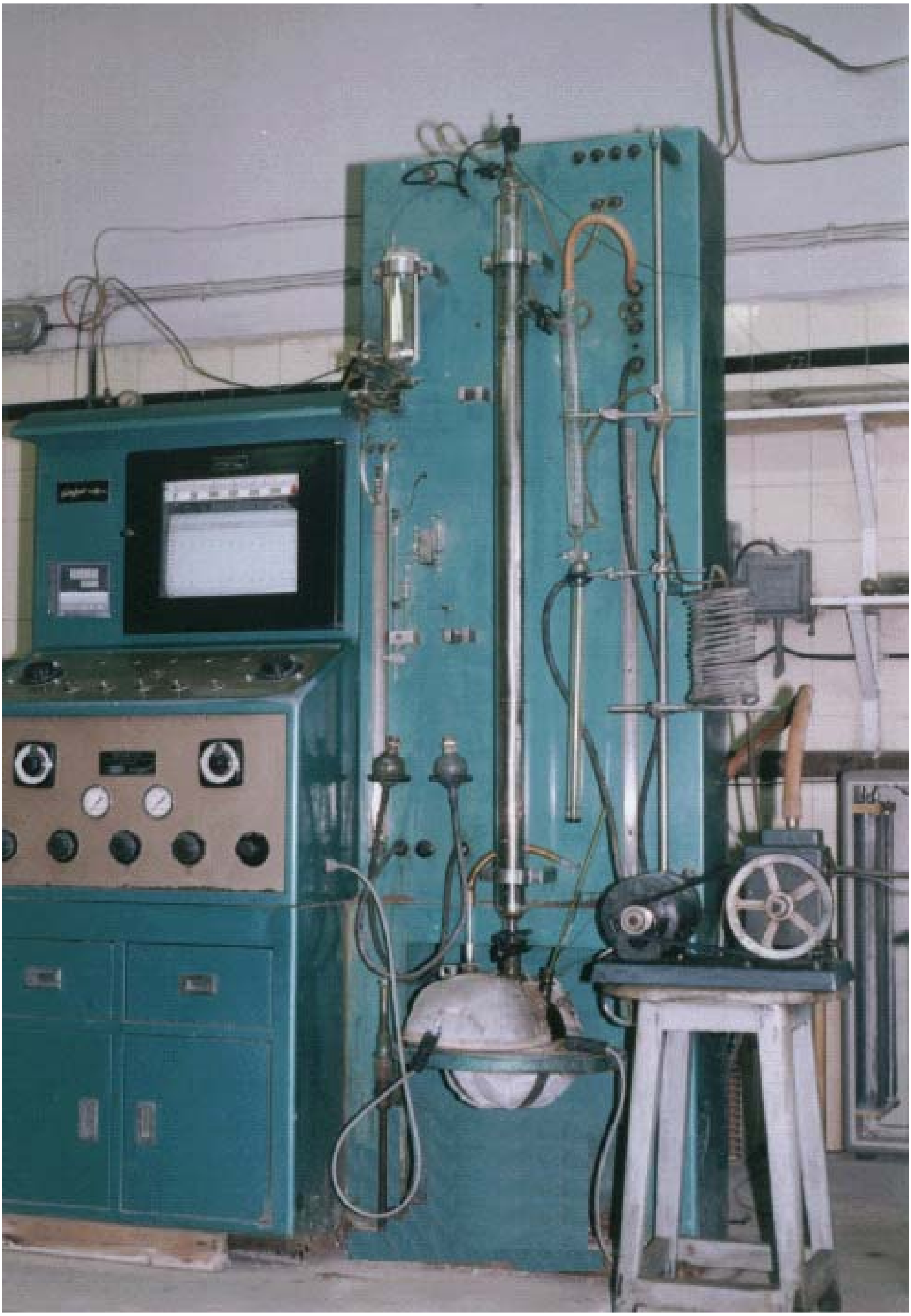

Figure 4-1 Photographic picture of the laboratory distillation unit

Item	Descriptions
1	Distillation flask
2	Thermocouple for measurement bottom temperature
3	Mantel heater
4	Paced bed of helipak packing materials
5	Multiple metal reflectors
6	Reflux condenser
7	Cool in and cool out
8	Thermocouple for measurement vapor temperature
9	Automatic distillate take of solenoid
10	To distillate take-off timer
11	Double expansion coil
12	Vapor trap
13	Refrigerant
14	Vacuum pump
15	Throttling valve
16	Pressure gauge
17	Surge drum
18	U type manometer
19	Top vent valve
20	Receiver vent valve
21	Distillate cooler
22	Cool in and cool out
23	Receivers changer
24	Distillate receiver (or burettes)
25	Control panel

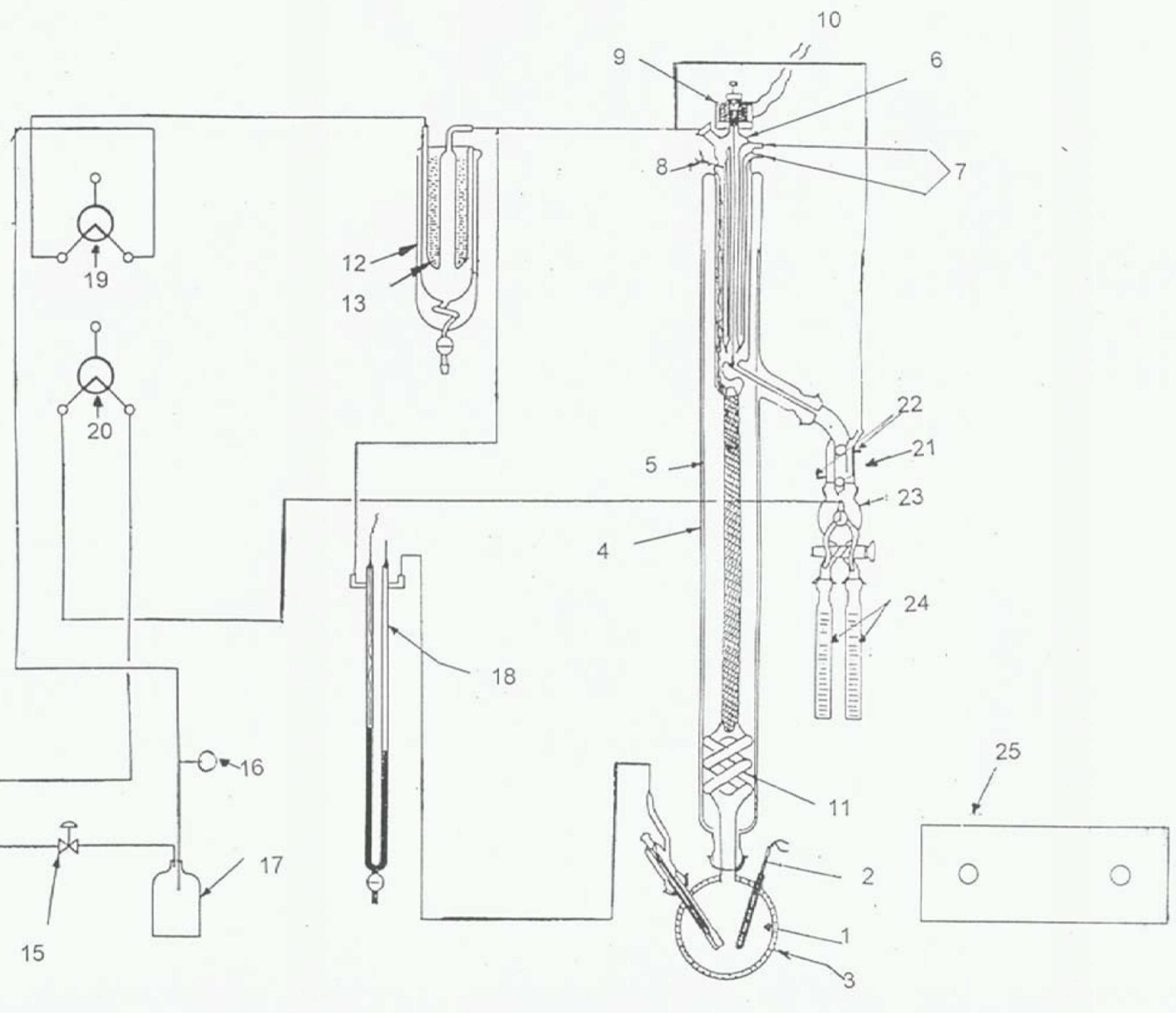

Figure 4-2 Schematic diagram of the laboratory distillation unit

When the temperature of crude oil inside distillation flask reached 300 °C, the distillation column was then connected to the vacuum system for producing the suitable vacuum pressure. The vacuum system was consisted of the vacuum pump (14), throttling valve (15), pressure gauge (16), surge drum (17), U – tube manometer (18), top vent valve (19) and receiver vent valve (20). The vacuum pressure was achieved by using 1/3 HP vacuum pump of general electric type. The vacuum pump can provide a vacuum pressure of 60mmHg.

The liquid distillate from reflux condenser was collected by distillate cooler (21). The distillate cooler was furthermore cooled the distillate fraction {i.e. by side streams (22)} by using ethylene glycol alcohol or ordinary trap water (the same as the cooling method that described in the reflux condenser). The aim of cooling the distillate in the distillate cooler is to reduce the light hydrocarbons loss from the light fractions (*i.e.* those cuts that have temperature less than 75 °C). The vacuum line of the distillate cooler, and reflux condenser were gathered by T shape joint to produce 60mmHg pressure.

The bottom of the distillate cooler was connected to receiver changer valve (22), which can be opened in two positions, the first position (the normal position) in which the distillate can be collected in one distillate receiver (23), while in the second position two distillate receivers can be used. The distillate receiver has a capacity of 200ml.

When the distillation unit is operated at vacuum pressure, the distillate receiver must be vented to avoid interrupting column equilibrium during taking the samples. The distillate receiver can be vented by using receiver vent valve (20). When the operation under vacuum is finished all distillation unit can be vented by using top vent valve (19).

The distillation column was mounted in the column panel of 2.20m length and 0.71m width as shown in Fig. 4-1.

The simple control panel (25), of 1.72m length and 0.726m width was mounted besides the column panel (as shown in Fig. 4-1) and consisting of the following items:

1. Selector switch with small screen for reading the vapor and bottom temperatures that measured by using thermocouples.

2. Electronic recording potentiometer for measuring the vapor temperature (not used).
3. Starting and off electrical switches for heating mantel and vacuum pump.
4. Variable resistance for controlling the input heat to heating mantel.
5. The solenoid valve timer for controlling the reflux ratio for atmospheric and vacuum distillation operations.
6. Gauge pressure for reading the vacuum pressure of the system.

The connection lines between the distillation column and other parts of distillation unit was achieved by using the double coated rubber tubing suitable for high temperature operations.

The utility requirement of the distillation units can be given in Table C-4.

4.4 Density and specific gravity

Density and specific gravity of all distillation fractions from Kirkuk, Basrah, Jambour and Bai – Hassan crude oils were determined according to *ASTM D12980 – 80* by using 25cm^3 pycnometer. The calibration of pycnometer was performed according to *ASTM D12980 – 80*.

Chapter Five

Selected data and estimation methods

The calculation of vapor – liquid equilibria for petroleum fractions is important because of the difficulty of obtaining experimental values or data. The most important vapor – liquid equilibria calculation for petroleum fractions is well known as the equilibrium flash vaporization curve (*EFV*) calculation. The applicability and limitations of the prediction of the *EFV* curve for petroleum fractions by means of graphical methods, and the pseudo – component (computer) methods had been studied. Both methods are based on converting the true boiling point curve (*TBP*) into the *EFV* curve.

In the present work, the results were divided into two parts. The first part has two folds, firstly, the graphical methods and pseudo – component (computer) methods were tested to decide, which approach shows the greatest promise. Secondly, various methods for improving existing methods were investigated. The first part can be considered as testing and improving part.

In the second part of the present work, the improved methods were used for predicting or calculating the *EFV* curves for four types of Iraqi crude oils (Kirkuk, Basrah, Jambur and Bai – Hassan). The second part can be considered as an application part.

5.1 Data sources

5.1.1 Data sources for part one (testing and improving part)

For the first part of the present work, the flash data examined which come from chemical engineering literatures. Table 5-1 gives the general characterization of these data. For simplicity, the petroleum stock name will be eliminated and just the stocks number will be used. Petroleum stocks of number 1 to 15 of Table 5-1 are presented with incomplete *TBP* curves and overall specific gravity. The *TBP* curves for these petroleum stocks are illustrated in Figs. 5-1 through 5-15, respectively, while the *EFV* curves for these stocks are given in Figs. 5-16 through 5-30, respectively. Tables D-1 through D-15 in Appendix D give the numerical values for *TBP* and *EFV* of these petroleum stocks.

The petroleum stocks of numbers 16, 17 and 18 of Table 5-1 contain more complete *TBP* distillation curves (generally from 0 to 80 vol.%). These petroleum stocks also have specific gravity curves. The *TBP* curves of number 16, 17 and 18 are illustrated in Figs. 5-31, 5-32 and 5-33, respectively, and their *EFV* curves are illustrated in Figs. 5-34, 5-35 and 5-36, respectively. The *EFV* curves for these stocks are given in Figs. 5-37, 5-38 and 5-39, respectively. Table D-16, D-17 and D-178 in Appendix D show the *TBP*, *EFV* and specific gravity values of these petroleum stocks.

Table 5-1 Literature sources and characterization of flash data

Stock no.	Stock name	*API*	Range of *TPB* distilled (Vol.%)	*Sp.gr* range of stock	Experimental Flash volume (Vol.%)	Number of *EFV* points	Ref.
1	Santa fe springs	32.4	5-70	overall	5-70	5	**[79]**
2	Eldwood	36.5	5-70	overall	5-70	5	**[79]**
3	Colombian	27.2	5-70	overall	5-70	5	**[79]**
4	Ranger	37.3	5-70	overall	5-70	5	**[79]**
5	Lulting	34.9	5-70	overall	5-70	5	**[79]**
6	50% COL.OH.	40.9	5-70	overall	5-70	5	**[79]**
7	Kansas	40.8	5-70	overall	5-70	5	**[79]**
8	Mid-continent	37.7	5-70	overall	5-70	5	**[79]**
9	Magnoland	28.2	5-70	overall	5-70	5	**[79]**
10	Mid-continent	38.2	5-70	overall	5-70	5	**[79]**
11	Hendricks	32.5	5-70	overall	5-70	5	**[79]**
12	Mid-continent	34.4	5-70	overall	5-70	5	**[79]**
13	Naphtha-kerosene blend	47.8	10-70	overall	10-70	7	**[4]**
14	California-research stock 7	37	10-70	overall	10-70	4	**[4]**
15	Middle east	38.6	4.4-80	overall	10-70	6	**[6]**
16	Intermediate-paraffin base	37.3	0-90	0.6769-0.9894	10-70	10	**[3]**
17	Asphaltic-naphthene base	20.2	0-80	0.8105-1.0186	10-70	10	**[3]**
18	Paraffin base	42.2	0-90	0.6951-0.9150	10-70	10	**[3]**

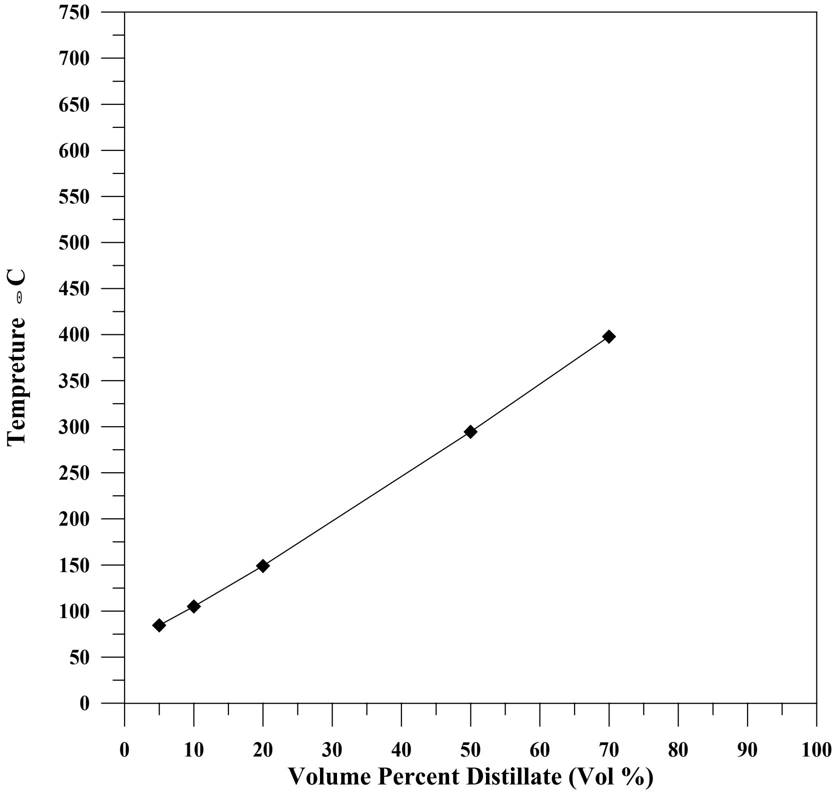

Figure 5-1 *TBP* curve for petroleum stock number 1

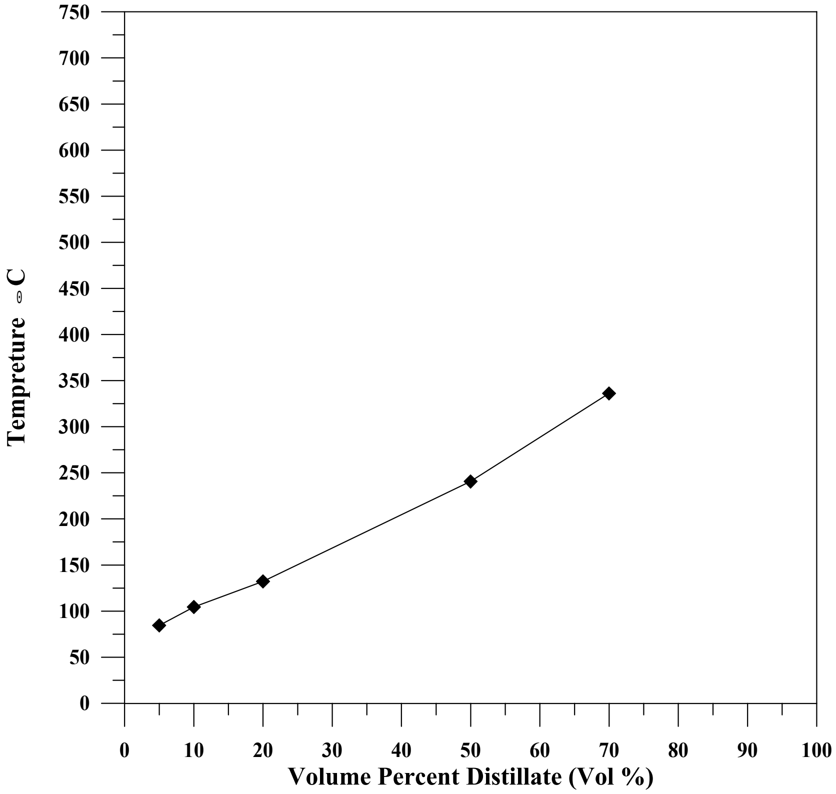

Figure 5-2 *TBP* curve for petroleum stock number 2

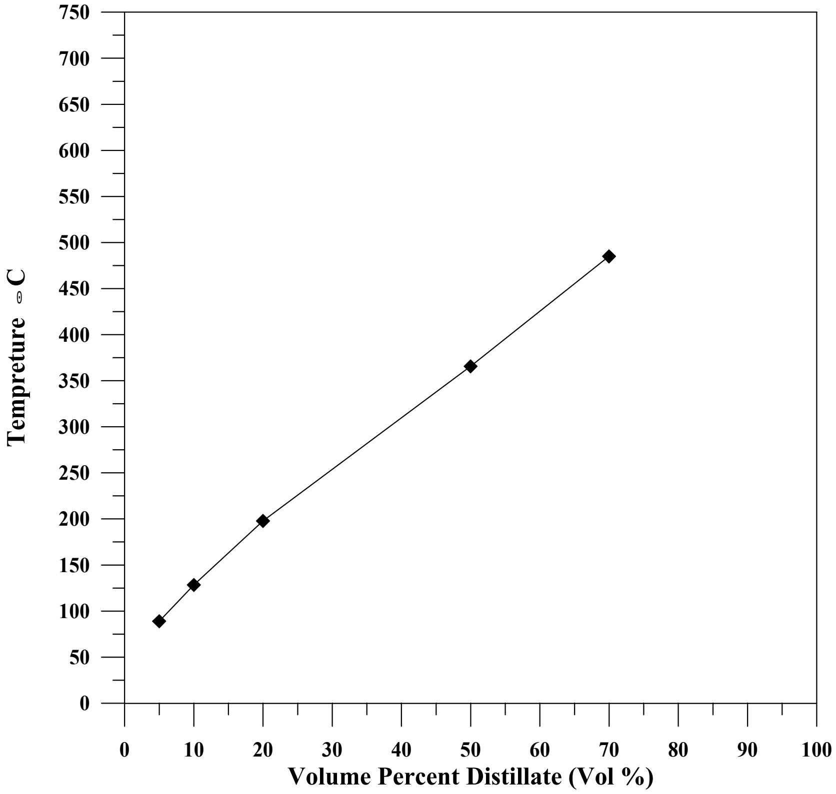

Figure 5-3 *TBP* curve for petroleum stock number 3

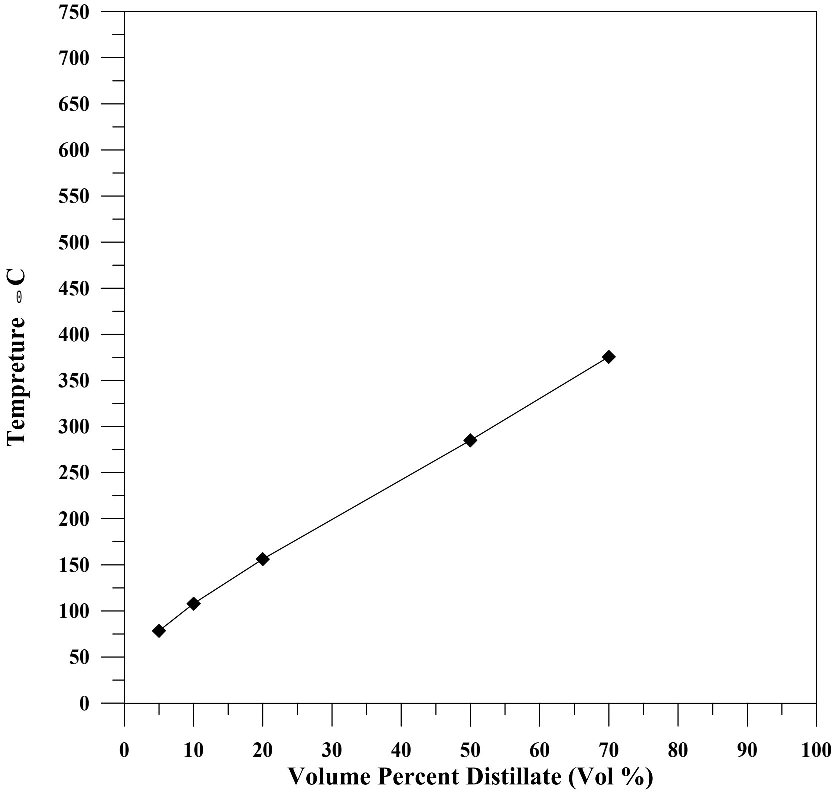

Figure 5-4 *TBP* curve for petroleum stock number 4

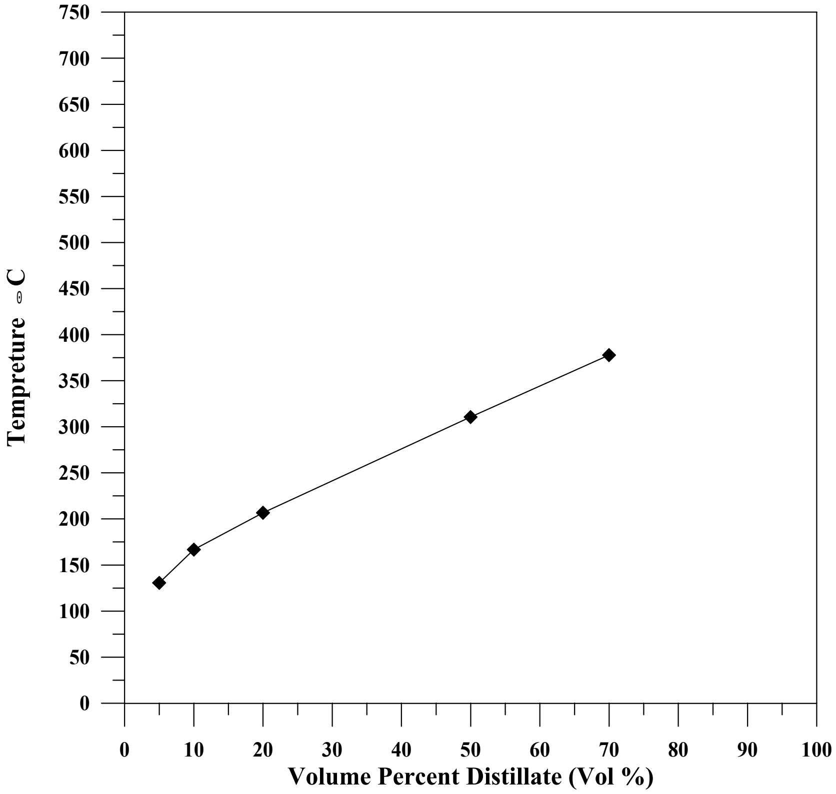

Figure 5-5 *TBP* curve for petroleum stock number 5

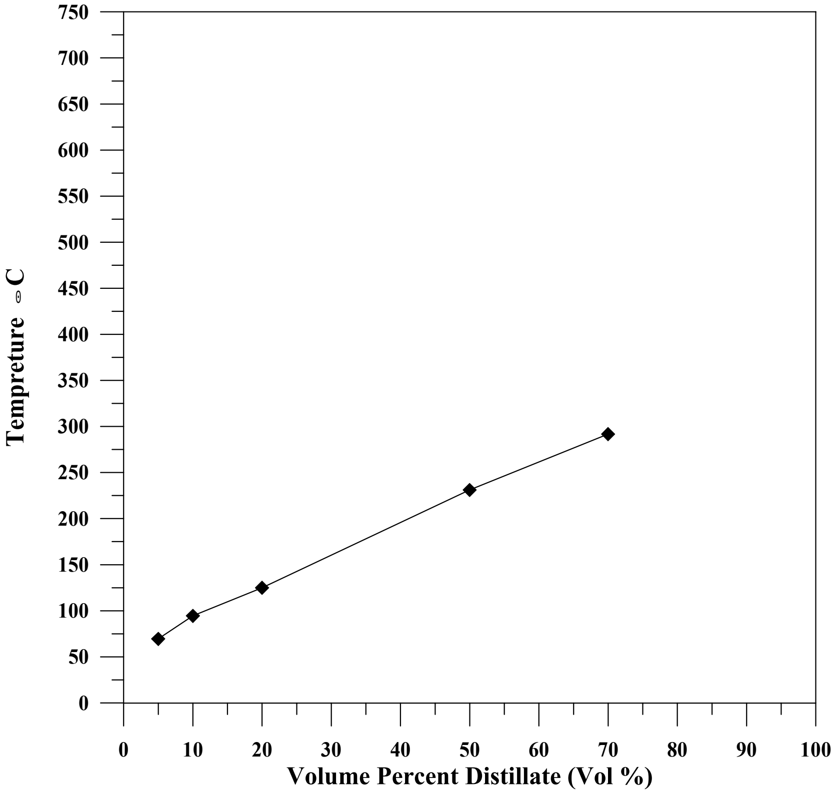

Figure 5-6 *TBP* curve for petroleum stock number 6

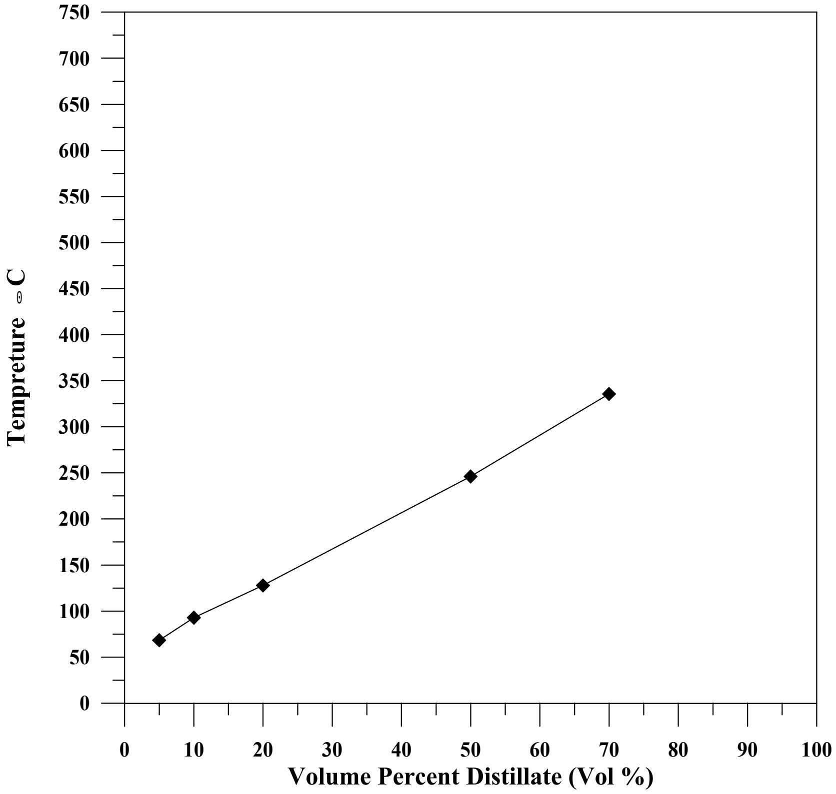

Figure 5-7 *TBP* curve for petroleum stock number 7

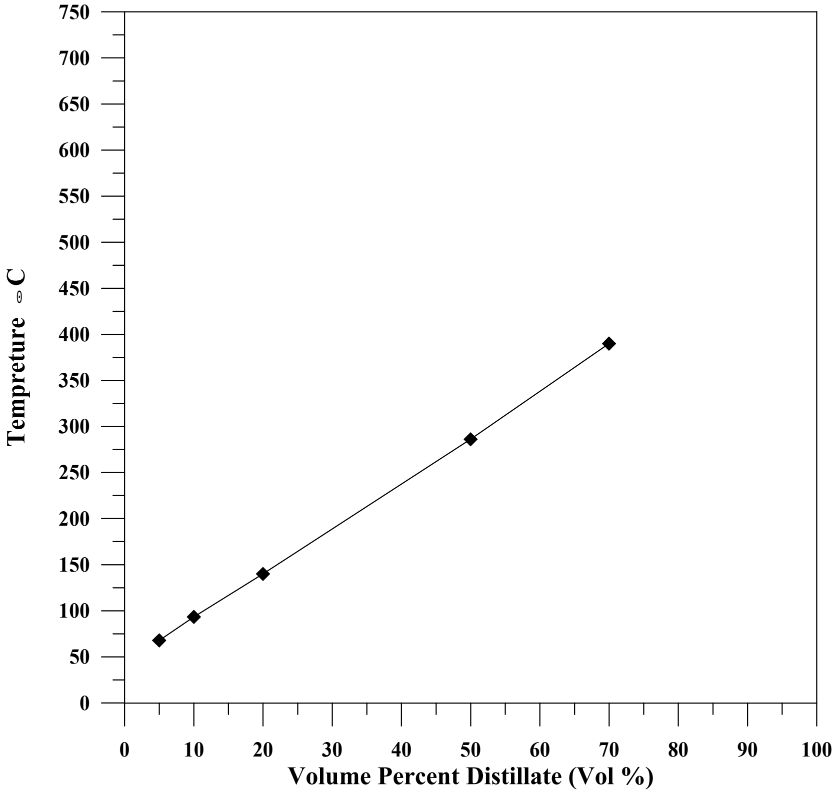

Figure 5-8 *TBP* curve for petroleum stock number 8

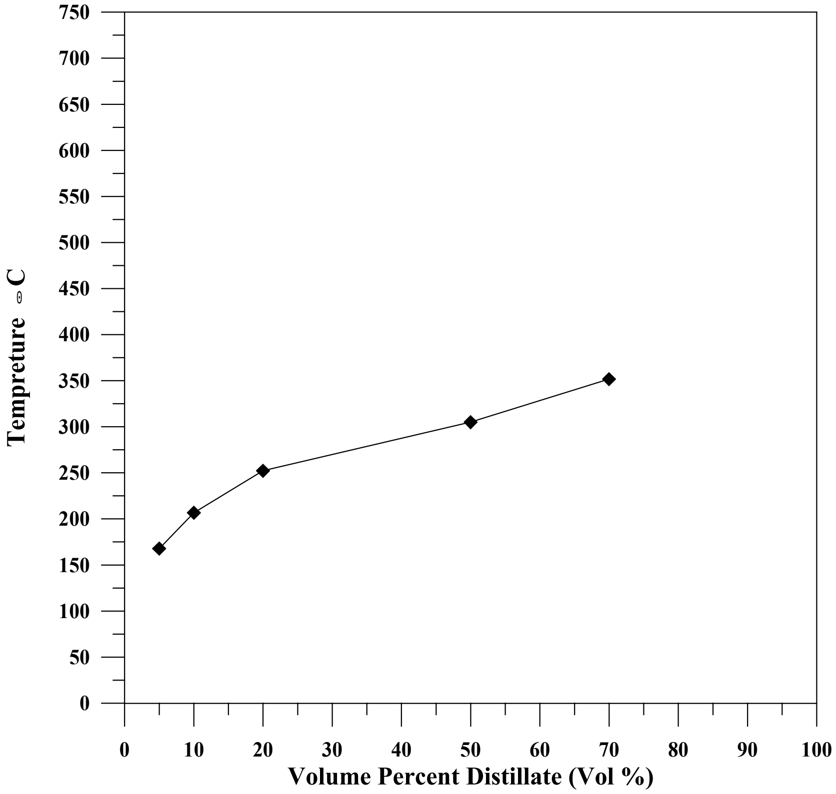

Figure 5-9 *TBP* curve for petroleum stock number 9

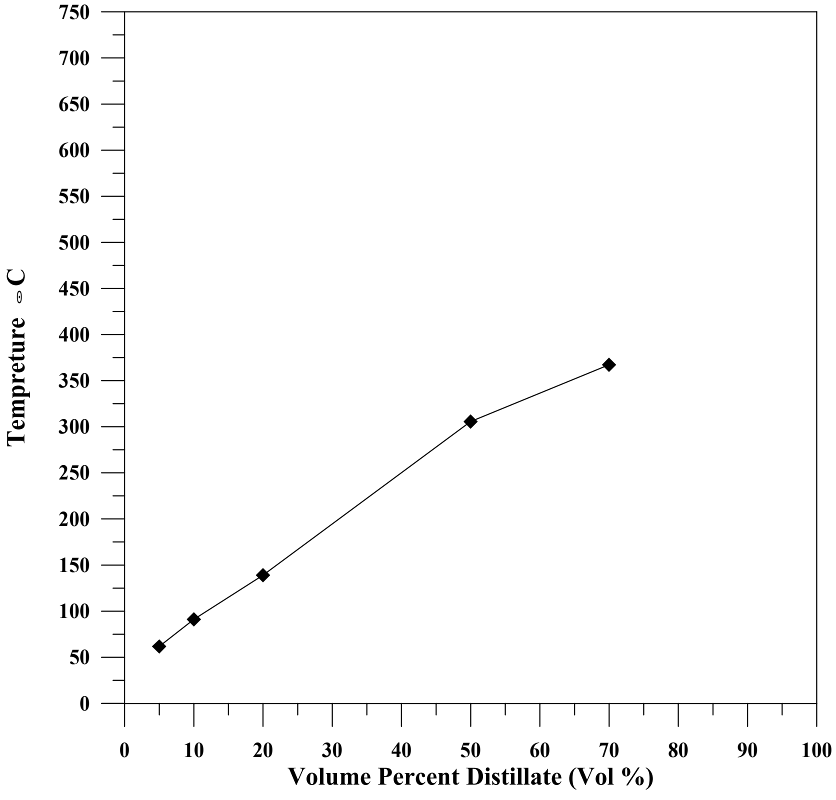

Figure 5-10 *TBP* curve for petroleum stock number 10

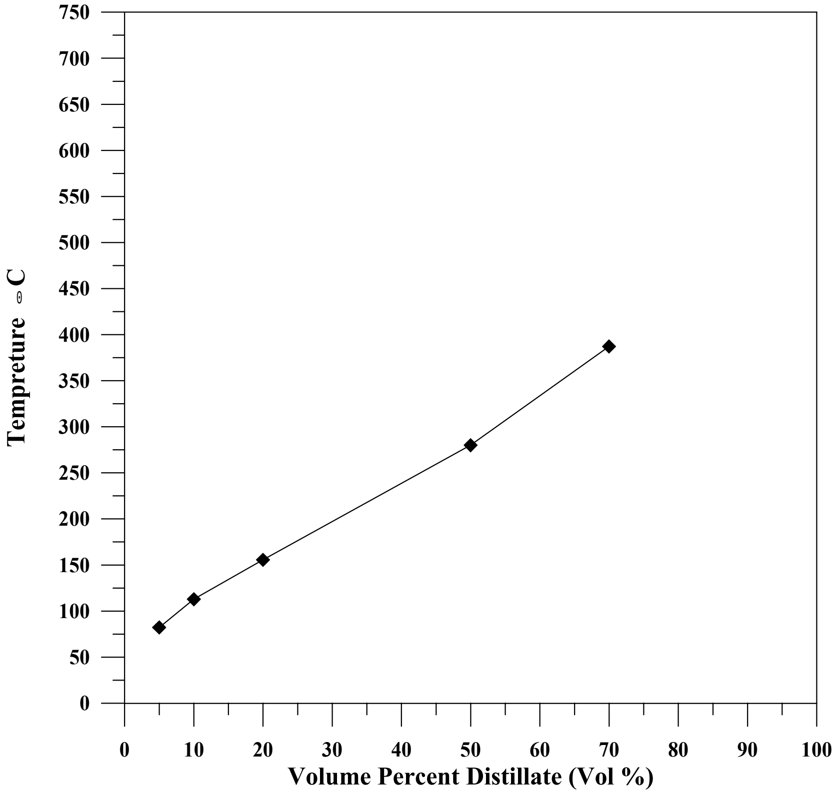

Figure 5-11 *TBP* curve for petroleum stock number 11

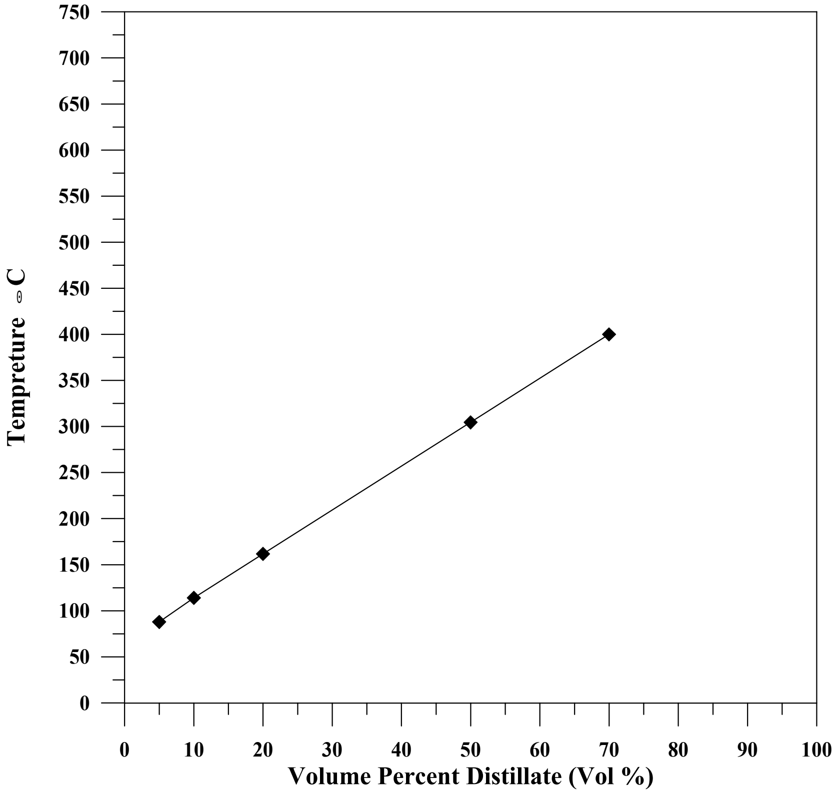

Figure 5-12 *TBP* curve for petroleum stock number 12

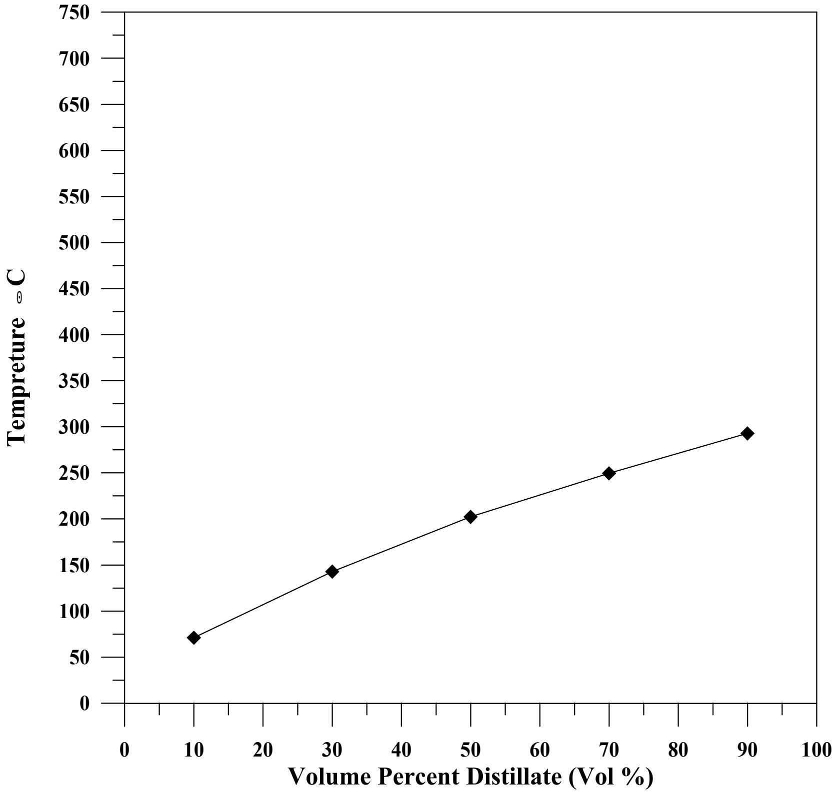

Figure 5-13 *TBP* curve for petroleum stock number 13

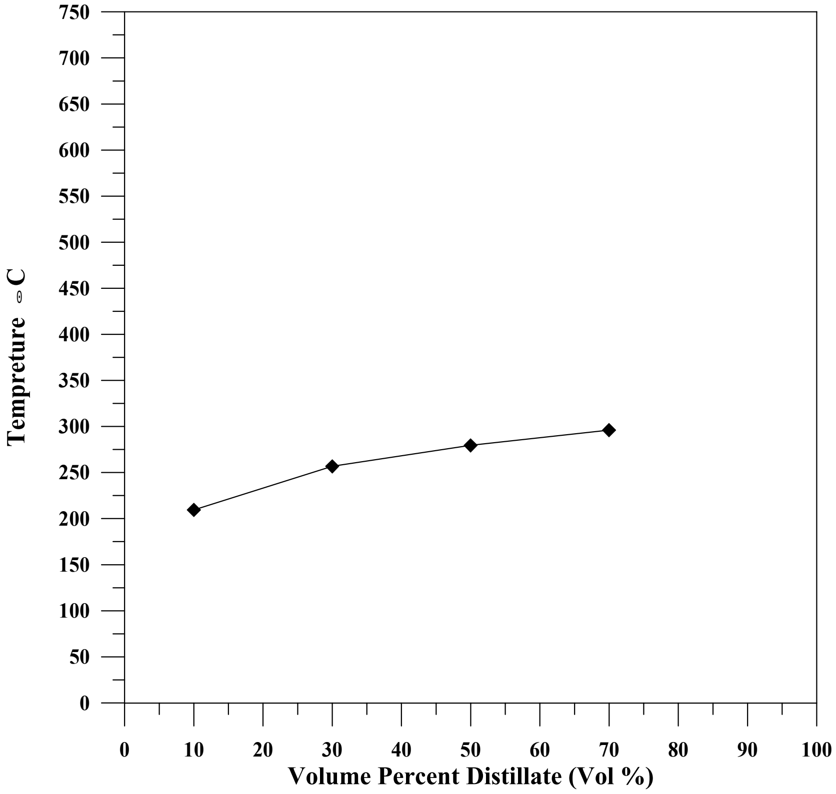

Figure 5-14 *TBP* curve for petroleum stock number 14

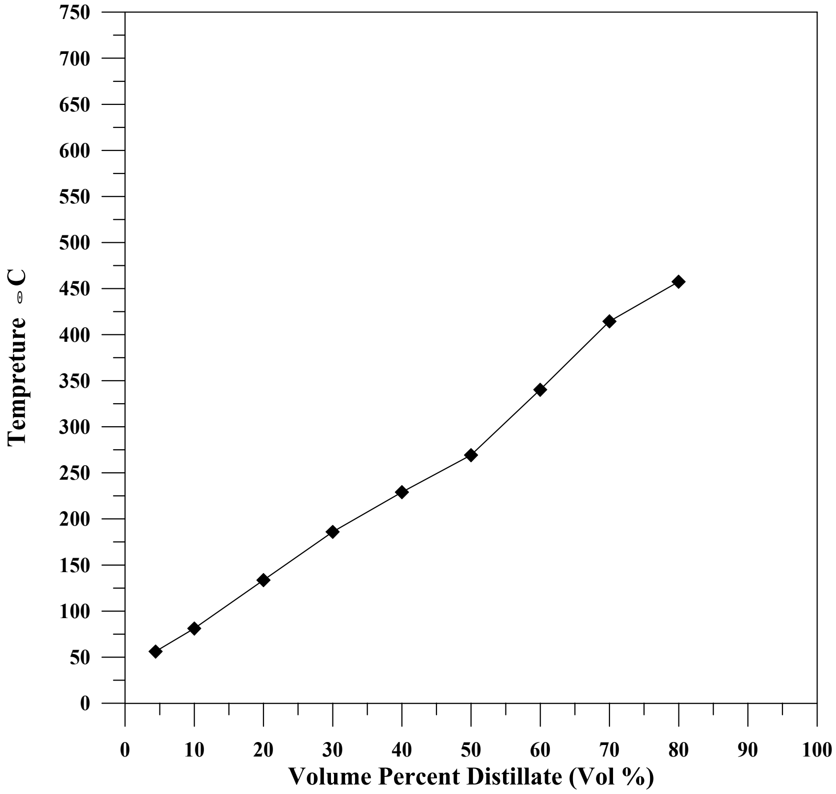

Figure 5-15 *TBP* curve for petroleum stock number 15

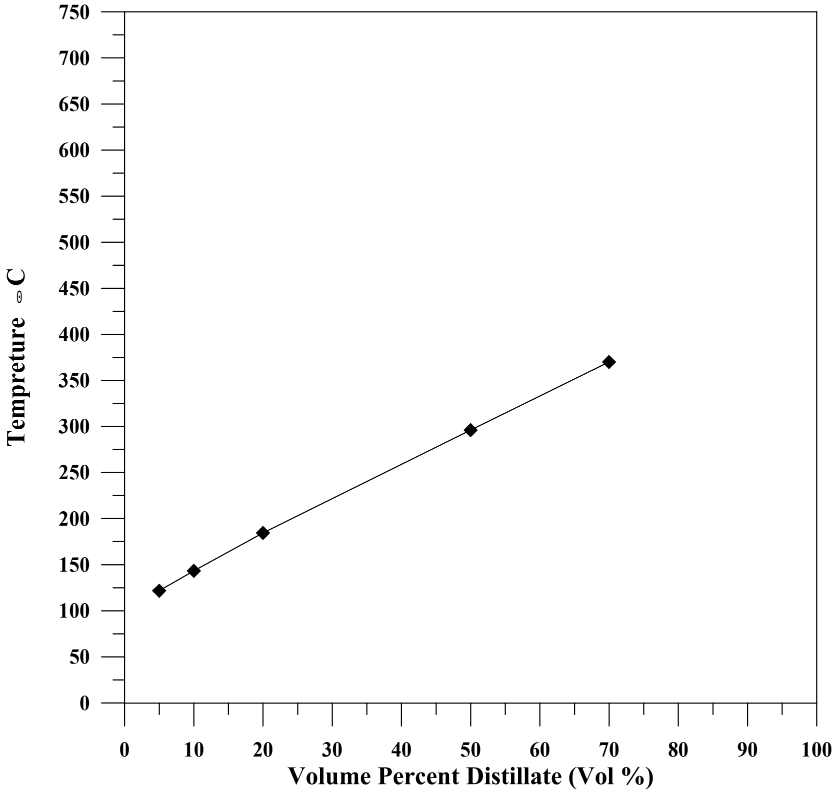

Figure 5-16 *EFV* curve for petroleum stock number 1

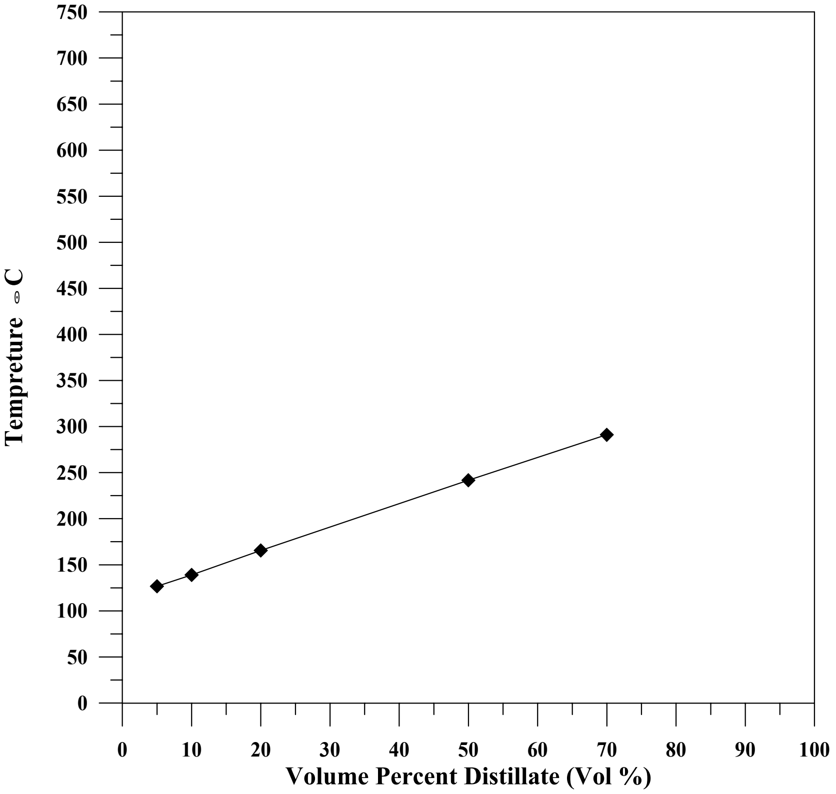

Figure 5-17 *EFV* curve for petroleum stock number 2

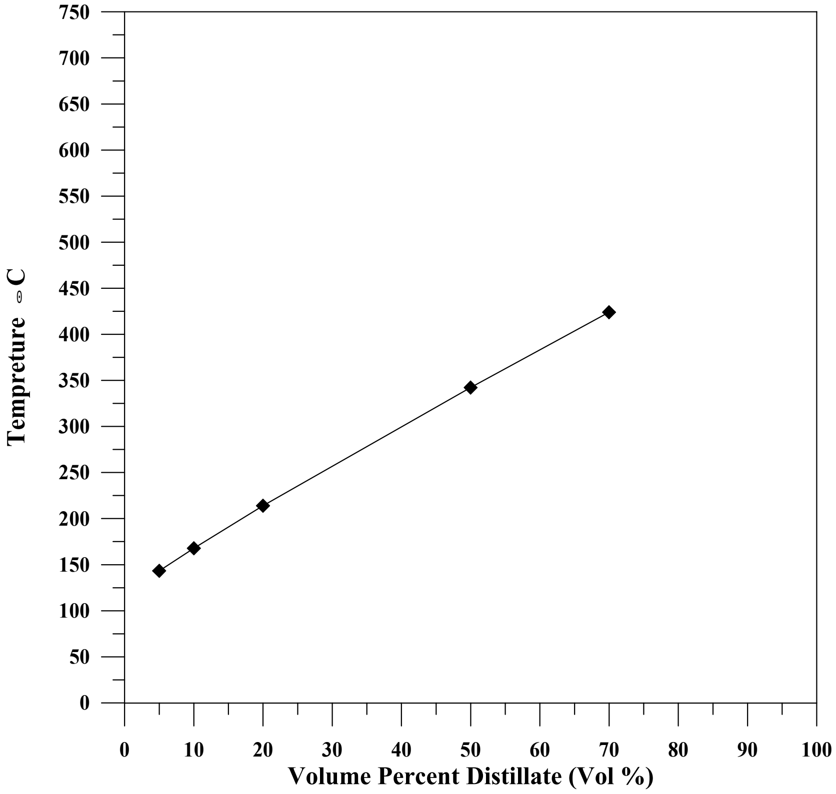

Figure 5-18 *EFV* curve for petroleum stock number 3

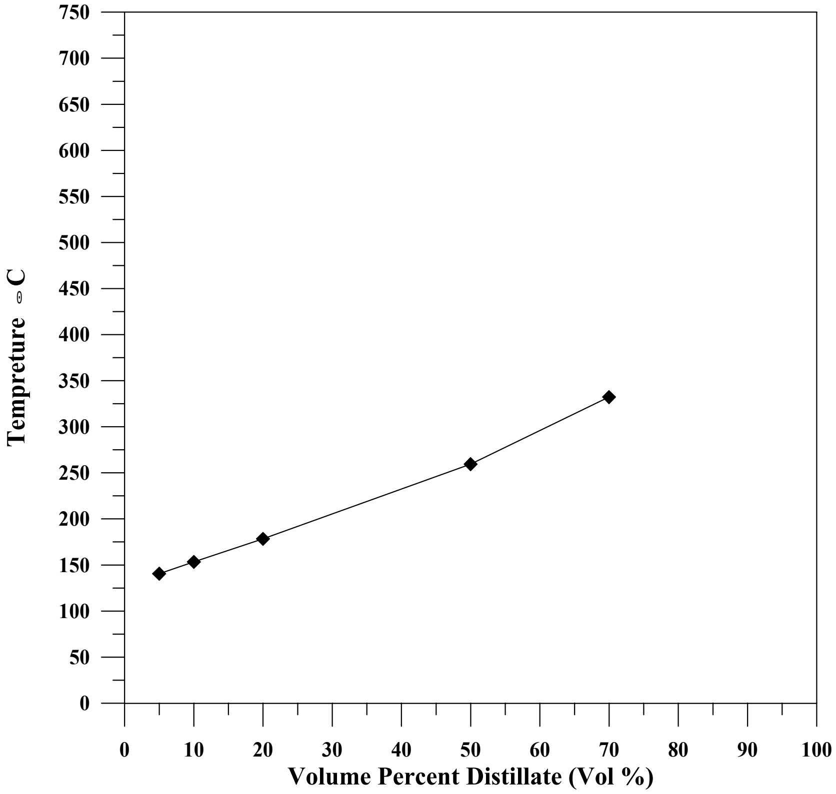

Figure 5-19 *EFV* curve for petroleum stock number 4

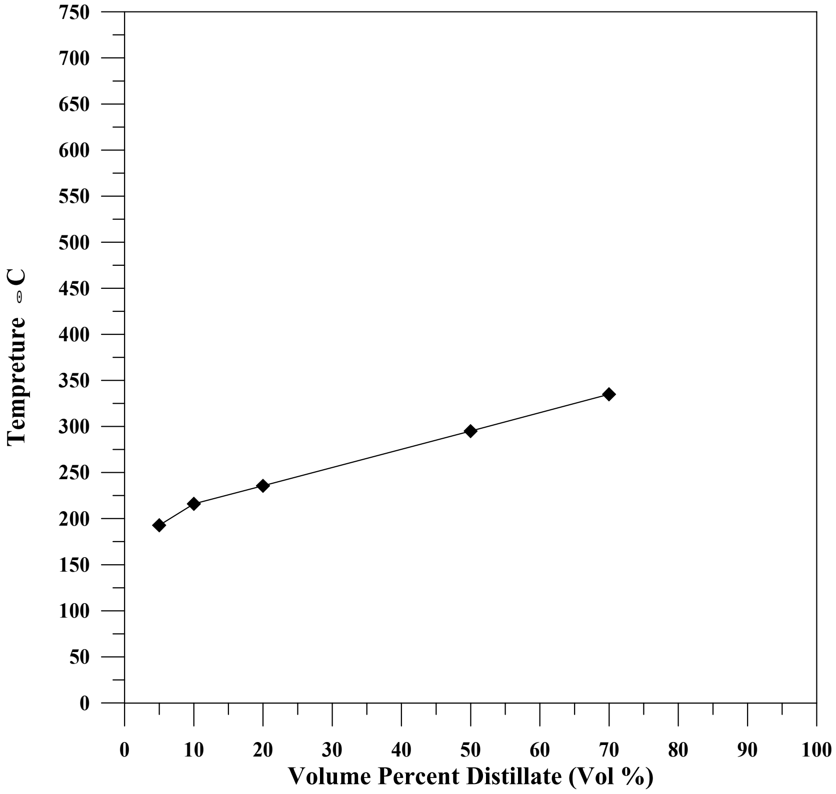

Figure 5-20 *EFV* curve for petroleum stock number 5

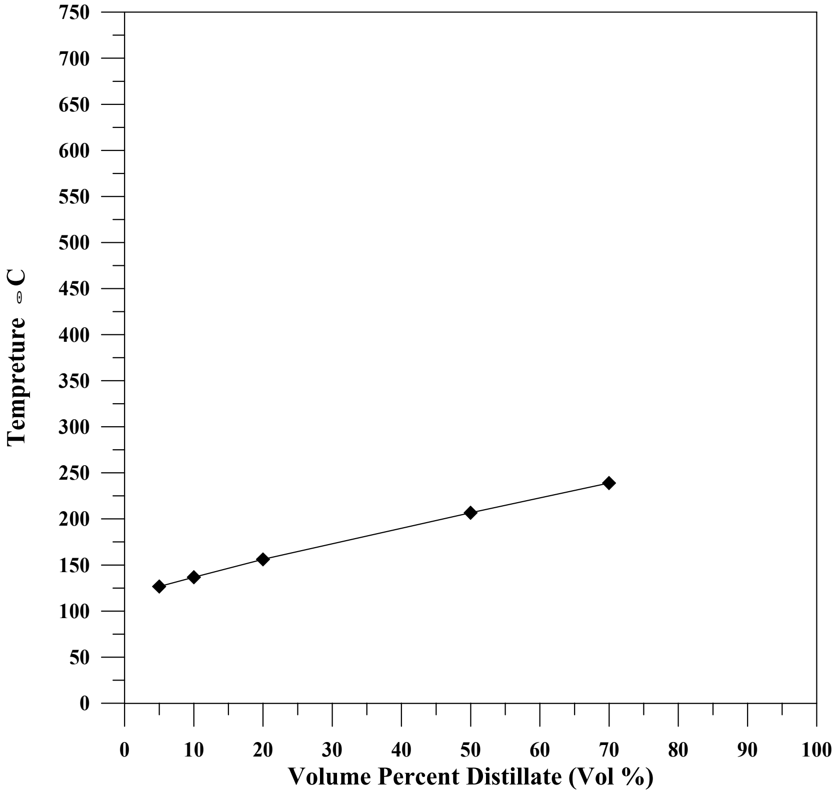

Figure 5-21 *EFV* curve for petroleum stock number 6

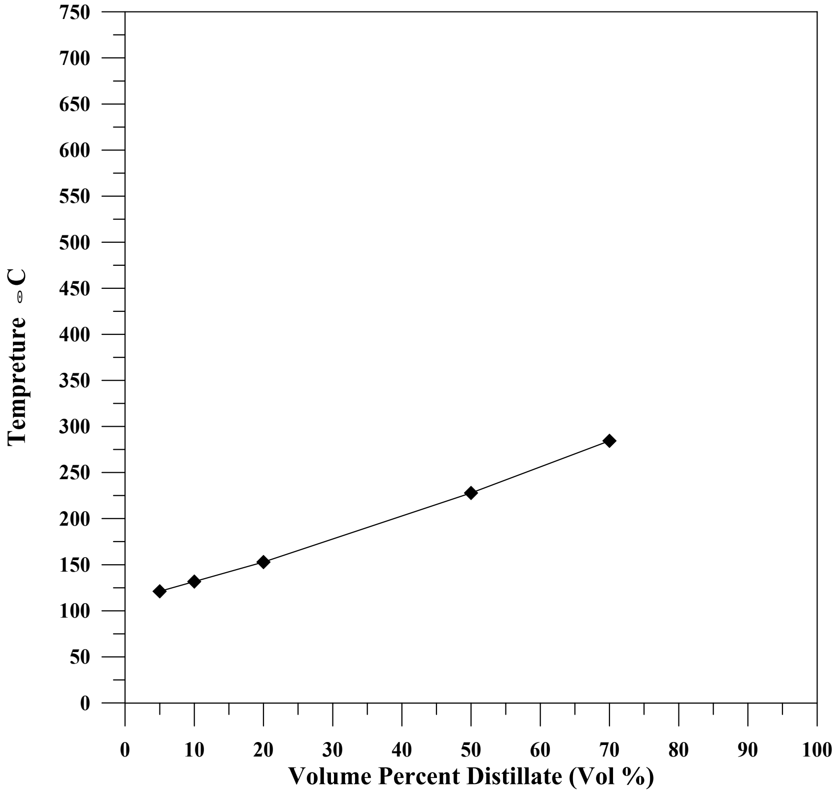

Figure 5-22 *EFV* curve for petroleum stock number 7

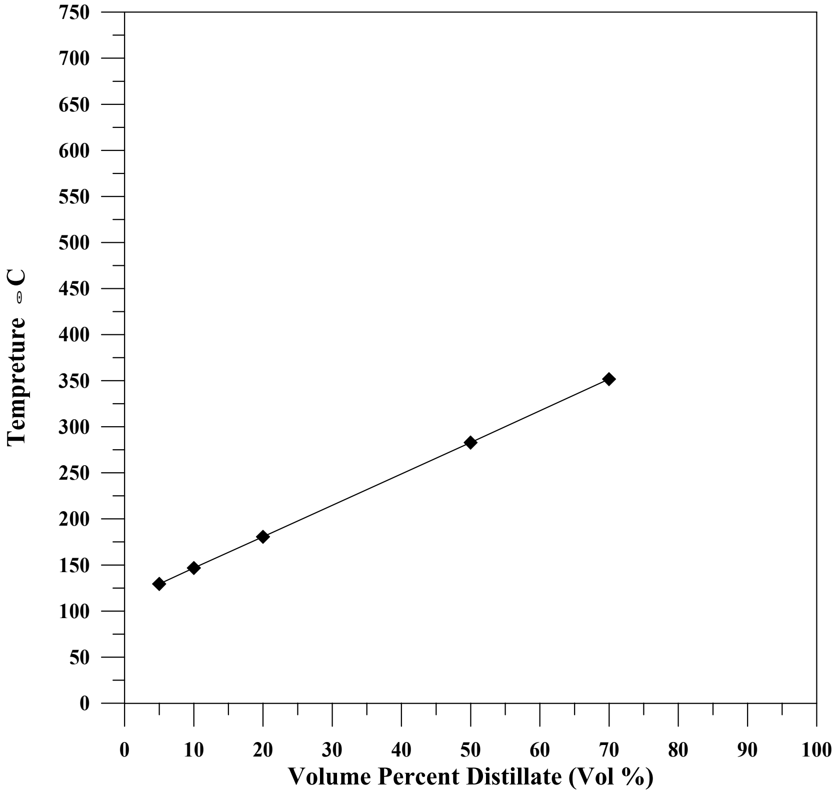

Figure 5-23 *EFV* curve for petroleum stock number 8

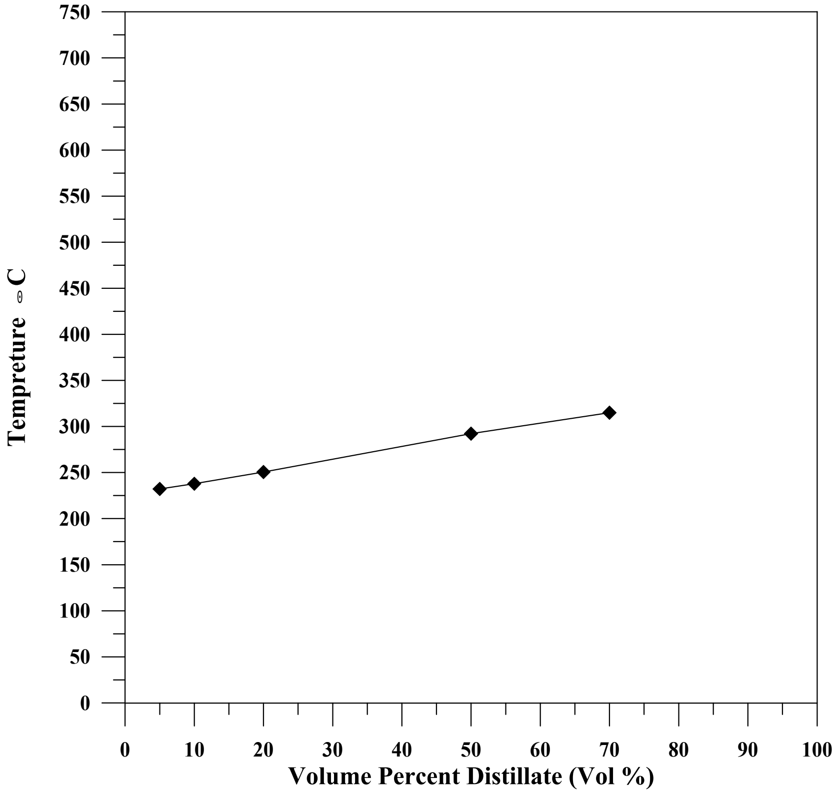

Figure 5-24 *EFV* curve for petroleum stock number 9

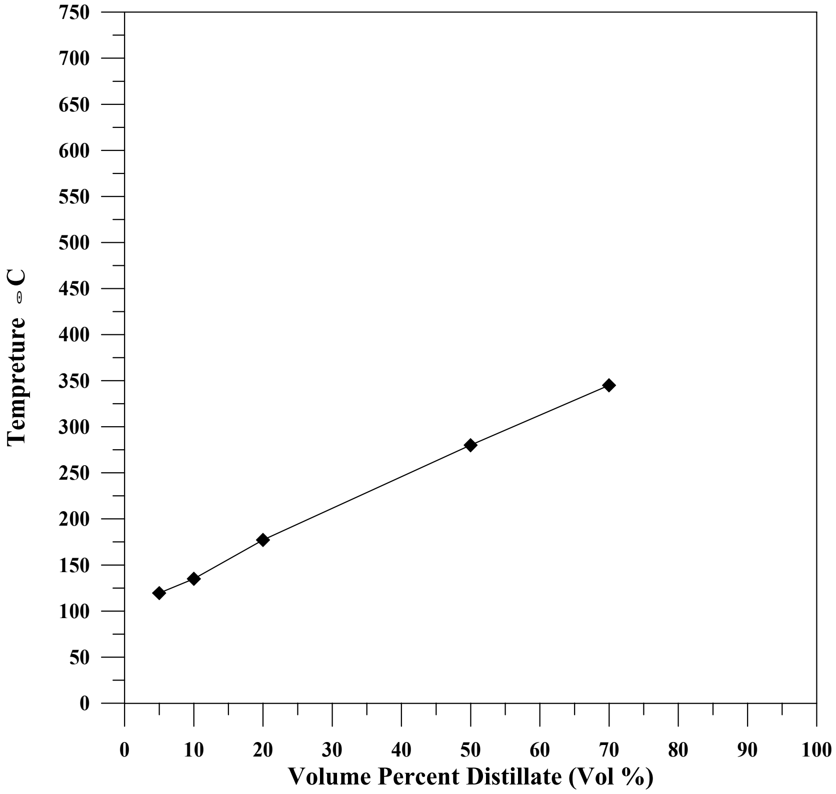

Figure 5-25 *EFV* curve for petroleum stock number 10

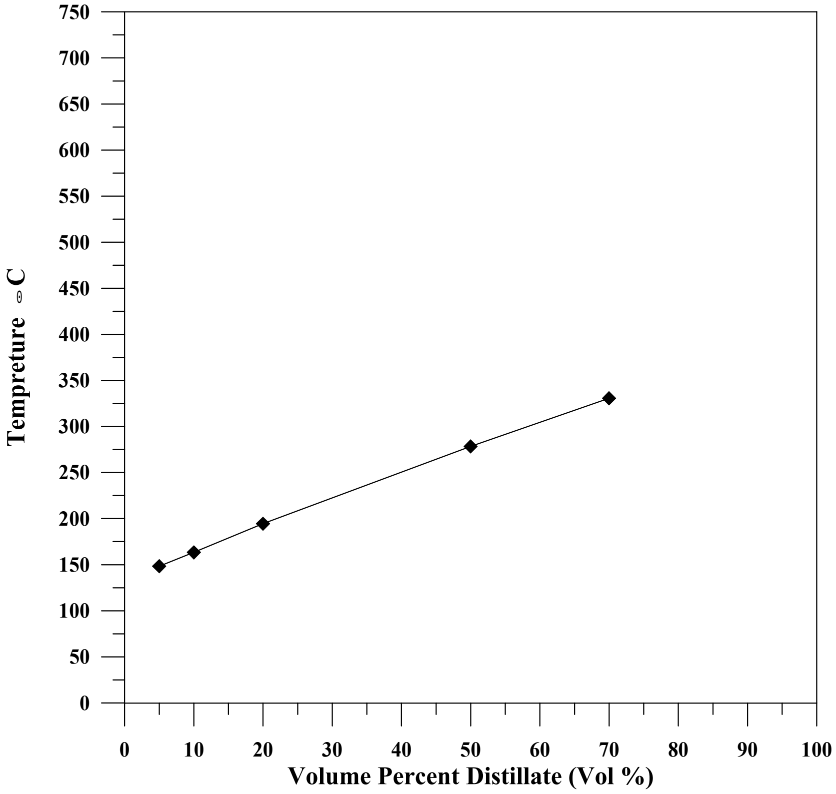

Figure 5-26 *EFV* curve for petroleum stock number 11

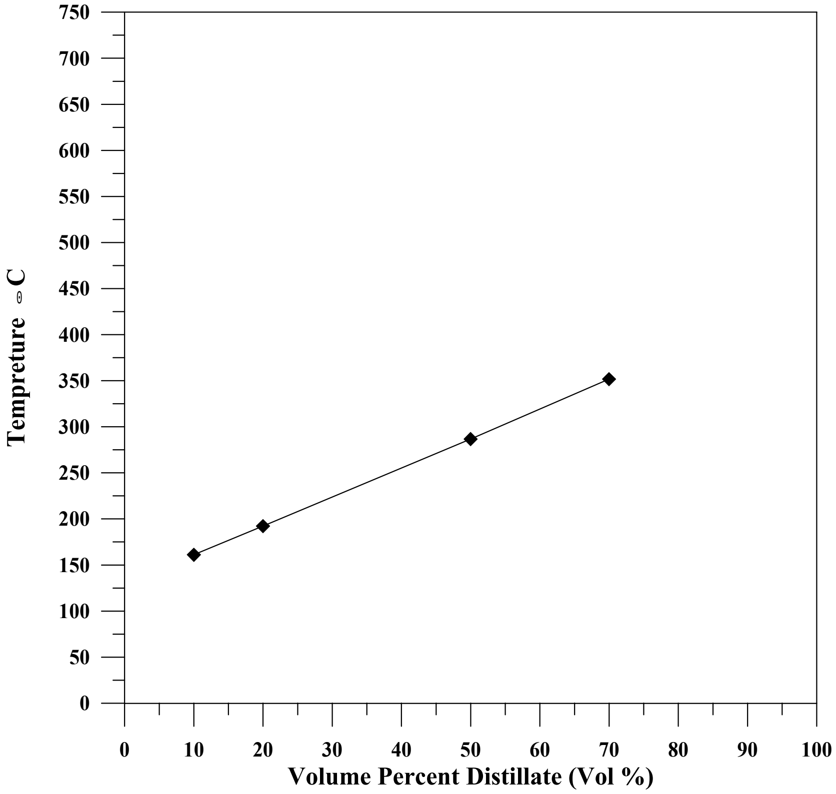

Figure 5-27 *EFV* curve for petroleum stock number 12

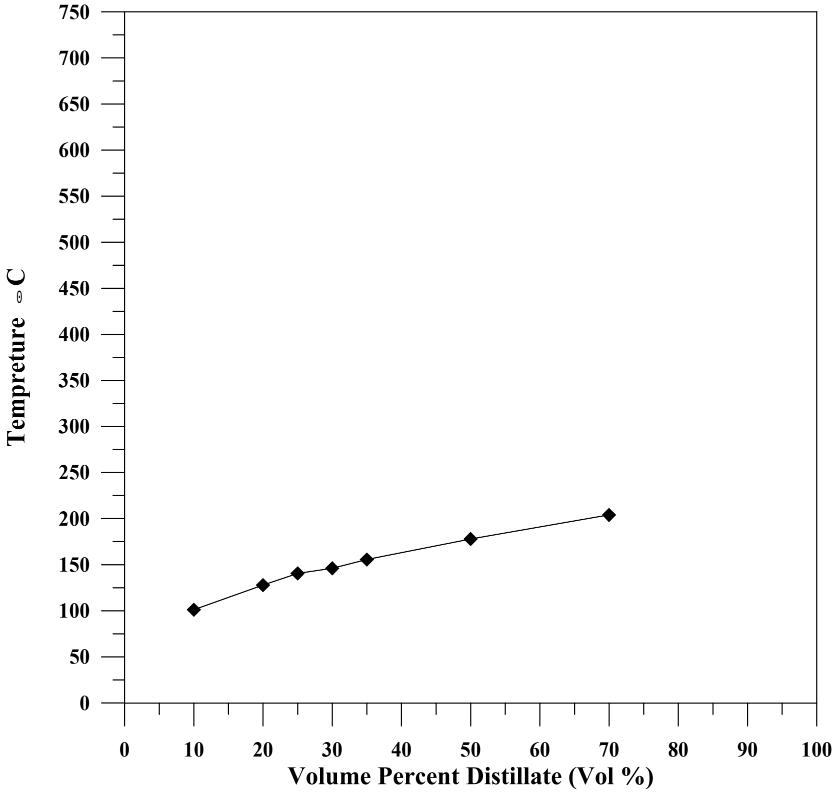

Figure 5-28 *EFV* curve for petroleum stock number 13

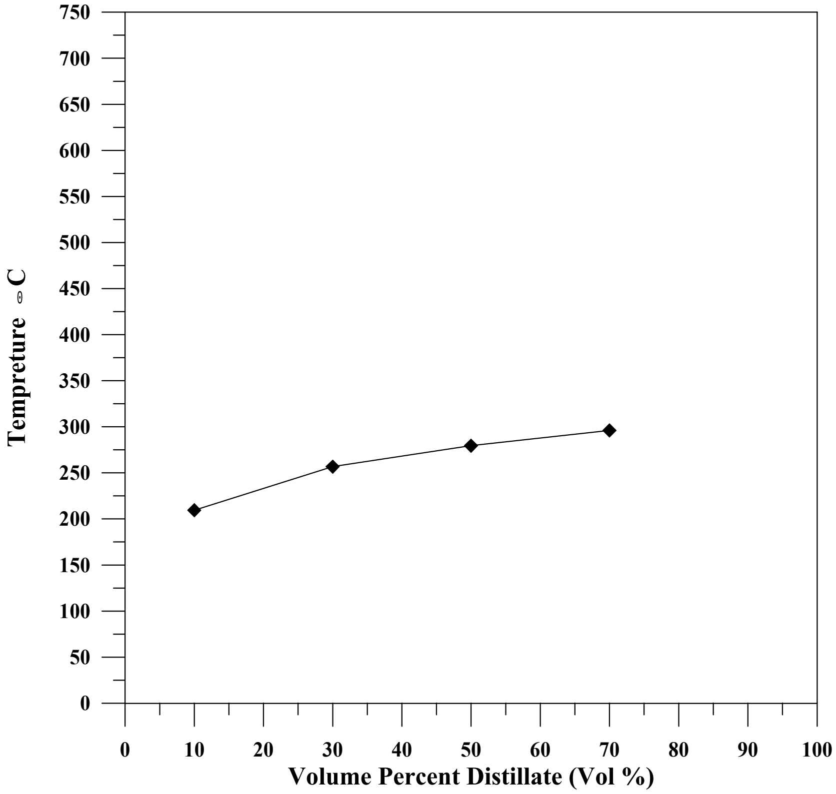

Figure 5-29 *EFV* curve for petroleum stock number 14

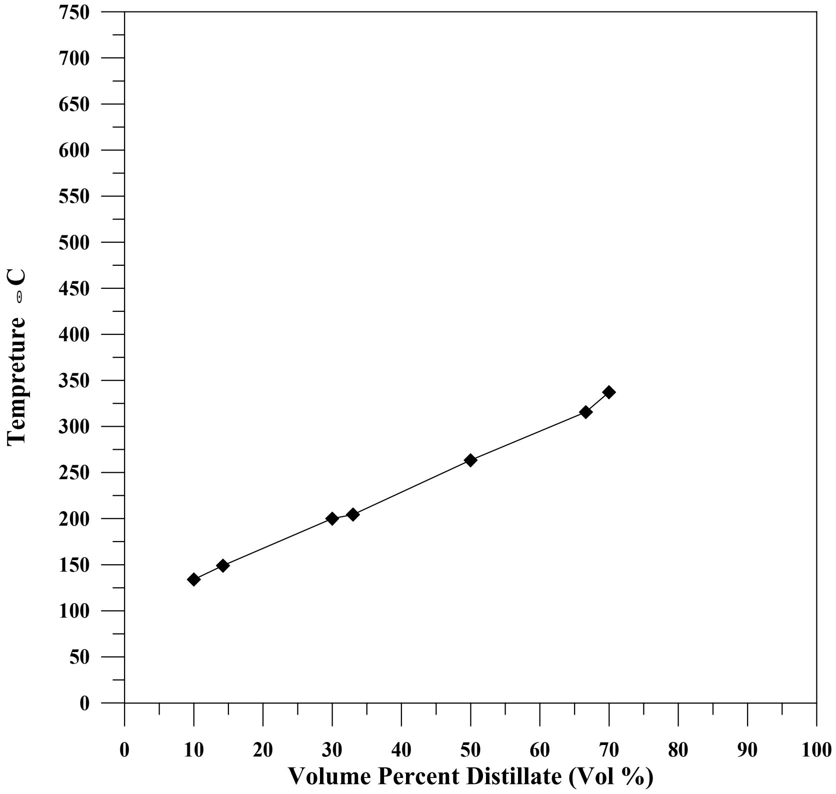

Figure 5-30 *EFV* curve for petroleum stock number 15

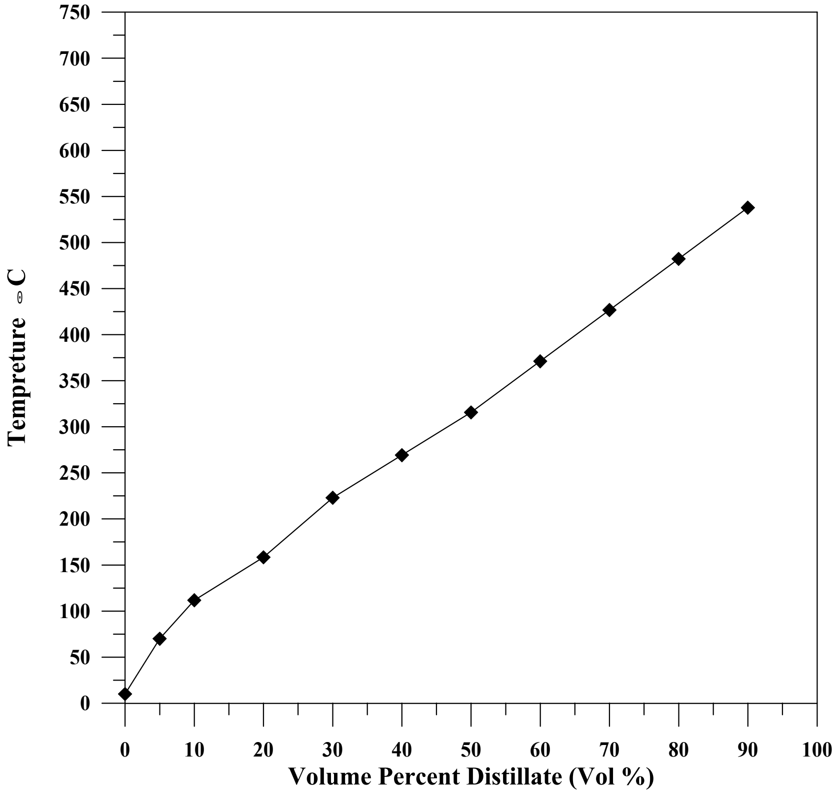

Figure 5-31 *TBP* curve for petroleum stock number 16

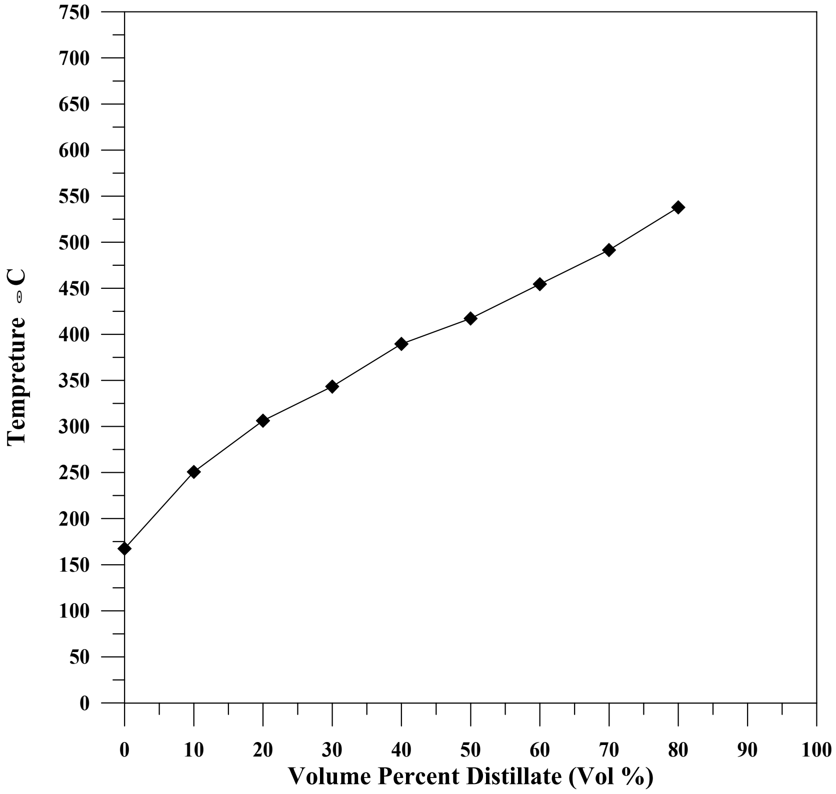

Figure 5-32 *TBP* curve for petroleum stock number 17

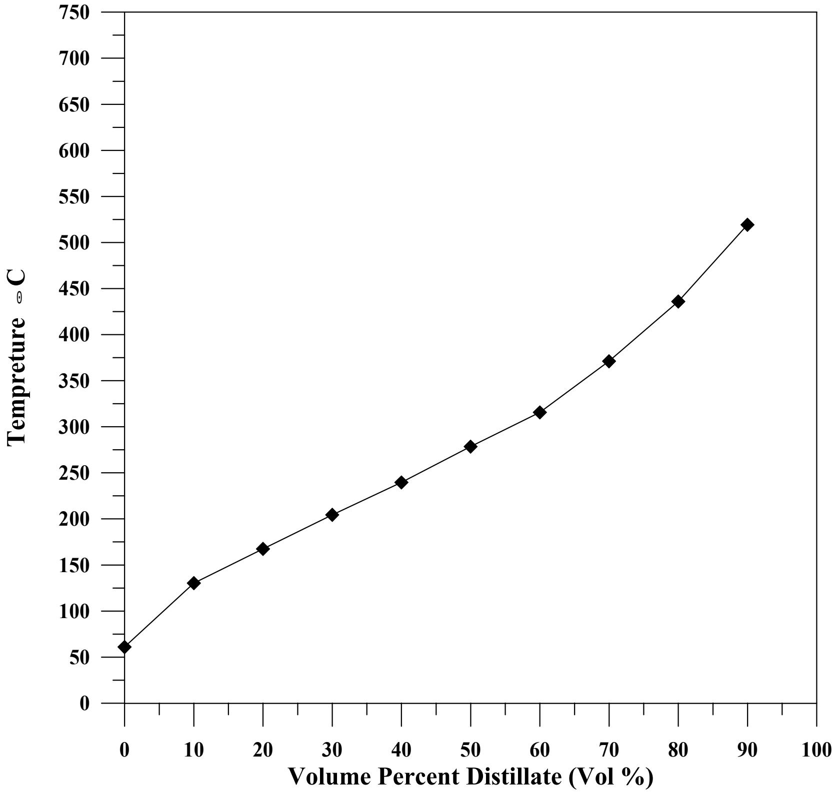

Figure 5-33 *TBP* curve for petroleum stock number 18

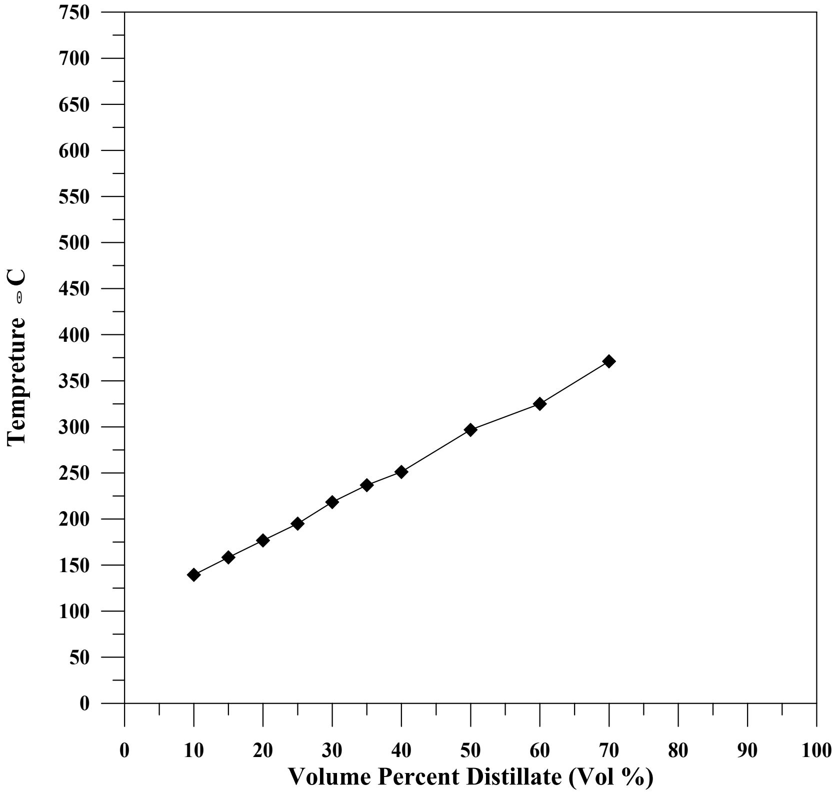

Figure 5-34 *EFV* curve for petroleum stock number 16

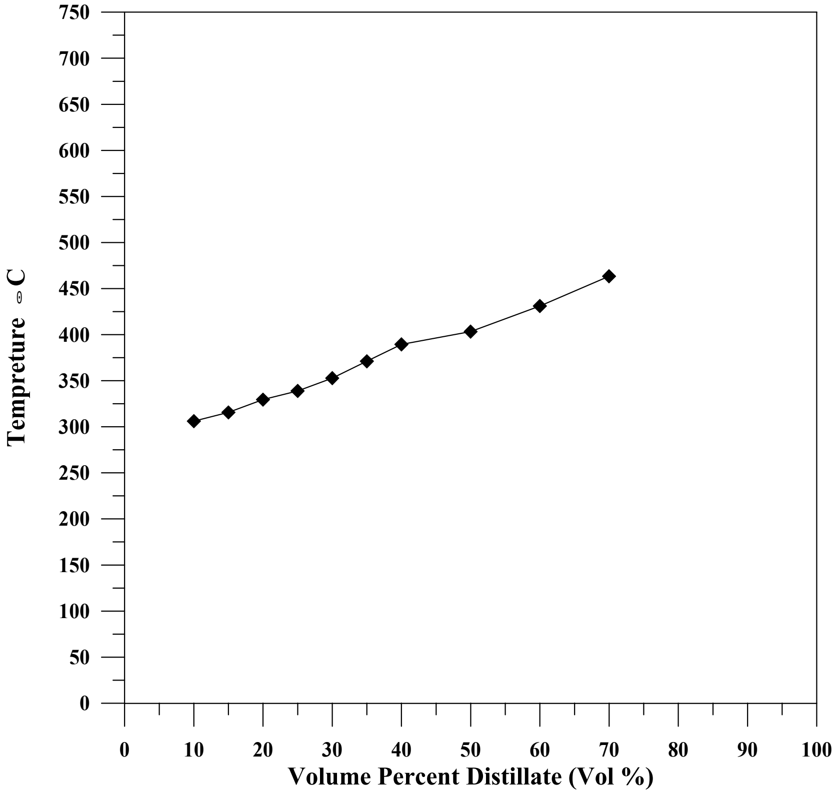

Figure 5-35 *EFV* curve for petroleum stock number 17

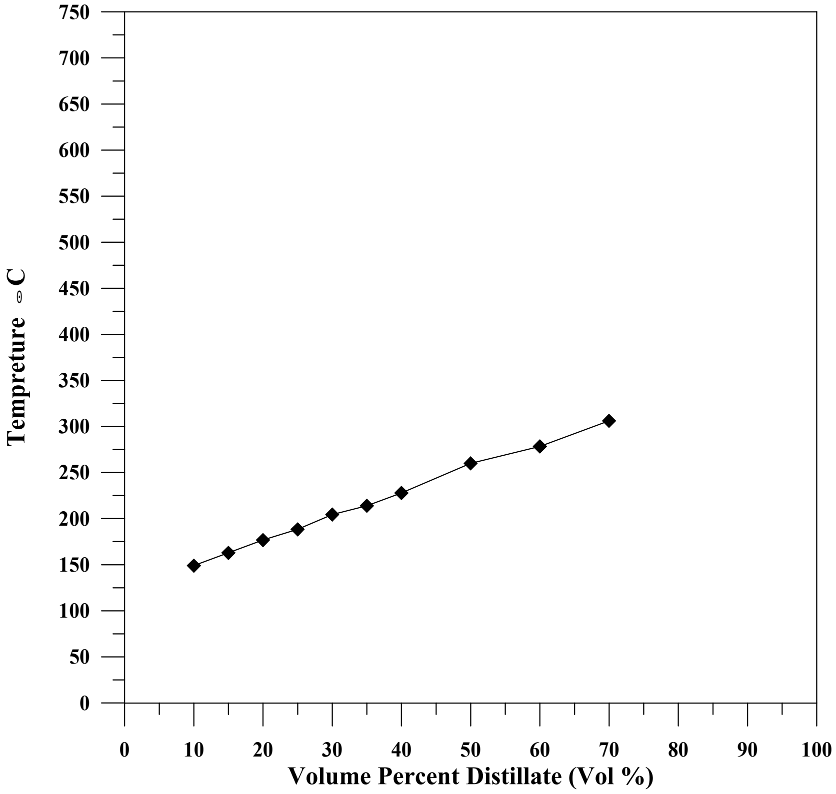

Figure 5-36 *EFV* curve for petroleum stock number 18

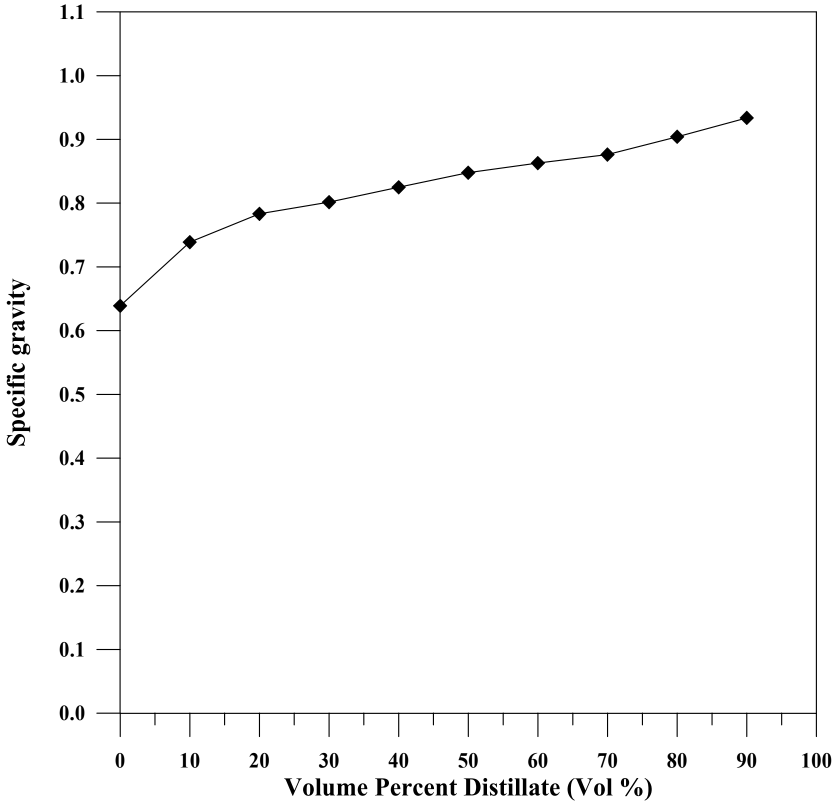

Figure 5-37 *Sp.gr* curve for petroleum stock number 16

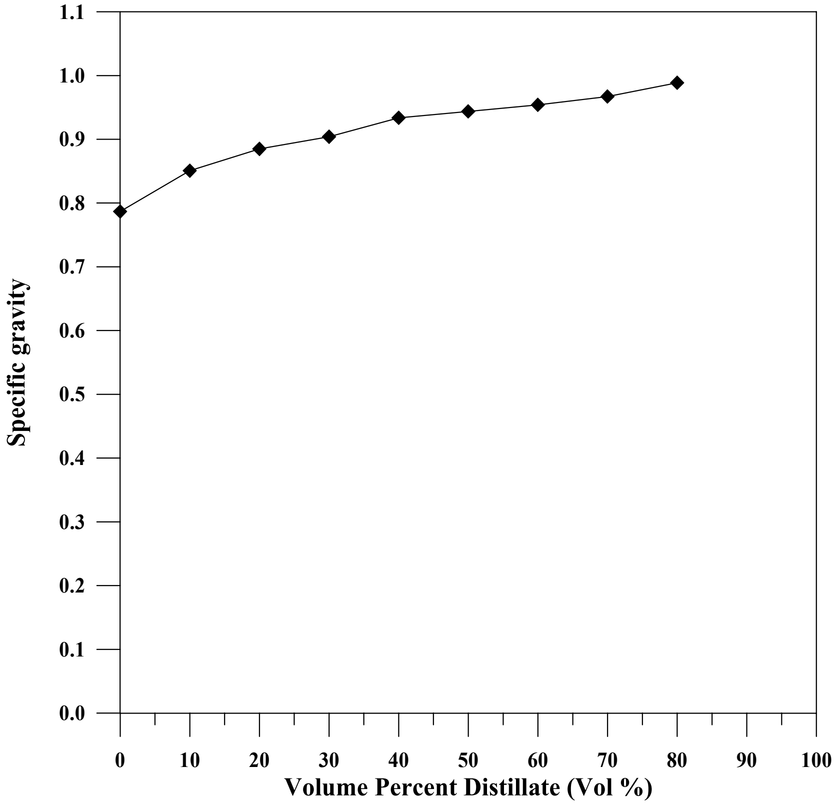

Figure 5-38 *Sp.gr* curve for petroleum stock number 17

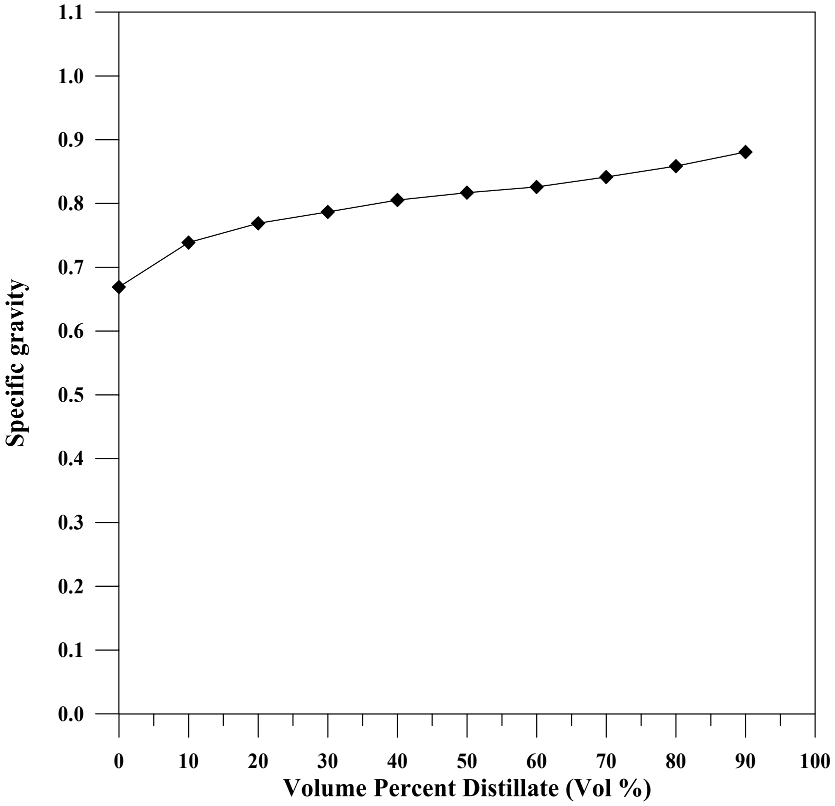

Figure 5-39 *Sp.gr* curve for petroleum stock number 18

5.1.2 Data sources for part two (application part)

The data for part two of the present work (application part) which includes the *TBP* and specific gravity curves for four types of Iraqi crude oils, Kirkuk, Basrah, Jambur and Bai – Hassan crude oils. Kirkuk, Basrah and Bai – Hassan crude oils were distilled into narrow fractions using laboratory distillation unit (as discussed in Chapter 4). Tables E-1, E-2, E-3 and E-4 in Appendix E show the material balance of Kirkuk, Basrah, Jambur and Bai – Hassan crude oils distillation, respectively. Figs. 5-40, 5-41, 5-42 and 5-43 show the true boiling point (*TBP*) curves of Kirkuk, Basrah, Jambur and Bai – Hassan crude oils, respectively.

Figures 5-44, 5-45, 5-46 and 5-47 show the specific gravity curves for Kirkuk, Basrah, Jambur and Bai – Hassan crude oils, respectively, while Tables E-5, E-6, E-7 and E-8 in Appendix E show the specific gravity of narrow fractions distilled from these crude oils.

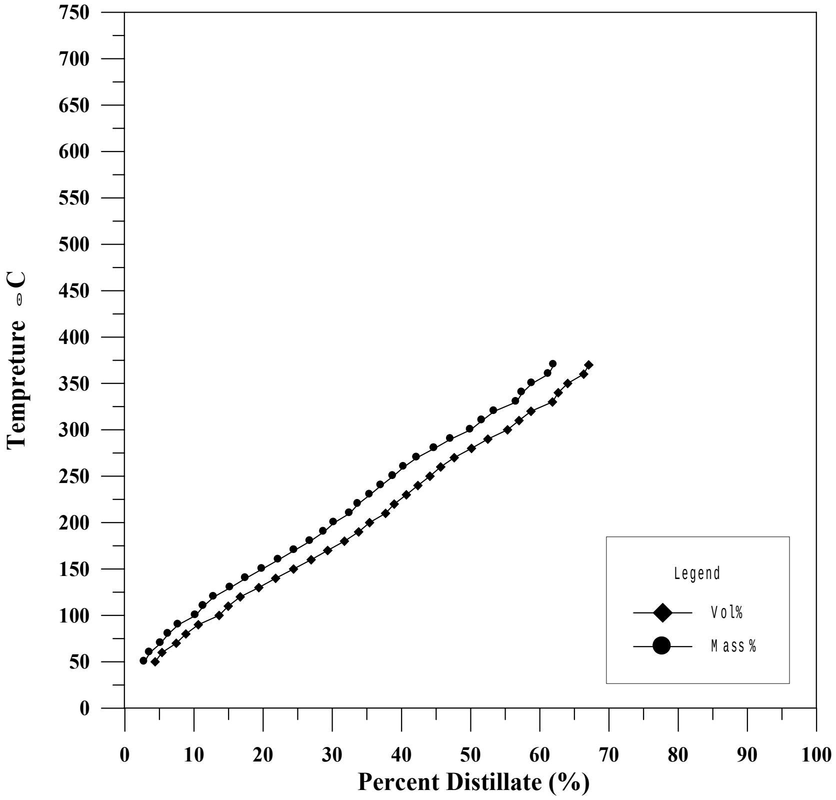

Figure 5-40 *TBP* curve for Kirkuk crude oil

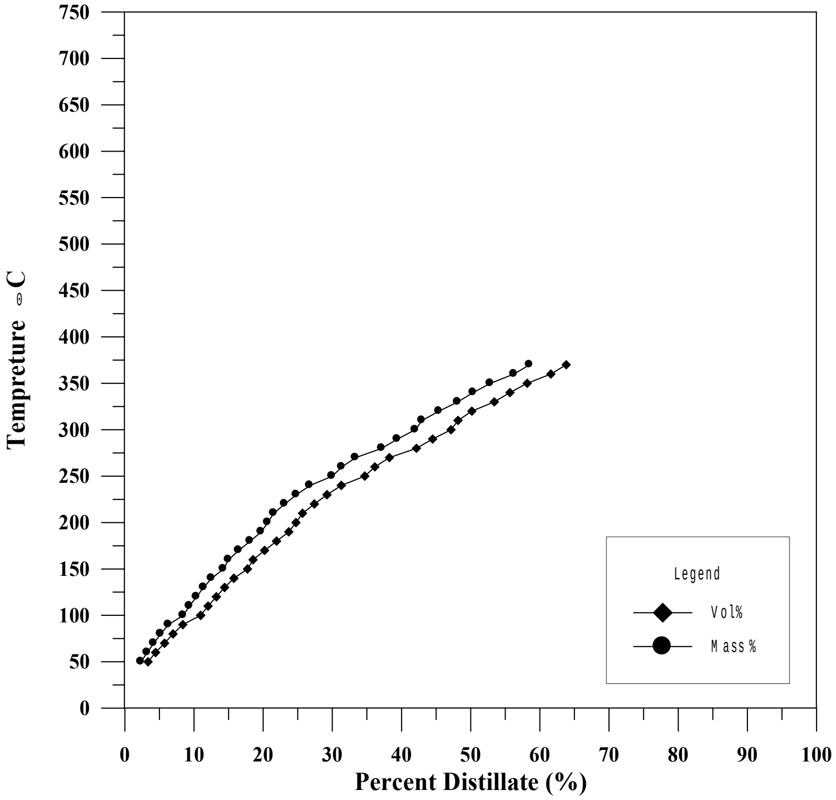

Figure 5-41 *TBP* curve for Basrah crude oil

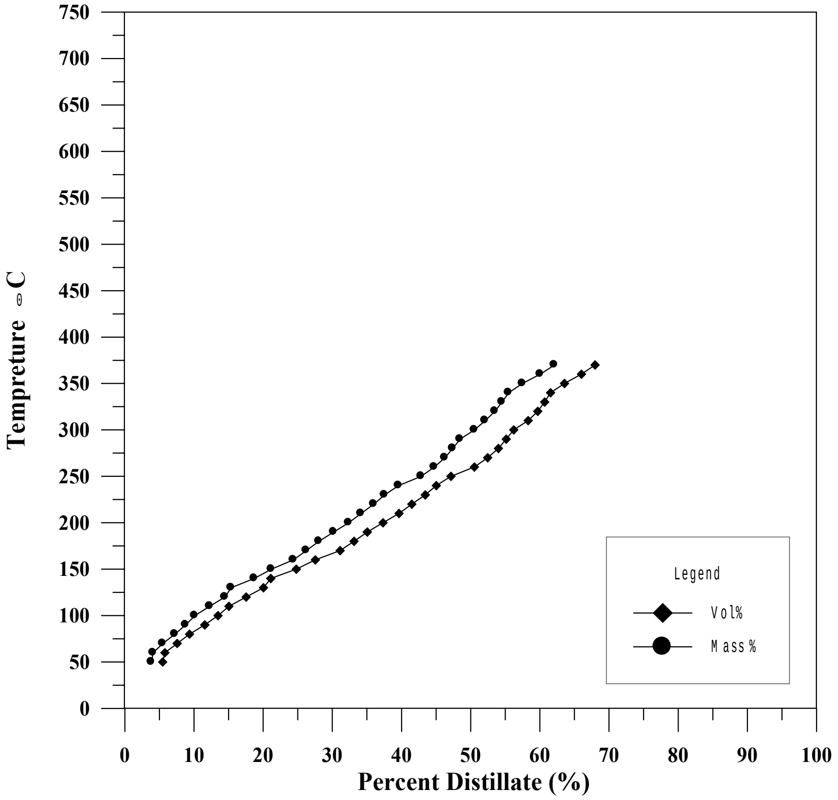

Figure 5-42 *TBP* curve for Jambur crude oil

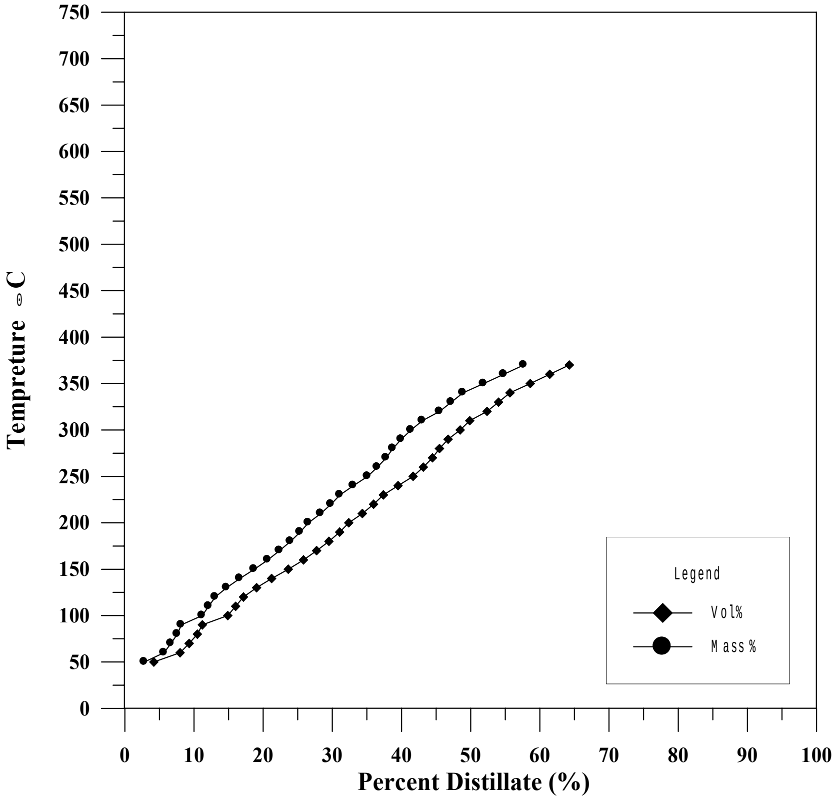

Figure 5-43 *TBP* curve for Bai-Hassan crude oil

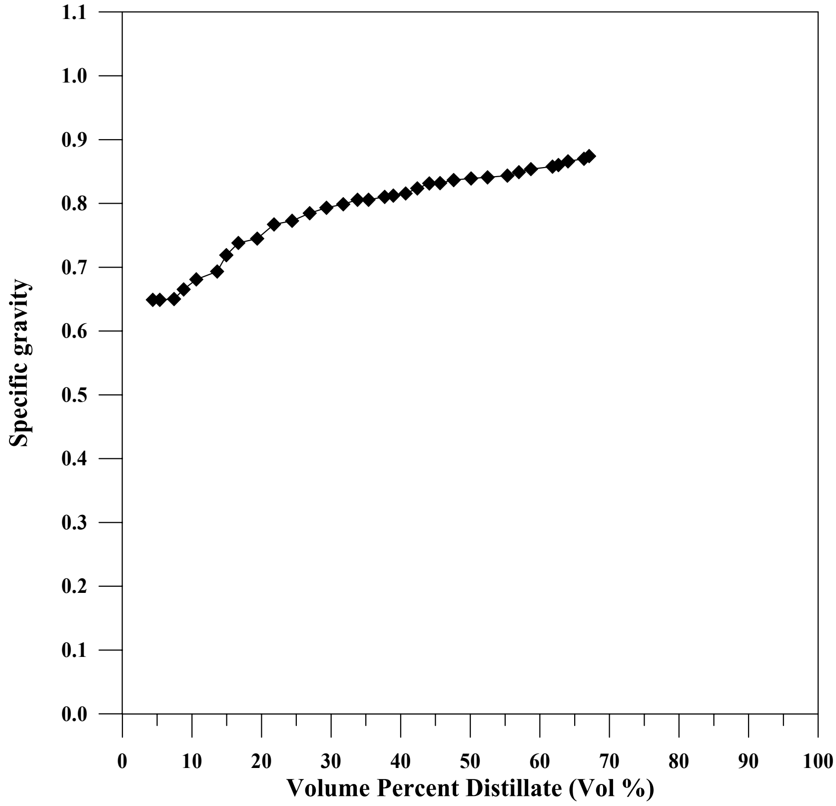

Figure 5-44 *Sp.gr* curve for Kirkuk crude oil

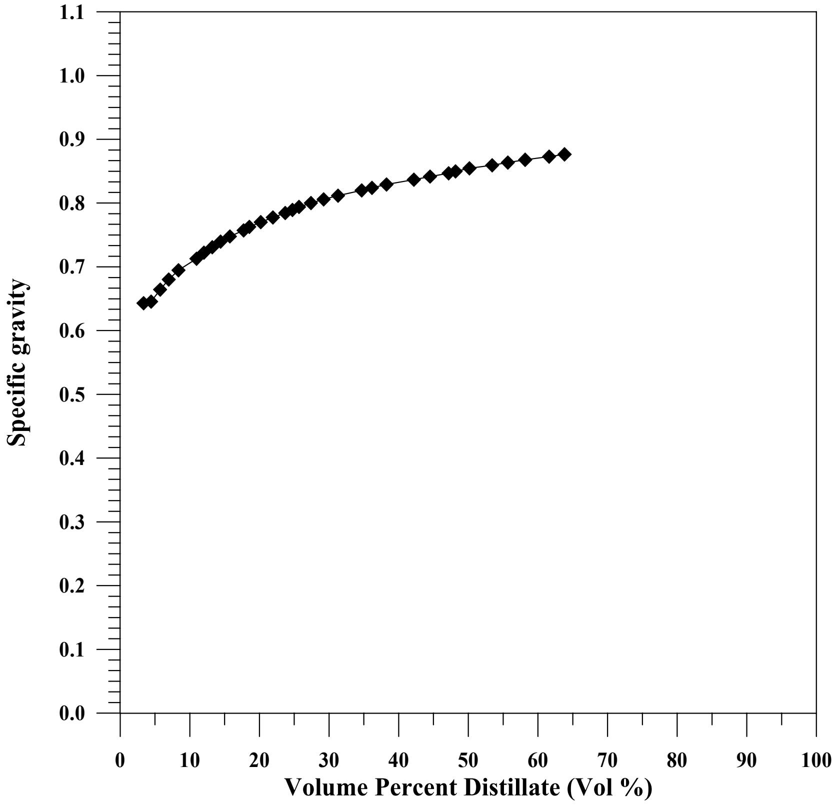

Figure 5-45 *Sp.gr* curve for Basrah crude oil

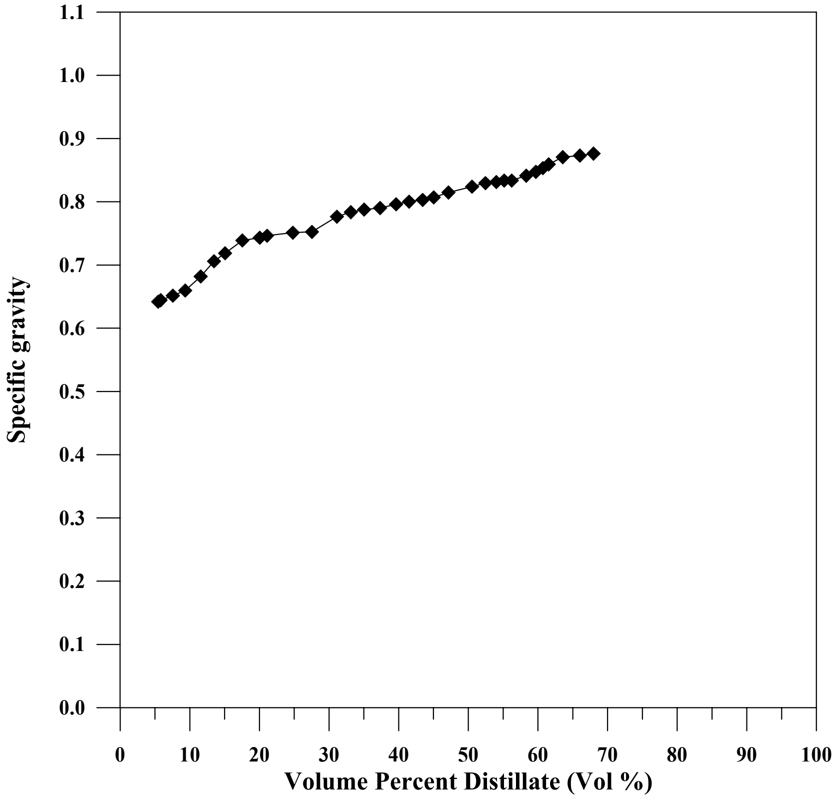

Figure 5-46 *Sp.gr* curve for Jambur crude oil

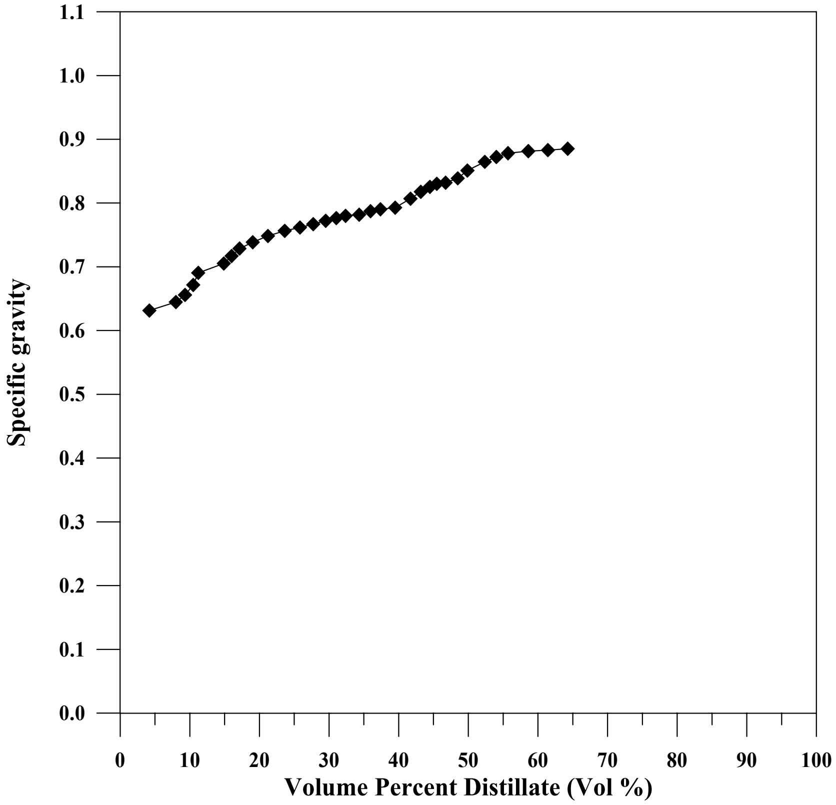

Figure 5-47 *Sp.gr* curve for Bai-Hassan crude oil

5.2 Part one: Testing and developing part

5.2.1 Calculational methods

5.2.1.1 Estimation the *TBP* and specific gravity curves

For the given data for part one and part two, both the *TBP* curves and *Sp.gr* curves (if available) are not covered the full range of the percent distilled (*i.e.* 0 to 100 vol.%). The use of graphical methods and pseudo – component methods require that both of the *TBP* and specific gravity curves must cover the full range of percent distilled. As a result, both curves must be interpolated, extrapolated and smoothed as necessary to complete the range from 0 to 100%. These full range curves will be referred to as working curves.

For *TBP* curves for the data sources for part one and part two, the following recommendations that collected from number of literatures **[6, 81, 105]** can be helpful for estimation the working curves of *TBP* curves.

♦ The initial boiling point (*IBP*) of *TBP* curve is obtained by extrapolation of the curve to 0 vol.%. All light ends (gases) will be assumed to boiling up at the estimated *IBP*.

♦ The vol.% at 593 °C (1100 °F) is equal to 100 minus three time the Conrad son carbon residue (wt.%) of the petroleum stocks.

♦ The 80 vol.% true boiling point temperature (*TBP* 80%) can be estimated by using the following artificially generated data point:

$$TBP_{80\%} = 10^{(-0.2127)} \times TBP_{50\%}^{(1.103)} \times Sp.gr^{(-0.6445)} \qquad \ldots(5.1)$$

Where *TBP* 80%, *TBP* 50% are the *TBP* at 80% and 50%, respectively in °K, *Sp.gr* is the stocks specific gravity.

♦ The end point of temperature of the *TBP* curve (*i.e.* at 100 vol.%) varies with the petroleum stock *API* gravity as follows:

API gravity	End point temperature (at 100 vol.%)
= 35	760 °C (1400 °F)
$20 \leq API < 35$	788 °C (1450 °F)
> 35	Less than 649 °C (1200 °F)

Using the above recommendations, the least square fitting performed using a fourth degree polynomial equation as follows:

$$TBP = A'_1V^4 + B'_1V^3 + C'_1V^2 + D'_1V + E'_1 \qquad \ldots(5.2)$$

where *TBP* is the true boiling point temperature, *V* is the volume percent distilled (Vol. %), and A'_1, B'_1, C'_1, D'_1 and E'_1 are constants.

A computer program package named Microsoft excel used for developing the necessary equation and their constants. The constants A'_1, B'_1, C'_1, D'_1 and E'_1 for data source of part one are given in Table F-1 in Appendix F, while Table F-2 in Appendix F gives the values of the constants A'_1, B'_1, C'_1, D'_1 and E'_1 for the data source of part two.

For specific gravity curves, the least square fitting using the power form equation gives:

$$Sp.gr_i = A'_2V^{(B'_2)} \qquad \ldots(5.3)$$

where A'_2 and B'_2 are constants, *V* is the volume percent distilled (Vol. %).

A Microsoft excel computer program used for developing the necessary equations and their constants. The constants $A^{'}$ and $B^{'}$ for petroleum stocks of number 16, 17 and 18 of the data source of part one are given in Table F-1 in Appendix F, while Table F-2 in Appendix F gives the values of constants $A^{'}$ and *B* for petroleum stocks of the data source of part two (*i.e.* four Iraqi types crude oils).

5.2.1.2 Graphical method

For the present work, the graphical method by Raizi – Dunbert is used for converting the *TBP* curve to *EFV* curve (hence it is called as RD – graph). The algorithm for this method can be given as follows:

1. Given *TBP* curve equation constants A'_1, B'_1, C'_1, D'_1 and E'_1, *Sp.gr* curve equation constants A'_2 and B'_2 (if *Sp.gr* curve available), the constants for equations (3.3) and (3.4), and the petroleum stock *API*.
2. Calculating *Sp.gr* using equation (5.3) for petroleum stocks in which the specific gravity curve is available, or by using equation (3.6) for the petroleum stocks in which just the overall specific gravity are available. Equation (3.6) need that *EFV 10%* and *EFV 50%* temperatures must be known.
3. Converting the *TBP* temperature to *ASTM D86* temperature by using equation (3.3).
4. Converting the *ASTM D86* temperature to *EFV* temperature by using equation (3.4).
5. Printing out the volumes distilled (Vol. %), *ASTM D86* temperatures and *EFV* temperatures.

In the above algorithm, the *EFV* temperature corresponding to 0, 10, 30, 50, 70 and 90% vol.% distilled can be estimated. Any other *EFV* temperatures between or above the given vol.% distilled must be interpolated or extrapolated. The above algorithm can be illustrated by flow sheet as shown in Fig. 5-48:

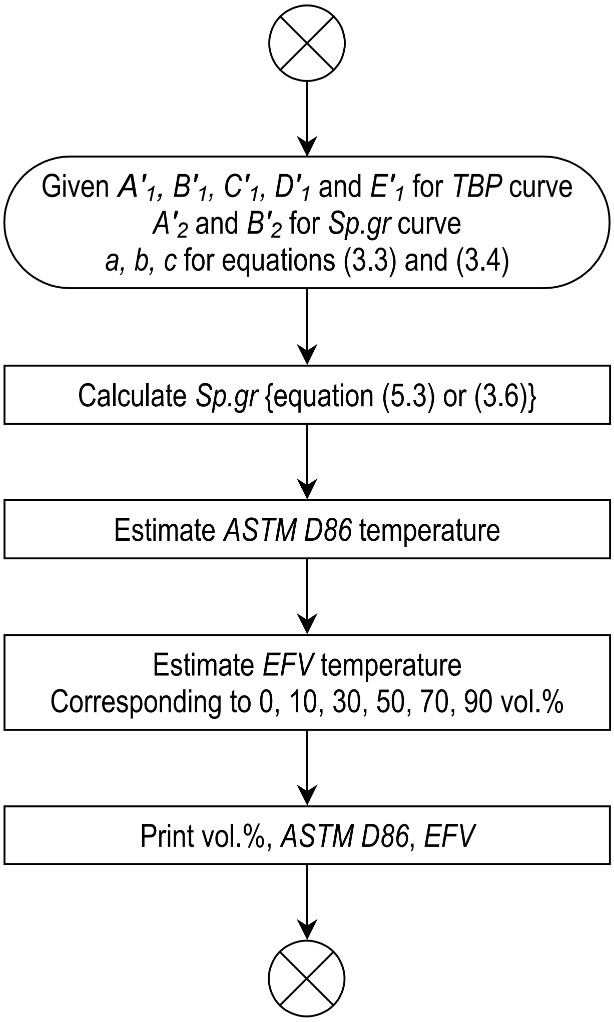

Figure 5-48 Flow sheet for algorithm of Raizi – Daubert graphical method (RD – graph)

5.2.1.3 Pseudo – component (computer) methods

Pseudo – component (computer) methods based on three thermodynamic models for predicting *K* – values used in the present work. These thermodynamic models are; equation of state model (*EOS*), activity coefficient models and the ideal solution *K* – value model. All these models discussed in details in Chapter three.

To obtain the *EFV* curve from *TBP* curve using the pseudo – component (computer) methods, there are four important steps that must be achieved. These steps were discussed previously in Chapter three, but because of their importance, they summarized here again to show the present work handling and treatments of the estimation. These steps are:

Step one: The *TBP* curve is divided into a suitable number of fractions or cuts. In the present work the available working *TBP* curves were divided into 40 cuts with volumes distilled range of 2.5% for each cuts. This suggested method of splitting the *TBP* curve into 40 cuts will ensure that the boiling point range of each cut has a good agreement with the literature boiling range of 5 – 25 °C (41 – 77 °F).

Step two: Using the mid – boiling point (*TB*) and specific gravity (*Sp.gr*), the basic characterization parameters for each cut can be estimated. The basic parameter including the critical properties (critical temperatures and critical pressures), acentric factor (ω) and the molecular weight (*MW*). In the present work the Raizi – Daubert correlations (*API* – method) was used for estimation the molecular weight (*MW*), critical temperature (*Tc*), critical pressure (*Pc*) (*i.e.* equations (3.41), (3.42) and (3.43) respectively of Table 3-3), while the Lee – Kesler correlations was used for estimation the acentric factor (ω) (*i.e.* equations (3.12) and (3.13) in Table 3-3).

The Raizi – Daubert correlations for estimation the critical properties (*Tc, Pc*) have a maximum *TB* limitation of 343 °C (650 °F). For the *TB* greater than 343 °C (650 °F), the present work suggested that using the Lee – Kesler correlations for estimation *Tc* and *Pc* for each cut (*i.e.* equations (3.9) and (3.10) respectively of Table 3-3). The Lee – Kesler correlations give a good accuracy for estimation the *Tc* and *Pc* for heavy cuts (*i.e.* $TB \geq 343$ °C (650 °F)) **[7]**.

The liquid volume basis for the cuts can then be converted to weight basis and finally to mole basis. The conversion procedure needs the specific gravity and molecular weight of each cut. The specific gravities for the given data in the present work were of two types, first type for those petroleum stocks in which just the overall specific gravities were available (petroleum stocks of number 1 to 15 in Table 5-1). In such case, the specific gravity for each cut can be estimated by using the Katz – Firoozabadi correlation {*i.e.* equation (3.7)}. For petroleum stocks in which the specific gravity curves were available, the specific gravity for each cut can be obtained by using the equation form of (5.3). The latter is true for petroleum stocks of number 16, 17 and 18 in Table 5-1, and also for four types of Iraqi crude oils. Using any input type of specific gravity, the specific gravity for each cuts must be adjusted to satisfy of the petroleum stocks the overall specific gravity. The latter must be done before estimation of the basic characterization constants (*i.e. MW, Tc,* *Pc, ω ...etc*). Using the adjusted specific gravity and the molecular weight for each cut, the feed compositions in mole basis can be obtained by performing the material balance (*i.e.* converting volume basis of *TBP* curve to weight and mole basis respectively).

Steps one and two of pseudo – component methods can be considered as characterization steps and they must be performed before proceeding in flash calculations for obtaining the flash volume at system temperature and pressure. In the present work the following algorithm used for performing the characterization steps:

1. Given *TBP* curve in form of equation (5.2), *API* gravity of petroleum stocks, overall feed volume basis (V_t).
2. Splitting the *TBP* curve into 40 cuts or pseudo – components. Each cut has a volume percent range of 2.5%. Estimate the *TB* for each cut by using the mid – boiling point concept.
3. Obtaining the specific gravity for each cut ($Sp.gr_i$) by using equation (3.7) for overall specific gravity type, or equations (5.3) and (5.4) for available specific gravity curve type. If equation (5.3) is used, the mid – point specific gravity can be obtained using mid – point concept.
4. Estimation of weight of each cut by the following equations:

$$W_i = Sp.gr_i \times V_i \qquad \text{...(5.4)}$$

$$W_t = \sum_{i=1}^{N} W_i \qquad \text{...(5.5)}$$

where, W_i is the weight for each cut, V_i is the volume of each cut and W_t is the total estimated weight.

For the present work, a basis of 4000 cm^3 of petroleum stock used for obtaining the material balance, thus each cut has a volume of 100 cm^3 (*i.e.* V_i = 100 cm^3). The overall petroleum weight (W_f) is obtained by using the petroleum stock specific gravity (*i.e.* W_f = 4000 × *Sp.gr* of feed).

5. Comparing the total estimated weight (W_t), with the overall petroleum stock weight (W_f). If W_t differs from W_f then the specific gravity for each cut must be adjusted to satisfy the overall.

6. Estimation of molecular weight (*MW*) and critical properties (*Tc, Pc*) and acentric factor (ω) using Raizi – Daubert and Lee – kasler correlations for material balance and the overall petroleum stock specific gravity.

7. If there is no differences between W_f and W_t, then the moles of each fraction can be estimated using the following equations:

$$N_i = \frac{W_i}{MW_i} \qquad \text{...(5.6)}$$

$$N_t = \sum_{i=1}^{N} N_i \qquad \text{...(5.7)}$$

8. Estimation of the feed compositions in mole basis as follows:

$$Z_i = \frac{N_i}{N_t} \qquad \text{...(5.8)}$$

The characterization algorithm can be illustrated also by the flow sheet diagram shown in Fig. 5-49.

Step three: In the third step, the *K* – values for cuts can be estimated using suitable thermodynamic models. In the present work, different types of thermodynamic models are used. Each of these thermodynamic models will be treated as a separate pseudo – component method. These different types of thermodynamic models can be summarized as follows:

1. *SPK* and *PR* equations of state (*EOS*) are used in both vapor and liquid phases. The working equation for estimation the *K* – values by using equation of state models is given by equation (3.65).

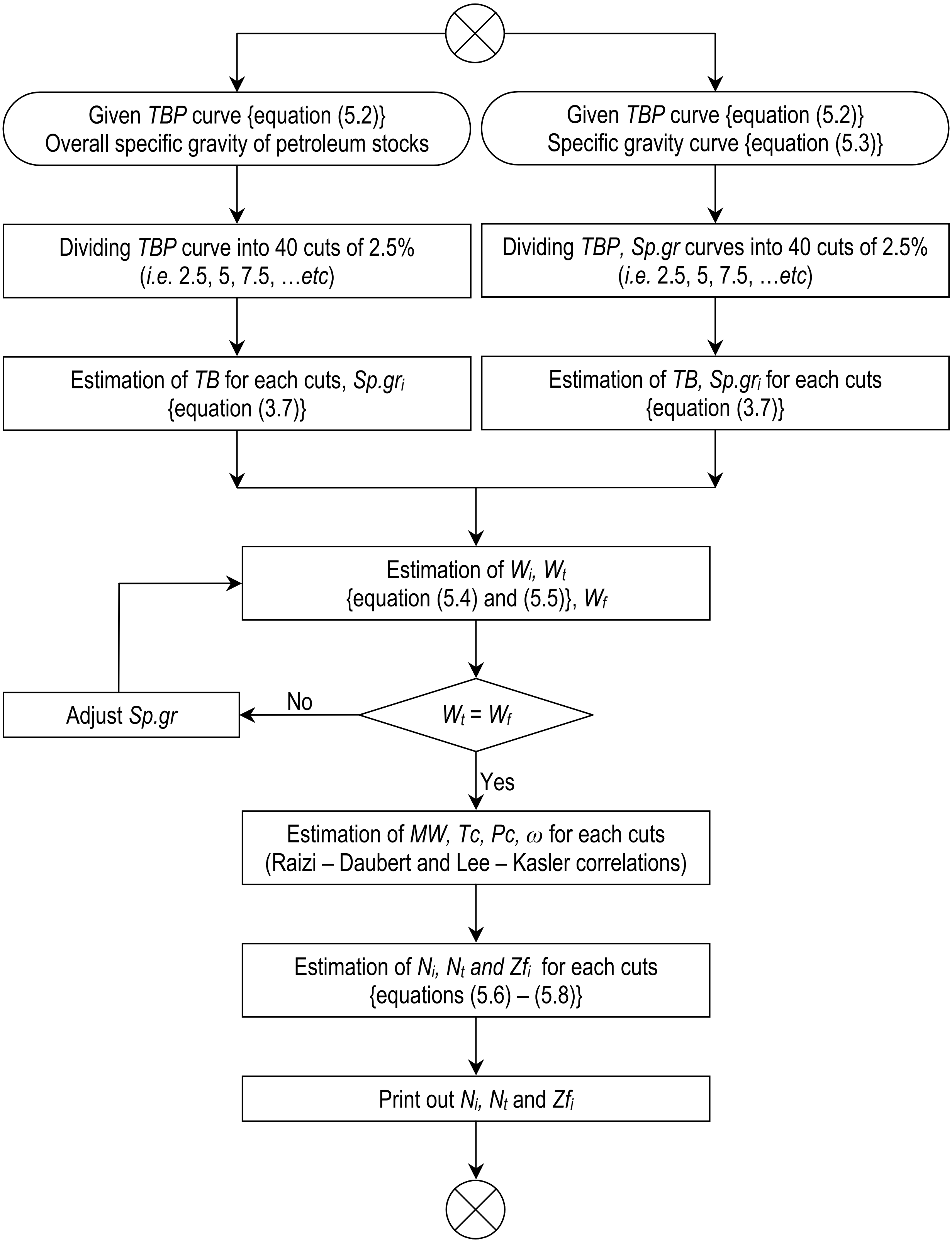

Figure 5-49 Flow sheet for algorithm of characterization steps of pseudo – components methods

2. The *SRK EOS* are used for vapor phase and the activity coefficient model by van – Laar {equation (3.145)} used for liquid phase (this model henceforth called as *SRK* + Van). Also the *PR EOS* is used for the vapor phase and the activity coefficient model by van – Laar used for the liquid phase (this model henceforth called as *RP* + Van). The working equation for prediction the *K* – values using the activity coefficient models is given by equation (3.147).

3. The ideal solution model is used in the present work, where both phases (vapor and liquid phases) are considered to form ideal solution. The working equation for estimation the *K* – values by ideal solution model is given by equation (3.160) (henceforth this model is called as Ideal K).

Step four: In this step, the flash volume at a given temperature, pressure and compositions can be estimated by performing the isothermal flash calculations (*P* – *T* flash process). The latter can be done by solving equation (3.177) for β by Newton – Raphson method. The β can then be converted to volume basis by using equation (3.181). The algorithm for performing (*P* – *T*) flash calculations will be summarized in the next sections.

5.2.1.4 Algorithms (procedures) for performing isothermal flash (*P* – *T*) calculations

Many algorithms or procedures for performing isothermal flash calculation can be found in literatures **[88, 89** and **91]**. All these algorithms can be divided into two categories, the first category in which the *K* – values of species are not depending on the system compositions. The ideal solution *K* – value equation {equation (3.160)} falls in such category. In the second category, the *K* – values are depending on the system compositions, the *EOS* and activity coefficient models {equations (3.65) and (3.147)} fall into such category. For the present work and since dealing with the bulk of petroleum fractions and hydrocarbons (more than 98% vol. %), the following two assumptions will be adopted:

a. All the interaction parameters (K_{ij}) for both *SRK* and *PR EOS* mixing rules assumed to be zero.

b. Testing the two phase region will be achieved using the ideal *K* – values only (*i.e.* using equation (3.177) for $\beta = 1$ and 0) and there is no need to perform the bubble and dew point calculations.

5.2.1.4.1 Isothermal flash calculation algorithm using ideal *K* – values models

The **Rachford – Rice [42, 88]** algorithm for isothermal flash calculations where the *K* – values are independent of the system compositions (first category) was adopted in the present work. The Rachford – Rice algorithm can be summarized as follows:

1. Input flash temperature (T) and flash pressure (P), feed molar rate (F), feed compositions (Zf_i), petroleum stock *API*, cut critical properties (Tc_i, Pc_i), acentric factors (ω_i), alfa functions (α_i), vapor pressures P_i^s and molar volumes at system temperature (V_i^L) for $Tr < 1$ and $Tr > 1$.
2. Calculating of *K* – values for each cut (K_i), using equation (3.160).
3. Testing for two phase by solution of equation (3.177) for $\beta = 0$ and $\beta = 1$ {*i.e.* *F(0)* and *F(1)*}. If $F(0) < 0$ and $F(1) > 0$, then the flash calculation can be achieved or if not the given feed composition is at the bubble point conditions and $\beta = 0$. Go to step 10.
4. If the flash calculation is achieved, equation (3.177) can be solved for β using Newton – Raphson method (see Appendix D).
5. Calculation of vapor flow rate (F_V) and liquid flow rate (F_L) by using the following equations:

$$F_V = \beta \times F \qquad \ldots(5.9)$$

$$F_L = F - F_V \qquad ..(5.10)$$

6. Calculation of vapor and liquid phases compositions (y_i, x_i) using equations (3.171) and (3.170), respectively.

7. Calculation of molal volume of feed and vapor phase by using equations (3.180) and (3.179), respectively.

8. Converting β to β_V using equation (3.181).

9. Printing out β, β_V, T and P. The *EFV* curve can be obtained by plotting T versus β_V.

The above algorithm for performing isothermal flash calculations using ideal *K* – values can be also illustrated by the flow sheet diagram shown in Fig. 5-50.

5.2.1.4.2 Isothermal flash calculations algorithm using equation of state (*EOS*) models

Equation of state (*EOS*) models are widely used in isothermal flash calculations. In the present work, the *SR* and *PR EOS* models used for performing isothermal flash calculation using the following selected algorithm **[88, 89]** shown in Fig. 5-50.

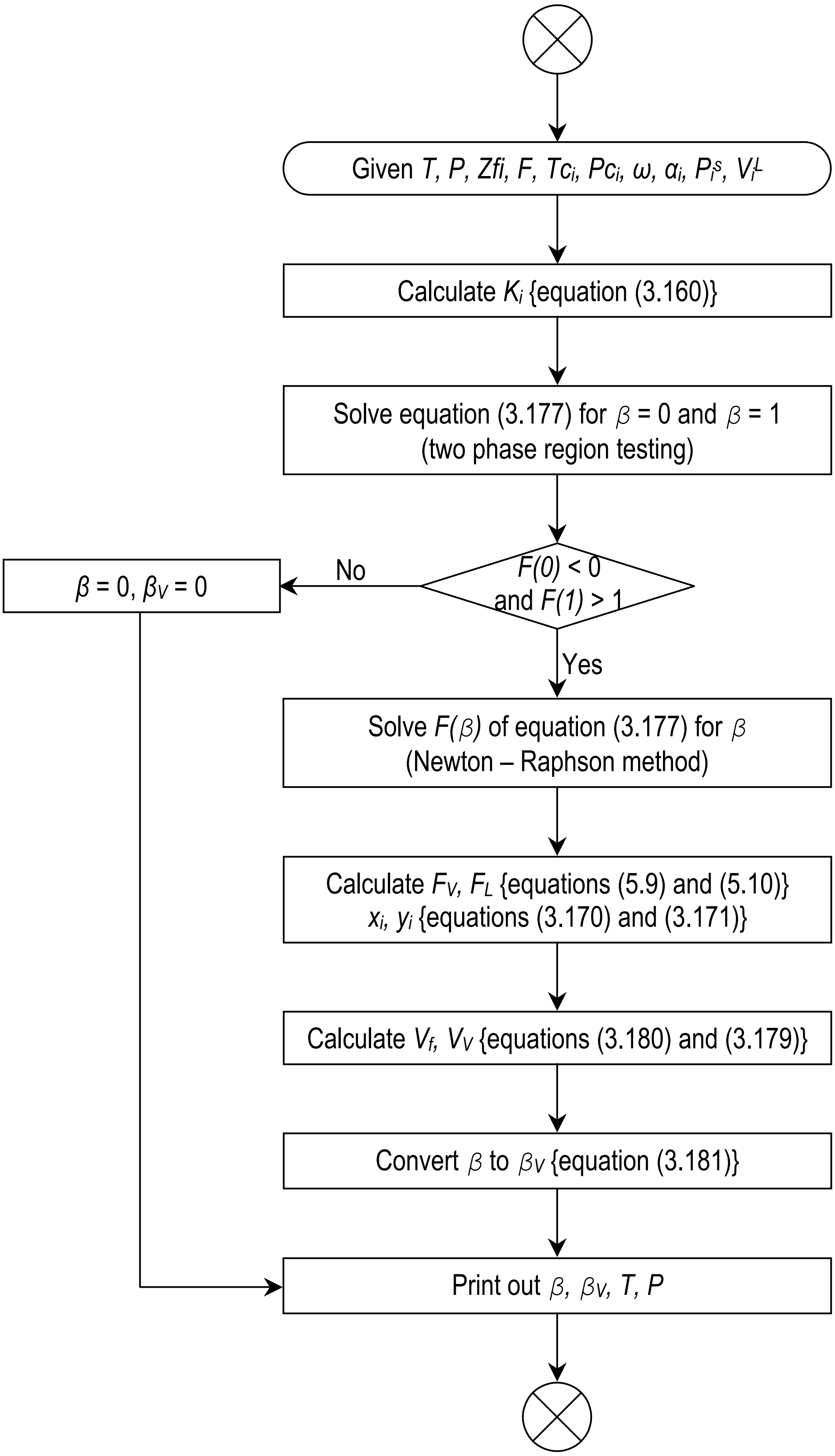

Figure 5-50 Flow sheet for algorithm for Rachford – Rice algorithm for isothermal flash calculations using ideal K – values equation

1. Input the flash temperature (T), flash pressure (P), feed rate (F), feed compositions (Zf_i), critical properties (Tc_i, Pc_i), acentric factors (ω_i), vapor pressures (P_i^S), alfa functions (α_i) and molar volumes (V_i^L) at system temperature for $Tr > 1$ and $Tr < 1$.
2. Assuming an initial value of K – values for each cut at a given flash temperature and flash pressure (T, P). The ideal K – values given by equation (3.160) can provide the initial K – values (K_i^A).
3. Testing for two phase region by solving equation (3.175) $\{F(\beta)\}$ with $\beta = 0$, and $\beta = 1$. If $F(0) < 0$ and $F(1) > 0$, then the flash calculation can be performed and proceeding to step 4. If the above conditions are not satisfied, then $\beta = 0$ and $\beta_V = 0$ and proceeding to step 12.
4. Performing flash calculations by solving equation (3.175) for β by Newton – Raphson method (as shown in Appendix D).
5. Calculation of vapor and liquid compositions (y_i, x_i) using equations (3.170) and (3.171), respectively.
6. Calculation of liquid and vapor phase compressibility factors (Z^V, Z^L) using equation (3.79) for *SRK EOS* or equation (3.92) for *PR EOS* {using Newton – Raphson method (as shown in Appendix D)}. Calculation of partial molal fugacity coefficients for liquid and vapor phases ($\bar{\phi}_i^L$, $\bar{\phi}_i^V$) using equations (3.85) and (3.87) for *SRK EOS*, or equations (3.98) and (3.100) for *PR EOS*.
7. Calculation of new K – values (K_i), using equation (3.65).
8. Checking for the solution by applying the following constraint:

$$\sum_{i=1}^{N}\left[\frac{K_i}{K_i^A - 1}\right]^2 \leq \epsilon \qquad ..(5.11)$$

where ϵ is the preset error tolerance (*e.g.* 0.0001), and N is the number of components or cuts in the system.

9. If the constraint of equation (5.11) is satisfied, then the solution has been reached for both (β) and (K_i) and then proceeding to step 10. If not steps 2 through 7 must be repeated using the calculated K – values (K_i) as initial values.

10. Calculation of F_V and F_L using equations (5.9) and (5.10). Also calculation of vapor and liquid phase compositions (y_i and x_i) using equations (3.171) and (3.170).

11. Calculation of molar density for feed and vapor phase streams by using equations (3.180) and (3.179).

12. Calculation of β_V using equation (3.181).

13. Printing out β, β_V, T and P. The *EFV* curve can be obtained by plotting T versus β_V.

The above algorithm can be also illustrated in the flow sheet diagram shown in Fig. 5-51.

5.2.1.4.3 Isothermal flash calculation algorithm using activity coefficients models

Activity coefficients models are widely used in isothermal flash calculations. In the present work, the *SRK* and *PR EOS* used for vapor phase, while the van – Laar activity coefficient model used for the liquid phase. The following algorithm used in the present work for performing isothermal flash calculations **[88, 91]**:

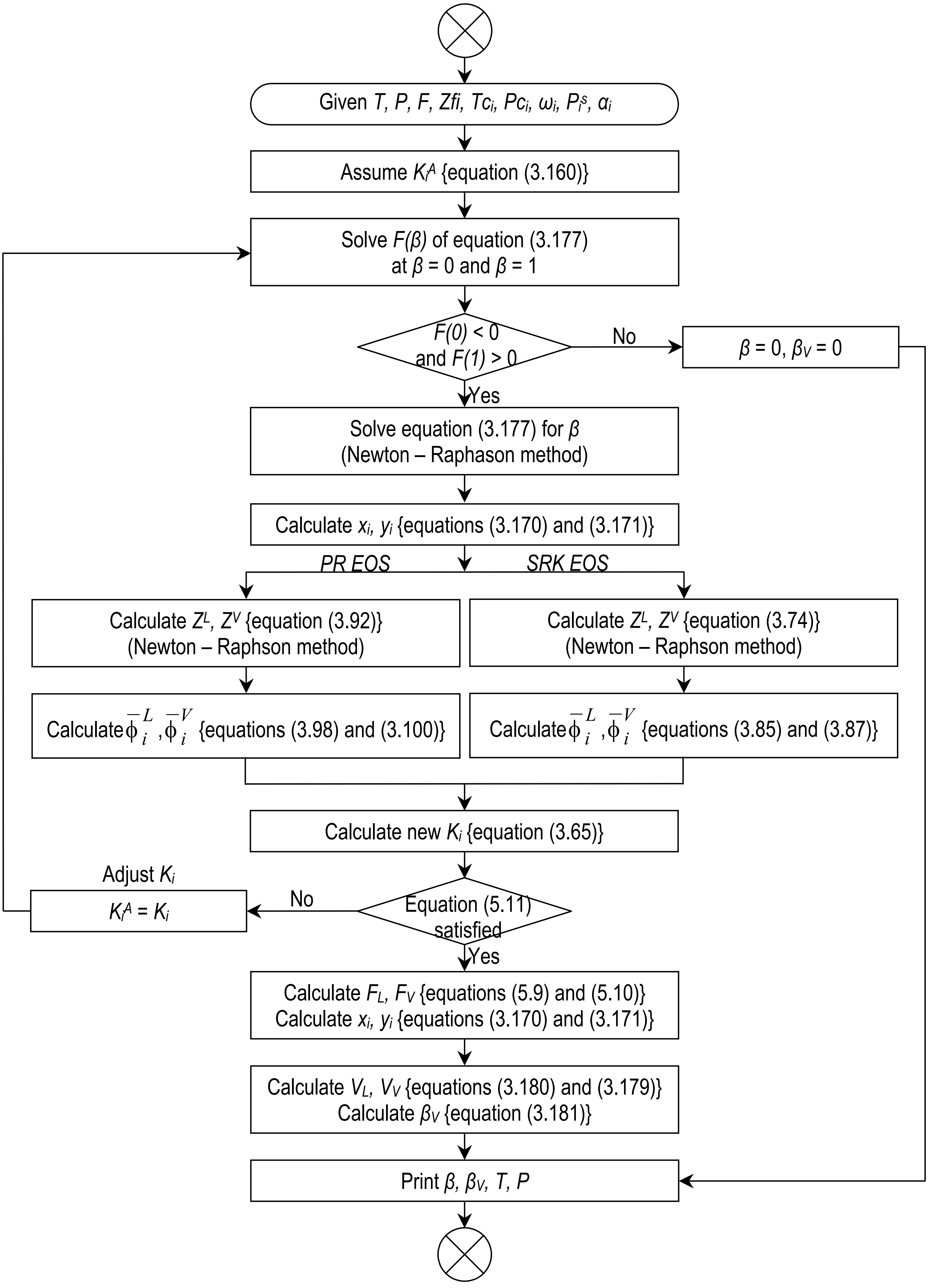

Figure 5-51 Flow sheet algorithm for isothermal flash calculations using *EOS* models (*SRK* or *PR*)

1. Given flash temperature (T), flash pressure (P), feed rate (F), feed compositions (Zf_i), critical properties (Tc_i, Pc_i), acentric factors (ω_i), vapor pressures (P_i^s), alfa functions (α_i), solubility parameters (δ_i) and molar volume (V_i^L) at a system temperature for $Tr > 1$ and $Tr < 1$.
2. Assuming initial values of K – values for each cuts (K_i^A) at a given flash temperature (T), and flash pressures (P). The latter can be done using equation (3.160).
3. Testing for two phase region by solving equation (3.177) $\{F(\beta)\}$ with $\beta = 0$ and $\beta = 1$. If $F(0) < 0$ and $F(1) > 0$, then the flash calculation can be performed and proceeding to step 4. If the above conditions are not satisfied then $\beta = 0$, $\beta_V = 0$ and proceeding to step ?.
4. Performing flash calculations, by solving equation (3.177) for β using Newton – Raphson method (as shown in Appendix D).
5. Calculation of vapor and liquid phases compositions (y_i and x_i) using equations (3.170) and (3.171).
6. Calculation of activity coefficient (γ_i^L) using van – Laar model {equation (3.145)}.
7. Calculation of vapor phase compressibility factor (Z^V) by using equation (3.79) for *SRK EOS* or (3.92) for *PR EOS* (Newton – Raphson method, as shown in Appendix D). partial molal fugacity coefficients $\bar{\phi}_i^V$ can be estimated using equation (3.87) for *SRK EOS* or equation (3.98) for *PR EOS*.
8. Checking of supercritical region ($Tr > 1$). If $Tr_i > 1$, the new K – values for each species (K_i), can be calculated by using equation (3.68). The liquid phase partial molal fugacity coefficients (ϕ_i^L) of equation (3.66) can be estimated by using Choa – Sender correlation {equations (3.121) – (3.123)}. For the case of $Tr < 1$ proceeding to step 9.
9. For $Tr_i < 1$, the new K – values can be estimated by using equation (3.147). The saturated fugacity coefficients (ϕ_i^{Vs}) for equation (3.147) can be obtained from equation (3.118) for *SRK EOS*, or (3.120) for *PR EOS*. The saturated

compressibility factor (Z_i^{Vs}) can be estimated by solving equation (3.79) for *SRK EOS* or (3.92) for *PR EOS* (using Newton – Raphson method).

10. Checking for solution by applying equation (5.11). If the constraint of (5.11) ($\epsilon \leq 0.0001$) is reached then the solutions for both β and K_i are achieved and proceeding to step 11. If not, then steps 2 through 10 must be repeated using the calculated (K_i) as initial values.
11. When the solutions for (β) and (K_i) are achieved, then calculation of vapor and liquid compositions (x_i, y_i) can be done using equations (3.171) and (3.170). F_V and F_L also can be obtained using equations (5.9) and (5.10).
12. Calculation of molar volumes for feed stream (V_f) and vapor phase stream (V_L) using equations (3.180) and (3.179).
13. Calculation of β_V using equation (3.181).
14. Printing out β, β_V, T and P. The *EFV* curve can be obtained by plotting T versus β_V.

The above mentioned algorithm for isothermal flash calculations using the activity coefficients models can be illustrated by the following flow sheet diagram:

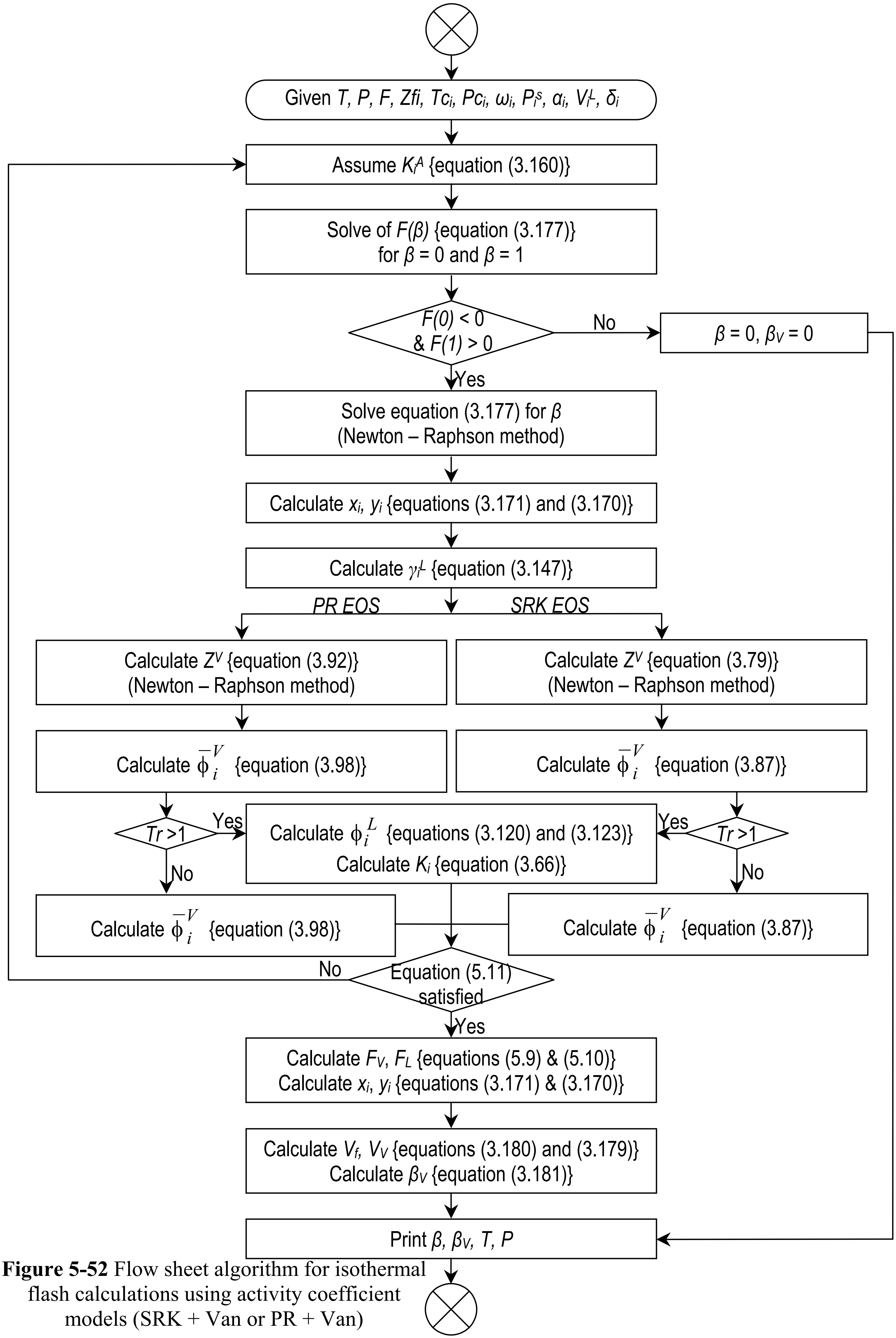

Figure 5-52 Flow sheet algorithm for isothermal flash calculations using activity coefficient models (SRK + Van or PR + Van)

5.2.1.5 Statistical measurement and analysis dispersion

To know the applicability and accuracy of any proposed correlation, it is very important to know how this correlation fits the experimental data which is done by comparing the obtained results from the proposed correlation with the experimental data.

The various measurement of dispersion or variation are available, the most common being the average absolute percent deviation (*AAD%*) and the average percent deviation or bais (*AD%*).

The average absolute percent deviation (*AAD%*) is a more tangible element indicating the overall goodness of the fit of the data by the correlation and it reads:

$$AAD\% = \frac{\sum_{i=1}^{N} \left| \frac{M_i^{exp} - M_i^{calcd}}{M_i^{exp}} \right|}{N} \times 100 \qquad ..(5.12)$$

where M is an intensive property and N is the number of data points.

The average percent deviation (*AD%*) gives an indication about how the calculated data centered about the experimental data. The *AD%* can be written as follows:

$$AD\% = \frac{\sum_{i=1}^{N} \frac{M_i^{exp} - M_i^{calcd}}{M_i^{exp}}}{N} \times 100 \qquad ..(5.13)$$

The above two equations {equations (5.12) and (5.13)} are used for the *AAD%* and *AD%* for experimental data for part one of the present work. The flash volume in (vol.%) used for calculations of *AAD%* and *AD%*, consequently equations (5.12) and (5.13) can be written as follows:

$$AAD\% = \frac{\sum_{i=1}^{N}\left|\frac{V_i^{exp} - V_i^{calcd}}{V_i^{exp}}\right|}{N} \times 100 \quad ..(5.14)$$

$$AD\% = \frac{\sum_{i=1}^{N}\frac{V_i^{exp} - V_i^{calcd}}{V_i^{exp}}}{N} \times 100 \quad ..(5.15)$$

5.2.1.6 Improvement on the existing thermodynamic models used with pseudo – component methods

For pseudo – component methods, the thermodynamic models have an important rule in performing the flash calculation to obtain the flash volume at a given flash temperature and pressure. Thus, knowledge and judgment are required to select the most appropriate method by which to estimate the required flash volume under the conditions in which the two phases will be in equilibrium.

In the present work, there are five thermodynamic models used for prediction the *K* – values and thus for performing the flash calculations, these models are *SRK, PR, SRK* + Van, *PR* + Van and the Ideal *K* models. By taking of deep observations on the above thermodynamic models and with the help of published literature, the following important points may be observed **[88, 87, 106]**:

1. The most important terms for *EOS* models (*SRK* and *PR*) is the alfa function (α) (also known as attractive term).
2. For the activity coefficient models (*SRK* + Van and *PR* + Van), the most important terms are the activity coefficient (γ^L), alfa function (α) and the vapor pressure term (P^s).
3. For the ideal solution model, the most important terms are the alfa function (α) and the vapor pressure (P^s).
4. Selection the correction for estimation the alfa functions (α), vapor pressure (P^s), activity coefficient leads to fix the mode of used thermodynamic models (unmodified or modified modes).

Based on the above observation, the present work suggested three modes of thermodynamic models based on the selection of the alfa function (α), vapor pressure (P^s) and activity coefficient (γ_i^L) terms, these modes are:

a. Unmodified models mode.

b. Modified models No. 1 mode (existing in the literature).

c. Present work suggested modification mode (modified models No. 2 mode).

The above mentioned thermodynamic modes are tested and investigated for obtaining the *EFV* curve from *TBP* curve using 18 petroleum stock of Table 5-1. The total number of *EFV* data points that tested were 106 points.

5.2.1.6.1 Unmodified models mode

In this mode, the following correlations for alfa functions (α), vapor pressure (P^s) and activity coefficients model (γ^L) are used:

- The original alfa functions correlations for *SRK* and *PR EOS* used {equations (3.76) and (3.90) for *SRK* and *PR EOS* respectively}.
- The Lee – Kasler correlations {equations (113 – 115)}.
- The van – Laar model for activity coefficient model {equation (3.145)}.

5.2.1.6.2 Modified models No.1 mode

In this mode, the following correlations for alfa functions (α), vapor pressure (P^s) and activity coefficient model (γ^L), are used:

- For *SRK EOS*, the modified alfa function given by Sim – Daubert is used {equation (3.102)}.
- For *PR EOS*, the modified alfa function given by Twa et al. is used {equations (3.103) – (3.105)}.
- The Lee – Kasler correlation is used for estimation the vapor pressure (P^s).
- The van – Laar model is used for estimation the activity coefficient (γ^L).

The present work suggested a modification (modified models No. 2 mode) and will be discussed in the next chapter.

Chapter Six

Present work suggested modification

6.1 Suggested modification mode (modified models No. 2 mode)

In the present work, the ideal solution model {equation (3.160)} is used for improving the prediction of the K – values and thus, the predicted flash volumes. The reasons behind selection of ideal solution model are:

a. Its composition is independent, thus the flash calculations can be performed more easily than the other models (*EOS* and activity models).

b. Since the bulk of the petroleum fraction is hydrocarbons , it is expected that both vapor and liquid phase obey the ideal solution concept especially at atmospheric pressure.

Recalling equation (3.160), thus:

$$K_{i(ideal)} = \frac{P_i^s}{P} exp\left[\left(\frac{0.08664}{Tr_i Pc_i} - \frac{0.4178\alpha_i}{Tr_i^2 Pc_i} - \frac{V_i^L}{RT}\right)\left(P_i^s - P\right)\right] \qquad (3.160)$$

In the present work the vapor pressure (P_i^s) is selected as a most important term, and it is modified to improve the performance of equation (3.160) in flash calculation and thus the estimation of the *EFV* curve. Consequently, the Lee – Kasler correlation for estimation of vapor pressure is replaced by a new suggested correlation. The new suggested correlation is based on the perturbation theory. In perturbation theory, any physical property (including vapor pressure) can be estimated by using Taylor series expansion as follows:

$$\theta(x_1,...,x_n)=\theta^{ref}(x_1,...,x_n)+\sum_i\theta_i(x_1,...,x_n)\left(x_i-x_i^{ref}\right)$$
$$+\sum_{ij}\theta_{ij}(x_1,...,x_n)\left(x_i-x_i^{ref}\right)\left(x_j-x_j^{ref}\right) \quad ...(6.1)$$

where θ is any physical properties, $(x_1, ...,x_n)$ are the independent variable such as *TB, Sp.gr ...etc,* θ_i, θ_{ij} are the first and second partial derivatives with respect to the difference variables $(x_i - x_i^{ref})$ evaluated for the reference system, the superscript (*ref*) denotes the reference system properties.

Equation (6.1) represents the general form of Taylor series expansion of the property θ about its value in some reference state. The normal alkane hydrocarbons are widely used as a reference property (θ_{ref}) **[37]**.

For the purpose of empirically correlating the deviations between n – alkane and non – alkane hydrocarbons Lee and Kasler and Sandler **[107]** suggested the following simpler, first order perturbation expansion:

$$\theta(Tb,Sp.gr,\omega_s)=\theta^A(TB)+\theta_1(TB)\left(Sp.gr-Sp.gr^A\right)$$
$$+\theta_2(TB)\left(\omega-\omega^A\right) \quad ...(6.2)$$

where $(Sp.gr - Sp.gr^A)$ is the difference between the non – hydrocarbon specific gravity and n – alkane specific gravity measured at same *TB* of non – alkane hydrocarbons and $(\omega - \omega^A)$ is the difference between the acentric factor of non – alkane hydrocarbons and the acentric factor of n – alkane hydrocarbons measured at same non – alkane hydrocarbons *TB*. θ_1 and θ_2 are derivations and must be calculated by back calculation from experimental data. For the vapor pressure property they suggested to terminate equation (6.2) to second term and they obtain the following equation:

$$ln\,P^s = ln\,P^{sA}+\left(\omega-\omega^A\right)F_1F_2 \quad ...(6.3)$$

where P^s and P^{sA} are the vapor pressure in (atm) for non – alkane and n – alkane hydrocarbons and F_1 and F_2 are functions and have the following forms:

$$F_1 = 1.21864(3.8 + TBr)\left[\frac{1}{C+1} - \frac{1}{C+TBr}\right] \quad (6.3a)$$

and $$C = \left(0.0953 + 3.197 \times 10^{-4}\,TB\right)(TBr - 0.85) \quad ...(6.4)$$

$$F_2 = 0.6828 + \left(1.2532 - 4.3574 \times 10^{-3}\,TB\right)\left(1 - \frac{0.85}{TBr}\right) \quad ...(6.5)$$

with $TBr = T/TB$

Equation (6.3) is limited to pure components non – alkane hydrocarbons, and it is expected to be useful for calculation the petroleum fractions vapor pressures **[107]**.

In the present work, equation (6.3) is modified and extended for petroleum fractions by achieving the following modifications:

1. The term ($\omega - \omega^A$) is replaced by ($Sp.gr - Sp.gr^A$) terms, since *Sp.gr* can be measured easily for petroleum fraction rather than ω.
2. The correction term (*CF*) is used for extending equation (6.3) for petroleum fractions. The correction factor term is given as follows:

$$CF = Ac - \frac{Bc}{TBr} \quad ...(6.6)$$

where *Ac* and *Bc* are the adjustable parameters that must be calculated using experimental data.

Consequently, the modified form of equation (6.3) can be written as follows:

$$\ln P^s = \ln P^{sA} + \left(Sp.gr - Sp.gr^A\right)F_1 F_2 + \left(Ac - \frac{Bc}{TBr}\right) \quad ...(6.7)$$

The P^{sA} and $Sp.gr^{A}$ of equation (6.7) can be obtained by using the following equation **[107]**:

$$ln\,P^{sA} = \left(0.9665 + 2.3021\times10^{-3}TB - 5.4728\times10^{-7}TB^{2} + \frac{89.301}{TB}\right)\times F_{1} \quad \ldots(6.8)$$

$$Sp.gr^{A} = 1.25386 - 6.42922\times10^{-4}TB + 4.5328\times10^{-7}TB^{2} - \frac{144.605}{TB} \quad \ldots(6.9)$$

The adjustable parameters *Ac* and *Bc* of equation (6.7) are calculated by using optimization technique using the *EFV* data for 18 petroleum stocks (106 data points). The optimization technique performed by using the solver program of Microsoft excel package. The optimization technique including the following two steps:

1. The flash calculation using equation (3.160) with conjunction of equation (6.7) is performed to obtain the flash volume.
2. The adjustable parameters are selected in such a way that the *AAD%* of flash volume be in a minimum case {equation (5.14)}.

Consequently, the value of *Ac* was 1.0202 (≈ 1) and *Bc* was 0.8498 (≈ 0.85). The working form of equation (6.3) is:

$$ln\,P^{s} = ln\,P^{sA} + \left(Sp.gr - Sp.gr^{A}\right)F_{1}F_{2} + \left(1 - \frac{0.85}{TBr}\right) \quad ..(6.10)$$

The constants F_1 and F_2 (equations 6.3a-6.5)were also used ,since the max. abslute diffreince between($\omega - \omega^{A}$) ,and($Sp.gr - Sp.gr^{A}$) did not exceed than 10^{-3}

It must be noted here, that the improved vapor pressure correlation can be applied under the following two conditions:

a. When the *TMEP* is negative, the *TMEP* can be defined as follows:

TMEP = 10 – The calculated flash volume {using equation (3.160)} when 20% TBP temperature is used as flash temperature

b. When the *TMEP* is positive and has the value of greater than 4 (*TMEP* > 4). The *TMEP* term suggested by **Sim – Daubert [1]** for improving the alfa function (α) of *SRK EOS* model. It is extended in the present work for improving the ideal *K* model.

The improved vapor pressure correlation with the above conditions can also be used for improving the *EOS* models (*SRK* and *PR*), and the activity coefficient models (*SRK* + Van and *PR* + Van) as follows:

1. for *SRK* and *PR* models, the improved vapor pressure correlations {equation (5.126)} can be used for improving the acentric factor (ω) prediction by replacing the Lee – Kasler correlations {equations (3.12) and (3.13)} by Pitzer et al. equation (3.78) with using the improved vapor pressure correlation for calculation the vapor pressure at $Tr = 0.7$. The latter will improve the alfa function (α) {*i.e.* $\alpha = f\,(Tr,\ \omega)$}.
2. For (*SRK* + Van) and (*PR* +Van) models, the improved vapor pressure correlation is used instead of Lee – Kasler correlation.

6.2 Computer implementation

A computer program is designed and developed by using quick basic language for the purpose of this work. The computer program is designed to obtain the *EFV* curve from the input *TBP* curve using the graphical method by Raizi – Daubert and the *SRK, PR, SRK* + Van, PR + Van and Ideal *K* pseudo – components methods. The remark statements are available at the beginning, and throughout the computer program. These statements help the user to understand the calculations used in the program. The computer program consists of three main parts. These parts are, input part, calculational part and printout part.

6.2.1 Input part

In this part all the necessary data for estimation the *EFV* curve from the *TBP* curve must be supplied. These data includes the following items:

a. Flash temperature (*T*), flash pressure (*P*), petroleum stocks *API*, constants for *TBP* (A_1', B_1', C_1', D_1' and E_1') and specific gravity equations (A_2' and B_2'), constants for Raizi – Daubert graphical method, total feed volume, and feed molar rate.

b. Type of specific gravity input data. There are two choices of specific gravity data input:

- Overall data input type (choice number 1).
- Specific gravity equation input type (choice number 2).

c. Type of vapor pressure correlations. There are two choices of vapor pressure correlations:

- Lee – Kasler correlation (choice number 1).
- Modified method suggested by the present work (choice number 2). The modified method will be discussed later.

d. Modes of thermodynamic models used with pseudo – components methods. There are three choices for modes of thermodynamic models used in computer program, those are:

- Unmodified models (choice number 1).
- Modified models No. 1 (choice number 2).
- Present work suggested modification (modified models No. 2).

6.2.2 Calculational part

This part of computer program is responsible for the calculations used for estimation the *EFV* curve from *TBP* curve. It is consisted of the following items:

a. Graphical methods for estimation the *EFV* curve from *TBP* curve. The latter can be achieved using the Raizi – Daubert algorithm (Fig. 5-48).

b. Pseudo – components methods for estimation the *EFV* curve from *TBP* curve. It consists of the following items:

1. Characterization steps using characterization algorithm (Fig. 5-49).
2. Calculation of molar volume (V_i^L) using Rackett equation {equation (3.110) for $Tr < 1$ and Cavett equation (3.111) for $Tr > 1$}.

3. Calculation of vapor pressure (P_i^s) depending on the choices of vapor pressure correlations. For choice 1, the vapor pressure (P_i^s) is calculated using Lee – Kasler correlation {equations (3.113) – (3.115)}, while for choice 2, the modified method suggested by the present work is used.

4. Calculation of alfa functions (α_i) for *EOS* models depending on the choices of thermodynamic modes. Since there are three modes of thermodynamic models, thus there are three types of alfa functions (α_i) that can be used in computer program, these models are:

   - Unmodified models {equations (3.76) for *SRK* and (3.90) for *PR*}.
   - Modified models No. 1 {equations (3.102) for *SRK* and (3.103) for *PR*}.
   - Modified models No. 2 {equations (3.76) for *SRK* and (3.90) for *PR*}.

5. Calculation of flash volume by performing flash calculations using the flash calculations algorithms that discussed previously and with conjunction of the five thermodynamic models as follows:

   - *SRK* thermodynamic model using *EOS* model algorithm (Fig. 5-51).
   - *PR* thermodynamic model using *EOS* model algorithm (Fig. 5-51).
   - *SRK* + Van thermodynamic model using activity coefficient model algorithm (Fig. 5-52).
   - *PR* + Van thermodynamic model using activity coefficient model algorithm (Fig. 5-52).
   - Ideal *K* thermodynamic model using Rachford – Rice model algorithm (Fig. 5-50).

6. Calculation of *AAD%* and *AD%* using equations (5.14) and (5.15).

6.2.3 Printout part

This part of computer program is responsible on the printing of the calculated results that performed by computer program. It consists of the following items:

1. Printing of flash temperature (*T*), flash pressure (*P*) and flash volume (Vol.%) for each pseudo – components methods.
2. Printing of error analysis (*i.e. AAD%* and *AD%*).
3. Printing of physical properties for each cuts including the critical properties (Tc_i, Pc_i), molecular weights (MW_i), acentric factors (ω_i), molar volumes at 15.5 °C (60 °F) (V_i^L), solubility parameters at 25 °C (77 °F) (δ_i), specific gravity ($Sp.gr_i$), …*etc*.
4. Printing of material balance (*MB*) for each cut including volumes (V_i), weights (W_i), moles (N_i) and the feed compositions (Zf_i) in mole basis.
5. Printing of Raizi – Daubert graphical method *EFV* temperatures at a corresponding volume percent (Vol.%).
6. Printing of vapor and liquid phases compositions for each cut (x_i and y_i) using the five thermodynamic models (*SRK, PR, SRK* + Van, *PR* + Van and Ideal *K*).
7. Printing of *K* – values for each components (K_i) using the five thermodynamic models.

For items 3 – 7, the printing results is converted to data files. These data files can be opened with other computer package such as Microsoft excel, and Microsoft grapher.

Items 6 – 7 can be considered as optional choices since the present work interested in *EFV* data rather than other calculated data.

The list of the computer program is given in Appendix G, while its flow sheet diagram is given in Fig. 6-1.

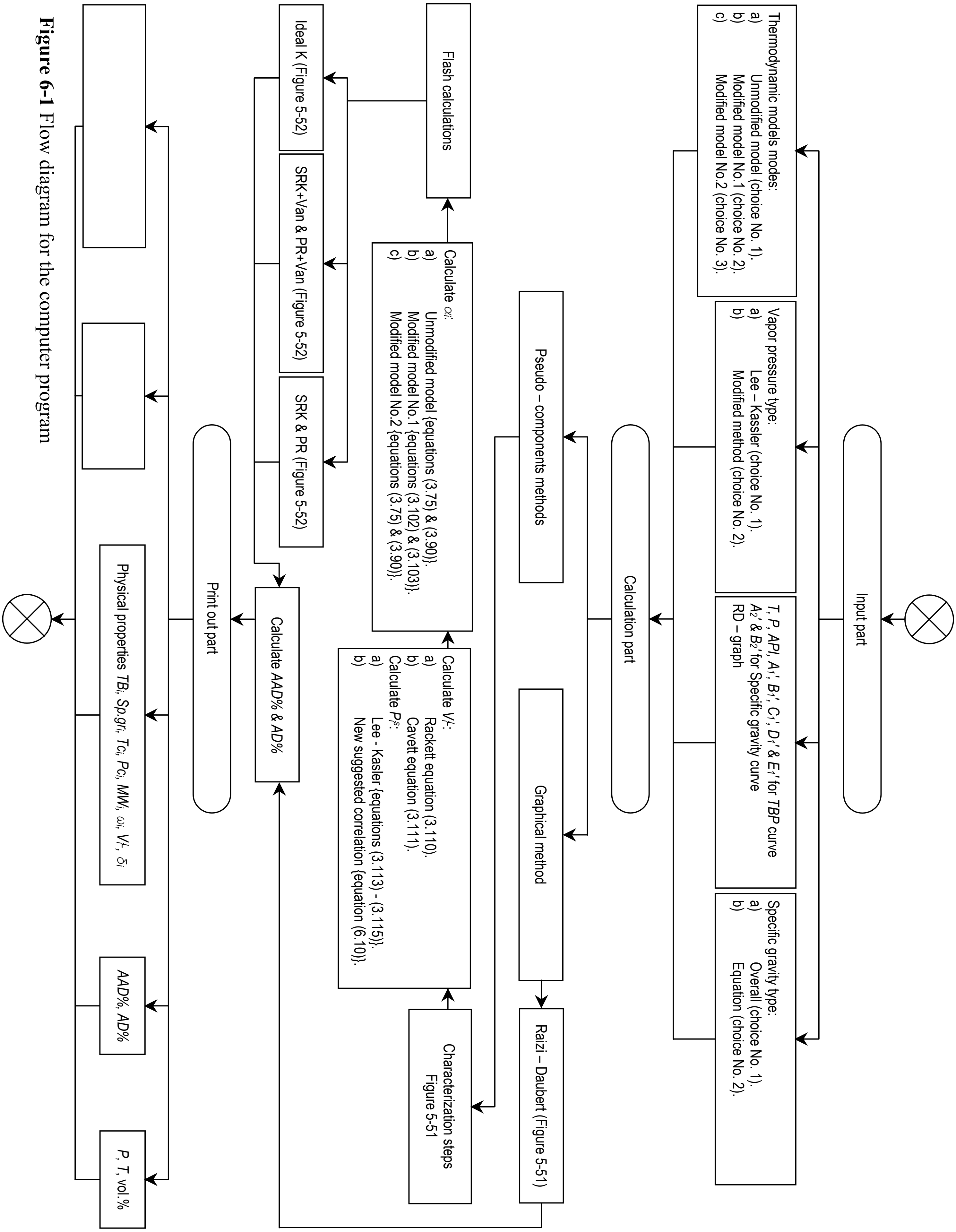

Figure 6-1 Flow diagram for the computer program

Chapter Seven

Results and discussion

7.1 Discussion of results

7.1.1 Selected data for part one(testing & developing part) and part two (application part)of the present work

For part one of the present work, 18 petroleum stocks are used for estimation the *EFV* curve from *TBP* curve. As shown in Table 5-1, the *API* gravity of these petroleum stocks were varies from 20.2 to 47.8. Petroleum stocks of number 1 to 15 were available with just overall specific gravity and *TBP* curve, while petroleum stocks number 16, 17 and 18 were available with specific gravity curve and *TBP* curve, consequently these petroleum stocks can be considered as industrial data type, while the first 15 petroleum stocks can be considered as a classical chemical engineering literature data type. Both data types were available with *EFV* curves.

Figures 5-1 – 5-15 illustrate the *TBP* curves for petroleum stocks of number 1 through 15, while Figs. 5-31 – 5-33 illustrate the *TBP* curves for petroleum stocks of number 16, 17 and 18, respectively. As shown by these figures, volume percent distilled (vol.%) of cuts or fractions increase with increasing the temperature of the fractions. This is due to the increase of the aromatic content and decrease of paraffinic content of the fractions(i.e. increasing the TB, and MW of cuts). Petroleum stocks that have low *API* gravity have much flatter distillation curves than those petroleum stocks of high *API* gravity. This is due to the highly naphthenic contents of low *API* petroleum stocks that characterized by their high boiling point, while the high *API* petroleum stocks have highly contents of paraffinic that can be characterized as low boiling point materials. Because of the close relations between the *TBP* curves and *EFV* curves. It is expected that the behavior of the *TBP* curves that mentioned above for the 18 petroleum stocks are also true for the *EFV* curves for these petroleum stocks. This is shown by Figs. 5-16 – 5-30 for *EFV* curves for petroleum stocks of number 1 to 15, and Figs. 5-33 – 5-

36 for *EFV* curves for petroleum stocks of number 16, 17 and 18. It is also noted that the *EFV* curves have flatter slopes, than the *TBP* curves.

For petroleum stocks of number 16, 17 and 18, Figs. 5-37 – 5-39 illustrate the specific gravity curves for these petroleum stocks. As shown by these curves, the specific gravity for each cut or fraction increases with increasing the volume percent distilled and the *TBP* of the fractions. This is due to the increase of the aromatic content and decrease of the paraffinic content of the fractions(i.e increasing the MW of cuts). Usually, the specific gravity of aromatic and naphthenic hydrocarbons are higher than those for paraffinic hydrocarbons having the same number of atoms (and also the same molecular weight).

For data of part two of the present work, four Iraqi crude oils were used for obtaining the *TBP* and specific gravity curves. These crudes are Kirkuk, Basrah, Jambour and Bai – Hassan crude oils. The *API* gravity of these crudes were 36.1, 30.1, 37.7 and 31.4, respectively. These crudes oil can be considered as paraffinic class **[22]**.

Figures 5-40 – 5-43 illustrate the *TBP* for Kirkuk, Basrah, Jambour and Bai – Hassan crude oils. As shown by these figures, that the total distillate from Kirkuk, Basrah, Jambour and Bai – Hassan (for IBP-370 ^{0}C)were 67.07 vol.% (63 wt. %), 63.93 vol.% (57.94 wt. %), 67.76 vol.% (62.19 wt. %) and 64.28 vol.% (57.34 wt. %), respectively. Also the figures show that the volume percent distilled increases with increasing the vapor temperature of each fraction, this is due to the increasing of the aromatic and naphthenic contents and decreasing of paraffinic contents. The *TBP* curves for these crudes have also a steepest distillation slopes due to the highly content of paraffin compounds. The slope of distillation curve usually measured at 10% and 70% distillation temperatures. The general shapes of the obtained *TBP* curves for the four Iraqi crude oils have a good agreement with the general shapes of *TBP* curves given by literature **[3, 22]**.

Figures 5-44 – 5-47 illustrate the specific gravity curves for Kirkuk, Basrah, Jambour and Bai – Hassan crude oils. As shown by the above figures, that the specific gravity for each cut or fraction increases with increasing the volume percent distilled (or TB &MW), this is due the increasing of aromatic and naphthenic contents and decreasing the paraffinic contents. The specific gravity of aromatic and naphthenic hydrocarbons are higher than those for paraffinic hydrocarbons having the same number of atoms (or molecular weight). The obtained specific gravity curve shapes for the four Iraqi crude oils have a good agreement with the general shapes of specific gravity curves observed in literature **[22]**.

7.1.2 Estimated physical properties and material balance for cuts or fractions

For pseudo – components methods, the physical properties and material balance must be obtained. Both physical properties and material balance are performed in the characterization steps that discussed previously. The physical properties including the estimation of basic properties such as molecular weight (*MW*), critical temperatures (*Tc*), critical pressures (*Pc*), acentric factor (ω) and other physical properties such as molar volume (V^L) and solubility parameters (δ). The material balance includes the conversion of the volume for each cut to weight and finally to moles. The number of cuts were 40.

Table 7-1 gives the physical properties for the 40 cuts of petroleum stock of number 1, while Tables H-1 – H-17 in Appendix H give the physical properties of the 40 cuts of the petroleum stocks of number 2 to 18. As shown in Table 7-1 and Tables H-1 – H-17 that the molecular weight (*MW*), critical temperature (*Tc*), acentric factors (ω) and molal volumes V^L for each cut increase with increasing the *TB* and the specific gravity for each cut, while the critical pressures (*Pc*) and solubility parameters (δ) for each cut decrease with increasing the *TB* and specific gravity of each cut. The reason behind this behavior is that when the *TB* and the specific gravity are increase the aromatic and naphthenic contents are increased and the paraffinic contents are decreased. The latter behavior for the cuts have a good agreement with the published physical properties for pure hydrocarbons of different family types (paraffins, aromatics, …*etc*) **[88, 91]**.

Table 7-2 gives the material balance for 40 cuts of the petroleum stock of number 1, while Tables H-18 – H-34 in Appendix H give the material balance for 40 cuts of the petroleum stocks of number 2 to 18. As shown in Table 7-2 and

Tables H-18 – H-34, that the weight of each cut increases due to increasing the specific gravity and *TB* of each cut. This is due to the proportional relations between the specific gravity and the estimated weight for each cut {as indicated by equation (5.4)}. The estimated moles for each cut decreases with the increasing of the specific gravity and weight for each cut, this is due to reverse proportional between the specific gravity and weight with the estimated moles for each cut {as indicated by equation (5.6)}. The volume percent (vol.%), weight percent (wt.%) and mole percent (mol.%) also are given in these tables. The volume percent (vol.%) for each cut remains constant since each petroleum stock is divided into 40 cuts of equal volume percent of 2.5% (100 cm^3). The weight percent (wt.%) and mole percent (mol.%) have the same behavior of estimated weights and moles for each cut that discussed above.

For the four Iraqi crude oils (data for part two of the present work), the above mentioned behaviors of the physical properties and the material balance for each cut are also observed. Table 7-3 gives the physical properties for Kirkuk crude oil, while Tables H-35 – H-37 of Appendix H give the physical properties for Basrah, Jambour and Bai – Hassan crude oils respectively, while Table 7-4 gives the material balance for Kirkuk crude oil and Tables H-38 – H-40 give the material balance for Basrah, Jambour and Bai – Hassan crude oils respectively.

Table 7-1 Physical properties for petroleum stock No. 1

Cut	*TB*, °C	*Sp.gr*	*MW*	*Tc*, °C	*Pc*, kPa	ω	V^L, cm^3/mol$^{(15)}$	δ, J/cm$^{3(25)}$
1	66.56	0.7038	85.04	242.33	3376.82	0.2546	120.83	29.05
2	75.88	0.7157	89.33	254.18	3312.29	0.2640	124.81	29.08
3	86.65	0.7283	94.37	267.56	3230.17	0.2755	129.58	29.09
4	98.63	0.7411	100.11	282.09	3133.16	0.2889	135.08	29.09
5	111.57	0.7538	106.49	297.42	3025.05	0.3039	141.28	29.06
6	125.24	0.7660	113.46	313.27	2909.86	0.3204	148.12	29.01
7	139.44	0.7777	120.99	329.39	2791.27	0.3381	155.57	28.93
8	153.97	0.7888	129.02	345.56	2672.49	0.3567	163.56	28.82
9	168.68	0.7993	137.51	361.63	2555.97	0.3761	172.04	28.69
10	183.40	0.8091	146.40	377.43	2443.61	0.3960	180.94	28.55
11	198.01	0.8183	155.63	392.86	2336.71	0.4163	190.19	28.39
12	212.40	0.8268	165.15	407.81	2236.04	0.4367	199.74	28.21
13	226.45	0.8347	174.87	422.21	2142.10	0.4571	209.50	28.03
14	240.09	0.8420	184.74	436.01	2054.99	0.4774	219.40	27.85
15	253.28	0.8488	194.69	449.18	1974.59	0.4974	229.38	27.66
16	265.96	0.8550	204.67	461.69	1900.66	0.5171	239.37	27.46
17	278.11	0.8608	214.62	473.55	1832.87	0.5363	249.33	27.28
18	289.72	0.8661	224.52	484.77	1770.69	0.5551	259.21	27.09
19	300.82	0.8711	234.32	495.40	1713.64	0.5733	268.99	26.91
20	311.43	0.8757	244.03	505.46	1661.15	0.5911	278.67	26.73
21	321.60	0.8800	253.65	515.03	1612.68	0.6084	288.25	26.55
22	331.40	0.8840	263.24	524.19	1567.58	0.6255	297.78	26.38
23	340.91	0.8878	272.84	533.01	1525.27	0.6423	307.32	26.21
24	350.25	0.8915	282.56	527.24	1509.88	0.8167	316.95	26.05
25	359.54	0.8951	292.52	535.23	1465.95	0.8396	326.82	25.88
26	368.91	0.8986	302.89	543.25	1422.77	0.8629	337.07	25.71
27	378.52	0.9021	313.86	551.41	1379.66	0.8871	347.91	25.53
28	388.56	0.9058	325.69	559.88	1335.92	0.9127	359.58	25.34
29	399.23	0.9095	338.70	568.81	1290.81	0.9403	372.38	25.14
30	410.73	0.9135	353.23	578.38	1243.73	0.9662	386.67	24.92
31	423.30	0.9178	369.76	588.76	1194.00	0.9967	402.89	24.68
32	437.19	0.9224	388.83	600.13	1141.16	1.0301	421.56	24.41
33	452.68	0.9273	411.14	612.71	1084.70	1.0672	443.37	24.11
34	470.04	0.9327	437.54	629.69	1024.38	1.1083	469.09	23.77
35	789.60	0.9386	469.13	642.28	960.00	1.1542	499.80	23.39
36	511.66	0.9451	507.28	659.69	891.67	1.2053	536.76	22.95
37	536.57	0.9521	553.82	679.14	819.65	1.2623	581.70	22.46
38	564.71	0.9597	611.14	700.86	744.45	1.3256	636.82	21.90
39	596.42	0.9679	682.42	725.05	666.87	1.3956	705.08	21.28
40	632.15	0.9767	772.10	751.97	587.86	1.4728	790.52	20.57

Table 7-2 Material balance for petroleum stock No. 1

Cut	*TB*, °C	*Sp.gr*	*MW*	Vol., cm^3	Wt., gm	Mole, g-mole	Z_i, vol.%	Z_i, wt.%	Z_i, mol.%
1	66.56	0.7038	85.04	100	70.38	0.8276	2.5	2.04	5.12
2	75.88	0.7157	89.33	100	71.57	0.8012	2.5	2.07	4.95
3	86.65	0.7283	94.37	100	72.83	0.7718	2.5	2.11	4.77
4	98.63	0.7411	100.11	100	74.11	0.7403	2.5	2.15	4.58
5	111.57	0.7538	106.49	100	75.38	0.7078	2.5	2.19	4.38
6	125.24	0.7660	113.46	100	76.60	0.6751	2.5	2.22	4.18
7	139.44	0.7777	120.99	100	77.77	0.6428	2.5	2.25	3.98
8	153.97	0.7888	129.02	100	78.88	0.6114	2.5	2.29	3.78
9	168.68	0.7993	137.51	100	79.93	0.5813	2.5	2.32	3.59
10	183.40	0.8091	146.40	100	80.91	0.5527	2.5	2.35	3.42
11	198.01	0.8183	155.63	100	81.83	0.5258	2.5	2.37	3.25
12	212.40	0.8268	165.15	100	82.68	0.5007	2.5	2.40	3.10
13	226.45	0.8347	174.87	100	83.47	0.4773	2.5	2.42	2.95
14	240.09	0.8420	184.74	100	84.20	0.4558	2.5	2.44	2.82
15	253.28	0.8488	194.69	100	84.88	0.4360	2.5	2.46	2.70
16	265.96	0.8550	204.67	100	85.50	0.4178	2.5	2.48	2.58
17	278.11	0.8608	214.62	100	86.08	0.4011	2.5	2.50	2.48
18	289.72	0.8661	224.52	100	86.61	0.3858	2.5	2.51	2.39
19	300.82	0.8711	234.32	100	87.11	0.3718	2.5	2.53	2.30
20	311.43	0.8757	244.03	100	87.57	0.3588	2.5	2.54	2.22
21	321.60	0.8800	253.65	100	88.00	0.3469	2.5	2.55	2.15
22	331.40	0.8840	263.24	100	88.40	0.3358	2.5	2.56	2.08
23	340.91	0.8878	272.84	100	88.78	0.3254	2.5	2.57	2.01
24	350.25	0.8915	282.56	100	89.15	0.3155	2.5	2.58	1.95
25	359.54	0.8951	292.52	100	89.51	0.3060	2.5	2.60	1.89
26	368.91	0.8986	302.89	100	89.86	0.2967	2.5	2.61	1.83
27	378.52	0.9021	313.86	100	90.21	0.2874	2.5	2.62	1.78
28	388.56	0.9058	325.69	100	90.58	0.2781	2.5	2.63	1.72
29	399.23	0.9095	338.70	100	90.95	0.2685	2.5	2.64	1.66
30	410.73	0.9135	353.23	100	91.35	0.2586	2.5	2.65	1.60
31	423.30	0.9178	369.76	100	91.78	0.2482	2.5	2.66	1.54
32	437.19	0.9224	388.83	100	92.24	0.2372	2.5	2.67	1.47
33	452.68	0.9273	411.14	100	92.73	0.2255	2.5	2.69	1.39
34	470.04	0.9327	437.54	100	93.27	0.2132	2.5	2.70	1.32
35	789.60	0.9386	469.13	100	93.86	0.2001	2.5	2.72	1.24
36	511.66	0.9451	507.28	100	94.51	0.1863	2.5	2.74	1.15
37	536.57	0.9521	553.82	100	95.21	0.1719	2.5	2.76	1.06
38	564.71	0.9597	611.14	100	95.97	0.1570	2.5	2.78	0.97
39	596.42	0.9679	682.42	100	96.79	0.1418	2.5	2.81	0.88
40	632.15	0.9767	772.10	100	97.67	0.1265	2.5	2.83	0.78
			Total	**4000**	**3449.1**	**16.17**	**100**	**100**	**100**

Table 7-3 Physical properties for Kirkuk crude oil

Cut	*TB*, °C	*Sp.gr*	*MW*	*Tc*, °C	*Pc*, kPa	ω	V^L, cm^3/mol$^{(15)}$	δ, J/cm$^{3(25)}$
1	35.16	0.5217	58.97	165.34	2079.82	0.3344	113.05	28.04
2	50.02	0.6342	75.84	209.80	2987.62	0.2690	119.58	28.24
3	64.19	0.6758	83.62	233.52	3143.25	0.2679	123.74	28.56
4	77.72	0.7043	90.24	253.32	3167.78	0.2745	128.14	28.78
5	90.70	0.7262	96.42	270.98	3137.89	0.2841	132.77	28.94
6	103.21	0.7442	102.39	287.20	3081.96	0.2951	137.58	29.04
7	115.31	0.7595	108.27	302.34	3013.02	0.3069	142.55	29.11
8	127.09	0.7729	114.13	316.67	2937.56	0.3192	147.67	29.14
9	138.59	0.7847	120.03	330.33	2859.06	0.3318	152.95	29.14
10	149.90	0.7954	126.01	343.48	2779.21	0.3448	158.41	29.12
11	161.08	0.8052	132.11	356.23	2699.09	0.3580	164.08	29.08
12	172.18	0.8141	138.39	368.66	2618.99	0.3717	169.99	29.01
13	183.27	0.8225	144.90	380.87	2539.15	0.3857	176.18	28.93
14	194.41	0.8302	151.68	392.92	2459.63	0.4002	182.71	28.83
15	205.64	0.8374	158.79	404.88	2380.37	0.4153	189.62	28.72
16	217.03	0.8443	166.30	416.81	2301.22	0.4311	196.98	28.58
17	228.62	0.8507	174.25	428.75	2222.23	0.4475	204.84	28.43
18	240.48	0.8568	182.74	440.76	2143.22	0.4649	213.28	28.26
19	252.63	0.8626	191.82	452.88	2064.28	0.4832	222.37	28.07
20	265.12	0.8682	201.59	465.13	1985.36	0.5026	232.20	27.87
21	278.01	0.8735	212.13	477.56	1906.52	0.5232	242.86	27.64
22	291.33	0.8785	223.55	490.19	1827.75	0.5452	254.46	27.39
23	305.11	0.8834	235.96	503.05	1749.26	0.5687	267.10	27.13
24	319.40	0.8881	249.48	516.15	1671.12	0.5939	280.91	26.84
25	334.22	0.8926	264.25	529.52	1593.50	0.6210	296.04	26.54
26	349.61	0.8970	280.42	528.76	1544.26	0.8066	312.63	26.21
27	365.61	0.9012	298.17	541.83	1457.92	0.8487	330.87	25.87
28	382.23	0.9052	317.68	555.20	1372.19	0.8937	350.94	25.51
29	399.51	0.9092	339.18	568.87	1287.38	0.9418	373.07	25.12
30	417.46	0.9130	362.91	582.85	1203.76	0.9871	397.49	24.72
31	436.11	0.9167	389.14	597.17	1121.64	1.0363	424.50	24.30
32	455.47	0.9203	418.18	611.83	1041.30	1.0871	454.39	23.87
33	475.57	0.9238	450.38	626.83	963.01	1.1395	487.52	23.42
34	496.42	0.9272	486.14	642.18	887.04	1.1934	524.30	22.95
35	518.03	0.9305	525.91	657.89	813.64	1.2487	565.16	22.47
36	540.42	0.9338	570.19	673.95	743.05	1.3055	610.62	21.98
37	563.58	0.9369	619.57	690.39	675.47	1.3636	661.27	21.47
38	587.52	0.9400	674.68	707.18	611.10	1.4229	717.72	20.95
39	612.26	0.9430	736.32	724.34	550.05	1.4833	780.79	20.42
40	637.79	0.9460	805.31	741.87	492.47	1.5448	851.29	19.89

Table 7-4 Material balance for Kirkuk crude oil

Cut	*TB*, °C	*Sp.gr*	*MW*	Vol., cm^3	Wt., gm	Mole, g-mole	Z_i, vol.%	Z_i, wt.%	Z_i, mol.%
1	35.16	0.5217	58.97	100	52.17	0.8846	2.5	1.54	5.01
2	50.02	0.6342	75.84	100	63.42	0.8362	2.5	1.88	4.73
3	64.19	0.6758	83.62	100	67.58	0.8082	2.5	2.00	4.57
4	77.72	0.7043	90.24	100	70.43	0.7804	2.5	2.09	4.42
5	90.70	0.7262	96.42	100	72.62	0.7532	2.5	2.15	4.26
6	103.21	0.7442	102.39	100	74.42	0.7268	2.5	2.20	4.11
7	115.31	0.7595	108.27	100	75.95	0.7015	2.5	2.25	3.97
8	127.09	0.7729	114.13	100	77.29	0.6772	2.5	2.29	3.83
9	138.59	0.7847	120.03	100	78.47	0.6538	2.5	2.32	3.70
10	149.90	0.7954	126.01	100	79.54	0.6313	2.5	2.36	3.57
11	161.08	0.8052	132.11	100	80.52	0.6095	2.5	2.38	3.45
12	172.18	0.8141	138.39	100	81.41	0.5883	2.5	2.41	3.33
13	183.27	0.8225	144.90	100	82.25	0.5676	2.5	2.44	3.21
14	194.41	0.8302	151.68	100	83.02	0.5473	2.5	2.46	3.10
15	205.64	0.8374	158.79	100	83.74	0.5274	2.5	2.48	2.99
16	217.03	0.8443	166.30	100	84.43	0.5077	2.5	2.50	2.87
17	228.62	0.8507	174.25	100	85.07	0.4882	2.5	2.52	2.76
18	240.48	0.8568	182.74	100	85.68	0.4689	2.5	2.54	2.65
19	252.63	0.8626	191.82	100	86.26	0.4497	2.5	2.55	2.55
20	265.12	0.8682	201.59	100	86.82	0.4307	2.5	2.57	2.44
21	278.01	0.8735	212.13	100	87.35	0.4118	2.5	2.59	2.33
22	291.33	0.8785	223.55	100	87.85	0.3930	2.5	2.60	2.22
23	305.11	0.8834	235.96	100	88.34	0.3744	2.5	2.62	2.12
24	319.40	0.8881	249.48	100	88.81	0.3560	2.5	2.63	2.02
25	334.22	0.8926	264.25	100	89.26	0.3378	2.5	2.64	1.91
26	349.61	0.8970	280.42	100	89.70	0.3199	2.5	2.66	1.81
27	365.61	0.9012	298.17	100	90.12	0.3022	2.5	2.67	1.71
28	382.23	0.9052	317.68	100	90.52	0.2849	2.5	2.68	1.61
29	399.51	0.9092	339.18	100	90.92	0.2680	2.5	2.69	1.52
30	417.46	0.9130	362.91	100	91.30	0.2516	2.5	2.70	1.42
31	436.11	0.9167	389.14	100	91.67	0.2356	2.5	2.71	1.33
32	455.47	0.9203	418.18	100	92.03	0.2201	2.5	2.73	1.25
33	475.57	0.9238	450.38	100	92.38	0.2051	2.5	2.74	1.16
34	496.42	0.9272	486.14	100	92.72	0.1907	2.5	2.75	1.08
35	518.03	0.9305	525.91	100	93.05	0.1769	2.5	2.76	1.00
36	540.42	0.9338	570.19	100	93.38	0.1638	2.5	2.77	0.93
37	563.58	0.9369	619.57	100	93.69	0.1512	2.5	2.77	0.86
38	587.52	0.9400	674.68	100	94.00	0.1393	2.5	2.78	0.79
39	612.26	0.9430	736.32	100	94.30	0.1281	2.5	2.79	0.72
40	637.79	0.9460	805.31	100	94.60	0.1175	2.5	2.80	0.66
			Total	**4000**	**3377.1**	**17.67**	**100**	**100**	**100**

7.1.3 Part one (testing and developing part)

7.1.3.1 Estimated *EFV* curve using unmodified models mode

The *EFV* curve (or flash volumes) for 18 petroleum stocks estimated by using the Raizi – Daubert graphical method and five pseudo – component methods using unmodified thermodynamic models mode. These models are SRK, PR, SPK + Van, PR + Van and Ideal *K* models. The total number of examined points were 106. The error analysis results are performed by using the *AAD%* and *AD%*, respectively (as shown by equation (5.14) for *AAD%* and (5.15) for *AD%*). The results of error analysis (*ADD%* and *AD%*) are divided into three regions, first region for the flash volume that are below or equal 25% vol.% (low flash volumes region) and the second region for the flash volumes that are above than 25% vol.% (high flash volumes region). Finally, the third region represents all flash volumes (including both low and high flash volumes). The reason behind this divisions of error analysis results, is to show the performance of all flash methods in prediction the *EFV* curves for each of these three regions. Each of Raizi – Daubert (RD graph) method and the five pseudo – components methods (SRK, PR, SRK + Van, PR + Van and Ideal K) have been handled as a separate flash method that are used for predication the *EFV* curve from the *TBP* curve. The above mentioned division of error analysis results will be used also with the other thermodynamic models modes (modified models No. 1 mode and the present work suggested modifications mode).

Table 7-5 gives the error analysis for 18 petroleum stocks using the *ADD%* and *AD%* for the three regions of the flash volumes. A more details including the predicted flash volumes, *ADD%* and *AD%* for each petroleum stock and for the three regions of the flash volumes are given in Tables I-1, I-2 and I-3 in Appendix I, respectively.

Table 7-5 Error analysis for 18 petroleum stocks using unmodified models mode flash methods

Flash method	Low flash volumes region		High flash volumes region		All flash volumes region	
	AAD%	*AD%*	*AAD%*	*AD%*	*AAD%*	*AD%*
SRK	37.04	33.94	8.08	5.98	22.56	19.96
SRK + Van	38.36	35.63	9.71	8.60	24.03	22.12
PR	36.75	33.63	8.16	1.35	22.45	17.47
PR + Van	38.82	36.15	9.65	8.56	24.24	22.35
Ideal K	37.58	34.73	8.03	2.85	22.80	18.78
RD graph	33.35	13.82	10.27	-7.39	21.81	3.22
No. of points	53		53		106	

Table 7-5 indicates the fact that while nearly all of the flash methods can adequately predict the flash volumes (*EFV* curve) in the region of high flash volumes, on the other hand non of the flash methods are very reliable at low flash volumes. The above mentioned behavior of the used flash methods are due to the following reasons:

- For the Raizi – Daubert flash method (RD graph), the empirical nature of that method causes inadequate prediction of the data that are out of range of the data base that are used for developing the method, however, it works slightly better than the other flash methods since approximately 65% of the used data are included in the data base that are used in the developing the method (as shown in Table 5-1). Another source of poor performance of RD graph method is that the original method is developed for prediction the flash temperature at 10, 30, 50, 70 and 90 vol.%, thus any point out of that range must be interpolated or extrapolated to obtain the desired flash volumes and flash temperatures. In the present work, some of data points used have to be extrapolated or interpolated since they have volume percent differs than the original RD graph method (those points of 5 vol.%, 15 vol.%, 25 vol.%, …, *etc*). The above mentioned reason is one of the important limitations of the graphical method **[26]**.
- For SRK, PR, SRK + Van, PR + Van and Ideal K flash methods or pseudo – components methods, the important source of bad performance of these flash methods comes from the application of the original alfa function (α) correlations for both SRK and PR equations of state and also the original vapor pressure correlation

of Lee – Kasler. Since both of alfa function correlations (α) and Lee – Kasler vapor pressure correlation were developed by using the pure hydrocarbon of low molecular weight, it is so unlikely that these correlations are suitable for high molecular weight petroleum fractions, specially for the region of low flash volumes (as shown in Table 5-6).

- Referring to Table 5-1, approximately more than 65% of the data that were used for estimation the *EFV* curve from *TBP* curve are presented with incomplete *TBP* curves which means that the initial and final segments of the *TBP* must be estimated. Thus the missing portions of the *TBP* curve would be expected to exert important effluence of the predicted flash volumes or *EFV* curves.

For pseudo – components flash methods (SRK, PR, SRK + Van and Ideal K), it must be noted here, that some of the used petroleum stocks show slightly a good performance, having slightly good values of AAD% and AD%. The latter can be shown in Tables 7-6 and 7-7 in which the petroleum stocks of number 4, 5, 8, 10, 11, 12, 15 and 17 show slightly good values for both AAD% and AD% for all flash volumes regions.

Table 7-6 *AAD%* for 18 petroleum stocks that used in part one of the present work (for all flash volumes regions)

Petroleum stock No.	*AAD%*				
	SRK	SRK + Van	PR	PR + Van	Ideal *K*
1	36.76	39.20	38.56	39.45	38.86
2	35.74	35.77	36.40	35.55	35.74
3	29.69	32.98	31.14	32.66	30.79
4	10.03	12.00	8.48	12.22	9.21
5	7.78	8.07	5.30	7.53	6.28
6	36.98	36.31	35.54	36.62	35.81
7	34.33	34.57	32.26	34.88	32.52
8	12.45	12.27	14.69	12.42	14.27
9	53.09	52.30	51.64	52.71	51.99
10	17.78	18.58	19.33	18.89	17.51
11	12.12	12.08	12.60	12.90	12.21
12	6.71	8.13	10.04	8.48	9.84
13	29.18	29.58	28.59	29.81	29.45
14	37.09	36.45	36.26	36.62	36.76
15	3.93	6.10	3.71	6.01	3.23
16	11.32	17.54	9.69	17.77	11.06
17	9.70	11.72	12.17	12.19	12.49
18	34.49	36.28	32.48	36.54	34.42

Table 7-7 *AD%* for 18 petroleum stocks that used in part one of the present work (for all flash volumes regions)

Petroleum stock No.	*AD%*				
	SRK	SRK + Van	PR	PR + Van	Ideal *K*
1	36.53	39.20	34.64	39.45	34.88
2	29.45	29.55	28.52	29.52	28.54
3	29.41	32.98	26.44	32.66	27.83
4	10.03	12.00	7.70	12.22	8.89
5	7.74	8.07	4.42	7.53	6.04
6	36.98	36.31	35.54	36.62	35.81
7	34.33	34.57	32.26	34.88	32.52
8	-2.77	-0.59	-5.49	1.20	-4.11
9	53.09	52.30	51.64	52.71	51.99
10	13.98	14.78	8.31	15.63	7.65
11	-2.35	-0.33	-4.60	-0.42	-3.65
12	5.79	8.13	3.18	8.48	4.06
13	29.18	29.58	28.59	29.81	29.45
14	37.09	36.45	36.26	36.62	36.76
15	-0.21	2.07	-3.60	2.28	-2.80
16	11.32	17.54	8.36	17.77	10.47
17	5.13	10.86	1.03	11.36	5.81
18	34.49	36.28	32.48	36.54	34.42

7.1.3.2 Estimated *EFV* curve using modified models No. 1 mode (existing in literature)

For the modified models No. 1 mode (existing in literature), the improvements of the SRK, SRK + Van and Ideal *K* flash methods are accomplished using the Sim – Daubert correlation {equation (3.108)} for alfa function (α) calculation, while the Twu et al. alfa function correlations {equations (3.103) – (3.105)} are used with the PR and PR + Van flash methods.

For SRK, SRK + Van and Ideal *K*, the application of Sim – Daubert alfa function (α) modification required that the *TMEP* term (defined in section 3.7.3) be negative. As mentioned by **Sim – Daubert [1]**, that any petroleum stock has negative values of *TMEP* and displays a serious values of *AD%* or bais indicating that the original correlation of alfa function given by Soave {equation (3.76)} did not properly centered about the experimental data. For the 18 petroleum stocks only 5 petroleum stocks were found satisfied the Sim – Daubert requirements (representing 45 flash data points from 106 flash data points used). The latter means that only 43% of the flash data points will be modified. Table 7-8 gives the *TEMP* values, 20% *TBP* temperature and the *AD%* of all flash volumes region for the 5 petroleum stocks. As shown by Table 7-8, that the 5 petroleum stocks are really have a serious values of *AD%*.

Table 7-9 gives the error analysis for the five petroleum stocks using unmodified SRK, SRK + Van and Ideal *K* flash methods and for the three regions of flash volumes (low, high and all flash volumes). Table 7-10 gives the error analysis for the same petroleum stocks but using the modified SRK, SRK + Van and Ideal *K* flash methods (using Sim – Daubert alfa modification), while Tables I-4 – I-6 in Appendix I give the more details about these petroleum stocks including the predicted flash volumes, *AAD%* and *AD%* for each petroleum stock and for the three regions of flash volumes (low, high and all flash volumes).

Table 7-8 *TMEP* values, 20% *TBP* and *AD%* values for five petroleum stocks that satisfy the Sim – Daubert requirements

Petroleum stock No.	20% *TBP* temperature, °C	20% *TBP* temperature, °F	*TEMP*	*AD%*		
				SRK	SRK + Van	Ideal *K*
3	197.78	388	-4.01	29.41	32.98	27.83
4	156.11	313	-0.01	10.03	12.00	8.89
9	252.22	486	-0.39	33.09	52.30	51.99
16	158.33	317	-1.9	11.32	17.54	10.07
18	177.22	351	-0.45	34.44	36.28	34.42

Table 7-9 Error analysis for the five petroleum stocks using unmodified models mode

Flash method	Low flash volumes region		High flash volumes region		All flash volumes region	
	AAD%	*AD%*	*AAD%*	*AD%*	*AAD%*	*AD%*
SRK	44.06	44.06	6.18	6.13	26.35	26.31
SRK + Van	46.21	46.21	8.54	8.54	29.28	29.28
Ideal - *K*	45.07	45.07	5.30	4.51	26.14	25.50
RD graph	30.65	-3.80	5.69	-4.85	15.12	-4.5
No. of points	17		28		45	

Table 7-10 Error analysis for the five petroleum stocks using modified models No. 1

Flash method	Low flash volumes region		High flash volumes region		All flash volumes region	
	AAD%	*AD%*	*AAD%*	*AD%*	*AAD%*	*AD%*
SRK	28.54	12.61	1.95	0.99	15.40	6.91
SRK + Van	45.49	45.49	8.48	8.48	28.88	28.88
Ideal K	44.29	44.29	5.28	4.51	25.73	25.12
No. of points	17		28		45	

As shown by Tables 7-9 and 7-10, that the modified SRK flash method has a reliable ability for prediction of flash volumes for the three regions of flash volumes (low, high and all flash volumes regions). Using the modified SRK flash method improves the values for *AAD%* and *AD%* for the three regions of flash volumes by more than 30% and 60% for *AAD%* and *AD%* respectively (especially for the low flash volumes regions) as compared with Tables 7-10 and 7-9. Also, it indicates that the performance of the modified SRK flash method was some what the same as the RD graph flash method.

It can be seen also from above mentioned error analysis of Tables 7-9 and 7-10, that the modified Sim – Daubert alfa function correlation has slightly little effect on the performance of SRK + Van and Ideal *K* flash methods as compared with unmodified flash methods. This is due to the following reasons:

– For the SRK + Van flash method, and since the flash pressure used was atmospheric pressure, it is expected that the ratio of the partial vapor fugacity coefficient to the saturation vapor fugacity coefficient of equation (3.147) for each cut (ϕ_i^V / ϕ_i^{Vs}) is approximately closer to unity, consequently this makes the effect of the modified alfa function correlation given by Sim – Daubert has a slightly little effect on the performance of the SRK + Van flash method.

– For the Ideal *K* flash method, the vapor pressure term (P_i^s) of equation (3.160) is the most important term, thus the other terms of equation (3.160) including the alfa function term have a miner effect. Consequently, the modified alfa function correlation given by Sim – Daubert has a slightly little effect on the performance of the Ideal *K* flash method.

For the PR and PR + Van flash methods, the Twu et al. modified alfa function correlation is used. All the 18 petroleum stocks are included in the Twn et al. modification of the alfa function (*i.e.* 106 flash data points used).

Table 7-11 gives the error analysis using *AAD%* and *AD%* for the 18 petroleum stocks using the unmodified PR and PR + Van flash methods and for the three categories of flash volumes (low, high and all flash volumes regions respectively).

Table 7-12 gives the error analysis using the *AAD%* and the *AD%* for the 18 petroleum stocks using the modified PR and PR + Van flash methods (*i.e.* using Twu alfa function modification) and for the three regions of the flash volumes. A complete error analysis for each of the 18 petroleum stocks, including the predicted flash volumes, *AAD%* and *AD%* are given in Tables I-7, I-8 and I-9 in Appendix I. As shown in Tables 7-11 and 7-12 show that there is no significant improvement of the modified Twu et al. alfa function correlation on the performance of PR and PR + Van flash methods as compared to unmodified flash methods. This is due to the following reasons:

– For PR flash method, Twu et al. suggested a linear function of alfa function to the acentric factor {*i.e.* equation (3.103)} and they used the vapor pressure data from the DIPPR data bank **[78]**, to obtain the developed alfa function correlation. The vapor pressure data used for their developing include the vapor pressure of hydrocarbons corresponding to C_1 through C_{16}. Unfortunately, the latter hydrocarbons still can be classified as low molecular weight hydrocarbons as compared to high molecular weight of petroleum fractions. For petroleum the carbon number (C_N) and the molecular weight (MW) can reach to more than C_{35} and 700, respectively **[7]**.

– For PR + Van flash method, the Twu et al. alfa function correlation have the same effect of the Sim – Daubert alfa function effect on the SRK + Van flash method that discussed previously.

Table 7-11 Error analysis for the 18 petroleum stocks using unmodified models mode

Flash Method	Low flash volumes region		High flash volumes region		All flash volumes region	
	AAD%	*AD%*	*AAD%*	*AD%*	*AAD%*	*AD%*
PR	38.64	35.48	8.16	1.35	23.40	18.42
PR + Van	40.71	38.04	9.65	8.56	25.18	23.30
No. of points	53		53		106	

Table 7-12 Error analysis for the 18 petroleum stocks using modified models No. 1 mode

Flash Method	Low flash volumes region		High flash volumes region		All flash volumes region	
	AAD%	*AD%*	*AAD%*	*AD%*	*AAD%*	*AD%*
PR	38.46	35.25	8.46	1.32	23.46	19.52
PR + Van	40.30	38.00	9.44	7.94	24.90	23.10
No. of points	53		53		106	

7.1.3.3 Estimated *EFV* curve using the present work of suggested modifications mode (modified models No. 2 mode)

For the present work of suggested modifications mode (modified models No. 2 mode), the improvement of the SRK, SRK + Van, PR, PR + Van and Ideal *K* flash methods were accomplished using the suggested a new vapor pressure correlation {*i.e.* equation (6.10)}. The application of the suggested new vapor pressure required that the *TEMP* for the interested petroleum stocks be negative or positive higher or equal to 4. For the 18 petroleum stocks investigated, only 10 petroleum stocks (represented 61 flash data points out of 106 flash data points) were found to satisfy the above requirements. The latter means that 58% of the used flash data points will be modified. The *TEMP* values and the 20% *TBP* temperatures for these petroleum stocks are given in Table 7-13.

Table 7-13 *TEMP* values and 20% *TBP* temperature for ten petroleum stocks that satisfy the suggested vapor pressure correlation requirements

Petroleum stock No.	20% *TBP* temperature, °C	20% *TBP* temperature, °F	*TEMP*	*AD%*
				Ideal *K*
1	148.89	300.0	4.80	34.88
2	132.22	270.0	10.00	28.54
3	197.78	388.0	-4.01	27.83
6	125.00	257.0	10.00	35.81
7	127.78	262.0	6.50	32.52
9	252.22	486.0	-0.39	51.99
13	108.00	226.4	9.21	29.45
14	232.78	451.0	10.00	36.76
16	158.33	317.0	-1.59	10.47
18	177.22	351.0	-0.14	34.42

Table 7-14 gives the error analysis for the ten petroleum stocks using the unmodified flash methods (*i.e.* SRK, SRK + Van, PR, PR + Van and Ideal *K* flash methods). While Table 7-15 gives the error analysis for the same ten petroleum stocks using the present work of suggested modifications (modified models No. 2) with the SRK, SRK + Van, PR, PR + Van and Ideal *K* flash methods. The complete information about the predicted flash volumes and error analysis (including *AAD%* and *AD%*) for each petroleum stock are given in details in Tables I-10, I-11 and I-12 in Appendix I.

Table 7-14 Error analysis for ten petroleum stocks using unmodified models mode

Flash Method	Low flash volumes region		High flash volumes region		All flash volumes region	
	AAD%	*AD%*	*AAD%*	*AD%*	*AAD%*	*AD%*
SRK	53.90	53.59	10.53	9.74	23.51	31.31
SRK + Van	55.30	55.07	12.51	11.73	24.98	33.04
PR	53.76	53.48	9.08	6.27	23.40	29.49
PR + Van	55.55	55.34	12.62	11.85	25.18	33.24
Ideal K	54.59	54.35	9.64	7.40	23.75	30.49
RD graph	25.95	-5.69	10.92	-7.83	21.81	-7.42
No. of points	30		31		61	

Table 7-15 Error analysis for ten petroleum stocks using the present work suggested modification mode (modified models No. 2 mode)

Flash method	Low flash volumes region		High flash volumes region		All flash volumes region	
	AAD%	*AD%*	*AAD%*	*AD%*	*AAD%*	*AD%*
SRK	35.35	32.96	8.48	7.26	21.69	19.90
SRK + Van	24.33	21.16	8.68	4.95	16.38	12.92
PR	35.40	33.69	6.89	3.42	20.91	18.31
PR + Van	25.03	22.20	8.79	5.09	17.00	13.50
Ideal *K*	23.42	20.08	8.07	0.12	15.62	9.94
No. of points	30		31		61	

As shown in Tables 7-14 and 7-15, the performance of the modified flash method (using the suggested vapor pressure correlation) were improved significantly as compared with the unmodified flash methods and the RD graph method using the same data points. The most improvement occurred in the low region of flash volumes, in which the values of *AAD%* and *AD%* improved by more than 30% for SRK and PR flash methods and by more than 50% for SRK + Van, PR + Van flash methods. Improvements can be also shown in the high region of flash volumes, in which the values of *AAD%* and *AD%* improved by more than 20% for SRK and PR flash methods and by more than 30% for the SRK + Van and PR + Van flash methods (however the *AD%* showed more than 45% improvement for SRK + Van). For the region of all flash volumes, the improvements of *AAD%* and *AD%* were by more than 10% and 30% respectively for both SRK and PR flash methods, while the improvements of the *AAD%* and *AD%* were by more than 30% and 50% respectively for both SRK + Van and PR + Van flash methods.

The important improvement in *AAD%* and *AD%* values occurred by using the modified Ideal *K* flash method (as compared with unmodified flash methods and RD graph method). The improvements include the three regions of flash volumes. Using the modified Ideal *K* flash method, the *AAD%* and *AD%* values improved by more than 50% for the low flash volumes region. For the high flash volumes region the improvements in *AAD%* and *AD%* values were by more than 10% and 70% respectively, while for the all flash volumes region, the improvement of *AAD%* and *AD%* values were by more than 30% and 60% respectively. The above mentioned error analysis indicates that the Ideal *K* flash method was most accurate method for estimation the *EFV* curves as compared with the other unmodified flash methods (SRK, PR, SRK + Van, PR + Van and Ideal *K*) and the RD graph flash method.

The reasons behind the above mentioned improvements in the values of *AAD%* and *AD%* for the modified flash methods (SRK, PR, SRK + Van, PR + Van and Ideal *K*) can be summarized as follows:

- For the Ideal *K* flash method, the ideal solution *K* – value equation is used with this method {equation (3.160)}. The vapor pressure term of equation (3.160) is the most important term of that equation. For the unmodified Ideal K flash method, the Lee – Kasler correlation {equation (3.113)}, the Lee – Kasler correlation was developed by using the vapor pressure of pure low molecular weight hydrocarbons, consequently it is expected that this correlation will not be suitable for the high molecular weight petroleum fractions. In the suggested new vapor pressure correlation, the flash data points of the 106 petroleum stocks were used with conjunction of the Ideal K solution equation for developing the coefficients of the new vapor pressure correlation {equation (6.10)}, consequently this methodology improved the performance of the correlation for high molecular weight petroleum fractions.
- For SRK and PR flash methods, the SRK and PR EOS were used for estimation the *K* – values by using equation (3.60). As mentioned previously that the most important term of SRK and PR EOS is the alfa function term. For the unmodified SRK and PR flash method, the alfa function terms were calculated by

using equations (3.76) and (3.90) respectively. The m terms for the above mentioned equations were correlated by using the acentric factor for each cut, that estimated by using the Lee – Kasler correlations {equations (3.12) and (3.13)}. Both equations (3.12) and (3.13) are correlated by using the vapor pressure of the low molecular weight hydrocarbons, consequently, it is expected that the m terms for original alfa functions (α) (and thus the alfa function terms) for both SRK and PR EOS will not be suitable for high molecular weight petroleum fractions. For modified SRK and PR flash methods the m terms for the alfa functions of the SRK and PR EOS were calculated using the suggested modified acentric factors for each cut (ω). The suggested modified acentric factor (ω) was calculated using Pitzer et al. equation {equation (3.78)} with the using of the suggested new vapor pressure correlation {equation (6.10)}. Table 7-16 gives the comparison between the Lee – Kasler acentric factors and the modified acentric factors for petroleum stock No. 1, while Tables J-1 to J-9 in Appendix J give the same comparison for the petroleum stocks of Table 7-13. Tables 7-16 and J-1 to J-9 indicate that the using of suggested new vapor pressure correlation improved the estimation of the acentric factors for each cut by reducing their values (comparing to Lee – Kasler correlation for ω) for those cuts that have approximately of 450 °C (≈ 842 °F), while it increases their values for heavier cuts {above 450 °C (842 °F)}. The heavier cuts have the values of acentric factor greater than 1, the latter is expected for petroleum fractions **[20]**.

– For SRK + Van and PR + Van flash methods, since the flash calculation was accomplished at atmospheric pressure, and as discussed in section 5.4.4.2, the most important term that affects the performance of the calculated *K* – values using equation (3.147) of the vapor pressure. Since the suggested new vapor pressure correlation was used instead of Lee – Kasler correlation the performance for both flash methods for estimation the flash volumes improved.

– For all modified flash methods, the above mentioned improvements in the values of *AAD%* and *AD%* represent the resultant of the addition of the second condition of the *TEMP* term that used in the improving the suggested new vapor pressure correlation in which the positive values of the *TEMP* term were also included (not just the negative values of *TEMP* term). To understand the reason behind the addition of the positive *TEMP* term in the present work which includes the developing the vapor pressure correlation, it must first understood that the philosophy of the *TEMP* term that originally used by Sim – Daubert alfa function developing. As mentioned by **Sim – Daubert [1]**, that any petroleum stocks that have negative values of *TEMP* displays a serious value of *AD%* or bais. This fact is extended by the present work to cover also the positive values of *TEMP* (which have values of more than 4) because in spite of the petroleum stock has positive *TEMP* values it is still has a serious value of *AD%* or bais. The latter fact can be shown by referring to Table 7-13 which is including the *TEMP* and *AD%* values for the ten petroleum stocks that satisfy the present work of suggested modifications requirements. Table 7-13 indicates that the Ideal *K* flash method shows a serious *AD%* with the positive and negative values of *TEMP* term (not just negative values as suggested by Sim – Daubert modification).

Table 7-16 Comparison between Lee – Kasler acentric factors and modified acentric factors for petroleum stock No. 1

Cut	*TB*, °C	*TB*, °F	Lee – Kasler ω^{LK}	Modified ω
1	66.56	151.81	0.2540	0.1622
2	75.87	168.57	0.2634	0.1729
3	86.65	187.96	0.2749	0.1861
4	98.62	209.52	0.2883	0.2016
5	111.56	232.81	0.3033	0.2192
6	125.23	257.41	0.3197	0.2388
7	139.43	282.97	0.3374	0.2599
8	153.96	309.13	0.3560	0.2825
9	168.66	335.60	0.3753	0.3061
10	183.39	362.10	0.3952	0.3307
11	197.99	388.39	0.4154	0.3559
12	212.38	414.28	0.4358	0.3816
13	226.43	439.57	0.4562	0.4074
14	240.07	464.13	0.4764	0.4333
15	253.26	487.86	0.4964	0.4590
16	265.94	510.68	0.5160	0.4843
17	278.08	532.54	0.5352	0.5092
18	289.70	553.45	0.5538	0.5336
19	300.79	573.42	0.5720	0.5574
20	311.40	592.52	0.5898	0.5807
21	321.57	610.82	0.6071	0.6034
22	331.36	628.46	0.6240	0.6257
23	340.88	645.58	0.6408	0.6478
24	350.21	662.39	0.8150	0.8024
25	359.50	679.10	0.8378	0.8282
26	368.87	695.96	0.8610	0.8546
27	378.48	713.27	0.8852	0.8820
28	388.52	731.34	0.9108	0.9109
29	399.19	750.54	0.9382	0.9419
30	410.68	771.23	0.9643	0.9759
31	423.26	793.86	0.9947	1.0135
32	437.14	818.86	1.0281	1.0556
33	452.63	846.73	1.0651	1.1033
34	469.99	877.98	1.1062	1.1576
35	489.54	913.18	1.1520	1.2199
36	511.60	952.89	1.2031	1.2914
37	536.52	997.73	1.2601	1.3737
38	564.65	1048.37	1.3233	1.4683
39	596.37	1105.46	1.3933	1.5769
40	632.09	1169.76	1.4704	1.7010

7.1.3.4 Effect of measured or calculated parameters on the predicted flash volumes

It can be seen that even with the modification on the flash methods, there is a considerable *AAD%* and *AD%* (more than 25%) persist in the low flash volume predictions (first category of the flash volumes), while an acceptable *AAD%* and *AD%* (less than 10%) persist in the high flash volume predictions (second category of flash volumes). The considerable high *AAD%* and *AD%* persist in the low flash volume predictions arise the question whether any further improvement can be reached. In order to answer this question, it is first necessary to ensure that the accuracy of the flash methods used in the investigation are not limited by errors in the measured or calculated parameters. **Sim – Daubert [1]** achieved a useful study on the effect of the error of the measured or calculated parameters on the performance of the SRK flash method for prediction the *EFV* curve from the *TBP* curve. According to that study, the error in the prediction of flash volumes using SRK flash method can come from two sources, first the error in calculated basic characterization parameters such as molecular weight (*MW*), critical properties (*Tc, Pc*), acentric factor (ω) …etc. For petroleum fractions it is not possible to determine the error introduced through the uses of the characterization parameter correlations since experimental values for the molecular weight (*MW*), critical properties (*Tc, Pc*), acentric factors (ω) are unknowns. The estimated characterization parameters from the characterization correlations are usually compared to heavy n – alkane compared such as n – heptane and n – octane.

The other sources of error in the prediction of the flash volume can be introduced through the use of the measuring experimental parameter including flash temperature, flash pressure and the *TBP* curve. According to the *ASTM* standards part 18 (1971), the uncertainty in the thermocouple measurement is approximately ± 0.5 °C, while error in the recorded pressure ± 1%. What is more significant, however is that the repeatability of the *TBP* curve. According to *ASTM* D 287 – 82, the repeatability is defined as the difference between successive tests results obtained by the same operator with the same apparatus under constant operating conditions on identical test material, would in the long run. The sensitivity of the

SRK flash method to slight errors in the measured parameter was evaluated and the results indicate that at low flash volumes (first category of flash volumes) a 0.5 °C error in the flash temperature can alter the SRK flash method predicted flash volume by 15%, while a 1% error in the pressure alters the predicted flash volume by 11%. The major source of error is the *TBP* curve. For low flash volume (first category of the flash volumes) a 5 °C error in *TBP* curve will result in a 100% error in the predicted flash volumes, while the 2.5 °C error in *TBP* can alter the predicted flash volume by more than 50% (> 50%). For the high flash volumes (second category), the error resulting from in accuracies in *TBP* curve is approximately 8%. The effect of errors in the flash temperature and flash pressure are negligible at high flash volumes (second category of flash volumes). Sim – Daubert expected that the above error analysis of the input parameter can be extended to other flash methods including the graphical methods.

For the present work, the repeatability for the *TBP* curves for the 18 petroleum stocks that used in part one investigations was ± 5 °C, while for the *TBP* curve for part two (four Iraqi crude oils) was ± 2.3 °C. While it is not possible to demonstrate conclusively that the inconsistencies in the flash method results are due to experimental errors, it is at least reasonable to conclude that the error in the basic characterization parameters (*MW, Tc, Pc, ω, ...etc*), and experimental parameters are capable of fully explaining the behavior of the flash methods used in present work investigations.

It must be noted here, and because of the sensitivity of the error in *TBP* curve on the performance of the used flash methods in the low flash volumes region, one must be careful when the working TBP curves were obtained by using the interpolation and extrapolation techniques. For the present work the latter curves were obtained using a minimum equation factor values (R^2) of 0.9888, to ensure a good accuracy for the working *TBP* curve.

7.1.4 Part two (Application part)

In part two of the present work, the *EFV* curves for four Iraqi crude oils are estimated from the *TBP* curves. These crude oils are Kirkuk, Basrah, Jambour and

Bai – Hassan crude oils. To identify which thermodynamic models mode must be used, the *TEMP* terms must be calculated by using the unmodified SRK and Ideal K flash methods. Table 7-17 gives the values of the *TEMP* for the Kirkuk, Basrah, Jambour and Bai – Hassan crude oils. As indicated in Table 7-17 that the values of *TEMP* are negative, and since the Ideal *K* flash method of modified models No. 2 mode is superior to other flash methods (i.e. SRK, SRK + Van, PR and PR + Van). Thus it is selected by the present work for estimation of the *EFV* curve from the given *TBP* curve for the four Iraqi crude oils. Tables 7-18 – 7-21 give the results of *EFV* or flash volumes data in vol.% for Kirkuk, Basrah, Jambour and Bai – Hassan crude oils, while Figs. 7-1 – 7-4 illustrate the *EFV* curves for Kirkuk, Basrah, Jambour and Bai – Hassan crude oils respectively. As shown in these figures that the temperature of each cut increases with increasing the volume distilled (vol.%), this is due to the increasing of the aromatic and naphthenic contents and decreasing the paraffinic content. The shape of the predicted *EFV* curves are more flatter than the shape of *TBP* curves obtained by the laboratory distillation unit (as indicated by Figs. 5-40 – 5-43) and this represent a good agreement with the behavior of the *EFV* curves with their *TBP* curves given in the literature **[3]**.

Table 7-17 *TEMP* values and 20% *TBP* temperature for four Iraqi crude oils

Crude name	20% *TBP* temperature, °C	20% *TBP* temperature, °F	*TEMP* (SRK)	*TEMP* (Ideal K)
Kirkuk	134	274	-1.11	-0.08
Basrah	170	338	-4.57	-4.14
Jambour	171	339	-4.53	-4.05
Bai – Hassan	136	276	-1.5	-0.09

Table 7-18 Predicted flash volumes (*EFV* curves) for Kirkuk crude oil

Flash temperature, °C	Flash temperature, °F	Predicted flash volumes, vol. %
148.89	300	18.5
204.44	400	36.85
260.00	500	53.05
315.56	600	66.42
371.11	700	77.84
398.89	750	83.15

Table 7-19 Predicted flash volumes (*EFV* curves) for Basrah crude oil

Flash temperature, °C	Flash temperature, °F	Predicted flash volumes, vol. %
148.89	300	10.75
204.44	400	25.85
260.00	500	41.75
315.56	600	57.88
371.11	700	70.76
398.89	750	76.02

Table 7-20 Predicted flash volumes (*EFV* curves) for Jambour crude oil

Flash temperature, °C	Flash temperature, °F	Predicted flash volumes, vol. %
148.89	300	10.45
204.44	400	25.14
260.00	500	40.54
315.56	600	57.43
371.11	700	72.18
398.89	750	78.47

Table 7-21 Predicted flash volumes (*EFV* curves) for Bai – Hassan crude oil

Flash temperature, °C	Flash temperature, °F	Predicted flash volumes, vol. %
148.89	300	18.30
204.44	400	37.08
260.00	500	53.11
315.56	600	65.40
371.11	700	75.00
398.89	750	79.19

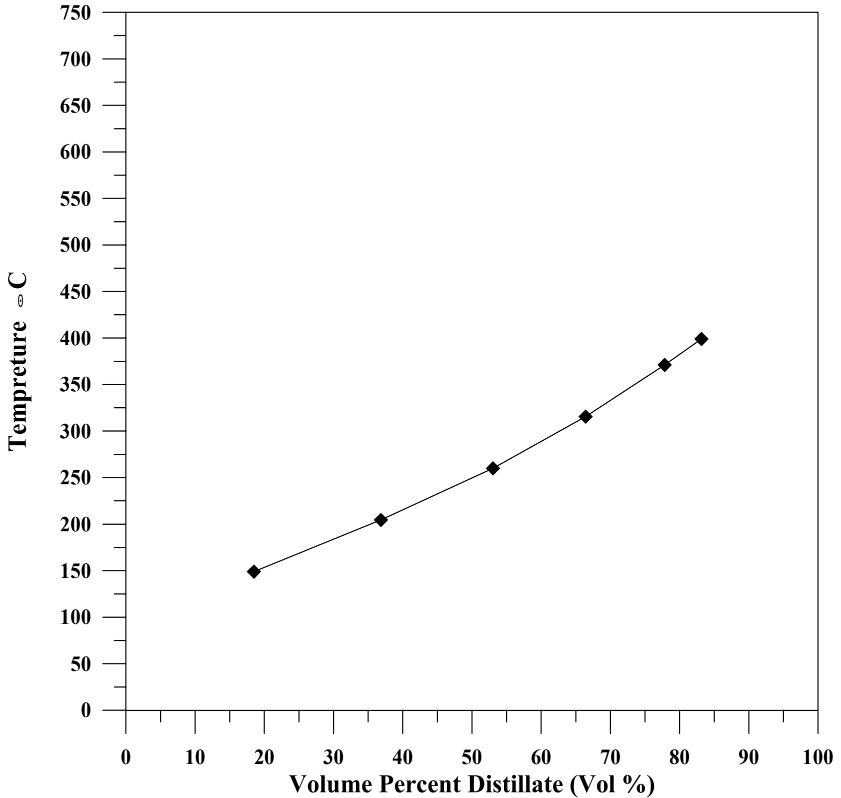

Figure 7-1 *EFV* curve for Kirkuk crude oil

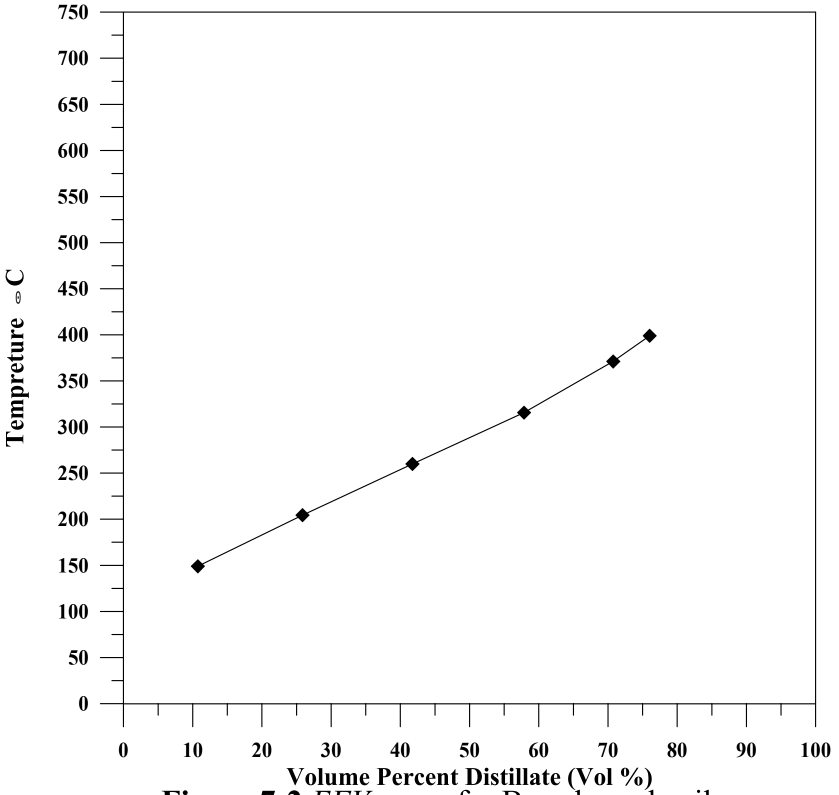

Figure 7-2 *EFV* curve for Basrah crude oil

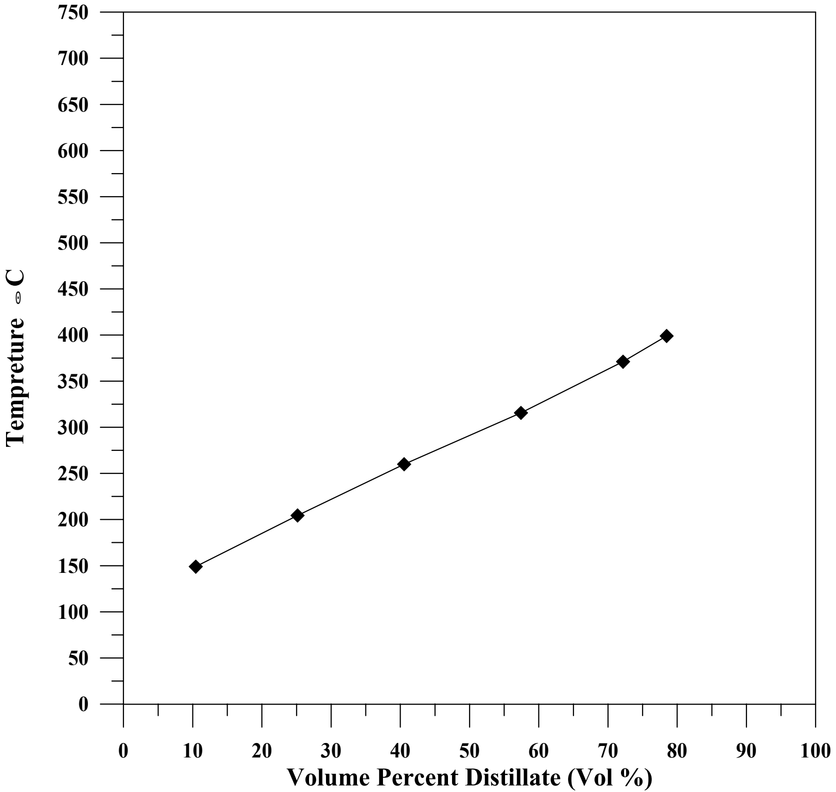

Figure 7-3 *EFV* curve for Jambur crude oil

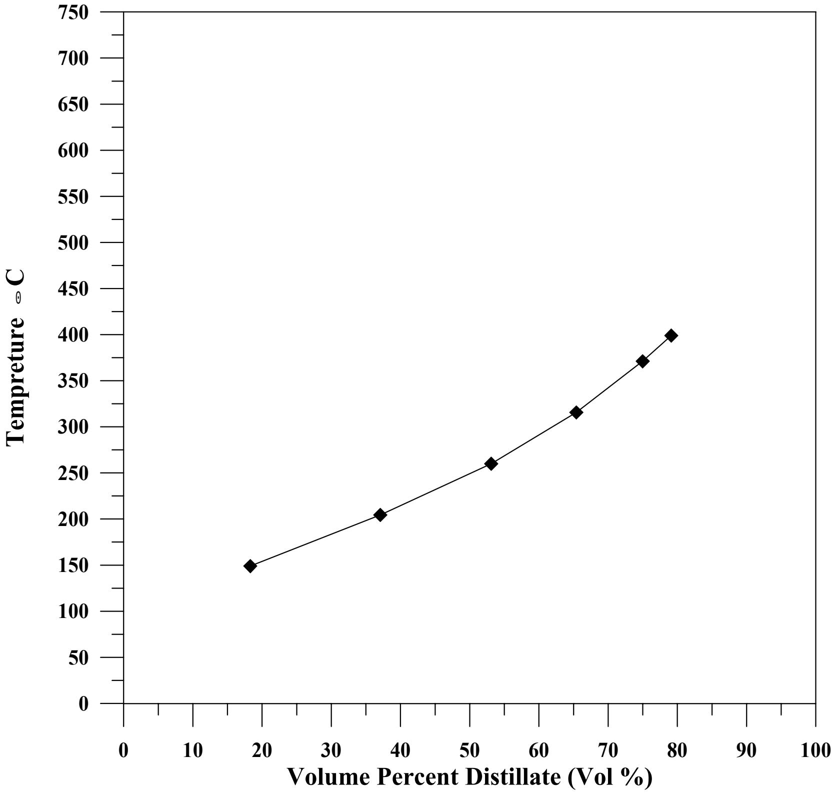

Figure 7-4 *EFV* curve for Bai – Hassan crude oil

After the *EFV* curves for Kirkuk, Basrah, Jambour and Bai – Hassan crude oils were predicted, the flash zone temperatures of these crude oils can also be predicted. This can be performed by using Nelson procedure **[3]**, and as follows:

1. The volume percent distilled for each crude oil at the end point of atmospheric gas oil. Usually this end point takes at 350 °C (≈ 660 °F) **[81, 103]**. The volume percent distilled at 350 °C can be obtained from the *TBP* curve. The values of volume distilled for Kirkuk, Basrah, Jambour and Bai – Hassan crude oils at 350 °C are 64.1%, 58.3%, 63.4% and 58.62% respectively.
2. The flash zone temperature can be read from the *EFV* curve by using the volume percent distilled at 350 °C. Consequently, the flash zone temperatures for Kirkuk, Basrah, Jambour and Bai – Hassan crude oils are 318 °C, 327 °C, 335 °C and 290 °C respectively. The predicted flash zone temperatures are reliable because they are under the cracking temperature. Usually the cracking temperature of petroleum stocks that have the range of 350 °C to 370 °C (662 °F – 698 °F) **[5, 22, 3]**. It must be noted here that the predicted flash zone temperatures for Kirkuk, Basrah, Jambour and Bai – Hassan crude oils must be considered as primary values. They are of the flash zone temperatures and they must be adjusted to the crude oil tower pressure and to the temperature, pressure and the amount of the stripping steam that usually used with the atmospheric crude oil tower **[3]**.

7.2 Conclusions

The purposes of the present work were divided into two parts: part one has two folds, the first one involves taking data of *TBP*, *EFV* and specific gravity for 18 petroleum stocks from literature and investigated the graphical method, and also the pseudo – component methods using three thermodynamic models modes to predict the *EFV* curve from *TBP* curve. Secondly, various attempts for improving the accuracy of the existing pseudo – component methods were investigated. In part two of this work, the most promised (greatest accuracy) method which was developed in this work was applied to four Iraqi crude oils in which their *TBP* and specific gravity data or curves were obtained experimentally to predict their *EFV* curves and flash zone temperature.

The conclusions are as follows:

For part one of this work, the Raizi – Daubert (RD graph) flash method was selected as a graphical method, also three thermodynamic models namely unmodified models, modified models No. 1, and suggested modified model that was developed in this work were selected to predict the *EFV* curve from the *TBP* and specific gravity curves or data. Each one of these thermodynamic models consists of five flash methods namely SRK, SRK + Van, PR, PR + Van and Ideal *K*.

From the present work, the following conclusions are indicated:

1. For unmodified models mode, while nearly all flash methods can adequately predicted the flash volumes or *EFV* curves in high flash volumes region, non of these flash methods were reliable for prediction the flash volumes at low flash volumes regions.
2. For modified models No. 1 mode, which involves two models, the first one suggested by Sim – Daubert, and was used with the SRK, SRK + Van, and Ideal *K* flash methods, and the second models suggested by Twu et al. was used with PR, PR + Van flash methods. The results indicate the following points:
   a. For the Sim – Daubert modification, only 5 petroleum stocks out of 18 petroleum stocks satisfied this model, this means that only 45 flash data points out of 106 flash data points used were modified (representing 43% from the total flash data points used). For those petroleum stocks that were satisfied by this modification, the results showed that when using with SRK flash method, the *AAD%* and *AD%* were improved by more than 30% and for all flash volumes regions as compared with unmodified flash methods and with RD Graph flash method. However, this modification had a little effect on improving the *AAD%* and *AD%*, when it is used with SRK + Van and Ideal *K* flash method, as compared with unmodified flash methods.
   b. The second modification that suggested by Twu et al. showed no significant improvements on *AAD%* and *AD%* when used with PR and PR + Van flash methods as compared with unmodified flash methods.
3. For the modified model suggested in this work using the new suggested vapor pressure correlation, 10 petroleum stocks out of 18 petroleum stocks were

satisfied by this suggested modification. This mean, that 61 flash data points out of 106 flash data points were modified. The results indicate the following points:

a. This modification when used with Ideal *K* flash method, the *AAD%* and *AD%* were improved by more than 50% for low flash volumes region, and more than 30% for all flash volumes region as compared with the unmodified flash methods, and RD graph method.

b. When the acentric factor was calculated using the vapor pressure correlation suggested in this work, and then this acentric factor was used with SRK and PR flash methods (using their original alfa function correlation), the *AAD%* and *AD%* were improved specially in the low flash region by more than 45%, while the improvements in the other regions relatively much less.

c. When using the new suggested vapor pressure correlation with the SRK + Van and PR + Van, the *AAD%* and *AD%* were improved more than 50% for low flash volumes region and more than 30% for all flash volumes region, as compared with the unmodified flash methods and RD Graph method.

d. Results showed that the Ideal *K* flash method was superior to other flash methods used in this investigation (having less values of *AAD%* and *AD%*).

4. A computer program was developed using Quick Basic language for estimation the *EFV* curve from available *TBP* and specific gravity curves, the computer program can estimate the *EFV* curve using any one of the three thermodynamic models.

5. For part two of this work, the Ideal *K* flash method which was developed in this work and was the most accurate prediction method for performing the following items:

a. Estimation of the *EFV* curves for four Iraqi crude oils (Kirkuk, Basrah, Jambur, and Bai – Hassan), from *TBP* and specific gravity data.

b. Using the *EFV* of these crude oils, the flash zone temperature were estimated. The values for these flash zone temperatures were 318 °C, 327 °C, 335 °C and 290 °C for Kirkuk, Basrah, Jambur and Bai – Hassan respectively. These flash zone temperatures were below their cracking temperatures and can be considered good values in view of design point procedures. However, these values of flash zone temperatures must be considered as primary values and must be adjusted to the temperature, pressure, and the amount of stripping steam that usually used with crude oil tower.

7.3 Recommendations for further work

Based on the conclusions presented, the following recommendations may be made for further work:

1. Improving the Lee – Kasler perturbation equation by extended it to cover another ready measurable physical properties such as viscosity, refractive index, *...etc*.
2. Because of the sensitivity of the pseudo – components flash methods to error in measured *TBP* curve the following points may be recommended:
    a) Using the *ASTM* curve instead of *TBP* curve for estimation *EFV* curve.
    b) Developing a new approach which utilizes only accessible fundamental properties of petroleum fractions (*e.g.* viscosity, specific gravity, refractive index, *...etc*) for estimation the basic characterization parameters (*MW, Tc, Pc, ω, ...etc*), instead of using the existing correlations which used the *TBP* as a basic input parameters.
3. Study the estimation of the *EFV* curves for sub atmospheric and super atmospheric pressures from available *TBP* or *ASTM* curves.

References

[1] Sim W.J. and Daubert T.E., *Ind. Eng. Chem. Process Des. Dev.*, **19**, 386 (1980).

[2] American petroleum institute, "*Technical data book – petroleum refining*", Vol. 1, Ch. 4, Washington D.C. (1988).

[3] Nelson W.L., "*Petroleum refining engineering*", 4th ed., Mc Graw – Hill book company (1958).

[4] Edmister W.C., "*Applied hydrocarbon thermodynamics*", Vol. 1, Gulf publishing company, Texas (1967).

[5] Gary J.H. and Handwerk G.E., "*Petroleum refining technology and economics*", 2nd ed., Marcel Dakker Inc. (1984).

[6] Hariu O. and Sage R.C., *Hydrocarbon processing*, **48** (4), 143 (1969).

[7] Raizi M.R., Aladwani H.A. and Marouf R., "*Selection of a characterization scheme for hydrocarbon systems*", Internet resource available at (http: \\www. OilIndustry. pdf. htm) 2003.

[8] Lion A.R. and Edmister W.C., *Hydrocarbon processing*, **58** (8), 119 (1975).

[9] Maxwell J.B., "*Data book of hydrocarbons*", 8th ed., Van Nostrand company Inc. (1950).

[10] Raizi M.R. and Daubert T.E., *Oil and Gas J.*, **25** (8), 50 (1986).

[11] American petroleum institute, "*API – Technical data book – petroleum refining*", Vol. 1, Ch. 3, Washington D.C. (1988).

[12] Kasler M.G. and Lee B.I., *AIChE J.*, **21**, 510 (1975).

[13] Raizi M.R. and Daubert T.E., *Hydrocarbon processing*, **59** (3), 115 (1980).

[14] Long R.B. and Speight J.G., "*Petroleum chemistry and refining*", 1st ed., Taylor and Eronics Inc. (2000).

[15] Speight J.G., "*The chemistry and technology of petroleum*", 2nd ed., Marcel Dakker Inc., New York (1991).

[16] Bestougeff M., "*Fundamental aspects of petroleum geochemistry*", Elsevier publishing company (1967).

[17] Rostler F.S., "*Bituminous materials, asphalts, tars and pitches*", Vol. 2, Hoibrg Editer Int., New York (1965).

[18] Altgelt K.H. and Gouw T.H., "*Chromatography in petroleum analysis*", Marcell Dekker Inc., New York (1976).

[19] Haak F.A. and Van Nes K., "*Investigation into the olefinic components of Pennsylvania crude oil*", *Inst. Petrol. J.*, **37**, 245 (1951).

[20] "*Refining – petrochemicals engineering*", rev. 4, ENSPM formation industries (2000).

[21] Marian P. and Gueret C., "*Hydrocracking technology – latest advances*", a paper presented by IFP industrial division (1995).

[22] Hobson G.D., "*Modern petroleum technology*", 4th ed., Applied science publisher LTD. (1973).

[23] "*Managerial seminar on oil refining documentation*", Dietsmann group comerint, S.P. Agip Petroli (2001).

[24] American petroleum institute, "*Technical data book – petroleum refining*", Vol. 1, Ch. 11, Washington D.C. (1985).

[25] Streeter V.L. and Benjamin W.E., "*Fluid mechanics*", Mc Graw – Hill book Co. (1983).

[26] Stichlmair J.G. and Fair J.R., "*Distillation principles and practices*", Wiley – Liss publication (1998).

[27] Attiya H.G., "*A method for characterization of petroleum fractions*", M.Sc. Thesis, College of Engineering, Baghdad University (2005).

[28] American petroleum institute, "*Technical data book – petroleum refining*", Vol. 1, Ch. 3, Washington D.C. (1977).

[29] Okamoto K.K. and Van Winkele M., *Petroleum Refiner*, **28** (8), 113 (1949).

[30] Smith R.L. and Watson K.M., *Ind. Eng. Chem.*, **25**, 808 (1933).

[31] Watson K.M., Nelson E.F. and Murphy G.B., *Ind. Eng. Chem.*, **27**, 1460 (1935).

[32] Smith R.L. and Watson K.M., *Ind. Eng. Chem.*, **29**, 1408 (1937).

[33] Winn F.W., *Petroleum Refiner*, **57** (2), 157 (1957).

[34] Schou K. and Fredenslund A., *Ind. Eng. Chem. Process Des. Dev.*, **23**, 163 (1984).

[35] Mathur B.C., Ibrahim S.H. and Kuloor N.R., *Chem. Eng.*, **76** (6), 182 (1969).

[36] Kasler M.G. and Lee B.I., *Hydrocarbon processing*, **3**, 153 (1976).

[37] Twu C.H., *Fluid Phase Equilibrium*, **16**, 137 (1984).

[38] Raizi M.R. and Daubert T.E., *Ind. Eng. Chem. Res.*, **26**, 755 (1987).

[39] Raizi M.R. and Shahhaf T.A., *Ind. Eng. Chem.*, **34**, 4145 (1995).

[40] Walas S.M., "*Phase equilibrium in chemical engineering*", Butterworth publisher, London (1985).

[41] Campbell J.M., "*Gas conditioning and processing*", Vol. 1, Gulf publishing company (1975).

[42] Seader J.D. and Henly E.J., "*Separation process principles*", John Wiley and Sons Inc. (1998).

[43] Nelson W.L. and Souders M., *Jr. Pet. Eng.*, **3** (1), 131 (1931).

[44] Packie J.W., *Trans. AIChE J.*, **37**, 51 (1941).

[45] Nelson W.C. Harvey R.J., *Oil and Gas J.*, **47** (7), 71 (1948).

[46] Edmister, Riedel and Marien, *Trans. AIChE J.*, **39** (4), 157 (1943).

[47] Edmister W.C. and Pollock D.H., *Chem. Eng. Prog.*, **44**, 905 (1948).

[48] Edmister W.C., *Petroleum Refiner*, **45** (10, 11, 12), (1949).

[49] American petroleum institute, "*API – Technical data book – petroleum refining*", Vol. 1, Ch. 3, Washington D.C. (1982).

[50] Arnold V.E., *Oil and Gas J.*, **11** (12), 55 (1985).

[51] PRO/ II, Key ward manual, Simulation science Inc., Fullerton, California (1992).

[52] Hysys. Plant, Version 2.0, "*Simulation basis*", Hyprotech Ltd., Alberta, Canada (1998).

[53] Katz D.L. and Brown G.G., *Ind. Eng. Chem.*, **28** (7), 1373 (1933).

[54] Pottman F.H. and Mayland J.B., *Petroleum Refiner*, **28** (7), 101 (1949).

[55] Smith J.M. and Van Ness H.C., "*Introduction to chemical engineering thermodynamics*", 4th ed., Mc Graw – Hill book company (1987).

[56] Chao K.C. and Seader J.D., *AIChE J.*, **7**, 598 (1961).

[57] Redlich D. and Kwong N.S., *Chem. Rev.*, **44**, 232 (1949).

[58] Hilderbrand J.H., Prausnitz J.M. and Scott R.L., "*Regular and related solution*", Van Nostrand Reinold company, New York (1970).

[59] Grayson H.G. and Streed C.W., "*Sixth world petroleum congress*", Frankfurt (1963).

[60] Hoffman H.G., *Chem. Eng. Sci.*, **23**, 957 (1968).

[61] Linden N.J., "*Vapor pressure charts for petroleum hydrocarbon*", Esso engineering and research company, April (1955).

[62] Starling K.E. and Han M.S., *Hydrocarbon Processing*, **51** (6), 107 (1972).

[63] Lee B.I., Erbar J.H. and Edmister W.C., *AIChE J.*, **19** (2), 349 (1973).

[64] Lion A.R. and Edmister W.C., *Hydrocarbon Processing*, **54** (8), 119 (1975).

[65] Graboski M.S. and Daubert T.E., *Ind. Eng. Chem. Process Des. Dev.*, **17**, 443 (1978a), 448 (1978b).

[66] Ibid, **18**, 3001 (1979).

[67] Soave G., *Chem. Eng. Sci.*, **27**, 1197 (1972).

[68] Daubert T.E., Graboski M.S. and Danner R.P., "*Documintation of the basis for selection of contents of chapter 8 – vapor – liquid equilibrium K – values*", American petroleum institute, Dept. of refining, Washington D.C. (1978).

[69] Peng D.Y. and Robinson D.B., *Ind. Eng. Chem. Fundam.*, **15**, 59 (1976).

[70] American petroleum institute, "*API – Technical data book – petroleum refining*", Ch. 8, Washington D.C. (1978).

[71] American petroleum institute, "*API – Technical data book – petroleum refining*", Vol. 1, Ch. 8, Washington D.C. (1982).

[72] Ibid, Vol. 1, Ch. 3 (1988).

[73] Ibid, Vol. 1, Ch. 8 (1992).

[74] Ibid, Vol. 1, Ch. 8 (1997).

[75] Mathias P.M., *Ind. Eng. Chem. Process Des. Dev.*, **22**, 385 (1983).

[76] Methem G.A. et al., *Fluid Phase Equilibrium*, **47**, 189 (1989).

[77] Twu C.H. et al., *Fluid Phase Equilibrium*, **69**, 33 (1991).

[78] Chorng H.T., Wayne D.S. and Tasson V., "*Getting a handle on advance cubic equation of state*", Internet resource available at (http: www. cepmagazine. org) (2002).

[79] Chu J.C. and Staffel E.J., *J. Indst. Petrol.*, **41**, 95 (1955).

[80] Lenoir J.M. and Hipkin H.G., *J. Chem. Eng. Data*, **18**, 18 (1973).

[81] OPEC world oil and energy study, Battele Geneva research center, Switzerland (1989).

[82] Katz D.L. and firoozabadi A., *Petroleum Technology*, **20**, 160 (1989).

[83] Gerald C.F. and Wheaty P.O., "*Applied numerical analysis*", 4th ed., Addison Wesley publishing company, 1982.

[84] Newman S.A., *Hydrocarbon Processing*, **10**, 133 (1981).

[85] Harold R.N., "*Phase equilibrium in process design*", Wiley – Interscience publisher, New York (1970).

[86] Chasib K.f., "*Vapor – liquid equilibrium of ternary systems involving experimental and theoretical correlations using cubic equation of state*", Ph.D. Thesis, College of Engineering, Saddam University (2001).

[87] Prausintz J.M., Liehtenthaler R.N. and De Azevedo E.G., "*Molecular thermodynamics of fluid phase equilibria*", 2nd ed., Prentice – Hall, Englewood Cliffs, N.J. (1986).

[88] Seader J.D. and Henley E.J., "*Equilibrium – stage separation operations in chemical engineering*", John Wiley and Sons Inc. (1981).

[89] Ahmed T., "*Reservoir engineering handbook*", 2nd ed., Gulf professional publishing (2001).

[90] Hasan O. and Sandler S.I., "*Modeling vapor – liquid equilibria – cubic equation of state and their mixing rules*", 1st ed., Cambridge University press (1998).

[91] Marc J.A., Martin J.P. and Thomas F.T., "*Thermophysical properties of fluid: An introduction to thin prediction*", Imperial college press, 1st ed. (1998).

[92] Pitzer K.S., Lippman D.Z., Curl R.F. and Huggins C.M., *J. Amer. Chem. Soc.*, **77**, 3433 (1955).

[93] Spencer C.F. and Danner R.P., *Chem. Eng. Data*, **17**, 236 (1972).

[94] Ried R.C., Prausnitz J.M. and Poling B.E., "*The properties of gases and liquids*", Mc Graw – Hill Prentice, Singapore (1988).

[95] Ewell R.H., Harrison J.M. and Berg L., *Ind. Eng. Chem.*, **36**, 871 (1944).

[96] Wilson G.M., *J. Amer. Chem. Soc.*, **86**, 127 (1964).

[97] Renon H. and Prausnitz J.M., *AIChE J.*, **19**, 135 (1968).

[98] Renon H. and Prausnitz J.M., *Ind. Eng. Chem. Process Des. Dev.*, **8**, 413 (1969).

[99] Abram D. and Prausnitz J.M., *AIChE J.*, **21**, 116 (1975).

[100] Prausnitz J.M., Edmister W.C. and Chao K.C., *AIChE J.*, **6**, 214 (1960).

[101] Paul G. and Lachhman D., *AIChE J.*, **17**, 343 (1971).

[102] Null H.R., "*Phase equilibrium in process design*", Interscience publisher Inc., New York (1970).

[103] Mechanical catalog for crude distillation unit, Vol. 1, Howe – Baker Engineers Inc., Tyler – Texas (1973).

[104] Norris F.A. and Terry D.E., *Oil and Soup*, **2**, 41 (1945).

[105] Poderson K.S., Thomas P. and Fredenslund A.G., *Ind. Eng. Chem. Process Des. Dev.*, **24**, 948 (1985).

[106] Valderrama J.O., *Ind. Eng. Chem. Res.*, **42**, 1603 (2003).

[107] Kasler M.G., Lee B.I. and Sandler S.I., *Ind. Eng. Chem. Fundam.*, **18**, 49 (1979).

Appendix A

Example of calculation

Example, A.1: Estimate the atmospheric *EFV* curve for petroleum fraction having the following atmospheric *TBP* curve and *API* = 32 °.

Distillation, vol.%	10	30	50	70	90
Temperature, °F	150	200	240	275	320

Solution: The Raizi – Dubert method is used with the following steps:

Step 1: Converting the *TBP* temperature to *ASTM D86* temperature using equation (3.3) as follows:

$$ASTM\ \ D86 = b_1^{-(1/b_2)} (TBP)^{(1/b_2)} \qquad \ldots(3.3)$$

Where *ASTM D86* and *TBP* are in °R, b_1 and b_2 obtained from Table 3-1.

For *ASTM D86 10%*: From Table 3-1, $b_1 = 0.5277$ and $b_2 = 1.090$.

Using equation (3.3), thus:

$$ASTM\ \ D86\ \ 10\% = (0.5277)^{-(1/1.09)} (150 + 460)^{(1/1.09)}$$

$$ASTM\ \ D86\ \ 10\% = 645.68°R\ \ or\ \ 185.55°F$$

Or by using Fig. A-1, the *ASTM D86 10%* = 200 °F. Using equation (3.3) with other vol.% distilled, the remaining *ASTM D86* temperature are obtained as follows:

Distillation, vol.%	10	30	50	70	90
ASTM D86, °F	185.5	213.4	239.2	267	304

Step 2: Obtaining the specific gravity (*Sp.gr*), using equation (3.5) or:

$$Sp.gr = 0.06711(ASTM\ \ D86\ \ 10\%)^{0.10731} \cdot (ASTM\ \ D86\ \ 50\%)^{0.26288}$$

so, $$Sp.gr = 0.06711(185.5 + 460)^{0.10731} \cdot (239.2 + 460)^{0.26288}$$

$$Sp.gr = 0.7517\ \ or\ \ \approx 57\,API°$$

Step 3: Converting the *ASTM D86* temperature to *EFV* temperature using equation (3.4):

$$EFV = c_1(ASTM\ \ D86)^{c_2}(Sp.gr)^{c_3} \qquad \ldots(3.4)$$

Where c_1, c_2 and c_3 are obtained from Table 3-2.
For *EFV 10%*: From Table 3-2, $c_1 = 3.2555$, $c_2 = 0.8466$ and $c_3 = 0.4208$.
Using equation (3.4):

$$EFV\ \ 10\% = 3.2555(185.5 + 460)^{0.8466}(0.7517)^{0.4208}$$

$$EFV\ \ 10\% = 674.8°R\ \ or\ \ 214.8°F$$

Or by using Fig. A-2, the *EFV 10%* = 220 °F

Using equation (3.4), with other vol.% distilled, the remaining *ASTM D86* temperatures are obtained as follows:

Distillation, vol.%	10	30	50	70	90
EFV, °F	214.8	214.4	223.8	245.8	265.6

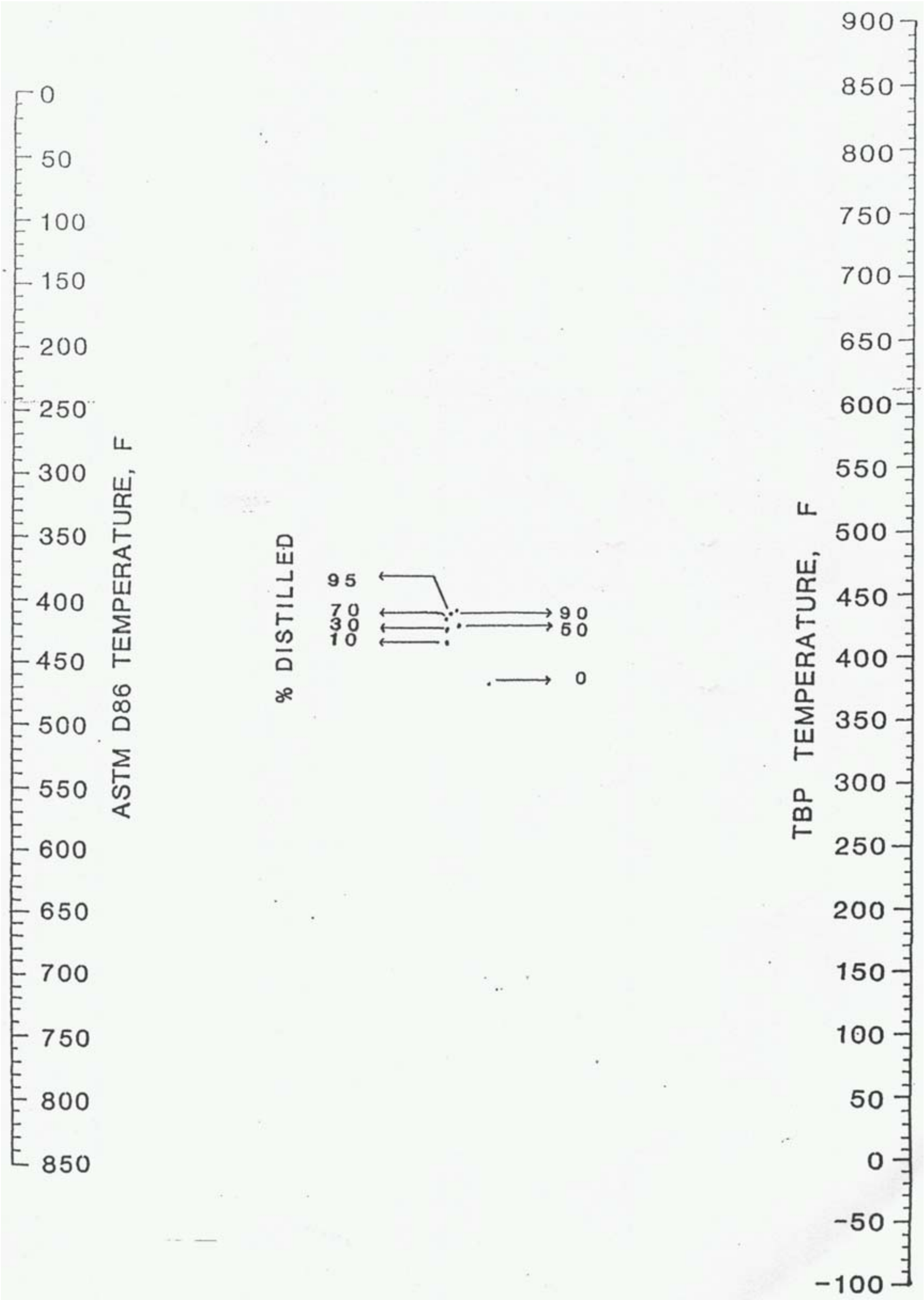

Figure A-1 Graphical form of equation (3.3)

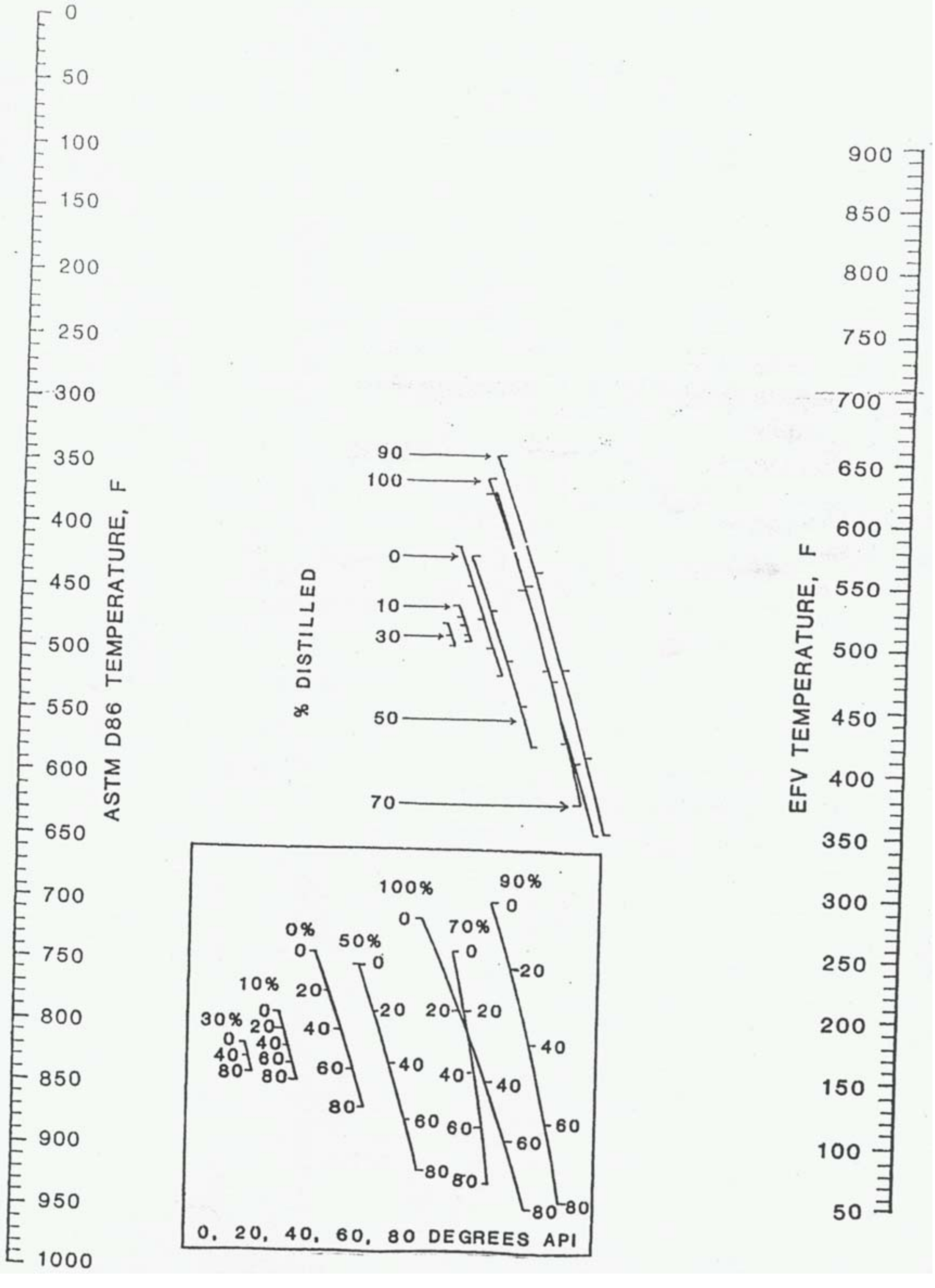

Figure A-2 Graphical form of equation (3.4)

Appendix B
Numerical technique

B.1 Newton – Raphson method

Numerical techniques are sometimes required in the solution of thermodynamics problems. Particularly useful is an iteration procedure that generates a sequence of approximations which rapidly converges on the exact solution of an equation. One of the most widely used methods of solving equations is the Newton – Raphson method, a technique for finding a root $x = x_r$ of the following equation **[55, 83]**.

$$F(x) = 0 \qquad \ldots(B.1)$$

The general form of Newton – Raphson method can be written as follows:

$$x_{j+1} = x_j + \frac{F(x_j)}{\overline{F}(x_j)}, \; x_j = x_j + \frac{F(x_j)}{\overline{F}(x_j)} \qquad \ldots(B.2)$$

where $F(x_j)$ is a nonlinear equation in x_j and $\overline{F}(x_j)$ is the derivative of $F(x_j)$ with respect to x_j. Equation (B.2) is the mathematical statement of Newton – Raphson method. Given estimate x_j to the solution of equation (B.1), it provides a better estimate x_{j+1}. The procedure is repeated until computed x_{j+1} differs from x_j by less than some preset tolerance error ϵ (*e.g.* $\epsilon = 0.0001$), where:

$$\epsilon = \left| \frac{x_{j+1} - x_j}{x_j} \right| \qquad \ldots(B.3)$$

In Newton – Raphson method, the initial estimate of x_j must be properly chosen. Fortunately, many problems in the thermodynamics involve function *F(x)*, that are monotonic in *x* and the Newton – Raphson method is usually suitable.

B.2 Newton – Raphson method for estimation the compressibility factor from equation of state

Newton – Raphson method is widely used for obtaining the vapor and liquid compressibility factors (Z^V and Z^L) from equation of state models. Equation (B.2) can be written for compressibility factor as follows:

$$Z_{j+1} = Z_j + \frac{F\left(Z_j\right)}{\overline{F}\left(Z_j\right)} \qquad \text{...(B.4)}$$

where *j* denotes the iteration number (*i.e. j = 1, 2, ...N*$_T$).

For SRK equation of state, the *F(Z)* can be obtained from equation (3.75) or:

$$F(Z) = Z^3 - (1-B)Z^2 + \left(A - B^2 - B\right)Z - AB = 0 \qquad \text{...(B.5)}$$

The derivative of equation (B.5) is:

$$\overline{F}(Z) = 3Z^2 - (1-B)Z + \left(A - B^2 - B\right) = 0 \qquad \text{...(B.6)}$$

Substituting expression for *F(Z)* and $\overline{F}(Z)$ into equation (B.4), the following equation is obtained:

$$Z_{j+1} = Z_j + \frac{Z_j^3 - (1-B)Z_j^2 + \left(A - B^2 - B\right)Z_j - AB}{3Z_j^2 - (1-B)Z_j + \left(A - B^2 - B\right)} \qquad \text{...(B.7)}$$

For PR equation of state, the *F(Z)* is obtained from equation (3.88), thus:

$$F(Z) = Z^3 - (1 - B)Z^2 - \left(A - 3B^2 - 2B\right)Z - \left(AB - B^2 - B^3\right) = 0 \qquad \ldots(\text{B.8})$$

Its derivative is :

$$\overline{F}(Z) = 3Z^2 - 2Z(1 - B) - \left(A - 3B^2 - 2B\right) = 0 \qquad \ldots(\text{B.9})$$

Substituting expression for *F(Z)* and $\overline{F}(Z)$ in equation (B.4), gives:

$$Z_{j+1} = Z_j + \frac{Z_j^3 - (1 - B)Z_j^2 + \left(A - 3B^2 - 2B\right)Z_j - \left(AB - B^2 - B^3\right)}{3Z_j^2 - 2Z_j(1 - B) + \left(A - 3B^2 - 2B\right)} \qquad ..(\text{B.10})$$

Equations (B.7) and (B.10), now can be solved iteratively for Z^V and Z^L, with the following recommendations:

1. For Z^V, the initial guess is preferred to be 1, (*i.e.* $Z_0^V = 1$).
2. For Z_L, the initial guess is preferred to be 0, (*i.e.* $Z_0^L = 0$).
3. The iteration procedure must be continued until the percent tolerance error {defined by equation (B.3)} not be less than 0.0001, (*i.e. € ≤ 0.0001*).

B.3 Newton – Raphson method for estimation the vapor fraction vaporized (*β*) in flash calculations

Newton – Raphson method is frequently used for estimating the vapor fraction vaporized (*β*) in flash. Equation (B.3) can be written for *β* as follows:

$$\beta_{j+1} = \beta_j + \frac{F\left(\beta_j\right)}{\overline{F}\left(\beta_j\right)} \qquad ..(\text{B.11})$$

where *j* denotes iteration number (*i.e.* $j = 1, 2, \ldots N_T$). The function $F(\beta_j)$ can be obtained from equation (3.175), as:

$$F(\beta)=\sum_{i=1}^{N}\frac{Z_i(1-K_i)}{1+\beta(K_i-1)} \qquad ..(B.12)$$

The derivative of equation (B.12) is:

$$\overline{F}(\beta)=\sum_{i=1}^{N}\frac{Z_i(1-K_i)^2}{[1+\beta(K_i-1)]^2} \qquad ..(B.13)$$

Substituting expressions for $F(\beta)$ and $\overline{F}(\beta)$ in equation (B.11), gives:

$$\beta_{j+1}=\beta_j+\frac{\sum_{i=1}^{N}\frac{Z_i(1-K_i)}{1+\beta_j(K_i-1)}}{\sum_{i=1}^{N}\frac{Z_i(1-K_i)^2}{[1+\beta_j(K_i-1)]^2}} \qquad ..(B.14)$$

Equation (B.14) can be solved iteratively for β_i with the following recommendations:

1. The initial guess for β_j is preferred to be 0.5 (*i.e.* $\beta_0 = 0.5$).
2. The iteration procedure must be continued until the percent tolerance error {defined by equation (B.3)} must not be less than 0.0001 (*i.e.* $\epsilon \leq 0.0001$).

Appendix C

Laboratory equipments specifications

C.1 Thermocouple specifications

The thermocouples that used in the experimental work for measurement of vapor temperature and bottom temperature have the following specifications:

Table C-1 Thermocouple specifications

Item	Specification
Thermocouple type	J
Alloys	Iron versus copper – nickel
Range of temperature	-210 °C to 1200 °C
Error	-0.05 to 0.03 °C if -210 °C < T < 0 °C -0.04 to 0.04 °C if 0 °C< T < 760 °C -0.04 to 0.03 °C if 760 °C < T < 1200 °C

The calibration curves for the thermocouples are shown in Fig. C-1.

C.2 Helipak packing materials specifications

The packing materials that was used in the experimental work for packing the distillation column was Helipak packing materials. The Helipak packing materials manufactured by Reliance Glass Works Inc., (USA), and have the following specifications:

Table C-2 Helipak packing materials specifications

Item	Specification
Dimensions, mm	1.27×2.54×2.54
Model number	2917
Materials	Nichrome
Porosity (volume%)	0.85
Specific area (m^2/m^3)	1200
Height equivalent to theoretical plate for operating pressure range of 50 – 760 mmHg, mm	23 – 61

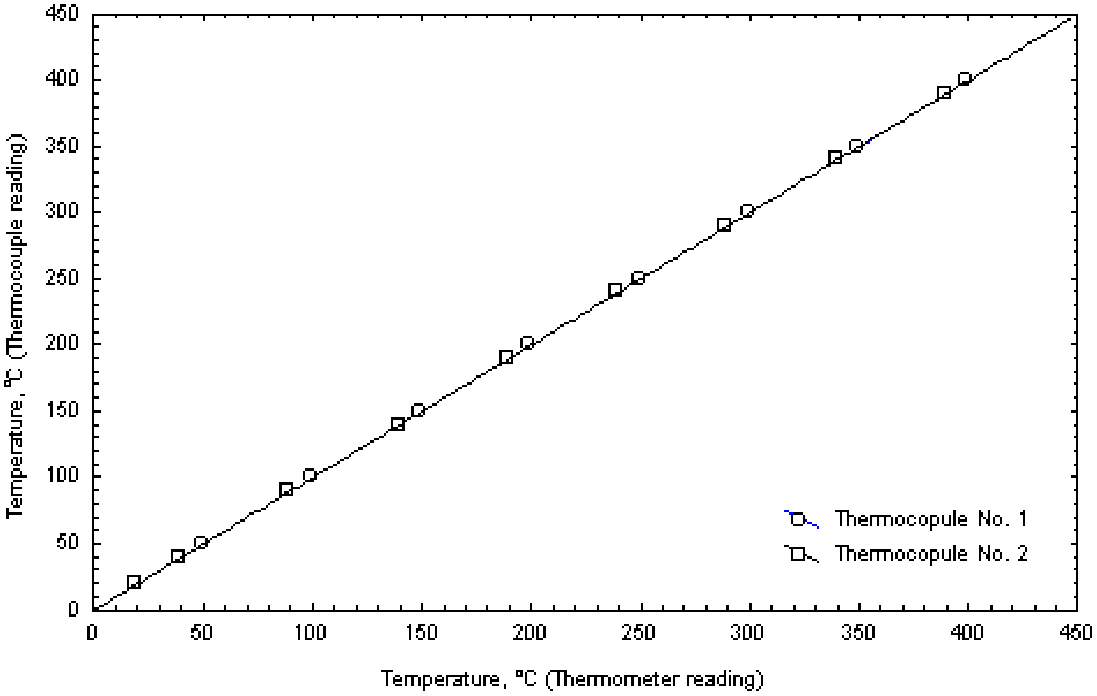

Figure C-1 Calibration curves for the thermocouples

C.3 Fractionating column components

The fractionating column that used in the experimental work consists of three main parts; these parts are:

a. Reflux condenser of 290mm high and 50mm inside diameter.

b. Packed bed column of 910mm high and 25mm inside diameter.

c. Double expansion coil of 250mm high.

The total length of the fractionating column was 1450mm and with outside diameter of 64mm. The fractionating column was manufactured by Podblelniak Inc., (USA), and it is satisfied the requirements of *ASTM D 2892 – 78*. The components of the fractionating column are shown in Fig. C-3.

C.4 Utility requirements

The utility that was required during the experimental work is given as follows:

1. Electricity of 115 V – 60 cy. A.C. for vacuum pump, heating mantle with variable resistance and timer.
2. Cooling water at pressure of 3atm, and at temperature of 15 °C. The cooling water is supplied from Dura – refinery utility unit in a 6.35 mm (1/4 inch) pipe.
3. Ethylene glycol alcohol at pressure of 5atm and temperature of below – 25 °C. The ethylene glycol alcohol was supplied from cooling machine of Dura – refinery laboratory in a 6.35 mm (1/4 inch) isolated pipe.
4. The power requirements at 115 V A.C., are as follows:

Table C-3 Power requirements

Item	Power requirements
Vacuum pump (1/3 HP)	690 W
Timers	13 W
Heating mantle with variable resistance	850 W

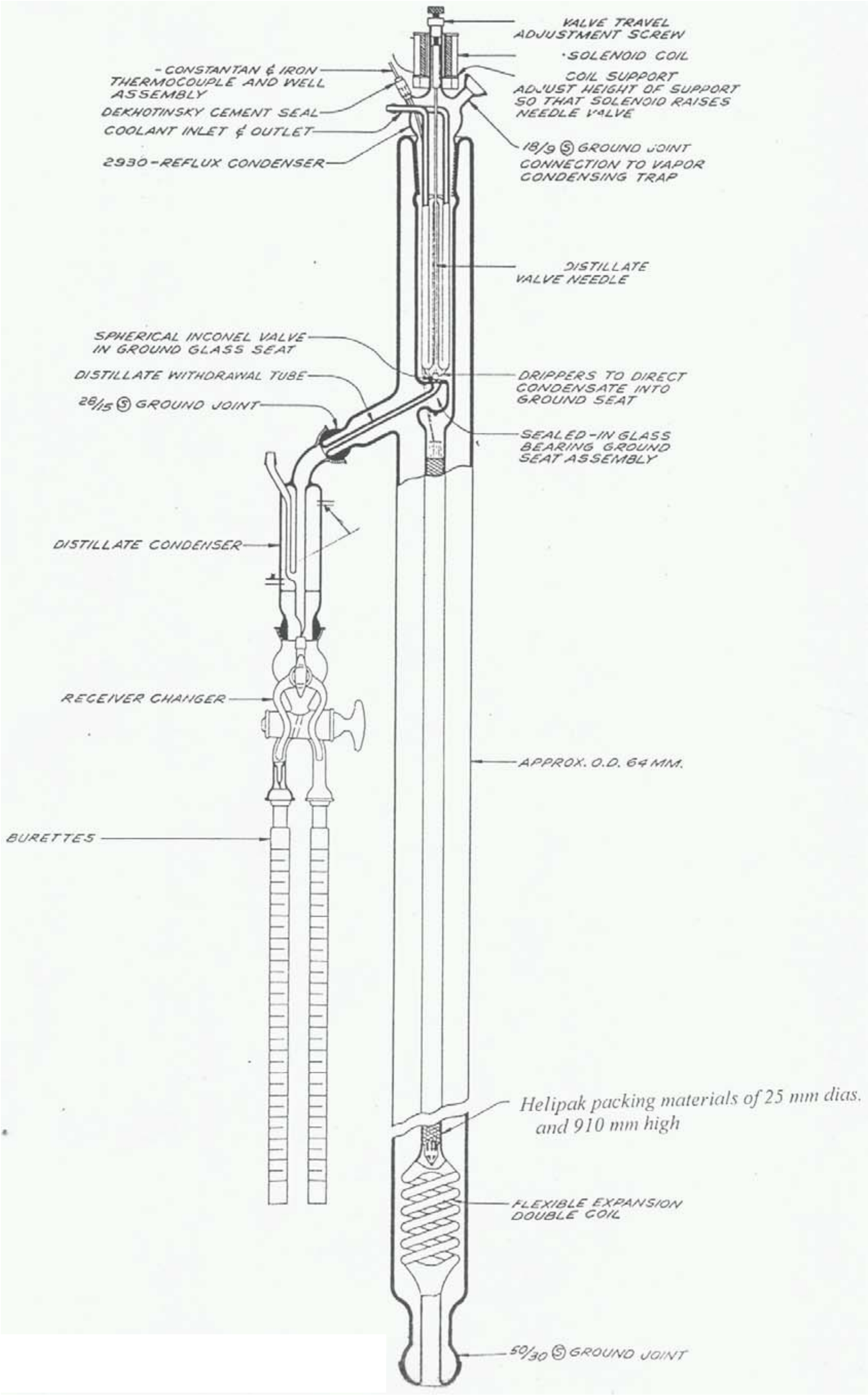

Figure C-2 Fractionating column components

Appendix D

Literature data for 18 petroleum stocks

Table D-1 *TBP, EFV* and *Sp.gr* data for Santa fe spring crude

API		32.4	
Sp.gr type		Overall	
TBP curve		*EFV* Curve	
Vol. distilled, %	Temperature, °C	Vol. distilled, %	Temperature, °C
5	84.4	5	125
10	105	10	145
20	148.8	20	200
50	294.4	50	289
70	397.7	70	350

Table D-2 *TBP, EFV* and *Sp.gr* data for Eldwood crude

API		36.5	
Sp.gr type		Overall	
TBP curve		*EFV* Curve	
Vol. distilled, %	Temperature, °C	Vol. distilled, %	Temperature, °C
5	84.4	5	126.6
10	104.4	10	138.8
20	132.2	20	165.5
50	240.5	50	241.6
70	336.1	70	291.1

Table D-3 *TBP, EFV* and *Sp.gr* data for Columbian crude

API		27.2	
Sp.gr type		Overall	
TBP curve		*EFV* Curve	
Vol. distilled, %	Temperature, °C	Vol. distilled, %	Temperature, °C
5	88.8	5	143.3
10	128.3	10	167.7
20	197.7	20	213.8
50	365.5	50	342.2
70	485	70	423.8

Table D-4 *TBP, EFV* and *Sp.gr* data for Ranger crude

API		37.3	
Sp.gr type		Overall	
TBP curve		*EFV* Curve	
Vol. distilled, %	Temperature, °C	Vol. distilled, %	Temperature, °C
5	78.3	5	140.1
10	107.7	10	153.3
20	156.1	20	178.3
50	285	50	259.4
70	375.5	70	332.2

Table D-5 *TBP, EFV* and *Sp.gr* data for Lulting crude

API		34.9	
Sp.gr type		Overall	
TBP curve		*EFV* Curve	
Vol. distilled, %	Temperature, °C	Vol. distilled, %	Temperature, °C
5	130.5	5	192.7
10	166.6	10	216.1
20	206.6	20	235.5
50	310.5	50	295
70	377.7	70	335

Table D-6 *TBP, EFV* and *Sp.gr* data for 50% COL. OH crude

API		40.9	
Sp.gr type		Overall	
TBP curve		*EFV* Curve	
Vol. distilled, %	Temperature, °C	Vol. distilled, %	Temperature, °C
5	69.4	5	126.6
10	94.4	10	136.6
20	125	20	156.1
50	231.1	50	206.6
70	291.6	70	238.8

Table D-7 *TBP, EFV* and *Sp.gr* data for Kansas crude

API		40.8	
Sp.gr type		Overall	
TBP curve		*EFV* Curve	
Vol. distilled, %	Temperature, °C	Vol. distilled, %	Temperature, °C
5	68.3	5	121.1
10	92.7	10	131.6
20	127.7	20	152.7
50	246.11	50	227.7
70	335.6	70	282.2

Table D-8 *TBP, EFV* and *Sp.gr* data for Mid – continent crude

API		37.1	
Sp.gr type		Overall	
TBP curve		*EFV* Curve	
Vol. distilled, %	Temperature, °C	Vol. distilled, %	Temperature, °C
5	67.7	5	129.4
10	93.3	10	146.6
20	140	20	180.5
50	286.1	50	282.7
70	390	70	351.6

Table D-9 *TBP, EFV* and *Sp.gr* data for Magnoland crude

API		28.2	
Sp.gr type		Overall	
TBP curve		*EFV* Curve	
Vol. distilled, %	Temperature, °C	Vol. distilled, %	Temperature, °C
5	1s67.7	5	232.2
10	206.6	10	237.7
20	252.2	20	250.5
50	305	50	292.2
70	351.6	70	315

Table D-10 *TBP, EFV* and *Sp.gr* data for Mid – continent crude

API		38.2	
Sp.gr type		Overall	
TBP curve		*EFV* Curve	
Vol. distilled, %	Temperature, °C	Vol. distilled, %	Temperature, °C
5	61.6	5	119.4
10	91.1	10	135
20	138.8	20	177.2
50	305.5	50	280
70	367.2	70	345

Table D-11 *TBP, EFV* and *Sp.gr* data for Hendricks crude

API		38.2	
Sp.gr type		Overall	
TBP curve		*EFV* Curve	
Vol. distilled, %	Temperature, °C	Vol. distilled, %	Temperature, °C
5	82.2	5	148.3
10	112.7	10	163.3
20	155.5	20	194.4
50	280	50	278.3
70	387.22	70	330.5

Table D-12 *TBP, EFV* and *Sp.gr* data for Mid – continent crude

API		34.4	
Sp.gr type		Overall	
TBP curve		*EFV* Curve	
Vol. distilled, %	Temperature, °C	Vol. distilled, %	Temperature, °C
5	87.7	5	-
10	113.8	10	161.1
20	161.6	20	192.2
50	304.4	50	286.6
70	400	70	351.6

Table D-13 *TBP, EFV* and *Sp.gr* data for Naphtha – kerosene blend

API		47.8	
Sp.gr type		Overall	
TBP curve		*EFV* Curve	
Vol. distilled, %	Temperature, °C	Vol. distilled, %	Temperature, °C
10	71.1	10	101
30	142.7	20	127.8
50	202.2	25	140.5
70	249.4	30	146.1
90	292.7	35	155.5
		50	177.7
		70	203.8

Table D-14 *TBP, EFV* and *Sp.gr* data for California research stock 7

API		37.0	
Sp.gr type		Overall	
TBP curve		*EFV* Curve	
Vol. distilled, %	Temperature, °C	Vol. distilled, %	Temperature, °C
10	209.4	10	246.1
30	256.6	30	260.6
50	279.4	50	268.8
70	296.1	70	277.7

Table D-15 *TBP, EFV* and *Sp.gr* data for Middle east crude

API		36.8	
Sp.gr type		Overall	
TBP curve		*EFV* Curve	
Vol. distilled, %	Temperature, °C	Vol. distilled, %	Temperature, °C
4.4	56.11	0	93.33
10	81.11	10	133.88
20	133.61	30	200
30	185.89	50	263.33
40	229.11	66.66	315.55
50	269.22	70	337.22
60	340.22		
70	414.44		
80	457.50		

Table D-16 *TBP, EFV* and *Sp.gr* data for Intermediate – paraffin base crude

API			37.3	
Sp.gr type			Curve	
TBP curve		*Sp.gr* curve	*EFV* Curve	
Vol. distilled, %	Temperature, °C	*Sp.gr*	Vol. distilled, %	Temperature, °C
5	70	0.6388	10	139.4
10	111.6	0.7389	15	158.3
20	158.3	0.7832	20	176.6
30	222.9	0.8017	25	195
40	269.2	0.825	30	218.3
50	315.5	0.8478	35	236.6
60	371.1	0.8628	40	251.1
70	426.6	0.8761	50	296.6
80	482.22	0.9042	60	325
90	537.7	0.9339	70	371.1

Table D-17 *TBP, EFV* and *Sp.gr* data for Asphaltic – naphthene base crude

API			20.2	
Sp.gr type			Curve	
TBP curve		*Sp.gr* curve	*EFV* Curve	
Vol. distilled, %	Temperature, °C	*Sp.gr*	Vol. distilled, %	Temperature, °C
5	213.7	0.7868	10	306.1
10	250.7	0.8508	15	315.6
20	306.3	0.8849	20	329.4
30	343.3	0.9041	25	338.8
40	389.6	0.9339	30	352.7
50	417.2	0.9439	35	371.1
60	454.4	0.9541	40	389.4
70	491.4	0.9671	50	403.3
80	537.8	0.9888	60	431.1
			70	463.3

Table D-18 *TBP, EFV* and *Sp.gr* data for Paraffin base crude

API			42.2	
Sp.gr type			Curve	
TBP curve		*Sp.gr* curve	*EFV* Curve	
Vol. distilled, %	Temperature, °C	*Sp.gr*	Vol. distilled, %	Temperature, °C
5	102.2	0.669	10	148.8
10	130.3	0.7389	15	162.7
20	167.4	0.769	20	176.6
30	204.4	0.7868	25	188.3
40	239.6	0.8055	30	204.4
50	278.5	0.8171	35	213.4
60	315.6	0.826	40	227.7
70	371.1	0.8415	50	260
80	435.9	0.8585	60	278.3
90	519.2	0.8806	70	306.1

Appendix E

Material balance and *Sp.gr* data for four types of Iraqi crude oils

Table E-1 Material balance of Kirkuk crude oil

Cut No.	Boiling range, °C	Volume, ml	Volume,%	Weight, gm	Weight, %
1	gas	106.8	2.67	58.83	1.75
2	30-50	100	1.7	64.87	1.93
3	50-60	40	1	25.95	0.77
4	60-70	82	2.05	53.30	1.58
5	70-80	55.6	1.39	36.97	1.102
6	80-90	72.4	1.81	49.28	1.47
7	90-100	120	3	83.19	2.481
8	100-110	52.8	1.32	37.952	1.132
9	110-120	69.2	1.73	51.06	1.523
10	120-130	108	2.7	80.43	2.39
11	130-140	97.2	2.43	74.54	2.22
12	140-150	103.6	2.59	80.04	2.38
13	150-160	101.6	2.54	79.71	2.37
14	160-170	95.6	2.39	75.82	2.261
15	170-180	97.2	2.43	77.62	2.314
16	180-190	82	2.05	66.05	1.97
17	190-200	62.8	1.57	50.59	1.50
18	200-210	92.8	2.32	75.18	2.24
19	120-220	50	1.25	40.6	1.211
20	220-230	70.4	1.76	57.41	1.712
21	230-240	66.8	1.67	55.00	1.64
22	240-250	70	1.75	58.191	1.73
23	250-260	62.4	1.56	51.89	1.54
24	260-270	77.6	1.94	64.91	1.93
25	270-280	100	2.5	83.9	2.50
26	280-290	94.8	2.37	79.71	2.37
27	290-300	114	2.85	96.14	2.86
28	300-310	66	1.65	56.03	1.67
29	310-320	69.6	1.74	59.41	1.71
30	320-330	124	3.1	106.34	3.17
31	330-340	33.6	0.84	28.89	0.86
32	340-350	55.2	1.38	47.79	1.42
33	350-360	92	2.3	80.03	2.38
34	360-370	28.8	0.72	25.17	0.75
35	above 370	1285.2	32.93	1240.90	37
	Total	**4000**	**100**	**3353.85**	**100**

Table E-2 Material balance of Basrah crude oil

Cut No.	Boiling range, °C	Volume, ml	Volume,%	Weight, gm	Weight, %
1	Gas	68	1.7	37.84	1.08
2	34-50	66.4	1.66	42.70	1.22
3	50-60	47.6	1.19	30.72	0.88
4	60-70	48	1.2	31.89	0.91
5	70-80	49.2	1.23	33.46	0.96
6	80-90	55.6	1.39	38.61	1.10
7	90-100	103.6	2.59	73.84	2.11
8	100-110	42.8	1.07	30.91	0.88
9	110-120	47.6	1.19	34.78	0.99
10	120-130	48.4	1.21	35.80	1.02
11	130-140	53.2	1.33	39.78	1.14
12	140-150	78.4	1.96	59.35	1.69
13	150-160	33.2	0.83	25.32	0.72
14	160-170	65.6	1.64	50.52	1.44
15	170-180	73.6	1.84	57.22	1.63
16	180-190	70.8	1.77	55.53	1.59
17	190-200	41.6	1.04	32.84	0.94
18	200-210	37.6	0.94	29.85	0.85
19	120-220	68.4	1.71	54.71	1.56
20	220-230	73.2	1.83	58.98	1.68
21	230-240	83.2	2.08	67.54	1.93
22	240-250	135.2	3.38	112.75	3.22
23	250-260	58.8	1.47	48.45	1.38
24	260-270	84	2.1	69.65	1.99
25	270-280	157.2	3.93	131.51	3.75
26	280-290	93.2	2.33	78.43	2.24
27	290-300	106.8	2.67	90.43	2.58
28	300-310	40	1	34.00	0.97
29	310-320	100	2.5	85.46	2.44
30	320-330	110	2.75	94.54	2.70
31	330-340	90	2.25	77.72	2.22
32	340-350	100	2.5	86.78	2.48
33	350-360	137.2	3.43	119.74	3.42
34	360-370	88.8	2.22	77.83	2.22
35	above 370	1442.8	36.07	1472.97	42.06
	Total	**4000**	**100**	**3502.48**	**100**

Table E-3 Material balance of Jambur crude oil

Cut No.	Boiling range, °C	Volume, ml	Volume,%	Weight, gm	Weight, %
1	Gas	132	3.3	73.46	2.20
2	37-50	86.4	2.16	55.47	1.66
3	50-60	13.6	0.34	8.76	0.26
4	60-70	71.2	1.78	46.38	1.39
5	70-80	88.8	2.22	58.57	1.75
6	80-90	76.8	1.92	52.37	1.57
7	90-100	62.8	1.57	44.33	1.33
8	100-110	100	2.5	71.85	2.15
9	110-120	100	2.5	73.87	2.21
10	120-130	40	1	29.73	0.89
11	130-140	150	3.75	111.95	3.35
12	140-150	110	2.75	82.61	2.47
13	150-160	141.6	3.54	106.53	3.18
14	160-170	81.2	2.03	63.04	1.88
15	170-180	77.2	1.93	60.49	1.81
16	180-190	90.8	2.27	71.52	2.14
17	190-200	92.4	2.31	73.01	2.18
18	200-210	74.8	1.87	59.54	1.78
19	120-220	77.6	1.94	62.09	1.86
20	220-230	64.4	1.61	51.71	1.55
21	230-240	84.4	2.11	68.11	2.04
22	240-250	135.6	3.39	110.47	3.30
23	250-260	76.4	1.91	62.95	1.88
24	260-270	62.4	1.56	51.76	1.55
25	270-280	45.6	1.14	37.90	1.13
26	280-290	43.2	1.08	36.01	1.08
27	290-300	83.2	2.08	69.35	2.07
28	300-310	61.2	1.53	51.48	1.54
29	310-320	55.6	1.39	47.10	1.41
30	320-330	40	1	34.13	1.02
31	330-340	38	0.95	32.65	0.98
32	340-350	76.8	1.92	66.85	2.00
33	350-360	98	2.45	85.55	2.56
34	360-370	78.4	1.96	68.68	2.05
35	above 370	1289.6	32.24	1264.89	37.81
	Total	**4000**	**100**	**3465.98**	**100**

Table E-4 Material balance of Bai – Hassan crude oil

Cut No.	Boiling range, °C	Volume, ml	Volume,%	Weight, gm	Weight, %
1	Gas	120	3	66.78	1.93
2	33-50	48	1.2	30.31	0.87
3	50-60	152	3.8	97.99	2.83
4	60-70	52	1.3	34.10	0.98
5	70-80	48	1.2	32.24	0.93
6	80-90	28.56	0.71	19.72	0.57
7	90-100	146.4	3.66	103.24	2.98
8	100-110	45.6	1.14	32.70	0.94
9	110-120	45.2	1.13	32.94	0.95
10	120-130	76	1.9	56.13	1.62
11	130-140	87.6	2.19	65.57	1.89
12	140-150	95.6	2.39	72.30	2.09
13	150-160	88.4	2.21	67.33	1.94
14	160-170	76	1.9	58.29	1.68
15	170-180	71.2	1.78	54.99	1.59
16	180-190	61.6	1.54	47.83	1.38
17	190-200	52.8	1.32	41.18	1.19
18	200-210	78.4	1.96	61.28	1.77
19	120-220	65.2	1.63	51.34	1.48
20	220-230	56.4	1.41	44.57	1.29
21	230-240	84.8	2.12	67.23	1.94
22	240-250	88	2.2	71.01	2.05
23	250-260	59.2	1.48	48.40	1.40
24	260-270	53.2	1.33	43.92	1.27
25	270-280	40	1	33.21	0.96
26	280-290	50	1.25	41.60	1.20
27	290-300	58	1.45	48.65	1.40
28	300-310	66.8	1.67	56.84	1.64
29	310-320	100	2.5	86.46	2.49
30	320-330	66.8	1.67	58.26	1.68
31	330-340	66.4	1.66	58.30	1.68
32	340-350	116.8	2.92	102.95	2.97
33	350-360	112.8	2.82	99.60	2.87
34	360-370	113.2	2.83	100.22	2.89
35	above 370	1429.04	35.72	1478.50	42.66
	Total	**4000**	**100**	**3465.98**	**100**

Table E-5 Specific gravity and *API* of distillate fractions from Kirkuk crude oil

Cut No.	Boiling range, °C	*Sp.gr*	*API*
1	gas	-	-
2	30-50	0.6487	86.63
3	50-60	0.6488	86.59
4	60-70	0.6501	86.16
5	70-80	0.665	81.28
6	80-90	0.6808	76.34
7	90-100	0.6933	72.60
8	100-110	0.7188	65.36
9	110-120	0.738	60.23
10	120-130	0.7448	58.48
11	130-140	0.7669	53.01
12	140-150	0.7726	51.65
13	150-160	0.7846	48.85
14	160-170	0.7932	46.89
15	170-180	0.7986	45.69
16	180-190	0.8056	44.15
17	190-200	0.8056	44.15
18	200-210	0.8102	43.15
19	120-220	0.812	42.76
20	220-230	0.8156	41.99
21	230-240	0.8234	40.35
22	240-250	0.8313	38.72
23	250-260	0.8317	38.63
24	260-270	0.8365	37.66
25	270-280	0.8390	37.15
26	280-290	0.8409	36.77
27	290-300	0.8434	36.27
28	300-310	0.8490	35.17
29	310-320	0.8536	34.27
30	320-330	0.8576	33.50
31	330-340	0.8601	33.02
32	340-350	0.8658	31.93
33	350-360	0.8699	31.16
34	360-370	0.8740	30.40

Table E-6 Specific gravity and *API* of distillate fractions from Basrah crude oil

Cut No.	Boiling range, °C	*Sp.gr*	*API*
1	gas	-	-
2	30-50	0.6430	88.56
3	50-60	0.6623	82.16
4	60-70	0.6782	77.14
5	70-80	0.6914	73.15
6	80-90	0.7039	69.52
7	90-100	0.7201	65.01
8	100-110	0.7285	62.74
9	110-120	0.7367	60.56
10	120-130	0.7445	58.55
11	130-140	0.7522	56.61
12	140-150	0.7611	54.42
13	150-160	0.7665	53.10
14	160-170	0.7737	51.39
15	170-180	0.7806	49.76
16	180-190	0.7873	48.23
17	190-200	0.7922	47.12
18	200-210	0.7967	46.10
19	120-220	0.8025	44.82
20	220-230	0.8082	43.58
21	230-240	0.8141	42.31
22	240-250	0.8216	40.73
23	250-260	0.8260	39.80
24	260-270	0.8311	38.75
25	270-280	0.8383	37.29
26	280-290	0.8432	36.30
27	290-300	0.8484	35.29
28	300-310	0.8515	34.68
29	310-320	0.8556	33.88
30	320-330	0.8609	32.87
31	330-340	0.8649	32.10
32	340-350	0.8691	31.31
33	350-360	0.8740	30.40
34	360-370	0.8777	29.72

Table E-7 Specific gravity and *API* of distillate fractions from Jambur crude oil

Cut No.	Boiling range, °C	*Sp.gr*	*API*
1	gas	-	-
2	30-50	0.642	88.90
3	50-60	0.6444	88.08
4	60-70	0.6514	85.72
5	70-80	0.6596	83.02
6	80-90	0.6819	76.01
7	90-100	0.7059	68.95
8	100-110	0.7185	65.44
9	110-120	0.7387	60.05
10	120-130	0.7432	58.89
11	130-140	0.7463	58.10
12	140-150	0.7510	56.92
13	150-160	0.7523	56.59
14	160-170	0.7763	50.77
15	170-180	0.7835	49.10
16	180-190	0.7877	48.14
17	190-200	0.7901	47.59
18	200-210	0.7960	46.26
19	120-220	0.8001	45.35
20	220-230	0.8030	44.71
21	230-240	0.8070	43.84
22	240-250	0.8147	42.18
23	250-260	0.8239	40.24
24	260-270	0.8295	39.08
25	270-280	0.8311	38.76
26	280-290	0.8335	38.27
27	290-300	0.8336	38.25
28	300-310	0.8412	36.71
29	310-320	0.8472	35.52
30	320-330	0.8532	34.35
31	330-340	0.8592	33.19
32	340-350	0.8705	31.05
33	350-360	0.8730	30.58
34	360-370	0.8760	30.03

Table E-8 Specific gravity and *API* of distillate fractions from Bai – Hassan crude oil

Cut No.	Boiling range, °C	*Sp.gr*	*API*
1	gas	-	-
2	30-50	0.6314	92.61
3	50-60	0.6447	87.98
4	60-70	0.6558	84.27
5	70-80	0.6717	79.16
6	80-90	0.6906	73.39
7	90-100	0.7052	69.15
8	100-110	0.7170	65.85
9	110-120	0.7287	62.68
10	120-130	0.7386	60.08
11	130-140	0.7485	57.54
12	140-150	0.7563	55.60
13	150-160	0.7616	54.29
14	160-170	0.7670	52.99
15	170-180	0.7723	51.72
16	180-190	0.7765	50.73
17	190-200	0.7800	49.91
18	200-210	0.7816	49.54
19	120-220	0.7874	48.21
20	220-230	0.7903	47.55
21	230-240	0.7928	46.98
22	240-250	0.8069	43.86
23	250-260	0.8176	41.57
24	260-270	0.8255	39.91
25	270-280	0.8303	38.92
26	280-290	0.8319	38.59
27	290-300	0.8388	37.19
28	300-310	0.8509	34.79
29	310-320	0.8646	32.16
30	320-330	0.8722	30.73
31	330-340	0.8780	29.66
32	340-350	0.8814	29.04
33	350-360	0.8830	28.75
34	360-370	0.8853	28.33

Appendix F

Constants for *TBP* and *Sp.gr* equations

Table F-1 Constants for working *TBP* and *Sp.gr* equations for data sources of part one

Petroleum stock no.	*API*	Constants for *TBP* equation*					Constants for *Sp.gr* Equation**	
		$A^{'}$	$B^{'}$	$C^{'}$	$D^{'}$	$E^{'}$	$A^{'}$	$B^{'}$
1	32.4	0.00003516	-0.00572	0.2716 1	5.4706	144.44	overall	overall
2	36.5	0.00002843	-0.0004	0.1838	3.3991	155.89	overall	overall
3	27.2	0.00003045	-0.0041	0.1222	11.5959	135.69	overall	overall
4	37.3	0.0000090	-0.0004	-0.0487	10.7238	121.51	overall	overall
5	34.9	0.00001209	0.00016	-0.1482	13.013	208.52	overall	overall
6	40.9	0.00003687	-0.00512	0.2035	4.1413	138.09	overall	overall
7	40.8	0.00001271	-0.00109	0.01700	7.3032	120.21	overall	overall
8	37.1	0.00001863	-0.0028	0.1368	6.4295	121.08	overall	overall
9	28.2	0.000040	0.0029	-0.4074	19.045	248.81	overall	overall
10	38.2	0.00001	-0.0011	0.0091	10.285	90.11	overall	overall
11	32.5	0.00001240	-0.00119	0.01428	8.6287	141.19	overall	overall
12	34.4	0.00001809	-0.00145	0.04880	8.3455	148.07	overall	overall
13	47.8	0.00004349	-0.0007	0.0098	6.7759	91.91	overall	overall
14	37	0.00003574	-0.0050	0.1911	1.7281	371.0	overall	overall
15	38.6	0.0000020	0.0001	-0.019	9.2441	91.53	overall	overall
16	37.3	0.000005	0.0001	-0.085	13.914	84.254	0.5963	0.0923
17	20.2	0.00001553	-0.0006	-0.1389	15.544	330.38	0.7365	0.0639
18	42.2	0.00000277	0.0010	-0.1499	12.4372	146.63	0.6364	0.0662

* $TBP,\ °F = A'_1V^4 + B'_1V^3 + C'_1V^2 + D'_1V + E'_1$

** $Sp.gr = A'_2V^{B'2}$

Table F-2 Constants for working *TBP* and *Sp.gr* equations for data sources of part two

Petroleum stock name	*API*	Constants for *TBP* equation*					Constants for *Sp.gr* Equation**	
		A'	B'	C'	D'	E'	A'	B'
Kirkuk	36.1	-0.0000041	0.0016	-0.1136	11.267	81.46	0.5213	0.1216
Basrah	31.1	0.00000427	0.001136	-0.1907	16.7699	67.609	0.5478	0.1134
Jambur	37.7	0.000004	0.0007	-0.1501	15.904	72.899	0.5111	0.1229
Bai – Hassan	31.8	0.00000241	0.001	-0.1039	11.115	82.851	0.4901	0.1380

* $TBP, °F = A'_1V^4 + B'_1V^3 + C'_1V^2 + D'_1V + E'_1$

** $Sp.gr = A'_2V^{B'2}$

Appendix G

List of computer program

```
REM THIS PROGRAMME IS USED FOR CALCULATION EFV FOR PETROLUEM FRACTIONS AT ATM
PRESSURE
REM THE EFV CURVE IS ESTIMATED FROM TBP CURVE BY A) GRAPHICAL METHOD B) PSEDO-
COMPONENTS (COMPUTER) METHODS
REM-----------------------------------------------------------------------------
REM INSTRUCTION FOR USING THE PROGRAMME
REM------------------------------------
REM if TBP curve and s.gr curve equation are available then input chois =2
REM if TBP curves and just overall sp.gr available then input choise =1
REM if the LEE-KASLER (1975) correlation used for vapor pressure calculation then
input vap=1
REM if the modefied method of the present work for eatimation vapor pressure then
input vap=2
REM if the unmodefied thermodynamic models used then input typ=1
REM if the modefied model no.1 is used then input typ=2
REM if the modefied model no.2 is used then input typ=3
PRINT " if TBP curve and s.gr curve equation are available then input chois =2"
PRINT " if TBP curves and just overall sp.gr available then input choise =1"
PRINT " if the LEE-KASLER (1975) correlation used for vapor pressure calculation
then input vap=1"
PRINT " if the modefied method of the present work for eatimation vapor pressure
then input vap=2"
PRINT " if the unmodefied thermodynamic models used then input typ=1"
PRINT " if the modefied model no.1 is used then input typ=2"
PRINT " if the modefied model no.2 is used then input typ=3"

DIM x(100), t(100), spgr(100), mw(100), mol(100), v(100), w(100)
DIM ag(10), bg(10), astmd86(100), spgrg(10), efvgm(100), agg(10), bgg(10)
DIM vld(10), tg(100), spgrgm(10), tv(100), ac(100), zfg(100), tgg(100)
DIM ymol(100), xmol(100), xwight(100), tc(100), pc(100), acf(100), cgg(100)
DIM kuop(100), wi(100), vap(100), ps(100), kmr(100), vl(100), a(100)
DIM cf(100), tr(100), pr(100), ksrk(100), ksrknew(100), zf(100)
DIM b(100), alfa1(100), m(100), fiv(100), fil(100), wwv(100, 100)
DIM wwl(100, 100), spgrad(100), alfao(100), lamda(100), vl25(100)
DIM solp(100), aac(100, 100), fivs(100), pof(100), act(100), vapa(100)
DIM y(1001), ta2(1001), s(1001), xf(1001), midv(100), ms(100), ns(100)
DIM tbr(100), wa(100), spgra(100), CVAP(100), f1(100), vapnew(100), vaplk(100)
DIM f2(100), delspgr(100), pcw(100), tcw(100), ww(100), mww(100), alfasro(100)
DIM vc(100), pbr(100), vl60(100), filcs(100), zar(100), tess(100), filcss(100)
DIM trs(100), pcc(100), wnew(100), alfasr(100), alfapr(100), mp(100)
DIM prst(100), prpt(100), alfaos(100), spgrgm1(100), xid(100), yid(100)
DIM xsrk(100), ysrk(100), xpr(100), ypr(100), xsrkva(100), ysrkva(100)
DIM xprva(100), yprva(100), ksrkm(100), kpr(100), ksrkva(100), kprva(100)

REM INPUT PART
REM-----------
REM input system temp. and pressure
REM--------------------------------
INPUT " system tem (f)=", ts
INPUT "system pressure (pasia)=", psy
REM input petroleum stock API
INPUT " petroelum stock API", API
REM input number of cuts(nb)
REM-------------------------
INPUT "input number of cuts(nb)", nb
REM input the experimantail efv volume distilate(vol%)
INPUT "the experimantail efv volume distilate(vol%)="; efvd
INPUT " inpute choise", choise
INPUT "vap", vap
INPUT "typ", typ
ts = ts + 460: tco = 60
feed = 100
temp = 10
REM INPUT EFV10% ,EFV50%
REM----------------------
'INPUT "EFV10%="; VRP10
'INPUT "EFV50%="; VAP50
vpr10 = 475
vpr50 = 516
```

```
REM input total feed volume vt(cm3)
vt = 4000
REM graphical methode constants
REM-----------------------------
REM constants of equation (3-3),(ag,bg)
REM------------------------------------
FOR i = 1 TO 6
READ ag(i), bg(i)
PRINT ag(i), bg(i)
NEXT i
DATA .9167,1.0019,.5277,1.0900,.7429,1.0425
DATA .8920,1.0176,.8705,1.0226,.9490,1.0110

REM-----------------------------
REM constants of equation (3-4),(agg,bgg,cgg)
REM-----------------------------------------
FOR i = 1 TO 6
READ agg(i), bgg(i), cgg(i)
PRINT agg(i), bgg(i), cgg(i)
NEXT i
DATA 3.2555,.8466,.4208,1.4881,.9511,.1287
DATA .8350,1.0315,.0817,3.617,.8274,.6214
DATA 9.9607,.6871,.9340,13.0316,.6529,1.1025

REM read of volume persent distilled for graphical method 0,10,30,50,70,90
REM-----------------------------------------------------------------------
FOR i = 1 TO 6
READ vld(i)
PRINT vld(i)
NEXT i
DATA 0,10,30,50,70,90

REM read of 4th dergree polynomial constants for true boling point equation
REM TBP(F)=abf4*x^4+abf3*x^3+abf2^2+abf1*x+abfo
REM ------------------------------------------------------------------------
Rem input TBP eqution constants
Input “abfo”;abfo
Input “abf1”;abf1
Input “abf2:.abf2
Input “abf3”;abf3
Input :”abf4”.abf4
IF choise = 1 THEN 5
REM input type of sp.gr type
REM input sp.gr curve constants( a,b) if available
REM sp.gr(i)= a*v^b
INPUT "a="; a
INPUT "b="; b


5 REM CALCULATIONAL Parts
REM--------------------------
REM calculational methodes for estimation EFV curve from TBP curve
REM---------------------------------------------------------------

REM a- graphical methodes
REM-------------------
REM 1- graphical methode by using Raizi-Daubert method(1986)
REM---------------------------------------------------------------
        FOR i = 1 TO 6
        x = vld(i)
        TEM = abf4 * x ^ 4 + abf3 * x ^ 3 + abf2 * x ^ 2 + abf1 * x + abfo
        astmd86(i) = ag(i) ^ (-1 / bg(i)) * (TEM + 460) ^ (1 / bg(i))
         NEXT i
        FOR i = 1 TO 6
        IF choise = 1 THEN 8
        spgrgm1(i) = a * vld(i) ^ b: GOTO 9
8   spgrgm1(i) = .074251 * (vpr10 + 460) ^ -.01534 * (vpr50 + 460) ^ .36844
9   efvgm(i) = agg(i) * astmd86(i) ^ (bgg(i)) * spgrgm1(i) ^ cgg(i)
        PRINT vld(i), astmd86(i) - 460, efvgm(i) - 460
        NEXT i

REM b- pseudo-components (computer) methodes
REM-------------------------------------

REM chrachtrization steps (step 1 and 2)
REM-------------------------------------

REM divided petroleum stock to 40 cuts
REM------------------------------------
total = 100
inc = total / nb
nb1 = nb + 1
```

```
FOR i = 1 TO nb1
IF i = 1 THEN x(i) = 0: GOTO 10
x(i) = x(i - 1) + inc
10  PRINT x(i), inc
NEXT i

REM calculation of sp.gr of petroleum stock
REM-------------------------------------
spo = 141.5 / (API + 131.5)

REM estimation tbp curve by four degree polynomial equation
REM tbp=abf4 * X ^ 4 + abf3 * X ^ 3 + abf2 * X ^ 2 + abf1 * X + abfo
REM X is the vol% distilled
FOR i = 1 TO nb1
x = x(i)
TEM = abf4 * x ^ 4 + abf3 * x ^ 3 + abf2 * x ^ 2 + abf1 * x + abfo
t(i) = TEM
tgg(i) = TEM
PRINT x(i), t(i)
NEXT i

REM calculation of mid boiling point temp.
REM--------------------------------------
u = .001
FOR i = 1 TO nb1 - 1
FOR xo = x(i) TO (x(i) + inc) STEP u
IF xo = x(i) THEN 40
w = x(i) + inc
m = (xo + x(i)) / 2
m2 = (x(i + 1) + xo) / 2
x = xo
TEM = abf4 * x ^ 4 + abf3 * x ^ 3 + abf2 * x ^ 2 + abf1 * x + abfo
yo = TEM
x = w
TEM = abf4 * x ^ 4 + abf3 * x ^ 3 + abf2 * x ^ 2 + abf1 * x + abfo
y(i + 1) = TEM
x = x(i)
TEM = abf4 * x ^ 4 + abf3 * x ^ 3 + abf2 * x ^ 2 + abf1 * x + abfo
y(i) = TEM
x = m
TEM = abf4 * x ^ 4 + abf3 * x ^ 3 + abf2 * x ^ 2 + abf1 * x + abfo
ym = TEM
x = m2
TEM = abf4 * x ^ 4 + abf3 * x ^ 3 + abf2 * x ^ 2 + abf1 * x + abfo
ym2 = TEM
a1 = ((xo - x(i)) / 6) * (yo + 4 * ym + y(i))
a2 = (y(i + 1) - yo) * (xo - x(i))
at = (xo - x(i)) * y(i + 1)
a3 = at - (a1 + a2)
a11 = ((w - xo) / 6) * (yo + y(i + 1) + 4 * ym2)
a22 = (w - xo) * yo
a33 = a11 - a22
er = ((a3 - a33) / a3) * 100: PRINT ABS(er), xo
IF ABS(er) <= 1 THEN ta2(i) = yo: midv(i) = xo: GOTO 30
40 NEXT xo
30  PRINT ta2(i), ABS(er):
NEXT i
FOR i = 1 TO nb
t(i) = ta2(i)
PRINT i, t(i)
NEXT i
 IF choise = 2 THEN 50
 FOR i = 1 TO nb
 spgr(i) = .3067 * t(i) ^ .1605
 NEXT i
 GOTO 60

50 REM calculation of mid sp.gr
REM-----------------------
u = .001
FOR i = 1 TO nb1 - 1
FOR xo = x(i) TO (x(i) + inc) STEP u
IF xo = x(i) THEN 55
w = x(i) + inc
m = (xo + x(i)) / 2
m2 = (x(i + 1) + xo) / 2
   x = xo
   TEM = a * x ^ b
   yo = TEM
   x = w
   TEM = a * x ^ b
   y(i + 1) = TEM
```

```
    x = x(i)
    TEM = a * x ^ b
    y(i) = TEM
    x = m
   TEM = a * x ^ b
    ym = TEM
    x = m2
  TEM = a * x ^ b
    ym2 = TEM
    a1 = ((xo - x(i)) / 6) * (yo + 4 * ym + y(i))
    a2 = (y(i + 1) - yo) * (xo - x(i))
    at = (xo - x(i)) * y(i + 1)
    a3 = at - (a1 + a2)
    a11 = ((w - xo) / 6) * (yo + y(i + 1) + 4 * ym2)
    a22 = (w - xo) * yo
    a33 = a11 - a22
    er = ((a3 - a33) / a3) * 100: PRINT ABS(er), xo
IF ABS(er) <= 1 THEN ta2(i) = yo: xf(i) = xo: GOTO 54
55 NEXT xo:
54  PRINT ta2(i), ABS(er):
 NEXT i
 FOR i = 1 TO nb
 spgr(i) = ta2(i)
 'PRINT xf(i), spgr(i), t(i)
 NEXT i

60 REM calculation of ajusted sp.gr
REM--------------------------------
  spgrca = 0
  FOR i = 1 TO nb
  spgrca = spgrca + (inc / 100) * spgr(i)
  PRINT spgr(i)
  NEXT i

 wf = spo * vt
 PRINT spgrca, spo, wf
 wt = 0
  FOR i = 1 TO nb
  v(i) = (inc / 100) * vt
  wi(i) = v(i) * spgr(i)
  wt = wt + wi(i)
  NEXT i

 REM ajust the spgr  for material balance
 REM---------------------------------------
       FOR i = 1 TO nb
       wi(i) = wi(i) * (wf / wt)
       spgrad(i) = wi(i) / v(i)
       sum = sum + wi(i)
       sum2 = sum2 + (inc / 100) * spgrad(i)
       NEXT i
       PRINT sum, wf, spo, sum2
       FOR i = 1 TO nb
        spgr(i) = spgrad(i)
    PRINT i, spgr(i), t(i)
       NEXT i

 REM calculation of critical properties of crude oil
REM -------------------------------------------------
FOR i = 1 TO nb
REM RAZIE DUBERT (1987)
REM----------------------
mw(i) = 20.468 * (t(i) + 460) ^ 1.26007 * spgr(i) ^ 4.98308 * (EXP(1.165 * 10 ^ -
4 * (t(i) + 460) - 7.78712 * spgr(i) + 1.1582 * 10 ^ -3 * (t(i) + 460) *
spgr(i)))
IF t(i) > 650 THEN 61
tc(i) = 10.6443 * (t(i) + 460) ^ .81067 * spgr(i) ^ .53691 * (EXP(-5.1747 * 10 ^
-4 * (t(i) + 460) - .54444 * spgr(i) + 3.5995 * 10 ^ -4 * (t(i) + 460) *
spgr(i)))

pc(i) = 6.162 * 10 ^ 6 * (t(i) + 460) ^ -.4844 * spgr(i) ^ 4.0846 * (EXP(-4.725 *
10 ^ -3 * (t(i) + 460) - 4.8014 * spgr(i) + 3.1939 * 10 ^ -3 * (t(i) + 460) *
spgr(i)))

GOTO 62
61 REM LEE KASLER (1975)
REM----------------------
tc(i) = 341.7 + 811 * spgr(i) + (.4244 + .1174 * spgr(i)) * (t(i) + 460) + (.4669
- 3.2623 * spgr(i)) * (10 ^ 5 / (t(i) + 460))
a1 = 8.3634 - (.0566 / spgr(i))
a2 = (.24244 + 2.2898 * spgr(i) ^ -1 + .11857 * spgr(i) ^ -2) * (t(i) + 460) * 10
^ -3
```

```
a3 = (1.4685 + 3.648 * spgr(i) ^ -1 + .47227 * spgr(i) ^ -2) * (t(i) + 460) ^ 2 *
10 ^ -7
a4 = (.42019 + 1.6977 * spgr(i) ^ -2) * (t(i) + 460) ^ 3 * 10 ^ -10
pc(i) = EXP((a1 - a2 + a3 - a4))
62 tbr(i) = (t(i) + 460) / tc(i)
pbr(i) = psy / pc(i)
kuop(i) = ((t(i) + 460)) ^ .3333 / spgr(i)
IF tbr(i) < .8 THEN 63
w(i) = -7.904 + .1352 * kuop(i) - .007465 * kuop(i) ^ 2 + 8.359 * tbr(i) + (1.408
- .01063 * kuop(i)) * tbr(i) ^ -1
    GOTO 64
63  a1 = LOG(pbr(i)) - 5.92714 + 6.09648 * tbr(i) ^ -1 + 1.28862 * LOG(tbr(i)) -
.169347 * tbr(i) ^ 6
   a2 = 15.2518 - 15.6875 * tbr(i) ^ -1 - 13.4721 * LOG(tbr(i)) + .4377 * tbr(i)
^ 6
   w(i) = a1 / a2
64 PRINT t(i), tc(i), pc(i), mw(i), w(i)
NEXT i
REM calculation of feed compostions in mole basis (ZFi)
REM---------------------------------------------------
summol = 0
 FOR i = 1 TO nb
  mol(i) = wi(i) / mw(i)
  summol = summol + mol(i)
  NEXT i
  FOR i = 1 TO nb
  zf(i) = mol(i) / summol
  PRINT zf(i)
  NEXT i

REM calculation of molar density (Vl)at 15.5 C(60 F),25 C (77 F),and system temp.
REM ---------------------------------------------------------------------------
REM for tr<1 the ract equation is used,while for tr>1 then cavvt equation is used
FOR i = 1 TO nb
vl60(i) = (1 / spgr(i)) * mw(i)
  r = 10.73
   trs(i) = ts / tc(i)
    IF trs(i) >= 1 THEN vl60(i) = vl60(i) * .01601: cf(i) = vl60(i) / (5.7 + 3 *
((tco + 460) / tc(i))): vl(i) = cf(i) * (5.7 + (3 * (ts / tc(i)))): vl25(i) =
cf(i) * (5.7 + (3 * (77 / tc(i)))): GOTO 56
       vl60(i) = vl60(i) * .01601
       mr60 = (1 + (1 - ((tco + 460) / tc(i))) ^ .2857)
       arc = (r * tc(i)) / pc(i)
       zar(i) = EXP((LOG(vl60(i)) - LOG(arc)) / mr60)
       mrts = (1 + (1 - trs(i)) ^ .2857)
       vl(i) = arc * zar(i) ^ mrts
       mr25 = (1 + (1 - ((77 + 460) / tc(i))) ^ .2857)
       vl25(i) = arc * zar(i) ^ mr25
56  PRINT trs(i);
          NEXT i
REM calculation of cuts vapor pressures using LEE-KASLER method (1975)or
developted method
REM ------------------------------------------------------------------------
  'IF vap = 2 THEN GOTO 34
  REM LEE-KASLER METHOD (1975)
    FOR i = 1 TO nb
    trk = ts / tc(i)
    PRO = 5.92714 - 6.09648 / trk - 1.28862 * LOG(trk) + .169347 * trk ^ 6
    PR1 = 15.2518 - 15.6875 / trk - 13.4721 * LOG(trk) + .43577 * trk ^ 6
    pr = PRO + w(i) * PR1
    vaplk(i) = EXP(pr) * pc(i)
    'vap(i) = vaplk(i)
    NEXT i
      'GOTO 33
34 REM CALCULATION OF VAPOR PRESSURE USING DEVELOPTED LEE KASLER METHODE
  REM--------------------------------------------------------------------
  REM  VAP IN ATM,T IN KELVIEN
  REM VAP PRES IS CALCULATED BY VAP=A+B*TB+C*TB^2+D/TB
  REM RED OF ALKAN CONSTANT,FOR CALCULATION SPGR,VAP,W
  FOR i = 1 TO nb
tsyw = .7 * (((tc(i) - 460 - 32) / 1.8 + 273.15))
 pcc(i) = pc(i) / 14.7
  tv(i) = ((t(i)) - 32) / 1.8 + 273.15
  tbr(i) = tsyw / tv(i)
  spgra(i) = 1.2539 - 6.4292 * 10 ^ -4 * tv(i) + 4.5328 * 10 ^ -7 * tv(i) ^ 2 -
1.4461 * 10 ^ 2 / tv(i)
  wa(i) = -1.1435 + 3.3716 * 10 ^ -3 * tv(i) - 8.0152 * 10 ^ -7 * tv(i) ^ 2 +
(1.3079 * 10 ^ 2) / tv(i)
  CVAP(i) = (.0953 + 3.179 * 10 ^ -4 * tv(i)) * (tbr(i) - .85)
  AA = 1 / (CVAP(i) + 1)
  BB = 1 / (CVAP(i) + tbr(i))
  CC = AA - BB
```

```
  f1(i) = 1.21864 * (3.8 + tbr(i)) * CC
  f2(i) = .6828 + (1.2532 - 4.3574 * 10 ^ -3 * tv(i)) * (1 - .85 / tbr(i) ^ 2)
  vapa(i) = (.9665 + 2.3021 * 10 ^ -3 * tv(i) - 5.4728 * 10 ^ -7 * tv(i) ^ 2 +
89.301 / tv(i)) * f1(i)
  delspgr(i) = spgr(i) - spgra(i)

anew = 1: bnew = .85
vapnew(i) = vapa(i) + delspgr(i) * f1(i) * f2(i) + (anew - bnew / tbr(i))
vapnew(i) = (EXP(vapnew(i)))
vap(i) = vapnew(i)
a11 = LOG(vap(i) / pcc(i)): a11 = -a11 / 2.3025
wnew(i) = a11 - 1
tsy = (ts - 460 - 32) / 1.8 + 273.15
tbr(i) = tsy / tv(i)
spgra(i) = 1.2539 - 6.4292 * 10 ^ -4 * tv(i) + 4.5328 * 10 ^ -7 * tv(i) ^ 2 -
1.4461 * 10 ^ 2 / tv(i)
wa(i) = -1.1435 + 3.3716 * 10 ^ -3 * tv(i) - 8.0152 * 10 ^ -7 * tv(i) ^ 2 +
(1.3079 * 10 ^ 2) / tv(i)
CVAP(i) = (.0953 + 3.179 * 10 ^ -4 * tv(i)) * (tbr(i) - .85)
AA = 1 / (CVAP(i) + 1)
BB = 1 / (CVAP(i) + tbr(i))
CC = AA - BB
f1(i) = 1.21864 * (3.8 + tbr(i)) * CC
f2(i) = .6828 + (1.2532 - 4.3574 * 10 ^ -3 * tv(i)) * (1 - .85 / tbr(i))
vapa(i) = (.9665 + 2.3021 * 10 ^ -3 * tv(i) - 5.4728 * 10 ^ -7 * tv(i) ^ 2 +
89.301 / tv(i)) * f1(i)
delspgr(i) = spgr(i) - spgra(i)
anew = 1: bnew = .85
vapnew(i) = vapa(i) + delspgr(i) * f1(i) * f2(i) + (anew - bnew / tbr(i))
vapnew(i) = (EXP(vapnew(i))) * 14.7
'vap(i) = vapnew(i)
PRINT wnew(i)
NEXT i

33  REM ---------------------------------------
REM step 3
REM selection of types of thermodynamics models for performing flash
calculations(mode of operation)
REM--------------------------------------------------------------------------
FOR i = 1 TO nb
tr(i) = ts / tc(i)
pr(i) = psy / pc(i)
IF typ = 2 THEN GOTO 143
IF typ = 3 THEN GOTO 141
vap(i) = vaplk(i)
ms(i) = .48 + 1.574 * w(i) - .176 * w(i) ^ 2
mp(i) = .37646 + 1.5422 * w(i) - .26992 * w(i) ^ 2
alfasr(i) = (1 + ms(i) * (1 - tr(i) ^ .5)) ^ 2:
alfapr(i) = (1 + mp(i) * (1 - tr(i) ^ .5)) ^ 2:
GOTO 146
141  w(i) = wnew(i): vap(i) = vapnew(i)
ms(i) = .48 + 1.574 * w(i) - .176 * w(i) ^ 2
mp(i) = .37646 + 1.5422 * w(i) - .26992 * w(i) ^ 2
alfasr(i) = (1 + ms(i) * (1 - tr(i) ^ .5)) ^ 2:
alfapr(i) = (1 + mp(i) * (1 - tr(i) ^ .5)) ^ 2:
GOTO 146
143 vap(i) = vaplk(i)
ms(i) = .48 + 1.574 * w(i) - .176 * w(i) ^ 2
IF temp < 0 THEN 130
alfasr(i) = (1 + ms(i) * (1 - tr(i) ^ .5)) ^ 2:
GOTO 144
130 alfasro(i) = (1 + ms(i) * (1 - tr(i) ^ .5)) ^ 2
alfasr(i) = .0147 + (alfasro(i) * .939) - (.01 * temp)
144 REM ping-robinson alfa function using TWU method (2002)
IF tr(i) > 1 THEN 142
REM tr<1
lo = .272838: mo = .924779: no = 1.19764: l1 = .625701: m1 = .792014: n1 =
2.46022
alfao(i) = tr(i) ^ (no * (mo - 1)) * EXP(lo * (1 - tr(i) ^ (no * mo)))
alfa1(i) = tr(i) ^ (n1 * (m1 - 1)) * EXP(l1 * (1 - tr(i) ^ (n1 * m1)))
alfapr(i) = alfao(i) + w(i) * (alfa1(i) - alfao(i))
GOTO 146
142 REM tr>1
lo = .373949: mo = 4.7302: no = -.2: l1 = .0239035: m1 = 1.24615: n1 = -8
alfao(i) = trs(i) ^ (no * (mo - 1)) * EXP(lo * (1 - trs(i) ^ (no * mo)))
alfa1(i) = trs(i) ^ (n1 * (m1 - 1)) * EXP(l1 * (1 - trs(i) ^ (n1 * m1)))
alfapr(i) = alfao(i) + w(i) * (alfa1(i) - alfao(i))
146  PRINT alfapr(i);
NEXT i
REM supercritical fivs estimation using grayson-streed method(1962)
REM------------------------------------------------------------
```

```
ao = 2.05135: a1 = -2.10899: a2 = 0: a3 = -.19396: a4 = .02282: a5 = .08852: a6 =
0
a7 = -.00872: a8 = -.00353: a9 = .00203
a10 = -4.23893: a11 = 8.65808: a12 = -1.2206: a13 = -3.15224: a14 = -.025
FOR i = 1 TO nb
prs = psy / pc(i)
logfivso = ao + a1 / tr(i) + a2 * tr(i) + a3 * tr(i) ^ 2 + a4 * tr(i) ^ 3 + (a5 +
a6 * tr(i) + a7 * tr(i) ^ 2) * prs + (a8 + a9 * tr(i)) * prs ^ 2 - (LOG(prs)) /
2.3025
logfivs1 = a10 + a11 * tr(i) + a12 / tr(i) + a13 * tr(i) ^ 3 + a14 * (prs - .6)
logfivs = logfivso + w(i) * logfivs1
logfivs = logfivs / 2.3025
filcs(i) = EXP(logfivs)
PRINT filcs(i);
prs = vap(i) / pc(i)
logfivso = ao + a1 / tr(i) + a2 * tr(i) + a3 * tr(i) ^ 2 + a4 * tr(i) ^ 3 + (a5 +
a6 * tr(i) + a7 * tr(i) ^ 2) * prs + (a8 + a9 * tr(i)) * prs ^ 2 - (LOG(prs)) /
2.3025
logfivs1 = a10 + a11 * tr(i) + a12 / tr(i) + a13 * tr(i) ^ 3 + a14 * (prs - .6)
logfivs = logfivso + w(i) * logfivs1
logfivs = logfivs / 2.3025
filcss(i) = EXP(logfivs)

NEXT i

REM performing flash calculation for estimation of falsh volume(step 4)
REM flash calculation performed using five pseudo-components methods
REM ideak k,srk,pr,srk+van,pr+van pseudo-components methods
REM--------------------------------------------------------------------

REM 1- ideal solution k-values pseudo-componenet method (ideal k)
REM--------------------------------------------------------------
PRINT "flash calculations with modifed ideal k- value"
PRINT "--------------------------------------------"
REM estimatiom of ideak k-values(kmr)
REM----------------------------------
r = 10.73
FOR i = 1 TO nb
a1 = .08664 / ((ts / tc(i)) * pc(i))
a2 = (.42747 * alfasr(i)) / ((ts / tc(i)) ^ 2 * pc(i))
a3 = vl(i) / (r * ts)
a4 = vap(i) - psy
a5 = (a1 - a2 - a3) * a4
a6 = EXP(a5)
kmr(i) = (vap(i) / psy) * a6
PRINT kmr(i);
NEXT i
REM ckeck of two phase regions
REM---------------------------
su1 = 0
su2 = 0
FOR i = 1 TO nb
su1 = su1 + (zf(i) * (1 - kmr(i)))
e1 = 1 + kmr(i) - 1
IF e1 = 0 THEN e1 = .000001: GOTO 66
66 su2 = su2 + (zf(i) * (1 - kmr(i)) / e1)
NEXT i
PRINT su1, su2

IF su1 < 0 AND su2 > 0 THEN 334
PRINT "waring:it single phase accure": fr = 0: GOTO 202
334 PRINT " flash calculation can be accure"
REM performing flash calculations
REM-------------------------------
fr = .5
120 sum1 = 0
sum2 = 0: sum5 = 0
FOR i = 1 TO nb
s1 = zf(i) * (1 - kmr(i))
s2 = 1 + fr * (kmr(i) - 1)
sum1 = sum1 + (s1 / s2)
s3 = zf(i) * (i - kmr(i)) ^ 2
s4 = (1 + fr * (kmr(i) - 1)) ^ 2
sum2 = sum2 + (s3 / s4)
sum5 = sum5 + (s1 / s2)
NEXT i:
frn = fr - (sum1 / sum2)
IF frn < 0 THEN frn = fr / 2
eor = ABS(frn - fr) / fr
IF eor <= 10 ^ -4 AND fr > 0 THEN 200
fr = frn
PRINT eor, fr, "ideal k-value"
```

```
GOTO 120
200 PRINT "fraction vapor="; fr
REM calculation of vapor and liquid phases compostions(ymol,xmol)
REM--------------------------------------------------------------
 sumv = 0: suml = o
 FOR i = 1 TO nb
 xmol(i) = zf(i) / (1 + fr * (kmr(i) - 1))
 ymol(i) = kmr(i) * xmol(i)
 sumv = sumv + ymol(i): suml = suml + xmol(i)
 PRINT xmol(i), ymol(i)
 NEXT i

REM estimation of vapor and liquid molar flow rate(vf,vl)
REM------------------------------------------------------
Vf = feed * fr
vl = feed - Vf
FOR i = 1 TO nb
PRINT zf(i), ymol(i), xmol(i)
xid(i) = xmol(i): yid(i) = ymol(i)
NEXT i
REM conversion of mole bais fraction vaporized to volume bais fraction vaporized
REM-----------------------------------------------------------------------------
REM estimation of molar density for vapor phase,and feed (Vv,Vf)
sum = 0: sum1 = 0
FOR i = 1 TO nb
sum = sum + vl60(i) * zf(i)
sum1 = sum1 + vl60(i) * ymol(i)
NEXT i
Vf = sum: Vv = sum1
k1 = fr * (Vv / Vf) * 100: GOTO 203
202  k1 = 0
203 PRINT "fraction vaporized vol%="; k1, "frcaton vaporized mol%="; fr * 100
REM 2- srk pseudo-components method
REM----------------------------------
PRINT "falsh calculaions using srk equistion of state"
PRINT "---------------------------------------------"
REM first estimation of k-values
REM------------------------------
FOR i = 1 TO nb: ksrk(i) = kmr(i): NEXT i
su1 = 0
su2 = 0
FOR i = 1 TO nb
su1 = su1 + (zf(i) * (1 - ksrk(i)))
e1 = 1 + ksrk(i) - 1
IF e1 = 0 THEN e1 = .000001: GOTO 6
6 su2 = su2 + (zf(i) * (1 - ksrk(i)) / e1)
            NEXT i
            PRINT su1, su2
        IF su1 < 0 AND su2 > 0 THEN 3
           PRINT "waring:it single phase accure": fr = 0: GOTO 533
3 PRINT " flash calculation can be accure"
 REM performing flash calculations
 REM------------------------------
13  fr = .5: it = 1
1 sum1 = 0
    sum2 = 0
   FOR i = 1 TO nb
        s1 = zf(i) * (1 - ksrk(i))
        s2 = 1 + fr * (ksrk(i) - 1)
        sum1 = sum1 + (s1 / s2)
        s3 = zf(i) * (i - ksrk(i)) ^ 2
        s4 = (1 + fr * (ksrk(i) - 1)) ^ 2
        sum2 = sum2 + (s3 / s4)
        NEXT i:
        frn = fr - (sum1 / sum2)
        IF frn < 0 THEN frn = fr / 2: GOTO 11
        PRINT frn, fr
11 eor = ABS(frn - fr) / fr
  IF eor <= 10 ^ -4 AND fr > 0 THEN 2
        'IF fr < 0 THEN PRINT "negative root": END
        'IF fr > 1 THEN PRINT ">1 root": END
        PRINT it, fr, "srk"
        it = it + 1
        'IF it = 1000 THEN 2
        fr = frn
        GOTO 1
2 PRINT fr, eor

400 REM first estimation of vapor and liquid phases compostions(ymol,xmol)
REM------------------------------------------------------------------------
FOR i = 1 TO nb
  xmol(i) = zf(i) / (1 + fr * (ksrk(i) - 1))
```

```
  ymol(i) = ksrk(i) * xmol(i)
  'PRINT xmol(i), ymol(i)
  NEXT i
  sum = 0
  sum1 = 0
  FOR i = 1 TO nb
  sum = sum + ymol(i)
  sum1 = sum1 + xmol(i)
  NEXT i
  FOR i = 1 TO nb
  ymol(i) = ymol(i) / sum
  xmol(i) = xmol(i) / sum1
  'PRINT ymol(i), xmol(i)
  NEXT i
 REM k- value using srk question of state
 REM -----------------------------------
 PRINT "srk question of state k value"
 PRINT "-----------------------------------"
 REM estimation of parameters and mixing rules
 REM---------------------------------------------
   FOR i = 1 TO nb
   a(i) = (.42747 * alfasr(i) * pr(i)) / tr(i) ^ 2
   b(i) = (.08664 * pr(i)) / tr(i)
   'PRINT tr(i), pr(i), a(i), b(i)
       NEXT i
       FOR i = 1 TO nb
       PRINT i, alfasr(i)
       NEXT i

320   sum = 0: sum1 = 0
      FOR i = 1 TO nb
       sum = sum + ymol(i) * b(i)
       FOR j = 1 TO nb
       wwv(i, j) = (a(i) * a(j)) ^ .5
        sum1 = sum1 + ymol(i) * ymol(j) * wwv(i, j)
        NEXT j
        NEXT i
        aav = sum1: bbv = sum
          PRINT aav, bbv
 REM estimation vapor and lquid copressibility factors (zv,zl)using newton-
raphson method
REM-----------------------------------------------------------------------
    zv = 1
270  f = zv ^ 3 - zv ^ 2 + zv * (aav - bbv - bbv ^ 2) - (aav * bbv)
      ff = (3 * zv ^ 2) - (2 * zv) + (aav - bbv - bbv ^ 2)
      zvn = zv - (f / ff)
      eor = ABS(zvn - zv) / zv
      IF eor <= 10 - 4 THEN 280
        zv = zvn
        GOTO 270
280 PRINT eor, zv
        sum2 = 0: sum3 = 0
       FOR i = 1 TO nb
       sum2 = sum2 + xmol(i) * b(i)
       FOR j = 1 TO nb
       wwl(i, j) = (a(i) * a(j)) ^ .5
        sum3 = sum3 + xmol(i) * xmol(j) * wwl(i, j)
        NEXT j
        NEXT i
        aal = sum3: bbl = sum2
          'PRINT aal, bbl
      zl = 10 ^ -4
290 f = zl ^ 3 - zl ^ 2 + zl * (aal - bbl - bbl ^ 2) - (aal * bbl)
      ff = (3 * zl ^ 2) - (2 * zl) + (aal - bbl - bbl ^ 2)
      zln = zl - (f / ff)
      eor = ABS(zln - zl) / zl
      IF eor <= 10 ^ -4 THEN 300
         'PRINT eor, zl(k), zl(k + 1):
        zl = zln
        FOR i = 1 TO 1000: NEXT i
        'PRINT eor, zl
        GOTO 290
300 PRINT eor, zl
REM estimation of fugacity coefficients for vapor and liquid phases(fiv,fil)
REM-------------------------------------------------------------------------
FOR i = 1 TO nb
a1 = (zv - 1) * b(i) / bbv
a2 = ((2 * a(i) ^ .5 / aav ^ .5) - (b(i) / bbv))
a3 = LOG((zv + bbv) / zv)
a4 = aav / bbv
fiv(i) = EXP(a1 - LOG(zv - bbv) - (a4 * a2 * a3))
PRINT fiv(i)
```

```
NEXT i
FOR i = 1 TO nb
a1 = (zl - 1) * b(i) / bbl
a2 = ((2 * a(i) ^ .5 / aal ^ .5) - (b(i) / bbl))
a3 = LOG((zl + bbl) / zl)
a4 = aal / bbl
fil(i) = EXP(a1 - LOG(zl - bbl) - (a4 * a2 * a3))
PRINT fil(i)
NEXT i
REM estimation of new k-values(ksrknew)
REM------------------------------------
   FOR i = 1 TO nb
   ksrknew(i) = fil(i) / fiv(i)
   PRINT ksrknew(i);
   NEXT i

REM check for convergence in k-values
REM----------------------------------
r2 = 0
   FOR i = 1 TO nb
       r2 = r2 + (ksrknew(i) / ksrk(i) - 1) ^ 2
       NEXT i
     IF r2 <= 10 ^ -4 THEN 500
     PRINT "r2="; r2, "beta="; fr
     FOR i = 1 TO nb
     ksrk(i) = ksrknew(i)
     NEXT i
     GOTO 13
500 PRINT fr, "r2="; r2, "fr="; fr, it

REM estimation new of vapor and liquid compostions(ymol,xmol)
REM----------------------------------------------------------
sumv = 0: suml = o
FOR i = 1 TO nb
xmol(i) = zf(i) / (1 + fr * (ksrk(i) - 1))
ymol(i) = ksrk(i) * xmol(i)
sumv = sumv + ymol(i): suml = suml + xmol(i)
'PRINT xmol(i), ymol(i)
NEXT i
FOR i = 1 TO nb
ymol(i) = ymol(i) / sumv: xmol(i) = xmol(i) / suml
NEXT i
REM estimation of vapor and liquid molar flow rate
REM-----------------------------------------------
Vf = feed * fr
vl = feed - Vf
FOR i = 1 TO nb
PRINT zf(i), ymol(i), xmol(i)
xsrk(i) = xmol(i): ysrk(i) = ymol(i): ksrkm(i) = ksrk(i)
NEXT i
REM conversion of mole bais fraction vaporized to volume bais fraction vaporized
REM-----------------------------------------------------------------------------
REM estimation of molar density for vapor phase,and feed (Vv,Vf)
sum = 0: sum1 = 0
FOR i = 1 TO nb
sum = sum + vl60(i) * zf(i)
sum1 = sum1 + vl60(i) * ymol(i)
NEXT i
Vf = sum: Vv = sum1
PRINT sum, sum1
 k2 = (Vv / Vf) * fr * 100: GOTO 534
533 k2 = 0
534 PRINT "fraction vaporized vol%="; k2, "frcaton vaporized mol%"; fr * 100
                PRINT it

   REM 3- activity model psudo-components method(srk+van)
   REM ---------------------------------------------------
   REM calculation of solubility parameters for each cuts (solp)
   REM----------------------------------------------------------=
   REM heat of vaporization(lamda) usin Raizi -Daubert correlation
(1980),(BTU/BMOLE)
   FOR i = 1 TO nb
   lamda(i) = 8.48585 * (t(i) + 460) ^ 1.1347 * spgr(i) ^ .0214
   PRINT lamda(i)
   NEXT i:
   FOR i = 1 TO nb
   solp(i) = ((lamda(i) - (1.986 * 537)) / vl25(i)) ^ .5
   REM conversion to cal/cm3
   solp(i) = solp(i) * .09
   PRINT solp(i);
   NEXT i
   REM estimation of activity coefficents for each cuts
```

```
   REM--------------------------------------------------
   REM estimation of interaction parameters (aac)
   REM--------------------------------------------------
   FOR i = 1 TO nb
   FOR j = 1 TO nb
   aac(i, j) = ((vl25(i) * (solp(i) - solp(j)))) / (1.976 * ts)
   NEXT j
   NEXT i
   FOR i = 1 TO nb
   FOR j = 1 TO nb
   PRINT aac(i, j);
   NEXT j
   NEXT i
   REM calculation of pointing factor
   REM-----------------------------
   FOR i = 1 TO nb
    a1 = vl(i) / (r * ts)
    a2 = psy - vap(i)
    a3 = a1 * a2
    pof(i) = EXP(a3)
    PRINT pof(i)
 NEXT i
REM estimation of vapor phase fugacity coffecients(fiv)
 REM-----------------------------------------------------
 REM flash caculation using srk EOS
 REM-------------------------------
 REM test for two phase region
 REM---------------------------
 FOR i = 1 TO nb
 ksrk(i) = kmr(i)
 NEXT i
  su1 = 0
  su2 = 0
 FOR i = 1 TO nb
 su1 = su1 + (zf(i) * (1 - ksrk(i)))
 e1 = 1 + ksrk(i) - 1
 IF e1 = 0 THEN e1 = .000001: GOTO 700
700 su2 = su2 + (zf(i) * (1 - ksrk(i)) / e1)
 NEXT i
 PRINT su1, su2
        IF su1 < 0 AND su2 > 0 THEN 800
        PRINT "waring:it single phase accure": k3 = 0: GOTO 3001
800 PRINT " flash calculation can be accure"
REM performing flash calculations
REM------------------------------
950 fr = .5: it = 1
1000 sum1 = 0
    sum2 = 0
   FOR i = 1 TO nb
        s1 = zf(i) * (1 - ksrk(i))
        s2 = 1 + fr * (ksrk(i) - 1)
        sum1 = sum1 + (s1 / s2)
        s3 = zf(i) * (i - ksrk(i)) ^ 2
        s4 = (1 + fr * (ksrk(i) - 1)) ^ 2
        sum2 = sum2 + (s3 / s4)
        NEXT i:
        frn = fr - (sum1 / sum2)
        IF frn < 0 THEN frn = fr / 2
        eor = ABS(frn - fr) / fr
        IF eor <= 10 ^ -4 AND fr > 0 THEN 1100

        it = it + 1
        'IF it = 1000 THEN 1100
        fr = frn
        GOTO 1000
1100 PRINT fr, eor:

1200 REM estimation vapor and liquid compostions(y,x)
REM---------------------------------------------
FOR i = 1 TO nb
  xmol(i) = zf(i) / (1 + fr * (ksrk(i) - 1))
  ymol(i) = ksrk(i) * xmol(i)
  PRINT xmol(i), ymol(i)
  NEXT i
  sum = 0
  sum1 = 0
  FOR i = 1 TO nb
  sum = sum + ymol(i)
  sum1 = sum1 + xmol(i)
  NEXT i
  FOR i = 1 TO nb
  ymol(i) = ymol(i) / sum
```

```
  xmol(i) = xmol(i) / sum1
  PRINT ymol(i), xmol(i)
  NEXT i
REM calculation of actvity coefficints (act)
REM---------------------------------------
sum = 0: sum1 = 0
FOR i = 1 TO nb
FOR j = 1 TO nb
sum = sum + xmol(j) * aac(j, i)
sum1 = sum1 + xmol(j) * aac(i, j)
NEXT j
a1 = sum1 / (1 - xmol(i))
a2 = ((1 - ((xmol(i) * sum1) / ((xmol(i) * sum1) + (1 - xmol(i) * sum))))) ^ 2
a3 = a1 * a2
act(i) = EXP(a3)
PRINT act(i)
NEXT i
REM calculation of vapor phase fugacity coefficints(fiv)
REM---------------------------------------------------
REM calculation of srk EOS parameters and mixing rules
REM---------------------------------------------------
   FOR i = 1 TO nb
   a(i) = (.42747 * alfasr(i) * pr(i)) / tr(i) ^ 2
   b(i) = (.08664 * pr(i)) / tr(i)
   PRINT tr(i), pr(i), a(i), b(i):
       NEXT i
        sum = 0: sum1 = 0
      FOR i = 1 TO nb
       sum = sum + ymol(i) * b(i)
       FOR j = 1 TO nb
       wwv(i, j) = (a(i) * a(j)) ^ .5
        sum1 = sum1 + ymol(i) * ymol(j) * wwv(i, j)
        NEXT j
        NEXT i
        aav = sum1: bbv = sum
 REM estimation vapor phase copressibility factors (zv)using newton-raphson
method
REM---------------------------------------------------------------------------
      zv = 1
1500 f = zv ^ 3 - zv ^ 2 + zv * (aav - bbv - bbv ^ 2) - (aav * bbv)
      ff = (3 * zv ^ 2) - (2 * zv) + (aav - bbv - bbv ^ 2)
      zvn = zv - (f / ff)
      eor = ABS(zvn - zv) / zv
      IF eor <= 10 ^ -4 THEN 1400
        zv = zvn
        'PRINT eor, zv(k)
        GOTO 1500
1400 PRINT zv
REM calculation of fugacity coefficients for vapor phase(fiv)
REM---------------------------------------------------------
FOR i = 1 TO nb
a1 = (zv - 1) * b(i) / bbv
a2 = ((2 * a(i) ^ .5 / aav ^ .5) - (b(i) / bbv))
a3 = LOG((zv + bbv) / zv)
a4 = aav / bbv
fiv(i) = EXP(a1 - LOG(zv - bbv) - (a4 * a2 * a3))
PRINT fiv(i)
 NEXT i

REM calculation of saturation fugacity coffcients (fivs)
REM---------------------------------------------------
REM if tr>1 then the fugacity coefficints can be calculated using chao-seader
correlation
REM-----------------------------------------------------------------------
REM calculation of srk EOS parameters and mixing rules
REM---------------------------------------------------
   FOR i = 1 TO nb
   prst(i) = vap(i) / pc(i)
   a(i) = (.42747 * alfasr(i) * prst(i)) / tr(i) ^ 2
   b(i) = (.08664 * prst(i)) / tr(i)
   PRINT tr(i), pr(i), a(i), b(i)
   NEXT i
   sum = 0: sum1 = 0
   FOR i = 1 TO nb
   sum = sum + ymol(i) * b(i)
   FOR j = 1 TO nb
   wwv(i, j) = (a(i) * a(j)) ^ .5
   sum1 = sum1 + ymol(i) * ymol(j) * wwv(i, j)
        NEXT j
        NEXT i
        FOR i = 1 TO nb
        aav = a(i): bbv = b(i)
```

```
        IF tr(i) > 1 THEN fil(i) = filcs(i): ksrknew(i) = (act(i) * fil(i)) /
fiv(i): GOTO 2101
 REM estimation vapor copressibility factors at saturated conditions(zvs)using
newton-raphson method
 REM-------------------------------------------------------------------------
     zvs = 1
2000 f = zvs ^ 3 - zvs ^ 2 + zvs * (aav - bbv - bbv ^ 2) - (aav * bbv)
      ff = (3 * zvs ^ 2) - (2 * zvs) + (aav - bbv - bbv ^ 2)
      zvsn = zvs - (f / ff)
      eor = ABS(zvsn - zvs) / zvs
      IF eor <= 10 ^ -4 THEN 2100
        zvs = zvsn
        PRINT eor, zvs
        GOTO 2000
2100 PRINT zvs
IF zvs < 0 THEN fivs(i) = filcss(i): GOTO 2102
a1 = (zvs - 1)
a3 = LOG((zvs + bbv) / zvs)
a4 = aav / bbv
fivs(i) = EXP(a1 - LOG(zvs - bbv) - (a4 * a3))
PRINT "zvs="; zvs

REM calculation of new k-values(ksrknew)
REM----------------------------------------
2102 ksrknew(i) = (act(i) * fivs(i) * vap(i) * pof(i)) / (fiv(i) * psy)
2101 NEXT i

FOR i = 1 TO nb
PRINT ksrknew(i)
NEXT i

REM check for convergence in k-values
REM----------------------------------
REM
r2 = 0
FOR i = 1 TO nb
r2 = r2 + (ksrknew(i) / ksrk(i) - 1) ^ 2
NEXT i
IF r2 <= .0001 THEN 3000
PRINT "r2="; r2, "beta="; fr
FOR i = 1 TO nb
ksrk(i) = ksrknew(i): NEXT i
it = it + 1
PRINT it, r2
GOTO 950
3000 PRINT fr

REM calculation of vapor and lquid phase compostions(ymol,xmol)
REM------------------------------------------------------------
sumv = 0: suml = o
FOR i = 1 TO nb
xmol(i) = zf(i) / (1 + fr * (ksrk(i) - 1))
ymol(i) = ksrk(i) * xmol(i)
sumv = sumv + ymol(i): suml = suml + xmol(i)
PRINT xmol(i), ymol(i)
NEXT i

REM estimation of vapor and liquid molar flow rate (vf,vl)
REM-------------------------------------------------------
Vf = feed * fr
vl = feed - Vf
FOR i = 1 TO nb
PRINT zf(i), ymol(i), xmol(i)
ysrkva(i) = ymol(i): xsrkva(i) = xmol(i): ksrkva(i) = ksrk(i)
NEXT i
REM conversion of mole bais fraction vaporized to volume bais fraction vaporized
REM---------------------------------------------------------------------------
REM estimation of molar density for vapor phase,and feed (Vv,Vf)
sum = 0: sum1 = 0
FOR i = 1 TO nb
sum = sum + vl60(i) * zf(i)
sum1 = sum1 + vl60(i) * ymol(i)
NEXT i
Vv = sum1: Vf = sum
k3 = (Vv / Vf) * fr * 100: GOTO 3002
3001  k3 = 0
3002 PRINT "fraction vaporized vol%= "; k3, " frcaton vaporized mol%="; fr * 100
REM 4- PR EOS pseudo-components method
REM ------------------------------------
PRINT "falsh calculaions using pr equistion of state"
PRINT "-----------------------------------------------"
REM first estimation of k-values
```

```
REM------------------------------
FOR i = 1 TO nb: ksrk(i) = kmr(i)
NEXT i
REM ckeck of two phase regions
REM---------------------------
  su1 = 0
  su2 = 0
 FOR i = 1 TO nb
 su1 = su1 + (zf(i) * (1 - ksrk(i)))
 e1 = 1 + ksrk(i) - 1
 IF e1 = 0 THEN e1 = .000001: GOTO 336

336 su2 = su2 + (zf(i) * (1 - ksrk(i)) / e1)
            NEXT i
            PRINT su1, su2

        IF su1 < 0 AND su2 > 0 THEN 333
           PRINT "waring:it single phase accure": fr = 0: GOTO 5503

333 PRINT " flash calculation can be accure"

 REM performing flash calculations
 REM------------------------------
1333  fr = .5: it = 1
1113 sum1 = 0
    sum2 = 0
   FOR i = 1 TO nb
        s1 = zf(i) * (1 - ksrk(i))
        s2 = 1 + fr * (ksrk(i) - 1)
        sum1 = sum1 + (s1 / s2)
        s3 = zf(i) * (i - ksrk(i)) ^ 2
        s4 = (1 + fr * (ksrk(i) - 1)) ^ 2
        sum2 = sum2 + (s3 / s4)
        NEXT i:
        frn = fr - (sum1 / sum2)
        IF frn < 0 THEN frn = fr / 2: GOTO 1133
1133 eor = ABS(frn - fr) / fr
  IF eor <= 10 ^ -4 AND fr > 0 THEN 2333
        'IF fr < 0 THEN PRINT "negative root": END
        'IF fr > 1 THEN PRINT ">1 root": END
        it = it + 1
        'IF it = 1000 THEN 2333
        fr = frn
        PRINT eor, fr, it, "pr"
        GOTO 1113
2333 PRINT fr, eor
REM calculation of vapor and liquid phase compostions(y,x)
REM------------------------------------------------------
4400  FOR i = 1 TO nb
  xmol(i) = zf(i) / (1 + fr * (ksrk(i) - 1))
  ymol(i) = ksrk(i) * xmol(i)
  PRINT xmol(i), ymol(i)
  NEXT i
  sum = 0
  sum1 = 0
  FOR i = 1 TO nb
  sum = sum + ymol(i)
  sum1 = sum1 + xmol(i)
  NEXT i
  FOR i = 1 TO nb
  ymol(i) = ymol(i) / sum
  xmol(i) = xmol(i) / sum1
  'PRINT ymol(i), xmol(i)
  NEXT i
REM k- value using PR question of state
REM -------------------------------------
 PRINT "-----------------------------------"
 REM estimation of parameters and mixing rules
 REM------------------------------------------
PRINT "k- value using PR question of state "
PRINT "-----------------------------------"
 sum = 0: sum1 = 0: sum3 = 0: sum4 = 0
FOR i = 1 TO nb
a(i) = (.45724 * alfapr(i) * pr(i)) / tr(i) ^ 2
b(i) = (.0778 * pr(i)) / tr(i)
ac(i) = (.45724 * (10.73 * tc(i)) ^ 2) / pc(i)
NEXT i
sum11 = 0
FOR i = 1 TO nb
sum = sum + ymol(i) * b(i)
FOR j = 1 TO nb
wwv(i, j) = (a(i) * a(j)) ^ .5
```

```
sum1 = sum1 + ymol(i) * ymol(j) * wwv(i, j)
sum3 = sum3 + ymol(i) * ymol(j) * (ac(i) * alfapr(i) * ac(j) * alfapr(j)) ^ .5
NEXT j
NEXT i
aav = sum1: bbv = sum: aaj = sum3

REM estimation vapor and lquid copressibility factors (zv,zl)using newton-raphson method
REM---------------------------------------------------------------------
zv = 1
2230  f = zv ^ 3 - zv ^ 2 * (1 - bbv) + zv * (aav - 2 * bbv - 3 * bbv ^ 2) - (aav * bbv - bbv ^ 2 - bbv ^ 3)
ff = 3 * zv ^ 2 - 2 * zv * (1 - bbv) + (aav - 3 * bbv ^ 2 - 2 * bbv)
zvn = zv - (f / ff)
eor = ABS(zvn - zv) / zv
IF eor <= 10 ^ -4 THEN 2550
zv = zvn
PRINT eor, zv
GOTO 2230
2550 PRINT eor, zv
sum2 = 0: sum3 = 0: sum4 = 0
FOR i = 1 TO nb
sum2 = sum2 + xmol(i) * b(i)
FOR j = 1 TO nb
wwl(i, j) = (a(i) * a(j)) ^ .5
sum3 = sum3 + xmol(i) * xmol(j) * wwl(i, j)
sum4 = sum4 + xmol(i) * xmol(j) * (ac(i) * alfapr(i) * ac(j) * alfapr(j)) ^ .5
NEXT j
NEXT i
aal = sum3: bbl = sum2: bbj = sum4
zl = 10 ^ -4
2240  f = zl ^ 3 - zl ^ 2 * (1 - bbl) + zl * (aal - 2 * bbl - 3 * bbl ^ 2) - (aal * bbl - bbl ^ 2 - bbl ^ 3)
ff = 3 * zl ^ 2 - 2 * zl * (1 - bbl) + (aal - 3 * bbl ^ 2 - 2 * bbl)
zln = zl - (f / ff)
eor = ABS(zln - zl) / zl
IF eor <= 10 ^ -4 THEN 2260
'PRINT eor, zl(k)
zl = zln
PRINT eor, zl
GOTO 2240
2260 PRINT eor, zl
 PRINT zv, zl
FOR i = 1 TO nb
sum = 0
FOR j = 1 TO nb
sum = sum + ymol(j) * (ac(i) * alfapr(i) * ac(j) * alfapr(j)) ^ .5
NEXT j
a1 = (zv - 1) * (b(i) / bbv)
a2 = (((2 * sum) * (1 / aaj)) - b(i) / bbv)
'a2 = (((2 * a(i) ^ .5) * (1 / aav ^ .5)) - b(i) / bbv)
a3 = LOG((zv + bbv * 2.414) / (zv - bbv * .414))
a4 = aav / (2.828 * bbv)
'PRINT a1
'PRINT a2
'PRINT a3
'PRINT a4
fiv(i) = EXP(a1 - LOG(zv - bbv) - (a2 * a3 * a4))
PRINT fiv(i)
 NEXT i

REM estimation of fugacity coefficients for vapor and liquid phases(fiv,fil)
REM-------------------------------------------------------------------------
FOR i = 1 TO nb
sum = 0
FOR j = 1 TO nb
sum = sum + xmol(j) * (ac(i) * alfapr(i) * ac(j) * alfapr(j)) ^ .5
NEXT j
a1 = (zl - 1) * (b(i) / bbl)
a2 = (((2 * sum) * (1 / bbj)) - b(i) / bbl)
'a2 = (((2 * a(i) ^ .5) * (1 / aal ^ .5)) - b(i) / bbl)
a3 = LOG((zl + bbl * 2.414) / (zl - bbl * .414))
a4 = aal / (2.828 * bbl)
fil(i) = EXP(a1 - LOG(zl - bbl) - (a2 * a3 * a4))
PRINT fil(i), zl
PRINT "fil(i)="; fil(i)
NEXT i

REM estimation of new k-values(ksrknew)
REM------------------------------------
FOR i = 1 TO nb
   ksrknew(i) = fil(i) / fiv(i)
```

```
   PRINT ksrknew(i)
   NEXT i
REM check for convergence in k-values
REM-------------------------------
r2 = 0
FOR i = 1 TO nb
r2 = r2 + (ksrknew(i) / ksrk(i) - 1) ^ 2
       NEXT i
     IF r2 <= .0001 THEN 5500
     PRINT "r2="; r2, "beta="; fr
     FOR i = 1 TO nb
     ksrk(i) = ksrknew(i): NEXT i
     GOTO 1333
5500 PRINT fr, r2

REM calculation of vapor and lquid phase compostions(ymol,xmol)
REM------------------------------------------------------------
sumv = 0: suml = o
FOR i = 1 TO nb
xmol(i) = zf(i) / (1 + fr * (ksrk(i) - 1))
ymol(i) = ksrk(i) * xmol(i)
sumv = sumv + ymol(i): suml = suml + xmol(i)
NEXT i

REM estimation of vapor and liquid molar flow rate(vf,vl)
REM-----------------------------------------------------
Vf = feed * fr
vl = feed - Vf
FOR i = 1 TO nb
PRINT zf(i), ymol(i), xmol(i)
xpr(i) = xmol(i): ypr(i) = ymol(i): kpr(i) = ksrk(i)
NEXT i
REM conversion of mole bais fraction vaporized to volume bais fraction vaporized
REM----------------------------------------------------------------------------
REM estimation of molar density for vapor phase,and feed (Vv,Vf)
Vf = 0: Vv = 0
FOR i = 1 TO nb
Vf = Vf + vl60(i) * zf(i)
Vv = Vv + vl60(i) * ymol(i)
NEXT i
   k4 = (Vv / Vf) * fr * 100: GOTO 5504
5503 k4 = 0
5504 PRINT "fraction vaporized vol%"; k4, "frcaton vaporized mol%"; fr * 100


REM 5- activity model psudo-components method(pr+van)
REM -------------------------------------------------
PRINT "falsh calculaions using pr equistion of state"
REM -----------------------------------------------
REM heat of vaporization(lamda) usin Raizi -Daubert correlation
(1980),(BTU/BMOLE)
FOR i = 1 TO nb
lamda(i) = 8.48585 * (t(i) + 460) ^ 1.1347 * spgr(i) ^ .0214
PRINT lamda(i)
NEXT i

REM calculation of solubilty paramter(solp)
REM------------------------------------
FOR i = 1 TO nb
solp(i) = ((lamda(i) - (1.986 * 537)) / vl25(i)) ^ .5
REM conversion to cal/cm3
solp(i) = solp(i) * .09
PRINT solp(i)
NEXT i

REM calculation of interaction parameters(aac)
REM---------------------------------------
FOR i = 1 TO nb
FOR j = 1 TO nb
aac(i, j) = ((vl25(i) * (solp(i) - solp(j)))) / (1.976 * ts)
NEXT j
NEXT i
FOR i = 1 TO nb
FOR j = 1 TO nb
PRINT aac(i, j);
NEXT j
NEXT i

REM calculation of pointing factor(pof)
REM----------------------------------
FOR i = 1 TO nb
a1 = vl(i) / (r * ts)
```

```
a2 = psy - vap(i)
a3 = a1 * a2
pof(i) = EXP(a3)
PRINT pof(i)
NEXT i

REM calculation of vapor phase fugacity coefficints(fiv)
REM------------------------------------------------
PRINT "falsh calculaions using PR equistion of state"
PRINT "-----------------------------------------"
REM first estimation for k-values
REM-----------------------------
FOR i = 1 TO nb: ksrk(i) = kmr(i): NEXT i

 REM test for two phase region
 REM-------------------------
su1 = 0
su2 = 0
FOR i = 1 TO nb
su1 = su1 + (zf(i) * (1 - ksrk(i)))
e1 = 1 + ksrk(i) - 1
IF e1 = 0 THEN e1 = .000001: GOTO 3700
3700 su2 = su2 + (zf(i) * (1 - ksrk(i)) / e1)
NEXT i
PRINT su1, su2
IF su1 < 0 AND su2 > 0 THEN 3800
PRINT "waring:it single phase accure": fr = 0: GOTO 330001
3800 PRINT " flash calculation can be accure"

REM performing flash calculations
REM-------------------------------
3950 fr = .5: it = 1
31000 sum1 = 0
sum2 = 0
FOR i = 1 TO nb
s1 = zf(i) * (1 - ksrk(i))
s2 = 1 + fr * (ksrk(i) - 1)
sum1 = sum1 + (s1 / s2)
s3 = zf(i) * (i - ksrk(i)) ^ 2
s4 = (1 + fr * (ksrk(i) - 1)) ^ 2
sum2 = sum2 + (s3 / s4)
NEXT i
frn = fr - (sum1 / sum2)
IF frn < 0 THEN frn = fr / 2
eor = ABS(frn - fr) / fr
IF eor <= 10 ^ -4 AND fr > 0 THEN 31100
it = it + 1
'IF it = 1000 THEN 31100
fr = frn
PRINT eor, fr, it, "pr+gam"
GOTO 31000
31100 PRINT fr, eor

REM calculation of vapor and liquid phases compostions(ymol,xmol)
REM------------------------------------------------------------
31200  FOR i = 1 TO nb
xmol(i) = zf(i) / (1 + fr * (ksrk(i) - 1))
ymol(i) = ksrk(i) * xmol(i)
PRINT xmol(i), ymol(i)
NEXT i
sum = 0
sum1 = 0
FOR i = 1 TO nb
sum = sum + ymol(i)
sum1 = sum1 + xmol(i)
NEXT i
FOR i = 1 TO nb
ymol(i) = ymol(i) / sum
xmol(i) = xmol(i) / sum1
PRINT ymol(i), xmol(i)
NEXT i

REM calculation of actvity coefficints (act)
REM--------------------------------------
sum = 0: sum1 = 0
FOR i = 1 TO nb
FOR j = 1 TO nb
sum = sum + xmol(j) * aac(j, i)
sum1 = sum1 + xmol(j) * aac(i, j)
NEXT j
a1 = sum1 / (1 - xmol(i))
a2 = ((1 - ((xmol(i) * sum1) / ((xmol(i) * sum1) + (1 - xmol(i) * sum))))) ^ 2
```

```
a3 = a1 * a2
act(i) = EXP(a3)
PRINT act(i)
NEXT i

 REM estimation of vapor phase fugacity coffecients(fiv)
 REM-----------------------------------------------------
REM calculation of srk EOS parameters and mixing rules
REM----------------------------------------------------
sum = 0: sum1 = 0: r = 10.73
FOR i = 1 TO nb
ac(i) = .457235 * ((r * tc(i)) ^ 2 / pc(i))
a(i) = (.45724 * alfapr(i) * pr(i)) / tr(i) ^ 2
b(i) = (.0778 * pr(i)) / tr(i)
PRINT tr(i), pr(i), a(i), b(i):
NEXT i
sum11 = 0
FOR i = 1 TO nb
sum = sum + ymol(i) * b(i)
FOR j = 1 TO nb
wwv(i, j) = (a(i) * a(j)) ^ .5
sum1 = sum1 + ymol(i) * ymol(j) * wwv(i, j)
sum11 = sum11 + ymol(i) * ymol(j) * (ac(i) * ac(j) * alfapr(i) * alfapr(j)) ^ .5
NEXT j
NEXT i
aav = sum1: bbv = sum: aavv = sum1: aaj = sum11

REM estimation of vapor phase compessbility factores (zv)using newtone- raphsone
method
REM-----------------------------------------------------------------------
zv = 1
33231  f = zv ^ 3 - zv ^ 2 * (1 - bbv) + zv * (aav - 2 * bbv - 3 * bbv ^ 2) -
(aav * bbv - bbv ^ 2 - bbv ^ 3)
ff = 3 * zv ^ 2 - 2 * zv * (1 - bbv) + (aav - 3 * bbv ^ 2 - 2 * bbv)
zvn = zv - (f / ff)
eor = ABS(zvn - zv) / zv
IF eor <= 10 ^ -4 THEN 33251
zv = zvn
PRINT eor, zv
GOTO 33231
33251 PRINT eor, zv
REM estimation of vapor phase fugacity coeffidcients(fiv)
REM------------------------------------------------------
FOR i = 1 TO nb
sum = 0
FOR j = 1 TO nb
sum = sum + ymol(j) * (ac(i) * ac(j) * alfapr(i) * alfapr(j)) ^ .5
NEXT j
a1 = (zv - 1) * (b(i) / bbv)
a2 = (((2 * sum) * (1 / aaj)) - b(i) / bbv)
'a2 = (((2 * a(i) ^ .5) * (1 / aav ^ .5)) - b(i) / bbv)
a3 = LOG((zv + bbv * 2.414) / (zv - bbv * .414))
a4 = aav / (2.828 * bbv)
fiv(i) = EXP(a1 - LOG(zv - bbv) - (a2 * a3 * a4))
'PRINT fiv(i);
NEXT i
REM calculation of saturation fugacity coffecient(fivs)
REM-----------------------------------------------------
FOR i = 1 TO nb
prpt(i) = vap(i) / pc(i)
a(i) = (.45724 * alfapr(i) * prpt(i)) / tr(i) ^ 2
b(i) = (.0778 * prpt(i)) / tr(i)
ac(i) = (.45724 * (10.73 * tc(i)) ^ 2) / pc(i)
NEXT i
FOR i = 1 TO nb
aav = a(i): bbv = b(i)
IF tr(i) > 1 THEN fil(i) = filcs(i): ksrknew(i) = (act(i) * fil(i)) / fiv(i):
GOTO 32101
REM calcultion of saturates copressibily factores at saturation conditions
REM-----------------------------------------------------------------------
zvs = 1
32000 f = zvs ^ 3 - zvs ^ 2 * (1 - bbv) + zvs * (aav - 2 * bbv - 3 * bbv ^ 2) -
(aav * bbv - bbv ^ 2 - bbv ^ 3)
ff = 3 * zvs ^ 2 - 2 * zvs * (1 - bbv) + (aav - 3 * bbv ^ 2 - 2 * bbv)
zvsn = zvs - (f / ff)
eor = ABS(zvsn - zvs) / zvs
IF eor <= 10 ^ -4 THEN 32100
zvs = zvsn
GOTO 32000
32100 PRINT

REM calculation of saturted fugacity coefficinents(fivs)
```

```
REM-----------------------------------------------------
IF zvs < 0 THEN fivs(i) = filcss(i): GOTO 32102
a1 = (zvs - 1)
a3 = LOG((zvs + 2.414 * bbv) / (zvs - .414 * bbv))
a4 = aav / (2.828 * bbv)
fivs(i) = EXP(a1 - LOG(zvs - bbv) - (a3 * a4))
PRINT "fivs(i)="; zvs;

REM estimation of new k-values(ksrknew)
REM-------------------------------------
32102 ksrknew(i) = (act(i) * fivs(i) * vap(i) * pof(i)) / (fiv(i) * psy)
32101 NEXT i

REM check for convergence in k-values
REM----------------------------------
r2 = 0
FOR i = 1 TO nb
r2 = r2 + (ksrknew(i) / ksrk(i) - 1) ^ 2
NEXT i
IF r2 <= .0001 THEN 33000
PRINT "r2="; r2, "beta="; fr, it
FOR i = 1 TO nb
ksrk(i) = ksrknew(i): PRINT fr, "pr+van": NEXT i
GOTO 3950
33000 PRINT fr, r2

REM calculation of vapor and liquid phase compostions(ymol,xmol)
REM--------------------------------------------------------------
sumv = 0: suml = o
FOR i = 1 TO nb
xmol(i) = zf(i) / (1 + fr * (ksrk(i) - 1))
ymol(i) = ksrk(i) * xmol(i)
sumv = sumv + ymol(i): suml = suml + xmol(i)
'PRINT ymol(i), xmol(i), ksrk(i)
PRINT ksrk(i), tr(i)
NEXT i

REM estimation of vapor and liquid molar flow rate (vf,vl)
REM--------------------------------------------------------
Vf = feed * fr
vl = feed - Vf
FOR i = 1 TO nb
PRINT zf(i), ymol(i), xmol(i)
xprva(i) = xmol(i): yprva(i) = ymol(i): kprva(i) = ksrk(i)
NEXT i

REM conversion of mole bais fraction vaporized to volume bais fraction vaporized
REM-------------------------------------------------------------------------
REM estimation of molar density for vapor phase,and feed (Vv,Vf)
Vf = 0: Vv = 0
FOR i = 1 TO nb
Vf = Vf + vl60(i) * zf(i)
Vv = Vv + vl60(i) * ymol(i)
NEXT i
k5 = (Vv / Vf) * fr * 100: GOTO 330002
330001 k5 = 0
330002 PRINT "fraction vaporized vol%"; k5, "frcaton vaporized mol%"; fr * 100
PRINT
PRINT "------------------------------------------------------------"
REM  PRINT OUT PART
REM--------------------
REM print of flash volume vol%
REM-----------------------------
PRINT "srk vol%="; k2, "pr vol %="; k4, "ideal k vol%="; k1
PRINT "srk+van vol%="; k3, "pr+van vol%="; k5
PRINT "-----------------------------------------------"
REM eorr analysis
REM----------------
REM AAD % analysis
REM----------------
PRINT "AAD % analysis"
PRINT "-----------------------------------------------"
  PRINT "eor srk="; (ABS((k2 - efvd) / efvd)) * 100; "eor srk+gam="; (ABS((k3 -
efvd) / efvd)) * 100
    PRINT "eor pr="; (ABS((k4 - efvd) / efvd)) * 100; "eor pr+gam="; (ABS((k5 -
efvd) / efvd)) * 100
    PRINT "eor ideal k="; (ABS((k1 - efvd) / efvd)) * 100
REM AD % (bais) analysis
REM-----------------------
'PRINT "bias analysis"
'PRINT "---------------------------"
```

```
 'PRINT "bias srk="; (((k2 - efvd) / efvd)) * 100; "bias srk+gam="; (((k3 - efvd)
/ efvd)) * 100
 'PRINT "bias pr="; (((k4 - efvd) / efvd)) * 100; "bias pr+gam="; (((k5 - efvd) /
efvd)) * 100
 'PRINT "bias ideal k="; (((k1 - efvd) / efvd)) * 100
 REM system pressure and temp
 REM--------------------------
 PRINT "system tem in F="; ts - 460

   REM graphical method efv results
   REM------------------------------
    PRINT "graphical method EFV estimation using Raizi-Daubert (1986)"
    PRINT "-------------------------------------------------------"
    PRINT " vpl %", "astmd86", "efv"
    PRINT "-----------------------------"
    FOR i = 1 TO 6
    PRINT vld(i), astmd86(i) - 460, efvgm(i) - 460
    NEXT i
    END
    REM physical proprties for 40 cuts
    REM------------------------------
 OPEN "C:\C1neww.dat" FOR OUTPUT AS #1
    REM print out physical properties for cuts
    REM--------------------------------------
    FOR i = 1 TO nb
    PRINT i, t(i), w(i)
    PRINT #1, i, t(i), w(i)
    NEXT i
CLOSE #1
      END
   REM marerial balance for petroleum stock
   REM-------------------------------------
OPEN "C:\C22mb.dat" FOR OUTPUT AS #2
    REM print out material balance for petroleum stocks
    REM-----------------------------------------------
     FOR i = 1 TO nb
    PRINT i, t(i), spgr(i), v(i), wi(i), mol(i), zf(i)
    PRINT #2, i, t(i), spgr(i), mw(i), v(i), wi(i), mol(i), zf(i)
    NEXT i
    CLOSE #2
    END
    REM vapor and liquid compostions using five pseudo-components methods
    REM----------------------------------------------------------------

    REM liquid compostions
    REM------------------
    OPEN "C:\C6x.dat" FOR OUTPUT AS #3
    FOR i = 1 TO nb
    PRINT i, xid(i), xsrk(i), xpr(i), xsrkva(i), xprva(i)
    PRINT #3, i, xid(i), xsrk(i), xpr(i), xsrkva(i), xprva(i)
    NEXT i

    REM vapor compostions
    REM-----------------
    OPEN "C:\C6y.dat" FOR OUTPUT AS #4
    FOR i = 1 TO nb
    PRINT i, yid(i), ysrk(i), ypr(i), ysrkva(i), yprva(i)
    PRINT #4, i, yid(i), ysrk(i), ypr(i), ysrkva(i), yprva(i)
    NEXT i

    REM vapor and liquid k-values using five pseudo-components methods
    REM----------------------------------------------------------------
    OPEN "C:\C6k.dat" FOR OUTPUT AS #5
    FOR i = 1 TO nb
    PRINT i, kmr(i), ksrkm(i), kpr(i), ksrkva(i), kprva(i)
    PRINT #5, i, kmr(i), ksrkm(i), kpr(i), ksrkva(i), kprva(i)
    NEXT i
END
```

Appendix H

Physical properties and material balances for petroleum stocks for parts one and two of present work

Table H-1 Physical properties for petroleum stock No. 2

Cut	TB, °C	$Sp.gr$	MW	Tc, °C	Pc, kPa	ω	$V^{L(15)}$, cm^3/mol	$\delta^{(25)}$, J/cm^3
1	71.39	0.7118	87.24	248.90	3361.69	0.2583	122.56	29.10
2	77.26	0.7192	89.95	256.32	3319.27	0.2643	125.08	29.12
3	84.13	0.7273	93.15	264.87	3266.90	0.2716	128.08	29.13
4	91.79	0.7358	96.77	274.26	3205.79	0.2800	131.52	29.14
5	100.10	0.7445	100.76	284.28	3137.44	0.2894	135.35	29.13
6	108.90	0.7531	105.08	294.72	3063.69	0.2996	139.53	29.12
7	118.06	0.7616	109.68	305.44	2986.27	0.3104	144.01	29.09
8	127.45	0.7698	114.51	316.27	2906.87	0.3218	148.75	29.05
9	136.99	0.7777	119.55	327.10	2826.95	0.3337	153.72	28.99
10	146.56	0.7852	124.75	337.84	2747.71	0.3458	158.87	28.93
11	156.11	0.7924	130.08	348.42	2670.10	0.3581	164.16	28.86
12	165.58	0.7992	135.52	358.78	2594.75	0.3705	169.58	28.78
13	174.91	0.8056	141.04	368.88	2522.20	0.3830	175.08	28.69
14	184.09	0.8116	146.62	378.70	2452.63	0.3954	180.66	28.60
15	193.09	0.8173	152.25	388.24	2386.15	0.4078	186.29	28.50
16	201.91	0.8227	157.93	397.50	2322.69	0.4201	191.97	28.40
17	210.58	0.8278	163.67	406.52	2262.05	0.4324	197.71	28.30
18	219.12	0.8327	169.47	415.32	2203.93	0.4446	203.52	28.19
19	227.57	0.8374	175.38	423.97	2147.96	0.4569	209.43	28.08
20	236.00	0.8420	181.43	432.52	2093.70	0.4694	215.49	27.96
21	244.49	0.8464	187.69	441.05	2040.65	0.4821	221.74	27.84
22	253.11	0.8508	194.22	449.66	1988.28	0.4951	228.28	27.72
23	261.99	0.8552	201.14	458.45	1936.01	0.5088	235.19	27.58
24	271.23	0.8597	208.56	467.53	1883.26	0.5232	242.60	27.44
25	280.97	0.8643	216.63	477.03	1829.50	0.5386	250.64	27.29
26	291.37	0.8690	225.52	487.07	1774.13	0.5554	259.50	27.12
27	302.58	0.8740	235.45	497.81	1716.66	0.5738	269.39	26.94
28	314.78	0.8793	246.69	509.39	1656.62	0.5942	280.55	26.73
29	328.18	0.8849	259.54	521.97	1593.68	0.6171	293.31	26.50
30	342.97	0.8908	274.41	535.73	1527.51	0.6430	308.04	26.24
31	359.39	0.8972	291.78	535.92	1478.53	0.8358	325.19	25.94
32	377.68	0.9041	312.25	551.53	1394.91	0.8814	345.38	25.60
33	398.08	0.9114	336.57	568.71	1306.68	0.9334	369.29	25.22
34	420.86	0.9192	365.74	587.63	1214.08	0.9871	397.87	24.79
35	446.32	0.9276	401.01	608.47	1117.62	1.0481	432.31	24.29
36	474.74	0.9365	444.02	631.38	1018.07	1.1154	474.12	23.74
37	506.45	0.9459	496.98	656.56	916.29	1.1892	525.40	23.11
38	541.77	0.9559	562.85	684.18	813.52	1.2698	588.83	22.41
39	581.05	0.9663	645.63	714.40	711.11	1.3574	668.12	21.63
40	624.64	0.9773	750.89	747.42	610.59	1.4522	768.34	20.77

Table H-2 Physical properties for petroleum stock No. 3

Cut	*TB*, °C	*Sp.gr*	*MW*	*Tc*, °C	*Pc*, kPa	ω	$V^{L(15)}$, cm^3/mol	$\delta^{(25)}$, J/cm^3
1	65.77	0.7078	84.67	242.46	3433.39	0.2507	119.62	29.15
2	82.61	0.7290	92.38	263.78	3311.61	0.2679	126.72	29.21
3	99.99	0.7479	100.59	284.98	3170.19	0.2870	134.50	29.22
4	117.73	0.7650	109.34	305.93	3019.80	0.3077	142.93	29.18
5	135.68	0.7804	118.61	326.55	2867.63	0.3295	151.99	29.10
6	153.68	0.7944	128.41	346.70	2718.61	0.3523	161.64	28.98
7	171.60	0.8072	138.70	366.32	2575.78	0.3757	171.84	28.83
8	189.31	0.8188	149.45	385.31	2441.05	0.3995	182.51	28.65
9	206.72	0.8295	160.61	403.63	2315.29	0.4236	193.61	28.46
10	223.73	0.8393	172.12	421.22	2198.95	0.4479	205.08	28.24
11	240.29	0.8483	183.95	438.06	2091.85	0.4721	216.85	28.02
12	256.32	0.8565	196.02	454.12	1993.75	0.4961	228.85	27.79
13	271.80	0.8641	208.28	469.42	1904.07	0.5199	241.04	27.55
14	286.71	0.8711	220.68	483.96	1822.23	0.5434	253.34	27.32
15	301.02	0.8775	233.17	497.76	1747.57	0.5665	265.71	27.08
16	314.76	0.8835	245.72	510.85	1679.40	0.5892	278.12	26.85
17	327.94	0.8890	258.31	523.28	1617.03	0.6115	290.54	26.62
18	340.61	0.8942	270.92	535.11	1559.77	0.6333	302.98	26.40
19	352.82	0.8990	283.59	531.83	1533.09	0.8132	315.44	26.18
20	364.65	0.9036	296.34	542.02	1476.98	0.8421	327.97	25.96
21	376.17	0.9079	309.26	551.87	1424.05	0.8706	340.65	25.75
22	387.51	0.9120	322.45	561.48	1373.70	0.8991	353.56	25.53
23	398.77	0.9160	336.05	570.96	1325.25	0.9278	366.86	25.32
24	410.09	0.9200	350.24	580.41	1278.12	0.9538	380.70	25.11
25	421.62	0.9239	365.24	589.97	1231.66	0.9816	395.32	24.88
26	433.54	0.9279	381.35	599.78	1185.24	1.0102	410.99	24.65
27	446.01	0.9320	398.91	609.98	1138.34	1.0399	428.03	24.41
28	459.25	0.9362	418.35	620.73	1090.36	1.0712	446.86	24.15
29	473.46	0.9406	440.18	632.18	1040.87	1.1046	467.97	23.87
30	488.88	0.9453	465.03	644.51	989.45	1.1406	491.95	23.56
31	505.75	0.9503	493.72	657.89	935.74	1.1796	519.56	23.23
32	524.34	0.9556	527.24	672.52	879.54	1.2221	551.73	22.86
33	544.92	0.9613	566.79	688.57	820.78	1.2686	589.59	22.45
34	567.79	0.9675	614.01	706.24	759.51	1.3196	634.63	21.99
35	593.25	0.9741	670.94	725.73	695.95	1.3756	688.75	21.48
36	621.64	0.9813	740.28	747.25	630.50	1.4370	754.41	20.92
37	653.30	0.9889	825.61	770.99	563.76	1.5041	834.88	20.30
38	688.58	0.9971	931.79	797.18	496.50	1.5772	934.53	19.61
39	727.85	1.0058	1065.41	826.02	429.65	1.6566	1059.30	18.85
40	771.51	1.0150	1235.66	857.73	364.30	1.7424	1217.41	18.03

Table H-3 Physical properties for petroleum stock No. 4

Cut	TB, °C	$Sp.gr$	MW	Tc, °C	Pc, kPa	ω	$V^{L(15)}$, cm^3/mol	$\delta^{(25)}$, J/cm^3
1	57.10	0.6759	80.49	226.66	3282.77	0.2546	119.08	28.72
2	71.65	0.6954	87.34	245.38	3196.18	0.2690	125.59	28.75
3	85.83	0.7121	94.15	262.97	3094.20	0.2843	132.22	28.75
4	99.64	0.7265	100.95	279.57	2986.18	0.3001	138.95	28.72
5	113.06	0.7392	107.77	295.31	2877.36	0.3162	145.78	28.67
6	126.10	0.7506	114.62	310.26	2770.80	0.3325	152.71	28.60
7	138.76	0.7608	121.51	324.49	2668.16	0.3487	159.71	28.51
8	151.05	0.7701	128.44	338.06	2570.29	0.3650	166.78	28.41
9	162.97	0.7786	135.40	351.01	2477.54	0.3811	173.91	28.30
10	174.55	0.7864	142.41	363.41	2389.96	0.3971	181.09	28.19
11	185.80	0.7936	149.46	375.29	2307.38	0.4130	188.33	28.06
12	196.76	0.8003	156.56	386.71	2229.53	0.4288	195.62	27.94
13	207.45	0.8066	163.72	397.72	2156.01	0.4445	202.99	27.81
14	217.91	0.8125	170.97	408.37	2086.50	0.4601	210.43	27.67
15	228.17	0.8181	178.32	418.71	2020.52	0.4757	217.98	27.53
16	238.29	0.8234	185.80	428.80	1957.69	0.4914	225.66	27.39
17	248.31	0.8285	193.45	438.70	1897.55	0.5072	233.51	27.24
18	258.29	0.8334	201.32	448.45	1839.73	0.5232	241.57	27.09
19	268.28	0.8381	209.45	458.14	1783.80	0.5396	249.90	26.94
20	278.36	0.8428	217.92	467.81	1729.38	0.5563	258.57	26.78
21	288.57	0.8474	226.79	477.53	1676.14	0.5736	267.63	26.62
22	299.01	0.8520	236.17	487.38	1623.69	0.5916	277.20	26.45
23	309.75	0.8565	246.14	497.41	1571.76	0.6106	287.37	26.27
24	320.87	0.8611	256.84	507.70	1520.07	0.6305	298.25	26.08
25	332.45	0.8658	268.41	518.33	1468.33	0.6518	310.01	25.88
26	344.60	0.8706	281.01	515.61	1434.81	0.8304	322.79	25.66
27	357.39	0.8754	294.83	526.52	1376.06	0.8628	336.79	25.43
28	370.95	0.8804	310.11	537.98	1316.18	0.8978	352.23	25.19
29	385.37	0.8856	327.12	550.05	1255.10	0.9356	369.38	24.92
30	400.75	0.8909	346.17	562.80	1192.71	0.9725	388.55	24.64
31	417.23	0.8965	367.65	576.31	1129.01	1.0132	410.11	24.33
32	434.92	0.9022	392.03	590.68	1064.02	1.0567	434.52	23.99
33	453.93	0.9082	419.85	605.96	997.89	1.1029	462.29	23.63
34	474.40	0.9144	451.79	622.24	930.79	1.1521	494.08	23.24
35	496.47	0.9209	488.68	639.60	862.94	1.2045	530.68	22.81
36	520.28	0.9276	531.55	658.13	794.67	1.2602	573.05	22.35
37	545.96	0.9345	581.67	677.89	726.34	1.3195	622.41	21.85
38	573.66	0.9418	640.64	698.99	658.39	1.3823	680.25	21.32
39	603.54	0.9492	710.47	721.49	591.29	1.4488	748.46	20.74
40	635.76	0.9570	793.75	745.48	525.58	1.5191	829.44	20.13

Table H-4 Physical properties for petroleum stock No. 5

Cut	*TB*, °C	*Sp.gr*	*MW*	*Tc*, °C	*Pc*, kPa	ω	$V^{L(15)}$, cm^3/mol	$\delta^{(25)}$, J/cm^3
1	106.91	0.7265	104.74	286.41	2866.20	0.3136	144.18	28.53
2	123.97	0.7416	113.71	306.01	2729.02	0.3349	153.33	28.44
3	140.01	0.7544	122.52	323.98	2600.72	0.3558	162.40	28.32
4	155.06	0.7655	131.16	340.46	2483.00	0.3761	171.33	28.19
5	169.16	0.7752	139.61	355.60	2376.07	0.3956	180.09	28.05
6	182.33	0.7838	147.83	369.50	2279.56	0.4144	188.62	27.91
7	194.61	0.7913	155.80	382.27	2192.72	0.4323	196.89	27.76
8	206.05	0.7980	163.50	394.01	2114.67	0.4493	204.89	27.62
9	216.70	0.8040	170.92	404.81	2044.50	0.4655	212.60	27.48
10	226.62	0.8093	178.06	414.76	1981.30	0.4809	220.01	27.35
11	235.87	0.8142	184.92	423.94	1924.20	0.4954	227.13	27.22
12	244.53	0.8186	191.53	432.47	1872.36	0.5093	233.99	27.09
13	252.68	0.8226	197.91	440.41	1825.02	0.5225	240.60	26.97
14	260.39	0.8263	204.11	447.89	1781.40	0.5352	247.02	26.85
15	267.76	0.8298	210.18	454.98	1740.80	0.5476	253.30	26.74
16	274.89	0.8331	216.19	461.78	1702.56	0.5596	259.51	26.63
17	281.87	0.8362	222.21	468.41	1666.00	0.5716	265.72	26.52
18	288.82	0.8393	228.33	474.96	1630.52	0.5837	272.04	26.40
19	295.85	0.8424	234.67	481.55	1595.50	0.5961	278.58	26.29
20	303.09	0.8455	241.34	488.29	1560.37	0.6091	285.45	26.17
21	310.65	0.8486	248.49	495.29	1524.61	0.6228	292.81	26.04
22	318.69	0.8519	256.27	502.68	1487.68	0.6376	300.81	25.91
23	327.33	0.8554	264.86	510.56	1449.15	0.6538	309.64	25.76
24	336.72	0.8591	274.48	519.08	1408.58	0.6717	319.50	25.59
25	347.02	0.8631	285.37	514.64	1378.41	0.8488	330.65	25.41
26	358.39	0.8673	297.82	524.27	1327.48	0.8781	343.38	25.21
27	370.98	0.8719	312.15	534.86	1273.03	0.9111	358.01	24.98
28	384.99	0.8769	328.79	546.52	1214.87	0.9464	374.95	24.72
29	400.57	0.8822	348.21	559.37	1152.94	0.9856	394.69	24.44
30	417.92	0.8880	371.03	573.53	1087.32	1.0289	417.82	24.11
31	437.23	0.8942	397.97	589.12	1018.24	1.0766	445.04	23.75
32	458.70	0.9009	429.96	606.26	946.04	1.1290	477.28	23.34
33	482.53	0.9079	468.17	625.05	871.25	1.1865	515.64	22.89
34	508.93	0.9155	514.08	645.62	794.52	1.2492	561.55	22.38
35	538.10	0.9234	569.60	668.06	716.65	1.3174	616.84	21.82
36	570.29	0.9318	637.26	692.52	638.49	1.3911	683.90	21.21
37	605.72	0.9406	720.33	719.08	561.06	1.4704	765.83	20.53
38	644.62	0.9498	823.19	747.88	485.41	1.5554	866.73	19.80
39	687.21	0.9593	951.68	779.01	412.66	1.6459	992.04	19.01
40	733.79	0.9692	1113.94	812.62	343.84	1.7418	1149.32	18.15

Table H-5 Physical properties for petroleum stock No. 6

Cut	*TB*, °C	*Sp.gr*	*MW*	*Tc*, °C	*Pc*, kPa	ω	$V^{L(15)}$, cm^3/mol	$\delta^{(25)}$, J/cm^3
1	62.03	0.6875	82.87	234.17	3303.46	0.2563	120.54	28.83
2	69.05	0.6969	86.15	243.19	3259.98	0.2633	123.62	28.84
3	77.10	0.7069	89.95	253.33	3204.47	0.2717	127.25	28.85
4	85.96	0.7171	94.18	264.27	3138.41	0.2813	131.34	28.85
5	95.42	0.7272	98.78	275.73	3064.12	0.2920	135.84	28.84
6	105.29	0.7370	103.68	287.46	2984.12	0.3035	140.68	28.82
7	115.40	0.7464	108.83	299.26	2900.90	0.3157	145.80	28.78
8	125.60	0.7553	114.16	310.98	2816.70	0.3283	151.14	28.72
9	135.76	0.7636	119.61	322.45	2733.42	0.3411	156.63	28.66
10	145.75	0.7714	125.14	333.59	2652.44	0.3541	162.22	28.59
11	155.51	0.7786	130.69	344.31	2574.85	0.3670	167.84	28.51
12	164.93	0.7853	136.20	354.54	2501.41	0.3797	173.44	28.42
13	173.97	0.7914	141.64	364.25	2432.50	0.3920	178.98	28.33
14	182.60	0.7970	146.97	373.41	2368.29	0.4040	184.41	28.24
15	190.79	0.8021	152.17	382.02	2308.76	0.4156	189.71	28.15
16	198.54	0.8068	157.22	390.11	2253.68	0.4267	194.85	28.06
17	205.90	0.8112	162.11	397.71	2202.70	0.4374	199.84	27.97
18	212.87	0.8152	166.86	404.87	2155.39	0.4476	204.69	27.88
19	219.54	0.8189	171.50	411.67	2111.16	0.4575	209.42	27.80
20	225.98	0.8225	176.08	418.19	2069.37	0.4672	214.08	27.71
21	232.29	0.8258	180.65	424.53	2029.30	0.4768	218.74	27.62
22	238.58	0.8291	185.30	430.82	1990.18	0.4864	223.48	27.53
23	244.99	0.8324	190.14	437.18	1951.16	0.4964	228.41	27.44
24	251.68	0.8358	195.29	443.79	1911.35	0.5069	233.66	27.34
25	258.82	0.8393	200.92	450.79	1869.87	0.5182	239.38	27.24
26	266.61	0.8431	207.20	458.38	1825.79	0.5307	245.77	27.12
27	275.26	0.8471	214.37	466.74	1778.24	0.5448	253.05	26.98
28	285.00	0.8516	222.68	476.08	1726.40	0.5610	261.49	26.83
29	296.08	0.8565	232.46	486.62	1669.56	0.5797	271.41	26.65
30	308.78	0.8620	244.12	498.57	1607.10	0.6016	283.20	26.44
31	323.38	0.8681	258.12	512.16	1538.71	0.6274	297.36	26.19
32	340.21	0.8748	275.09	527.62	1464.24	0.6581	314.47	25.89
33	359.57	0.8822	295.82	530.56	1397.64	0.8593	335.31	25.54
34	381.82	0.8904	321.30	549.35	1299.88	0.9165	360.86	25.14
35	407.34	0.8993	352.88	570.55	1195.37	0.9791	392.41	24.66
36	436.51	0.9089	392.34	594.38	1085.19	1.0504	431.67	24.11
37	469.71	0.9192	442.07	621.03	970.84	1.1303	480.91	23.47
38	507.41	0.9303	505.45	650.74	854.05	1.2192	543.32	22.74
39	550.00	0.9420	587.08	683.70	737.02	1.3173	623.23	21.91
40	598.00	0.9544	693.71	720.16	622.02	1.4247	726.89	20.97

Table H-6 Physical properties for petroleum stock No. 7

Cut	*TB*, °C	*Sp.gr*	*MW*	*Tc*, °C	*Pc*, kPa	ω	$V^{L(15)}$, cm^3/mol	$\delta^{(25)}$, J/cm^3
1	54.08	0.6696	79.02	222.22	3277.44	0.2530	118.02	28.68
2	64.31	0.6840	83.85	235.59	3223.39	0.2627	122.58	28.70
3	74.58	0.6971	88.73	248.61	3157.06	0.2733	127.28	28.71
4	84.86	0.7090	93.68	261.30	3082.85	0.2845	132.13	28.71
5	95.08	0.7199	98.70	273.66	3004.06	0.2962	137.11	28.69
6	105.24	0.7299	103.81	285.69	2922.99	0.3082	142.22	28.65
7	115.31	0.7392	108.99	297.40	2841.35	0.3205	147.45	28.61
8	125.27	0.7478	114.25	308.79	2760.31	0.3329	152.78	28.55
9	135.11	0.7558	119.59	319.86	2680.69	0.3455	158.22	28.48
10	144.82	0.7633	125.00	330.65	2603.00	0.3583	163.76	28.41
11	154.41	0.7704	130.50	341.15	2527.55	0.3711	169.40	28.33
12	163.88	0.7770	136.09	351.41	2454.47	0.3840	175.14	28.24
13	173.27	0.7833	141.78	361.43	2383.74	0.3971	180.99	28.14
14	182.58	0.7893	147.59	371.28	2315.26	0.4102	186.98	28.04
15	191.84	0.7951	153.53	380.96	2248.89	0.4235	193.10	27.94
16	201.09	0.8006	159.64	390.53	2184.39	0.4371	199.40	27.83
17	210.38	0.8060	165.96	400.05	2121.47	0.4509	205.92	27.71
18	219.76	0.8112	172.53	409.56	2059.87	0.4650	212.68	27.59
19	229.27	0.8163	179.39	419.11	1999.28	0.4796	219.75	27.46
20	238.98	0.8214	186.61	428.77	1939.36	0.4948	227.19	27.32
21	248.97	0.8264	194.27	438.60	1879.82	0.5106	235.07	27.17
22	259.30	0.8315	202.46	448.67	1820.36	0.5273	243.49	27.02
23	270.05	0.8366	211.28	459.07	1760.67	0.5451	252.54	26.85
24	281.33	0.8418	220.85	469.85	1700.49	0.5640	262.37	26.67
25	293.22	0.8470	231.33	481.10	1639.63	0.5844	273.10	26.48
26	305.82	0.8525	242.89	492.90	1577.84	0.6066	284.92	26.27
27	319.25	0.8580	255.72	505.33	1515.04	0.6308	298.03	26.04
28	333.62	0.8638	270.09	518.48	1451.08	0.6574	312.67	25.79
29	349.04	0.8698	286.28	518.52	1400.98	0.8452	329.14	25.52
30	365.65	0.8760	304.64	532.60	1326.54	0.8879	347.77	25.22
31	383.59	0.8824	325.61	547.63	1250.17	0.9335	368.99	24.90
32	403.00	0.8892	349.71	563.68	1172.02	0.9820	393.31	24.54
33	424.02	0.8961	377.60	580.86	1092.30	1.0341	421.36	24.14
34	446.81	0.9034	410.05	599.25	1011.39	1.0899	453.90	23.71
35	471.54	0.9110	448.08	618.93	929.69	1.1496	491.88	23.24
36	498.36	0.9188	492.94	640.01	847.69	1.2134	536.50	22.72
37	527.46	0.9269	546.22	662.57	765.97	1.2815	589.28	22.16
38	559.00	0.9353	609.95	686.72	685.21	1.3539	652.13	21.55
39	593.20	0.9440	686.83	712.56	606.05	1.4308	727.56	20.89
40	630.23	0.9530	780.29	740.18	529.28	1.5122	818.79	20.18

Table H-7 Physical properties for petroleum stock No. 8

Cut	*TB*, °C	*Sp.gr*	*MW*	*Tc*, °C	*Pc*, kPa	ω	$V^{L(15)}$, cm^3/mol	$\delta^{(25)}$, J/cm^3
1	54.10	0.6746	79.15	223.39	3329.41	0.2498	117.34	28.77
2	63.89	0.6885	83.72	236.23	3277.05	0.2591	121.60	28.80
3	74.43	0.7021	88.68	249.63	3208.29	0.2698	126.31	28.82
4	85.59	0.7151	94.01	263.45	3126.43	0.2819	131.47	28.82
5	97.25	0.7274	99.71	277.53	3034.99	0.2951	137.06	28.80
6	109.30	0.7392	105.75	291.76	2937.11	0.3094	143.07	28.76
7	121.65	0.7503	112.13	306.04	2835.54	0.3245	149.46	28.71
8	134.20	0.7607	118.85	320.28	2732.66	0.3403	156.23	28.63
9	146.89	0.7706	125.87	334.40	2630.20	0.3568	163.35	28.54
10	159.63	0.7798	133.20	348.35	2529.64	0.3738	170.80	28.43
11	172.39	0.7886	140.81	362.08	2431.89	0.3912	178.57	28.30
12	185.09	0.7968	148.70	375.55	2337.73	0.4090	186.62	28.17
13	197.72	0.8046	156.84	388.75	2247.49	0.4270	194.94	28.02
14	210.23	0.8119	165.24	401.64	2161.45	0.4453	203.53	27.87
15	222.60	0.8188	173.88	414.23	2079.66	0.4638	212.36	27.71
16	234.84	0.8253	182.75	426.52	2002.04	0.4824	221.43	27.54
17	246.93	0.8316	191.87	438.53	1928.44	0.5012	230.74	27.36
18	258.89	0.8375	201.25	450.26	1858.62	0.5202	240.30	27.19
19	270.73	0.8431	210.89	461.76	1792.28	0.5394	250.12	27.00
20	282.49	0.8486	220.83	473.05	1729.09	0.5589	260.25	26.82
21	294.20	0.8538	231.12	484.19	1668.75	0.5787	270.70	26.63
22	305.91	0.8589	241.80	495.21	1610.84	0.5989	281.54	26.43
23	317.68	0.8638	252.96	506.18	1555.06	0.6197	292.84	26.23
24	329.58	0.8686	264.67	517.17	1500.99	0.6412	304.70	26.03
25	341.68	0.8734	277.06	528.23	1448.30	0.6635	317.21	25.82
26	354.07	0.8782	290.26	525.16	1412.41	0.8483	330.52	25.59
27	366.86	0.8830	304.44	536.02	1354.80	0.8809	344.80	25.36
28	380.14	0.8878	319.81	547.20	1297.20	0.9153	360.24	25.12
29	394.02	0.8927	336.61	558.78	1239.34	0.9493	377.08	24.86
30	408.65	0.8977	355.15	570.87	1180.90	0.9855	395.62	24.59
31	424.15	0.9029	375.78	583.56	1121.67	1.0236	416.21	24.29
32	440.66	0.9082	398.93	596.95	1061.51	1.0638	439.26	23.98
33	458.36	0.9137	425.16	611.16	1000.25	1.1066	465.30	23.64
34	477.38	0.9195	455.10	626.30	937.90	1.1521	494.95	23.27
35	497.92	0.9255	489.57	642.48	874.46	1.2006	528.97	22.88
36	520.17	0.9318	529.60	659.82	810.03	1.2525	568.36	22.44
37	544.30	0.9384	576.42	678.44	744.86	1.3080	614.26	21.97
38	570.52	0.9453	631.64	698.47	679.23	1.3674	668.20	21.46
39	599.05	0.9525	697.33	720.03	613.54	1.4309	732.11	20.91
40	630.11	0.9600	776.13	743.25	548.27	1.4987	808.43	20.31

Table H-8 Physical properties for petroleum stock No. 9

Cut	*TB*, °C	*Sp.gr*	*MW*	*Tc*, °C	*Pc*, kPa	ω	$V^{L(15)}$, cm^3/mol	$\delta^{(25)}$, J/cm^3
1	131.07	0.7763	116.20	321.22	2904.05	0.3240	149.69	29.12
2	154.78	0.7949	129.05	347.84	2707.31	0.3539	162.35	28.97
3	175.90	0.8098	141.29	370.88	2540.16	0.3816	174.48	28.78
4	194.57	0.8218	152.79	390.79	2400.13	0.4070	185.92	28.59
5	210.94	0.8317	163.45	407.93	2283.65	0.4299	196.53	28.40
6	225.19	0.8398	173.19	422.62	2187.13	0.4503	206.23	28.21
7	237.48	0.8465	181.95	435.12	2107.49	0.4682	214.96	28.05
8	247.96	0.8519	189.70	445.67	2042.17	0.4838	222.67	27.90
9	256.81	0.8564	196.45	454.50	1988.83	0.4972	229.38	27.77
10	264.18	0.8601	202.23	461.81	1945.60	0.5085	235.13	27.66
11	270.26	0.8630	207.09	467.80	1910.82	0.5179	239.96	27.57
12	275.21	0.8654	211.12	472.65	1883.04	0.5256	243.96	27.49
13	279.20	0.8673	214.42	476.54	1860.98	0.5319	247.24	27.43
14	282.41	0.8688	217.11	479.67	1843.43	0.5369	249.91	27.37
15	285.02	0.8700	219.32	482.21	1829.31	0.5411	252.10	27.33
16	287.22	0.8710	221.19	484.34	1817.56	0.5446	253.95	27.30
17	289.17	0.8719	222.86	486.23	1807.16	0.5477	255.61	27.27
18	291.08	0.8728	224.50	488.07	1797.11	0.5508	257.24	27.23
19	293.11	0.8737	226.27	490.04	1786.43	0.5541	258.99	27.20
20	295.47	0.8747	228.33	492.31	1774.17	0.5579	261.03	27.16
21	298.34	0.8760	230.86	495.06	1759.37	0.5625	263.54	27.12
22	301.91	0.8776	234.05	498.49	1741.14	0.5684	266.69	27.06
23	306.39	0.8796	238.08	502.77	1718.66	0.5757	270.69	26.98
24	311.96	0.8820	243.20	508.07	1691.15	0.5849	275.74	26.89
25	318.83	0.8849	249.63	514.58	1657.98	0.5964	282.10	26.77
26	327.19	0.8884	257.65	522.45	1618.68	0.6106	290.03	26.62
27	337.25	0.8925	267.61	531.86	1572.89	0.6279	299.85	26.45
28	349.22	0.8973	279.89	528.58	1548.63	0.8050	311.94	26.23
29	363.30	0.9027	294.96	540.74	1481.38	0.8393	326.76	25.98
30	379.70	0.9088	313.42	554.74	1406.37	0.8800	344.87	25.67
31	398.64	0.9156	336.00	570.71	1324.06	0.9281	366.96	25.31
32	420.32	0.9231	363.64	588.75	1235.15	0.9791	393.92	24.90
33	444.97	0.9313	397.55	608.99	1140.59	1.0380	426.89	24.42
34	472.79	0.9400	439.26	631.49	1041.66	1.1037	467.29	23.87
35	504.02	0.9494	490.87	656.37	939.71	1.1762	517.04	23.25
36	538.86	0.9593	555.04	683.69	836.41	1.2556	578.60	22.56
37	577.56	0.9697	635.49	713.57	733.34	1.3419	655.35	21.79
38	620.31	0.9805	737.11	746.07	632.35	1.4348	751.73	20.94
39	667.38	0.9918	866.79	781.30	535.06	1.5342	873.95	20.01
40	718.96	1.0034	1033.93	819.33	443.21	1.6396	1030.39	19.02

Table H-9 Physical properties for petroleum stock No. 10

Cut	TB, °C	$Sp.gr$	MW	Tc, °C	Pc, kPa	ω	$V^{L(15)}$, cm^3/mol	$\delta^{(25)}$, J/cm^3
1	39.43	0.6480	72.18	202.76	3348.29	0.2393	111.40	28.66
2	53.74	0.6716	78.93	222.36	3305.85	0.2510	117.52	28.72
3	68.04	0.6916	85.64	240.97	3226.67	0.2648	123.84	28.76
4	82.27	0.7088	92.42	258.78	3127.56	0.2799	130.40	28.77
5	96.41	0.7240	99.33	275.91	3018.42	0.2959	137.20	28.74
6	110.40	0.7375	106.38	292.40	2905.40	0.3125	144.24	28.70
7	124.22	0.7498	113.59	308.31	2792.33	0.3296	151.50	28.63
8	137.83	0.7609	120.96	323.65	2681.63	0.3470	158.98	28.54
9	151.23	0.7710	128.50	338.46	2574.66	0.3646	166.66	28.43
10	164.40	0.7804	136.20	352.76	2472.29	0.3824	174.54	28.31
11	177.32	0.7890	144.06	366.56	2374.95	0.4003	182.59	28.18
12	189.99	0.7970	152.07	379.89	2282.77	0.4183	190.81	28.04
13	202.41	0.8045	160.24	392.78	2195.69	0.4363	199.19	27.89
14	214.58	0.8114	168.56	405.24	2113.56	0.4544	207.72	27.73
15	226.52	0.8180	177.03	417.30	2036.10	0.4724	216.42	27.58
16	238.24	0.8242	185.66	429.00	1963.02	0.4905	225.27	27.41
17	249.76	0.8300	194.47	440.38	1893.97	0.5087	234.30	27.24
18	261.11	0.8356	203.47	451.47	1828.58	0.5269	243.51	27.07
19	272.31	0.8409	212.68	462.30	1766.53	0.5453	252.93	26.90
20	283.41	0.8459	222.14	472.92	1707.44	0.5639	262.59	26.72
21	294.46	0.8508	231.89	483.38	1650.94	0.5827	272.54	26.54
22	305.48	0.8556	241.97	493.73	1596.72	0.6019	282.81	26.36
23	316.54	0.8602	252.46	504.01	1544.41	0.6216	293.48	26.17
24	327.69	0.8648	263.42	514.29	1493.71	0.6419	304.61	25.98
25	338.99	0.8693	274.94	524.62	1444.36	0.6629	316.30	25.78
26	350.53	0.8737	287.14	520.99	1412.00	0.8441	328.65	25.58
27	362.35	0.8781	300.13	531.05	1358.47	0.8742	341.78	25.37
28	374.55	0.8826	314.07	541.33	1305.14	0.9058	355.84	25.14
29	387.21	0.8871	329.12	551.91	1251.83	0.9373	370.99	24.91
30	400.41	0.8917	345.49	562.86	1198.29	0.9702	387.46	24.67
31	414.26	0.8964	363.44	574.24	1144.36	1.0045	405.46	24.41
32	428.84	0.9012	383.23	586.11	1089.94	1.0403	425.26	24.13
33	444.27	0.9061	405.20	598.57	1034.90	1.0779	447.20	23.84
34	460.65	0.9112	429.79	611.69	979.15	1.1176	471.69	23.52
35	478.09	0.9164	457.44	625.53	922.73	1.1593	499.16	23.19
36	496.72	0.9219	488.76	640.18	865.65	1.2035	530.19	22.83
37	516.67	0.9275	524.46	655.72	808.02	1.2502	565.45	22.44
38	538.05	0.9334	565.39	672.23	749.96	1.2997	605.76	22.03
39	561.02	0.9394	612.65	689.80	691.66	1.3521	652.14	21.58
40	585.70	0.9458	667.51	708.50	633.42	1.4076	705.79	21.10

Table H-10 Physical properties for petroleum stock No. 11

Cut	TB, °C	$Sp.gr$	MW	Tc, °C	Pc, kPa	ω	$V^{L(15)}$, cm^3/mol	$\delta^{(25)}$, J/cm^3
1	66.65	0.7096	85.06	243.74	3433.71	0.2512	119.87	29.17
2	78.70	0.7250	90.56	259.06	3347.61	0.2634	124.91	29.22
3	90.76	0.7388	96.17	273.96	3252.34	0.2763	130.17	29.24
4	102.79	0.7514	101.92	288.48	3152.39	0.2898	135.64	29.23
5	114.74	0.7629	107.80	302.60	3050.88	0.3037	141.31	29.21
6	126.58	0.7734	113.81	316.32	2950.03	0.3179	147.15	29.17
7	138.27	0.7832	119.94	329.64	2851.30	0.3323	153.15	29.10
8	149.79	0.7922	126.19	342.55	2755.67	0.3468	159.30	29.03
9	161.13	0.8005	132.56	355.08	2663.64	0.3614	165.59	28.94
10	172.27	0.8083	139.03	367.23	2575.57	0.3760	172.00	28.84
11	183.22	0.8156	145.61	379.01	2491.56	0.3907	178.53	28.74
12	193.97	0.8225	152.29	390.44	2411.57	0.4054	185.16	28.62
13	204.54	0.8289	159.09	401.55	2335.47	0.4200	191.92	28.50
14	214.94	0.8350	166.00	412.37	2263.00	0.4347	198.79	28.38
15	225.18	0.8408	173.03	422.91	2193.96	0.4494	205.79	28.24
16	235.31	0.8464	180.22	433.24	2128.01	0.4641	212.93	28.11
17	245.35	0.8517	187.58	443.38	2064.79	0.4789	220.25	27.97
18	255.35	0.8568	195.14	453.38	2003.99	0.4940	227.76	27.82
19	265.35	0.8617	202.96	463.31	1945.23	0.5092	235.53	27.67
20	275.41	0.8666	211.09	473.20	1888.18	0.5248	243.59	27.52
21	285.59	0.8713	219.59	483.12	1832.45	0.5409	252.01	27.35
22	295.96	0.8761	228.54	493.15	1777.73	0.5575	260.87	27.19
23	306.59	0.8807	238.02	503.34	1723.70	0.5748	270.25	27.01
24	317.56	0.8855	248.17	513.76	1670.00	0.5930	280.28	26.82
25	328.95	0.8902	259.11	524.51	1616.38	0.6122	291.06	26.62
26	340.87	0.8951	270.99	535.64	1562.60	0.6328	302.76	26.41
27	353.40	0.9000	283.99	532.62	1534.52	0.8134	315.55	26.19
28	366.66	0.9051	298.35	544.04	1471.72	0.8458	329.63	25.94
29	380.77	0.9103	314.31	556.07	1407.47	0.8809	345.27	25.68
30	395.82	0.9158	332.19	568.78	1341.69	0.9189	362.74	25.40
31	411.97	0.9214	352.37	582.27	1274.24	0.9571	382.42	25.09
32	429.32	0.9273	375.29	596.63	1205.15	0.9988	404.72	24.75
33	448.03	0.9334	401.51	611.94	1134.44	1.0433	430.15	24.39
34	468.23	0.9398	431.70	628.30	1062.24	1.0910	459.35	23.99
35	490.09	0.9465	466.68	645.80	988.75	1.1420	493.08	23.56
36	513.75	0.9534	507.51	664.54	914.27	1.1965	532.31	23.09
37	539.39	0.9606	555.47	684.61	839.17	1.2547	578.23	22.58
38	567.16	0.9682	612.21	706.12	763.89	1.3167	632.34	22.02
39	597.26	0.9760	679.83	729.15	688.96	1.3828	696.55	21.42
40	629.86	0.9841	761.03	753.81	614.97	1.4529	773.31	20.77

Table H-11 Physical properties for petroleum stock No. 12

Cut	*TB*, °C	*Sp.gr*	*MW*	*Tc*, °C	*Pc*, kPa	ω	$V^{L(15)}$, cm^3/mol	$\delta^{(25)}$, J/cm^3
1	70.32	0.7035	86.77	245.95	3300.25	0.2615	123.34	28.95
2	82.20	0.7179	92.34	260.84	3214.53	0.2740	128.62	28.97
3	94.32	0.7312	98.15	275.62	3119.44	0.2874	134.23	28.96
4	106.58	0.7435	104.19	290.24	3018.93	0.3016	140.13	28.94
5	118.95	0.7549	110.46	304.66	2915.96	0.3164	146.33	28.89
6	131.36	0.7655	116.97	318.85	2812.71	0.3318	152.81	28.83
7	143.76	0.7754	123.71	332.77	2710.85	0.3476	159.55	28.74
8	156.10	0.7846	130.66	346.40	2611.55	0.3637	166.53	28.65
9	168.36	0.7932	137.82	359.72	2515.55	0.3801	173.75	28.54
10	180.50	0.8013	145.17	372.73	2423.39	0.3966	181.17	28.42
11	192.49	0.8089	152.72	385.40	2335.35	0.4134	188.80	28.28
12	204.32	0.8160	160.44	397.73	2251.56	0.4302	196.62	28.15
13	215.97	0.8227	168.33	409.73	2172.04	0.4471	204.60	28.00
14	227.45	0.8291	176.39	421.41	2096.64	0.4641	212.76	27.85
15	238.74	0.8351	184.62	432.77	2025.21	0.4811	221.08	27.69
16	249.85	0.8408	193.02	443.84	1957.51	0.4982	229.56	27.53
17	260.80	0.8462	201.58	454.62	1893.34	0.5153	238.21	27.37
18	271.60	0.8514	210.33	465.17	1832.39	0.5325	247.04	27.20
19	282.28	0.8564	219.29	475.49	1774.37	0.5498	256.07	27.03
20	292.87	0.8612	228.49	485.64	1718.95	0.5673	265.32	26.86
21	303.40	0.8658	237.95	495.64	1665.88	0.5850	274.83	26.69
22	313.92	0.8703	247.73	505.54	1614.81	0.6031	284.65	26.51
23	324.48	0.8747	257.88	515.40	1565.44	0.6215	294.84	26.33
24	335.13	0.8790	268.49	525.26	1517.48	0.6405	305.46	26.14
25	345.93	0.8832	279.63	521.13	1494.71	0.8159	316.59	25.95
26	356.95	0.8875	291.41	530.61	1442.76	0.8432	328.35	25.75
27	368.27	0.8917	303.94	540.25	1391.15	0.8717	340.85	25.55
28	379.96	0.8960	317.39	550.14	1339.56	0.9015	354.23	25.33
29	392.11	0.9003	331.93	560.33	1287.78	0.9330	368.67	25.10
30	404.81	0.9048	347.75	570.90	1235.60	0.9626	384.35	24.87
31	418.16	0.9093	365.10	581.92	1182.77	0.9953	401.52	24.61
32	432.27	0.9140	384.27	593.46	1129.19	1.0295	420.45	24.34
33	447.24	0.9188	405.62	605.61	1074.68	1.0656	441.48	24.05
34	463.19	0.9238	429.53	618.44	1019.21	1.1038	464.98	23.74
35	480.25	0.9289	456.52	632.04	962.71	1.1442	491.44	23.41
36	498.54	0.9343	487.18	646.51	905.20	1.1871	521.43	23.05
37	518.20	0.9399	522.24	661.91	846.79	1.2327	555.61	22.67
38	539.36	0.9458	562.59	678.34	787.59	1.2812	594.83	22.25
39	562.18	0.9519	609.35	695.89	727.82	1.3328	640.12	21.80
40	586.82	0.9583	663.88	714.66	667.73	1.3876	692.77	21.32

Table H-12 Physical properties for petroleum stock No. 13

Cut	*TB*, °C	*Sp.gr*	*MW*	*Tc*, °C	*Pc*, kPa	ω	$V^{L(15)}$, cm^3/mol	$\delta^{(25)}$, J/cm^3
1	37.99	0.6465	71.55	201.01	3363.15	0.2375	110.66	28.67
2	47.44	0.6630	76.01	214.17	3343.84	0.2448	114.65	28.72
3	56.91	0.6776	80.44	226.86	3303.97	0.2531	118.72	28.76
4	66.37	0.6907	84.87	239.14	3250.23	0.2623	122.88	28.78
5	75.78	0.7025	89.32	251.04	3187.39	0.2720	127.14	28.80
6	85.12	0.7133	93.79	262.59	3118.82	0.2822	131.48	28.79
7	94.36	0.7233	98.30	273.78	3047.02	0.2926	135.91	28.78
8	103.47	0.7324	102.83	284.63	2973.84	0.3032	140.41	28.75
9	112.45	0.7408	107.40	295.14	2900.54	0.3140	144.97	28.72
10	121.27	0.7487	111.98	305.30	2828.14	0.3249	149.58	28.68
11	129.92	0.7560	116.59	315.13	2757.32	0.3358	154.22	28.63
12	138.38	0.7627	121.19	324.63	2688.59	0.3466	158.89	28.57
13	146.63	0.7691	125.80	333.78	2622.29	0.3574	163.57	28.50
14	154.68	0.7750	130.40	342.61	2558.59	0.3681	168.26	28.44
15	162.51	0.7805	134.98	351.12	2497.64	0.3787	172.93	28.37
16	170.12	0.7857	139.54	359.30	2439.47	0.3891	177.59	28.29
17	177.51	0.7906	144.06	367.18	2384.09	0.3994	182.22	28.22
18	184.68	0.7952	148.55	374.75	2331.43	0.4095	186.81	28.14
19	191.63	0.7995	153.00	382.03	2281.41	0.4194	191.36	28.06
20	198.36	0.8036	157.40	389.03	2233.92	0.4291	195.87	27.98
21	204.88	0.8074	161.75	395.76	2188.83	0.4386	200.32	27.90
22	211.20	0.8111	166.05	402.24	2145.99	0.4480	204.74	27.82
23	217.34	0.8145	170.31	408.49	2105.25	0.4571	209.10	27.74
24	223.30	0.8178	174.53	414.52	2066.44	0.4661	213.42	27.66
25	229.11	0.8209	178.72	420.37	2029.38	0.4749	217.71	27.58
26	234.77	0.8239	182.88	426.03	1993.91	0.4836	221.96	27.50
27	240.32	0.8268	187.02	431.55	1959.85	0.4922	226.20	27.42
28	245.77	0.8296	191.17	436.94	1926.98	0.5008	230.44	27.34
29	251.15	0.8323	195.33	442.24	1895.16	0.5093	234.70	27.27
30	256.48	0.8349	199.54	447.47	1864.16	0.5178	238.99	27.19
31	261.80	0.8375	203.80	452.65	1833.82	0.5264	243.35	27.10
32	267.15	0.8400	208.15	457.83	1803.93	0.5351	247.79	27.02
33	272.54	0.8426	212.62	463.04	1774.31	0.5439	252.35	26.94
34	278.02	0.8451	217.25	468.31	1744.78	0.5530	257.07	26.85
35	283.64	0.8476	222.07	473.67	1715.14	0.5624	261.98	26.76
36	289.42	0.8502	227.12	479.17	1685.22	0.5722	267.13	26.67
37	295.41	0.8529	232.47	484.84	1654.84	0.5825	272.57	26.57
38	301.67	0.8556	238.15	490.73	1623.83	0.5933	278.35	26.47
39	308.23	0.8584	244.24	496.87	1592.03	0.6048	284.54	26.36
40	315.15	0.8613	250.80	503.31	1559.32	0.6170	291.20	26.24

Table H-13 Physical properties for petroleum stock No. 14

Cut	*TB*, °C	*Sp.gr*	*MW*	*Tc*, °C	*Pc*, kPa	ω	$V^{L(15)}$, cm^3/mol	$\delta^{(25)}$, J/cm^3
1	203.20	0.7951	161.66	390.75	2125.83	0.4461	203.32	27.63
2	202.77	0.7949	161.37	390.31	2128.75	0.4455	203.01	27.63
3	204.31	0.7958	162.42	391.88	2118.37	0.4478	204.10	27.61
4	207.44	0.7975	164.57	395.07	2097.41	0.4525	206.34	27.57
5	211.82	0.8000	167.60	399.51	2068.47	0.4592	209.50	27.52
6	217.12	0.8029	171.34	404.86	2033.96	0.4673	213.39	27.45
7	223.06	0.8062	175.60	410.82	1996.01	0.4765	217.82	27.37
8	229.37	0.8095	180.21	417.12	1956.49	0.4864	222.61	27.28
9	235.82	0.8129	185.03	423.51	1916.92	0.4966	227.62	27.19
10	242.22	0.8161	189.90	429.80	1878.57	0.5069	232.67	27.09
11	248.39	0.8192	194.69	435.84	1842.38	0.5168	237.65	27.00
12	254.18	0.8221	199.27	441.47	1809.09	0.5263	242.41	26.92
13	259.49	0.8246	203.55	446.60	1779.18	0.5351	246.84	26.84
14	264.23	0.8269	207.42	451.16	1752.94	0.5430	250.86	26.76
15	268.34	0.8288	210.84	455.11	1730.50	0.5500	254.40	26.70
16	271.81	0.8304	213.75	458.42	1711.85	0.5559	257.42	26.64
17	274.63	0.8317	216.15	461.11	1696.83	0.5607	259.90	26.60
18	276.85	0.8327	218.05	463.21	1685.15	0.5645	261.86	26.57
19	278.52	0.8334	219.48	464.80	1676.40	0.5673	263.35	26.54
20	279.74	0.8340	220.54	465.95	1670.05	0.5694	264.44	26.52
21	280.63	0.8344	221.31	466.80	1665.43	0.5710	265.24	26.50
22	281.34	0.8347	221.94	467.47	1661.73	0.5722	265.88	26.49
23	282.06	0.8350	222.56	468.15	1658.00	0.5735	266.53	26.48
24	283.00	0.8355	223.39	469.04	1653.17	0.5751	267.38	26.47
25	284.40	0.8361	224.61	470.36	1646.01	0.5775	268.65	26.44
26	286.53	0.8370	226.49	472.36	1635.18	0.5813	270.59	26.41
27	289.68	0.8384	229.30	475.33	1619.26	0.5868	273.49	26.36
28	294.20	0.8404	233.37	479.55	1596.80	0.5948	277.70	26.28
29	300.43	0.8430	239.08	485.36	1566.39	0.6059	283.59	26.18
30	308.77	0.8465	246.91	493.08	1526.74	0.6210	291.67	26.04
31	319.62	0.8510	257.42	503.06	1476.86	0.6411	302.49	25.86
32	333.46	0.8565	271.36	515.63	1416.08	0.6673	316.82	25.62
33	350.74	0.8631	289.67	517.32	1354.56	0.8603	335.60	25.31
34	371.97	0.8709	313.61	535.19	1262.15	0.9158	360.08	24.93
35	397.70	0.8799	344.90	556.50	1157.77	0.9805	391.97	24.46
36	428.48	0.8901	385.93	581.55	1043.09	1.0572	433.60	23.88
37	464.91	0.9013	440.08	610.62	920.51	1.1464	488.25	23.20
38	507.62	0.9137	512.23	644.03	793.16	1.2486	560.61	22.38
39	557.25	0.9270	609.60	682.04	664.74	1.3640	657.59	21.43
40	614.49	0.9413	743.12	724.97	539.28	1.4925	789.50	20.34

Table H-14 Physical properties for petroleum stock No. 15

Cut	*TB*, °C	*Sp.gr*	*MW*	*Tc*, °C	*Pc*, kPa	ω	$V^{L(15)}$, cm^3/mol	$\delta^{(25)}$, J/cm^3
1	39.45	0.6557	72.48	204.57	3433.22	0.2345	110.54	28.78
2	52.16	0.6771	78.37	222.08	3396.16	0.2447	115.74	28.86
3	64.76	0.6954	84.18	238.65	3328.79	0.2564	121.06	28.92
4	77.23	0.7113	90.00	254.48	3244.16	0.2691	126.53	28.95
5	89.59	0.7254	95.88	269.72	3149.91	0.2826	132.18	28.95
6	101.86	0.7381	101.86	284.46	3050.86	0.2966	138.01	28.93
7	114.04	0.7496	107.97	298.77	2950.00	0.3110	144.03	28.89
8	126.14	0.7603	114.25	312.71	2849.21	0.3259	150.27	28.83
9	138.18	0.7702	120.70	326.33	2749.78	0.3410	156.72	28.76
10	150.17	0.7794	127.34	339.66	2652.45	0.3565	163.39	28.67
11	162.13	0.7880	134.21	352.75	2557.66	0.3723	170.31	28.57
12	174.06	0.7962	141.31	365.62	2465.67	0.3885	177.48	28.46
13	185.99	0.8039	148.68	378.31	2376.59	0.4050	184.94	28.33
14	197.94	0.8113	156.33	390.85	2290.43	0.4218	192.69	28.20
15	209.92	0.8184	164.30	403.26	2207.12	0.4391	200.76	28.05
16	221.96	0.8252	172.61	415.57	2126.63	0.4567	209.18	27.90
17	234.06	0.8317	181.30	427.81	2048.81	0.4749	217.98	27.73
18	246.27	0.8381	190.41	439.99	1973.55	0.4935	227.20	27.56
19	258.59	0.8442	199.97	452.16	1900.69	0.5127	236.87	27.38
20	271.05	0.8502	210.04	464.33	1830.11	0.5326	247.03	27.19
21	283.69	0.8561	220.66	476.54	1761.65	0.5532	257.76	26.99
22	296.51	0.8618	231.90	488.79	1695.23	0.5745	269.08	26.78
23	309.56	0.8675	243.83	501.11	1630.70	0.5967	281.07	26.56
24	322.86	0.8730	256.51	513.54	1567.96	0.6199	293.81	26.33
25	336.43	0.8785	270.03	526.10	1506.90	0.6441	307.36	26.09
26	350.32	0.8840	284.50	524.57	1468.61	0.8281	321.84	25.85
27	364.54	0.8894	300.01	536.73	1402.89	0.8637	337.33	25.59
28	379.13	0.8947	316.69	549.08	1338.22	0.9009	353.95	25.32
29	394.13	0.9001	334.68	561.65	1274.56	0.9399	371.84	25.04
30	409.57	0.9054	354.15	574.46	1211.89	0.9759	391.15	24.75
31	425.48	0.9107	375.26	587.53	1150.19	1.0147	412.04	24.45
32	441.91	0.9161	398.24	600.90	1089.45	1.0545	434.73	24.13
33	458.89	0.9214	423.32	614.59	1029.72	1.0952	459.42	23.80
34	476.45	0.9268	450.76	628.62	970.99	1.1369	486.37	23.46
35	494.64	0.9322	480.90	643.02	913.31	1.1797	515.89	23.11
36	513.50	0.9376	514.09	657.81	856.71	1.2236	548.30	22.74
37	533.06	0.9431	550.76	673.03	801.24	1.2686	584.01	22.35
38	553.38	0.9486	591.39	688.70	746.97	1.3148	623.47	21.96
39	574.49	0.9541	636.58	704.85	693.97	1.3622	667.21	21.54
40	596.45	0.9597	686.99	721.50	642.32	1.4108	715.84	21.11

Table H-15 Physical properties for petroleum stock No. 16

Cut	*TB*, °C	*Sp.gr*	*MW*	*Tc*, °C	*Pc*, kPa	ω	$V^{L(15)}$, cm^3/mol	$\delta^{(25)}$, J/cm^3
1	38.57	0.5772	66.90	184.26	2597.00	0.2894	115.90	27.97
2	57.31	0.6755	80.57	226.77	3274.65	0.2552	119.27	28.71
3	75.47	0.7089	89.17	252.22	3254.40	0.2674	125.79	28.94
4	93.07	0.7315	97.51	274.48	3143.86	0.2850	133.31	29.00
5	110.10	0.7487	105.89	294.83	3005.99	0.3045	141.42	28.97
6	126.60	0.7628	114.39	313.74	2862.47	0.3250	149.97	28.89
7	142.57	0.7746	123.04	331.50	2722.11	0.3459	158.83	28.76
8	158.04	0.7850	131.84	348.26	2588.58	0.3670	167.96	28.60
9	173.03	0.7941	140.80	364.14	2463.40	0.3882	177.32	28.43
10	187.58	0.8023	149.92	379.26	2346.79	0.4093	186.87	28.24
11	201.70	0.8097	159.19	393.67	2238.50	0.4304	196.60	28.05
12	215.42	0.8166	168.63	407.46	2138.02	0.4514	206.51	27.85
13	228.80	0.8229	178.24	420.70	2044.62	0.4725	216.60	27.64
14	241.84	0.8288	188.02	433.43	1957.70	0.4935	226.87	27.43
15	254.61	0.8343	198.01	445.72	1876.55	0.5145	237.36	27.22
16	267.13	0.8394	208.23	457.62	1800.47	0.5357	248.07	27.01
17	279.46	0.8443	218.72	469.19	1728.81	0.5571	259.06	26.79
18	291.64	0.8489	229.50	480.47	1661.08	0.5788	270.36	26.57
19	303.72	0.8532	240.64	491.52	1596.63	0.6008	282.03	26.35
20	315.75	0.8574	252.18	502.38	1535.06	0.6234	294.13	26.12
21	327.79	0.8614	264.22	513.12	1475.85	0.6467	306.75	25.89
22	339.89	0.8651	276.82	523.76	1418.66	0.6709	319.97	25.66
23	352.12	0.8688	290.09	520.35	1375.40	0.8563	333.90	25.41
24	364.53	0.8723	304.13	530.44	1314.51	0.8900	348.66	25.16
25	377.20	0.8756	319.09	540.61	1254.38	0.9252	364.41	24.90
26	390.18	0.8789	335.10	550.89	1194.87	0.9592	381.28	24.63
27	403.55	0.8820	352.36	561.34	1135.69	0.9950	399.50	24.35
28	417.39	0.8850	371.05	572.01	1076.76	1.0320	419.26	24.06
29	431.76	0.8880	391.42	582.95	1017.94	1.0704	440.81	23.75
30	446.75	0.8908	413.75	594.21	959.13	1.1104	464.48	23.43
31	462.43	0.8935	438.34	605.83	900.38	1.1521	490.57	23.09
32	478.90	0.8962	465.57	617.87	841.68	1.1957	519.50	22.74
33	496.23	0.8988	495.90	630.39	783.10	1.2415	551.74	22.36
34	514.52	0.9013	529.81	643.42	724.81	1.2894	587.83	21.96
35	533.85	0.9038	567.94	657.02	666.96	1.3398	628.42	21.55
36	554.32	0.9061	611.01	671.24	609.77	1.3926	674.29	21.11
37	576.02	0.9085	659.88	686.14	553.49	1.4482	726.37	20.65
38	599.06	0.9107	715.62	701.76	498.44	1.5065	785.76	20.17
39	623.54	0.9130	779.47	718.17	444.91	1.5677	853.79	19.67
40	649.56	0.9151	852.98	735.41	393.27	1.6318	932.10	19.14

Table H-16 Physical properties for petroleum stock No. 17

Cut	*TB*, °C	*Sp.gr*	*MW*	*Tc*, °C	*Pc*, kPa	ω	$V^{L(15)}$, cm^3/mol	$\delta^{(25)}$, J/cm^3
1	176.38	0.7145	145.75	344.11	1876.78	0.4672	204.00	26.58
2	196.98	0.8041	156.37	387.98	2252.42	0.4260	194.46	28.03
3	216.59	0.8314	167.72	412.77	2221.76	0.4409	201.74	28.22
4	235.18	0.8496	179.61	434.10	2149.88	0.4610	211.40	28.21
5	252.76	0.8635	191.78	453.24	2068.27	0.4827	222.10	28.09
6	269.30	0.8747	204.04	470.66	1987.53	0.5046	233.28	27.93
7	284.83	0.8841	216.25	486.64	1911.60	0.5263	244.61	27.75
8	299.37	0.8922	228.31	501.32	1842.03	0.5474	255.89	27.55
9	312.94	0.8994	240.11	514.84	1779.22	0.5675	266.97	27.36
10	325.56	0.9058	251.57	527.31	1723.04	0.5867	277.73	27.17
11	337.30	0.9116	262.65	538.80	1673.02	0.6047	288.11	26.99
12	348.19	0.9169	273.29	534.95	1665.61	0.7725	298.04	26.82
13	358.29	0.9218	283.47	544.12	1619.79	0.7948	307.51	26.66
14	367.67	0.9264	293.21	552.61	1578.71	0.8155	316.51	26.51
15	376.40	0.9306	302.50	560.49	1541.78	0.8349	325.05	26.37
16	384.57	0.9346	311.41	567.85	1508.32	0.8530	333.20	26.24
17	392.25	0.9383	320.00	574.77	1477.68	0.8701	341.03	26.12
18	399.57	0.9419	328.35	581.33	1449.20	0.8865	348.61	26.00
19	406.61	0.9452	336.59	587.62	1422.18	0.9024	356.09	25.89
20	413.49	0.9484	344.84	593.72	1395.94	0.9181	363.60	25.78
21	420.34	0.9514	353.27	599.73	1369.81	0.9340	371.30	25.66
22	427.28	0.9544	362.07	605.74	1343.09	0.9505	379.39	25.53
23	434.46	0.9571	371.45	611.86	1315.09	0.9680	388.09	25.40
24	442.03	0.9598	381.67	618.20	1285.13	0.9813	397.66	25.25
25	450.13	0.9624	393.02	624.85	1252.57	1.0003	408.40	25.08
26	458.92	0.9648	405.82	631.93	1216.82	1.0213	420.62	24.90
27	468.59	0.9672	420.46	639.55	1177.33	1.0448	434.72	24.68
28	479.31	0.9695	437.38	647.84	1133.67	1.0713	451.15	24.43
29	491.27	0.9717	457.15	656.91	1085.47	1.1011	470.46	24.15
30	504.65	0.9738	480.37	666.88	1032.54	1.1348	493.28	23.83
31	519.68	0.9759	507.85	677.88	974.84	1.1729	520.39	23.46
32	536.55	0.9779	540.54	690.02	912.50	1.2157	552.74	23.05
33	555.49	0.9799	579.63	703.44	845.86	1.2638	591.53	22.58
34	576.72	0.9818	626.61	718.25	775.48	1.3174	638.24	22.07
35	600.49	0.9836	683.38	734.59	702.12	1.3771	694.75	21.50
36	627.02	0.9854	752.34	752.57	626.81	1.4431	763.46	20.87
37	656.59	0.9872	836.69	772.32	550.66	1.5157	847.55	20.19
38	689.45	0.9889	940.54	793.98	475.02	1.5951	951.11	19.45
39	725.86	0.9906	1069.36	817.66	401.33	1.6814	1079.56	18.65
40	766.08	0.9922	1230.40	843.49	331.12	1.7746	1240.10	17.81

Table H-17 Physical properties for petroleum stock No. 18

Cut	*TB*, °C	*Sp.gr*	*MW*	*Tc*, °C	*Pc*, kPa	ω	$V^{L(15)}$, cm^3/mol	$\delta^{(25)}$, J/cm^3
1	72.13	0.6185	84.09	226.35	2451.86	0.3272	135.96	27.59
2	88.40	0.6984	95.37	262.12	2923.96	0.2982	136.54	28.41
3	103.70	0.7230	103.10	282.56	2888.45	0.3100	142.59	28.54
4	118.10	0.7395	110.51	300.07	2800.68	0.3254	149.44	28.54
5	131.65	0.7519	117.73	315.71	2699.91	0.3419	156.57	28.48
6	144.40	0.7620	124.81	329.94	2598.89	0.3584	163.79	28.39
7	156.42	0.7705	131.75	343.01	2502.39	0.3748	170.98	28.28
8	167.77	0.7779	138.54	355.09	2412.06	0.3908	178.10	28.15
9	178.52	0.7844	145.21	366.34	2328.21	0.4064	185.13	28.03
10	188.71	0.7902	151.75	376.86	2250.64	0.4216	192.05	27.90
11	198.43	0.7954	158.19	386.75	2178.71	0.4363	198.87	27.77
12	207.73	0.8002	164.54	396.11	2111.80	0.4507	205.61	27.63
13	216.69	0.8047	170.84	405.01	2049.10	0.4648	212.32	27.50
14	225.37	0.8088	177.13	413.55	1989.93	0.4788	219.01	27.37
15	233.84	0.8126	183.45	421.78	1933.60	0.4927	225.75	27.23
16	242.17	0.8162	189.85	429.79	1879.40	0.5067	232.60	27.10
17	250.45	0.8196	196.39	437.64	1826.71	0.5209	239.62	26.96
18	258.75	0.8228	203.13	445.41	1774.97	0.5355	246.88	26.81
19	267.14	0.8258	210.15	453.16	1723.65	0.5506	254.47	26.66
20	275.69	0.8287	217.54	460.96	1672.26	0.5665	262.50	26.50
21	284.50	0.8315	225.38	468.86	1620.39	0.5833	271.06	26.33
22	293.64	0.8341	233.78	476.93	1567.67	0.6013	280.28	26.14
23	303.19	0.8366	242.86	485.22	1513.81	0.6207	290.29	25.95
24	313.24	0.8390	252.75	493.80	1458.54	0.6419	301.24	25.74
25	323.86	0.8413	263.60	502.71	1401.73	0.6651	313.31	25.51
26	335.17	0.8436	275.58	512.01	1343.23	0.6908	326.69	25.26
27	347.22	0.8457	288.90	508.52	1285.85	0.8744	341.60	25.00
28	360.13	0.8478	303.76	518.36	1217.27	0.9130	358.30	24.71
29	373.97	0.8498	320.46	528.76	1146.70	0.9532	377.09	24.40
30	388.85	0.8517	339.26	539.75	1074.44	0.9964	398.32	24.06
31	404.85	0.8536	360.55	551.40	1000.77	1.0428	422.37	23.70
32	422.07	0.8554	384.73	563.76	926.08	1.0925	449.75	23.31
33	440.61	0.8572	412.32	576.86	850.86	1.1457	481.00	22.90
34	460.56	0.8589	443.90	590.76	775.65	1.2025	516.80	22.45
35	482.03	0.8606	480.20	605.51	701.02	1.2631	557.97	21.98
36	505.12	0.8622	522.06	621.15	627.63	1.3276	605.46	21.48
37	529.92	0.8638	570.51	637.72	556.16	1.3959	660.44	20.95
38	556.55	0.8654	626.85	655.28	487.21	1.4682	724.37	20.39
39	585.11	0.8669	692.63	673.88	421.46	1.5444	798.98	19.80
40	615.70	0.8684	769.75	693.55	359.54	1.6245	886.43	19.19

Table H-18 Material balance for petroleum stock No. 2

Cut	*TB*, °C	*Sp.gr*	*MW*	Volume, cm^3	Weight, g	Mole, gmol	*Zf*, vol.%	*Zf*, wt.%	*Zf*, mol.%
1	71.39	0.7118	87.24	100	71.18	0.8159	2.5	2.11	4.37
2	77.26	0.7192	89.95	100	71.92	0.7995	2.5	2.13	4.28
3	84.13	0.7273	93.15	100	72.73	0.7807	2.5	2.16	4.18
4	91.79	0.7358	96.77	100	73.58	0.7603	2.5	2.18	4.07
5	100.10	0.7445	100.76	100	74.45	0.7388	2.5	2.21	3.95
6	108.90	0.7531	105.08	100	75.31	0.7167	2.5	2.24	3.84
7	118.06	0.7616	109.68	100	76.16	0.6944	2.5	2.26	3.72
8	127.45	0.7698	114.51	100	76.98	0.6723	2.5	2.28	3.60
9	136.99	0.7777	119.55	100	77.77	0.6505	2.5	2.31	3.48
10	146.56	0.7852	124.75	100	78.52	0.6295	2.5	2.33	3.37
11	156.11	0.7924	130.08	100	79.24	0.6091	2.5	2.35	3.26
12	165.58	0.7992	135.52	100	79.92	0.5897	2.5	2.37	3.16
13	174.91	0.8056	141.04	100	80.56	0.5712	2.5	2.39	3.06
14	184.09	0.8116	146.62	100	81.16	0.5535	2.5	2.41	2.96
15	193.09	0.8173	152.25	100	81.73	0.5368	2.5	2.43	2.87
16	201.91	0.8227	157.93	100	82.27	0.5209	2.5	2.44	2.79
17	210.58	0.8278	163.67	100	82.78	0.5058	2.5	2.46	2.71
18	219.12	0.8327	169.47	100	83.27	0.4914	2.5	2.47	2.63
19	227.57	0.8374	175.38	100	83.74	0.4775	2.5	2.49	2.56
20	236.00	0.8420	181.43	100	84.20	0.4641	2.5	2.50	2.48
21	244.49	0.8464	187.69	100	84.64	0.4510	2.5	2.51	2.41
22	253.11	0.8508	194.22	100	85.08	0.4381	2.5	2.53	2.34
23	261.99	0.8552	201.14	100	85.52	0.4252	2.5	2.54	2.28
24	271.23	0.8597	208.56	100	85.97	0.4122	2.5	2.55	2.21
25	280.97	0.8643	216.63	100	86.43	0.3990	2.5	2.57	2.14
26	291.37	0.8690	225.52	100	86.90	0.3854	2.5	2.58	2.06
27	302.58	0.8740	235.45	100	87.40	0.3712	2.5	2.59	1.99
28	314.78	0.8793	246.69	100	87.93	0.3564	2.5	2.61	1.91
29	328.18	0.8849	259.54	100	88.49	0.3409	2.5	2.63	1.82
30	342.97	0.8908	274.41	100	89.08	0.3246	2.5	2.64	1.74
31	359.39	0.8972	291.78	100	89.72	0.3075	2.5	2.66	1.65
32	377.68	0.9041	312.25	100	90.41	0.2895	2.5	2.68	1.55
33	398.08	0.9114	336.57	100	91.14	0.2708	2.5	2.71	1.45
34	420.86	0.9192	365.74	100	91.92	0.2513	2.5	2.73	1.35
35	446.32	0.9276	401.01	100	92.76	0.2313	2.5	2.75	1.24
36	474.74	0.9365	444.02	100	93.65	0.2109	2.5	2.78	1.13
37	506.45	0.9459	496.98	100	94.59	0.1903	2.5	2.81	1.02
38	541.77	0.9559	562.85	100	95.59	0.1698	2.5	2.84	0.91
39	581.05	0.9663	645.63	100	96.63	0.1497	2.5	2.87	0.80
40	624.64	0.9773	750.89	100	97.73	0.1302	2.5	2.90	0.70
			Total	**4000**	**3369.05**	**18.68**	**100**	**100**	**100**

Table H-19 Material balance for petroleum stock No. 3

Cut	*TB*, °C	*Sp.gr*	*MW*	Volume, cm^3	Weight, g	Mole, gmol	*Zf*, vol.%	*Zf*, wt.%	*Zf*, mol.%
1	65.77	0.7078	84.67	100	70.78	0.8360	2.5	1.98	5.94
2	82.61	0.7290	92.38	100	72.90	0.7892	2.5	2.04	5.60
3	99.99	0.7479	100.59	100	74.79	0.7435	2.5	2.10	5.28
4	117.73	0.7650	109.34	100	76.50	0.6996	2.5	2.14	4.97
5	135.68	0.7804	118.61	100	78.04	0.6579	2.5	2.19	4.67
6	153.68	0.7944	128.41	100	79.44	0.6186	2.5	2.23	4.39
7	171.60	0.8072	138.70	100	80.72	0.5820	2.5	2.26	4.13
8	189.31	0.8188	149.45	100	81.88	0.5479	2.5	2.30	3.89
9	206.72	0.8295	160.61	100	82.95	0.5165	2.5	2.33	3.67
10	223.73	0.8393	172.12	100	83.93	0.4876	2.5	2.35	3.46
11	240.29	0.8483	183.95	100	84.83	0.4611	2.5	2.38	3.27
12	256.32	0.8565	196.02	100	85.65	0.4370	2.5	2.40	3.10
13	271.80	0.8641	208.28	100	86.41	0.4149	2.5	2.42	2.95
14	286.71	0.8711	220.68	100	87.11	0.3947	2.5	2.44	2.80
15	301.02	0.8775	233.17	100	87.75	0.3763	2.5	2.46	2.67
16	314.76	0.8835	245.72	100	88.35	0.3596	2.5	2.48	2.55
17	327.94	0.8890	258.31	100	88.90	0.3442	2.5	2.49	2.44
18	340.61	0.8942	270.92	100	89.42	0.3301	2.5	2.51	2.34
19	352.82	0.8990	283.59	100	89.90	0.3170	2.5	2.52	2.25
20	364.65	0.9036	296.34	100	90.36	0.3049	2.5	2.53	2.17
21	376.17	0.9079	309.26	100	90.79	0.2936	2.5	2.55	2.08
22	387.51	0.9120	322.45	100	91.20	0.2828	2.5	2.56	2.01
23	398.77	0.9160	336.05	100	91.60	0.2726	2.5	2.57	1.94
24	410.09	0.9200	350.24	100	92.00	0.2627	2.5	2.58	1.87
25	421.62	0.9239	365.24	100	92.39	0.2530	2.5	2.59	1.80
26	433.54	0.9279	381.35	100	92.79	0.2433	2.5	2.60	1.73
27	446.01	0.9320	398.91	100	93.20	0.2336	2.5	2.61	1.66
28	459.25	0.9362	418.35	100	93.62	0.2238	2.5	2.62	1.59
29	473.46	0.9406	440.18	100	94.06	0.2137	2.5	2.64	1.52
30	488.88	0.9453	465.03	100	94.53	0.2033	2.5	2.65	1.44
31	505.75	0.9503	493.72	100	95.03	0.1925	2.5	2.66	1.37
32	524.34	0.9556	527.24	100	95.56	0.1812	2.5	2.68	1.29
33	544.92	0.9613	566.79	100	96.13	0.1696	2.5	2.70	1.20
34	567.79	0.9675	614.01	100	96.75	0.1576	2.5	2.71	1.12
35	593.25	0.9741	670.94	100	97.41	0.1452	2.5	2.73	1.03
36	621.64	0.9813	740.28	100	98.13	0.1326	2.5	2.75	0.94
37	653.30	0.9889	825.61	100	98.89	0.1198	2.5	2.77	0.85
38	688.58	0.9971	931.79	100	99.71	0.1070	2.5	2.80	0.76
39	727.85	1.0058	1065.41	100	100.58	0.0944	2.5	2.82	0.67
40	771.51	1.0150	1235.66	100	101.50	0.0821	2.5	2.85	0.58
			Total	**4000**	**3566.48**	**14.08**	**100**	**100**	**100**

Table H-20 Material balance for petroleum stock No. 4

Cut	*TB*, °C	*Sp.gr*	*MW*	Volume, cm^3	Weight, g	Mole, gmol	*Zf*, vol.%	*Zf*, wt.%	*Zf*, mol.%
1	57.10	0.6759	80.49	100	67.59	0.8398	2.5	2.02	5.14
2	71.65	0.6954	87.34	100	69.54	0.7962	2.5	2.07	4.88
3	85.83	0.7121	94.15	100	71.21	0.7563	2.5	2.12	4.63
4	99.64	0.7265	100.95	100	72.65	0.7197	2.5	2.17	4.41
5	113.06	0.7392	107.77	100	73.92	0.6860	2.5	2.20	4.20
6	126.10	0.7506	114.62	100	75.06	0.6549	2.5	2.24	4.01
7	138.76	0.7608	121.51	100	76.08	0.6261	2.5	2.27	3.84
8	151.05	0.7701	128.44	100	77.01	0.5996	2.5	2.30	3.67
9	162.97	0.7786	135.40	100	77.86	0.5750	2.5	2.32	3.52
10	174.55	0.7864	142.41	100	78.64	0.5522	2.5	2.35	3.38
11	185.80	0.7936	149.46	100	79.36	0.5310	2.5	2.37	3.25
12	196.76	0.8003	156.56	100	80.03	0.5112	2.5	2.39	3.13
13	207.45	0.8066	163.72	100	80.66	0.4926	2.5	2.41	3.02
14	217.91	0.8125	170.97	100	81.25	0.4752	2.5	2.42	2.91
15	228.17	0.8181	178.32	100	81.81	0.4588	2.5	2.44	2.81
16	238.29	0.8234	185.80	100	82.34	0.4431	2.5	2.46	2.71
17	248.31	0.8285	193.45	100	82.85	0.4282	2.5	2.47	2.62
18	258.29	0.8334	201.32	100	83.34	0.4140	2.5	2.49	2.54
19	268.28	0.8381	209.45	100	83.81	0.4002	2.5	2.50	2.45
20	278.36	0.8428	217.92	100	84.28	0.3867	2.5	2.51	2.37
21	288.57	0.8474	226.79	100	84.74	0.3736	2.5	2.53	2.29
22	299.01	0.8520	236.17	100	85.20	0.3608	2.5	2.54	2.21
23	309.75	0.8565	246.14	100	85.65	0.3480	2.5	2.55	2.13
24	320.87	0.8611	256.84	100	86.11	0.3353	2.5	2.57	2.05
25	332.45	0.8658	268.41	100	86.58	0.3226	2.5	2.58	1.98
26	344.60	0.8706	281.01	100	87.06	0.3098	2.5	2.60	1.90
27	357.39	0.8754	294.83	100	87.54	0.2969	2.5	2.61	1.82
28	370.95	0.8804	310.11	100	88.04	0.2839	2.5	2.63	1.74
29	385.37	0.8856	327.12	100	88.56	0.2707	2.5	2.64	1.66
30	400.75	0.8909	346.17	100	89.09	0.2574	2.5	2.66	1.58
31	417.23	0.8965	367.65	100	89.65	0.2438	2.5	2.67	1.49
32	434.92	0.9022	392.03	100	90.22	0.2301	2.5	2.69	1.41
33	453.93	0.9082	419.85	100	90.82	0.2163	2.5	2.71	1.33
34	474.40	0.9144	451.79	100	91.44	0.2024	2.5	2.73	1.24
35	496.47	0.9209	488.68	100	92.09	0.1884	2.5	2.75	1.15
36	520.28	0.9276	531.55	100	92.76	0.1745	2.5	2.77	1.07
37	545.96	0.9345	581.67	100	93.45	0.1607	2.5	2.79	0.98
38	573.66	0.9418	640.64	100	94.18	0.1470	2.5	2.81	0.90
39	603.54	0.9492	710.47	100	94.92	0.1336	2.5	2.83	0.82
40	635.76	0.9570	793.75	100	95.70	0.1206	2.5	2.85	0.74
			Total	**4000**	**3353.08**	**16.32**	**100**	**100**	**100**

Table H-21 Material balance for petroleum stock No. 5

Cut	*TB*, °C	*Sp.gr*	*MW*	Volume, cm^3	Weight, g	Mole, gmol	*Zf*, vol.%	*Zf*, wt.%	*Zf*, mol.%
1	106.91	0.7265	104.74	100	72.65	0.6936	2.5	2.14	4.97
2	123.97	0.7416	113.71	100	74.16	0.6522	2.5	2.18	4.67
3	140.01	0.7544	122.52	100	75.44	0.6158	2.5	2.22	4.41
4	155.06	0.7655	131.16	100	76.55	0.5837	2.5	2.25	4.18
5	169.16	0.7752	139.61	100	77.52	0.5553	2.5	2.28	3.98
6	182.33	0.7838	147.83	100	78.38	0.5302	2.5	2.30	3.80
7	194.61	0.7913	155.80	100	79.13	0.5079	2.5	2.33	3.64
8	206.05	0.7980	163.50	100	79.80	0.4881	2.5	2.35	3.50
9	216.70	0.8040	170.92	100	80.40	0.4704	2.5	2.36	3.37
10	226.62	0.8093	178.06	100	80.93	0.4545	2.5	2.38	3.26
11	235.87	0.8142	184.92	100	81.42	0.4403	2.5	2.39	3.15
12	244.53	0.8186	191.53	100	81.86	0.4274	2.5	2.41	3.06
13	252.68	0.8226	197.91	100	82.26	0.4156	2.5	2.42	2.98
14	260.39	0.8263	204.11	100	82.63	0.4048	2.5	2.43	2.90
15	267.76	0.8298	210.18	100	82.98	0.3948	2.5	2.44	2.83
16	274.89	0.8331	216.19	100	83.31	0.3853	2.5	2.45	2.76
17	281.87	0.8362	222.21	100	83.62	0.3763	2.5	2.46	2.70
18	288.82	0.8393	228.33	100	83.93	0.3676	2.5	2.47	2.63
19	295.85	0.8424	234.67	100	84.24	0.3590	2.5	2.48	2.57
20	303.09	0.8455	241.34	100	84.55	0.3503	2.5	2.49	2.51
21	310.65	0.8486	248.49	100	84.86	0.3415	2.5	2.49	2.45
22	318.69	0.8519	256.27	100	85.19	0.3324	2.5	2.50	2.38
23	327.33	0.8554	264.86	100	85.54	0.3230	2.5	2.51	2.31
24	336.72	0.8591	274.48	100	85.91	0.3130	2.5	2.53	2.24
25	347.02	0.8631	285.37	100	86.31	0.3024	2.5	2.54	2.17
26	358.39	0.8673	297.82	100	86.73	0.2912	2.5	2.55	2.09
27	370.98	0.8719	312.15	100	87.19	0.2793	2.5	2.56	2.00
28	384.99	0.8769	328.79	100	87.69	0.2667	2.5	2.58	1.91
29	400.57	0.8822	348.21	100	88.22	0.2534	2.5	2.59	1.81
30	417.92	0.8880	371.03	100	88.80	0.2393	2.5	2.61	1.71
31	437.23	0.8942	397.97	100	89.42	0.2247	2.5	2.63	1.61
32	458.70	0.9009	429.96	100	90.09	0.2095	2.5	2.65	1.50
33	482.53	0.9079	468.17	100	90.79	0.1939	2.5	2.67	1.39
34	508.93	0.9155	514.08	100	91.55	0.1781	2.5	2.69	1.28
35	538.10	0.9234	569.60	100	92.34	0.1621	2.5	2.71	1.16
36	570.29	0.9318	637.26	100	93.18	0.1462	2.5	2.74	1.05
37	605.72	0.9406	720.33	100	94.06	0.1306	2.5	2.77	0.94
38	644.62	0.9498	823.19	100	94.98	0.1154	2.5	2.79	0.83
39	687.21	0.9593	951.68	100	95.93	0.1008	2.5	2.82	0.72
40	733.79	0.9692	1113.94	100	96.92	0.0870	2.5	2.85	0.62
			Total	**4000**	**3401.44**	**13.96**	**100**	**100**	**100**

Table H-22 Material balance for petroleum stock No. 6

Cut	*TB*, °C	*Sp.gr*	*MW*	Volume, cm^3	Weight, g	Mole, gmol	*Zf*, vol.%	*Zf*, wt.%	*Zf*, mol.%
1	62.03	0.6875	82.87	100	68.75	0.8296	2.5	2.09	4.37
2	69.05	0.6969	86.15	100	69.69	0.8089	2.5	2.12	4.26
3	77.10	0.7069	89.95	100	70.69	0.7859	2.5	2.15	4.14
4	85.96	0.7171	94.18	100	71.71	0.7614	2.5	2.18	4.01
5	95.42	0.7272	98.78	100	72.72	0.7362	2.5	2.21	3.88
6	105.29	0.7370	103.68	100	73.70	0.7108	2.5	2.24	3.74
7	115.40	0.7464	108.83	100	74.64	0.6859	2.5	2.27	3.61
8	125.60	0.7553	114.16	100	75.53	0.6616	2.5	2.30	3.49
9	135.76	0.7636	119.61	100	76.36	0.6384	2.5	2.33	3.36
10	145.75	0.7714	125.14	100	77.14	0.6164	2.5	2.35	3.25
11	155.51	0.7786	130.69	100	77.86	0.5958	2.5	2.37	3.14
12	164.93	0.7853	136.20	100	78.53	0.5766	2.5	2.39	3.04
13	173.97	0.7914	141.64	100	79.14	0.5587	2.5	2.41	2.94
14	182.60	0.7970	146.97	100	79.70	0.5423	2.5	2.43	2.86
15	190.79	0.8021	152.17	100	80.21	0.5271	2.5	2.44	2.78
16	198.54	0.8068	157.22	100	80.68	0.5132	2.5	2.46	2.70
17	205.90	0.8112	162.11	100	81.12	0.5004	2.5	2.47	2.64
18	212.87	0.8152	166.86	100	81.52	0.4885	2.5	2.48	2.57
19	219.54	0.8189	171.50	100	81.89	0.4775	2.5	2.49	2.52
20	225.98	0.8225	176.08	100	82.25	0.4671	2.5	2.51	2.46
21	232.29	0.8258	180.65	100	82.58	0.4572	2.5	2.52	2.41
22	238.58	0.8291	185.30	100	82.91	0.4475	2.5	2.53	2.36
23	244.99	0.8324	190.14	100	83.24	0.4378	2.5	2.54	2.31
24	251.68	0.8358	195.29	100	83.58	0.4280	2.5	2.55	2.25
25	258.82	0.8393	200.92	100	83.93	0.4177	2.5	2.56	2.20
26	266.61	0.8431	207.20	100	84.31	0.4069	2.5	2.57	2.14
27	275.26	0.8471	214.37	100	84.71	0.3952	2.5	2.58	2.08
28	285.00	0.8516	222.68	100	85.16	0.3824	2.5	2.59	2.01
29	296.08	0.8565	232.46	100	85.65	0.3684	2.5	2.61	1.94
30	308.78	0.8620	244.12	100	86.20	0.3531	2.5	2.63	1.86
31	323.38	0.8681	258.12	100	86.81	0.3363	2.5	2.64	1.77
32	340.21	0.8748	275.09	100	87.48	0.3180	2.5	2.66	1.68
33	359.57	0.8822	295.82	100	88.22	0.2982	2.5	2.69	1.57
34	381.82	0.8904	321.30	100	89.04	0.2771	2.5	2.71	1.46
35	407.34	0.8993	352.88	100	89.93	0.2548	2.5	2.74	1.34
36	436.51	0.9089	392.34	100	90.89	0.2317	2.5	2.77	1.22
37	469.71	0.9192	442.07	100	91.92	0.2079	2.5	2.80	1.10
38	507.41	0.9303	505.45	100	93.03	0.1841	2.5	2.83	0.97
39	550.00	0.9420	587.08	100	94.20	0.1605	2.5	2.87	0.85
40	598.00	0.9544	693.71	100	95.44	0.1376	2.5	2.91	0.72
			Total	**4000**	**3283.06**	**18.98**	**100**	**100**	**100**

Table H-23 Material balance for petroleum stock No. 7

Cut	*TB*, °C	*Sp.gr*	*MW*	Volume, cm^3	Weight, g	Mole, gmol	*Zf*, vol.%	*Zf*, wt.%	*Zf*, mol.%
1	54.08	0.6696	79.02	100	66.96	0.8473	2.5	2.04	4.74
2	64.31	0.6840	83.85	100	68.40	0.8158	2.5	2.08	4.57
3	74.58	0.6971	88.73	100	69.71	0.7857	2.5	2.12	4.40
4	84.86	0.7090	93.68	100	70.90	0.7568	2.5	2.16	4.24
5	95.08	0.7199	98.70	100	71.99	0.7293	2.5	2.19	4.08
6	105.24	0.7299	103.81	100	72.99	0.7031	2.5	2.22	3.94
7	115.31	0.7392	108.99	100	73.92	0.6782	2.5	2.25	3.80
8	125.27	0.7478	114.25	100	74.78	0.6545	2.5	2.28	3.66
9	135.11	0.7558	119.59	100	75.58	0.6320	2.5	2.30	3.54
10	144.82	0.7633	125.00	100	76.33	0.6106	2.5	2.32	3.42
11	154.41	0.7704	130.50	100	77.04	0.5903	2.5	2.35	3.30
12	163.88	0.7770	136.09	100	77.70	0.5710	2.5	2.37	3.20
13	173.27	0.7833	141.78	100	78.33	0.5525	2.5	2.38	3.09
14	182.58	0.7893	147.59	100	78.93	0.5348	2.5	2.40	2.99
15	191.84	0.7951	153.53	100	79.51	0.5179	2.5	2.42	2.90
16	201.09	0.8006	159.64	100	80.06	0.5015	2.5	2.44	2.81
17	210.38	0.8060	165.96	100	80.60	0.4856	2.5	2.45	2.72
18	219.76	0.8112	172.53	100	81.12	0.4702	2.5	2.47	2.63
19	229.27	0.8163	179.39	100	81.63	0.4551	2.5	2.49	2.55
20	238.98	0.8214	186.61	100	82.14	0.4402	2.5	2.50	2.46
21	248.97	0.8264	194.27	100	82.64	0.4254	2.5	2.52	2.38
22	259.30	0.8315	202.46	100	83.15	0.4107	2.5	2.53	2.30
23	270.05	0.8366	211.28	100	83.66	0.3960	2.5	2.55	2.22
24	281.33	0.8418	220.85	100	84.18	0.3811	2.5	2.56	2.13
25	293.22	0.8470	231.33	100	84.70	0.3662	2.5	2.58	2.05
26	305.82	0.8525	242.89	100	85.25	0.3510	2.5	2.60	1.96
27	319.25	0.8580	255.72	100	85.80	0.3355	2.5	2.61	1.88
28	333.62	0.8638	270.09	100	86.38	0.3198	2.5	2.63	1.79
29	349.04	0.8698	286.28	100	86.98	0.3038	2.5	2.65	1.70
30	365.65	0.8760	304.64	100	87.60	0.2875	2.5	2.67	1.61
31	383.59	0.8824	325.61	100	88.24	0.2710	2.5	2.69	1.52
32	403.00	0.8892	349.71	100	88.92	0.2543	2.5	2.71	1.42
33	424.02	0.8961	377.60	100	89.61	0.2373	2.5	2.73	1.33
34	446.81	0.9034	410.05	100	90.34	0.2203	2.5	2.75	1.23
35	471.54	0.9110	448.08	100	91.10	0.2033	2.5	2.77	1.14
36	498.36	0.9188	492.94	100	91.88	0.1864	2.5	2.80	1.04
37	527.46	0.9269	546.22	100	92.69	0.1697	2.5	2.82	0.95
38	559.00	0.9353	609.95	100	93.53	0.1533	2.5	2.85	0.86
39	593.20	0.9440	686.83	100	94.40	0.1374	2.5	2.87	0.77
40	630.23	0.9530	780.29	100	95.30	0.1221	2.5	2.90	0.68
			Total	**4000**	**3284.97**	**17.86**	**100**	**100**	**100**

Table H-24 Material balance for petroleum stock No. 8

Cut	*TB*, °C	*Sp.gr*	*MW*	Volume, cm^3	Weight, g	Mole, gmol	*Zf*, vol.%	*Zf*, wt.%	*Zf*, mol.%
1	54.10	0.6746	79.15	100	67.46	0.8522	2.5	2.01	5.09
2	63.89	0.6885	83.72	100	68.85	0.8224	2.5	2.05	4.91
3	74.43	0.7021	88.68	100	70.21	0.7917	2.5	2.09	4.73
4	85.59	0.7151	94.01	100	71.51	0.7606	2.5	2.13	4.54
5	97.25	0.7274	99.71	100	72.74	0.7296	2.5	2.17	4.36
6	109.30	0.7392	105.75	100	73.92	0.6990	2.5	2.20	4.18
7	121.65	0.7503	112.13	100	75.03	0.6691	2.5	2.23	4.00
8	134.20	0.7607	118.85	100	76.07	0.6401	2.5	2.27	3.82
9	146.89	0.7706	125.87	100	77.06	0.6122	2.5	2.30	3.66
10	159.63	0.7798	133.20	100	77.98	0.5855	2.5	2.32	3.50
11	172.39	0.7886	140.81	100	78.86	0.5600	2.5	2.35	3.35
12	185.09	0.7968	148.70	100	79.68	0.5359	2.5	2.37	3.20
13	197.72	0.8046	156.84	100	80.46	0.5130	2.5	2.40	3.06
14	210.23	0.8119	165.24	100	81.19	0.4913	2.5	2.42	2.94
15	222.60	0.8188	173.88	100	81.88	0.4709	2.5	2.44	2.81
16	234.84	0.8253	182.75	100	82.53	0.4516	2.5	2.46	2.70
17	246.93	0.8316	191.87	100	83.16	0.4334	2.5	2.48	2.59
18	258.89	0.8375	201.25	100	83.75	0.4162	2.5	2.49	2.49
19	270.73	0.8431	210.89	100	84.31	0.3998	2.5	2.51	2.39
20	282.49	0.8486	220.83	100	84.86	0.3843	2.5	2.53	2.30
21	294.20	0.8538	231.12	100	85.38	0.3694	2.5	2.54	2.21
22	305.91	0.8589	241.80	100	85.89	0.3552	2.5	2.56	2.12
23	317.68	0.8638	252.96	100	86.38	0.3415	2.5	2.57	2.04
24	329.58	0.8686	264.67	100	86.86	0.3282	2.5	2.59	1.96
25	341.68	0.8734	277.06	100	87.34	0.3152	2.5	2.60	1.88
26	354.07	0.8782	290.26	100	87.82	0.3026	2.5	2.62	1.81
27	366.86	0.8830	304.44	100	88.30	0.2900	2.5	2.63	1.73
28	380.14	0.8878	319.81	100	88.78	0.2776	2.5	2.64	1.66
29	394.02	0.8927	336.61	100	89.27	0.2652	2.5	2.66	1.58
30	408.65	0.8977	355.15	100	89.77	0.2528	2.5	2.67	1.51
31	424.15	0.9029	375.78	100	90.29	0.2403	2.5	2.69	1.44
32	440.66	0.9082	398.93	100	90.82	0.2277	2.5	2.71	1.36
33	458.36	0.9137	425.16	100	91.37	0.2149	2.5	2.72	1.28
34	477.38	0.9195	455.10	100	91.95	0.2020	2.5	2.74	1.21
35	497.92	0.9255	489.57	100	92.55	0.1890	2.5	2.76	1.13
36	520.17	0.9318	529.60	100	93.18	0.1759	2.5	2.78	1.05
37	544.30	0.9384	576.42	100	93.84	0.1628	2.5	2.80	0.97
38	570.52	0.9453	631.64	100	94.53	0.1497	2.5	2.82	0.89
39	599.05	0.9525	697.33	100	95.25	0.1366	2.5	2.84	0.82
40	630.11	0.9600	776.13	100	96.00	0.1237	2.5	2.86	0.74
			Total	**4000**	**3357.06**	**16.74**	**100**	**100**	**100**

Table H-25 Material balance for petroleum stock No. 9

Cut	*TB*, °C	*Sp.gr*	*MW*	Volume, cm^3	Weight, g	Mole, gmol	*Zf*, vol.%	*Zf*, wt.%	*Zf*, mol.%
1	131.07	0.7763	116.20	100	77.63	0.6680	2.5	2.19	4.64
2	154.78	0.7949	129.05	100	79.49	0.6160	2.5	2.24	4.27
3	175.90	0.8098	141.29	100	80.98	0.5731	2.5	2.28	3.98
4	194.57	0.8218	152.79	100	82.18	0.5379	2.5	2.32	3.73
5	210.94	0.8317	163.45	100	83.17	0.5088	2.5	2.35	3.53
6	225.19	0.8398	173.19	100	83.98	0.4849	2.5	2.37	3.37
7	237.48	0.8465	181.95	100	84.65	0.4652	2.5	2.39	3.23
8	247.96	0.8519	189.70	100	85.19	0.4491	2.5	2.40	3.12
9	256.81	0.8564	196.45	100	85.64	0.4360	2.5	2.42	3.03
10	264.18	0.8601	202.23	100	86.01	0.4253	2.5	2.43	2.95
11	270.26	0.8630	207.09	100	86.30	0.4167	2.5	2.44	2.89
12	275.21	0.8654	211.12	100	86.54	0.4099	2.5	2.44	2.84
13	279.20	0.8673	214.42	100	86.73	0.4045	2.5	2.45	2.81
14	282.41	0.8688	217.11	100	86.88	0.4002	2.5	2.45	2.78
15	285.02	0.8700	219.32	100	87.00	0.3967	2.5	2.45	2.75
16	287.22	0.8710	221.19	100	87.10	0.3938	2.5	2.46	2.73
17	289.17	0.8719	222.86	100	87.19	0.3912	2.5	2.46	2.72
18	291.08	0.8728	224.50	100	87.28	0.3887	2.5	2.46	2.70
19	293.11	0.8737	226.27	100	87.37	0.3861	2.5	2.47	2.68
20	295.47	0.8747	228.33	100	87.47	0.3831	2.5	2.47	2.66
21	298.34	0.8760	230.86	100	87.60	0.3795	2.5	2.47	2.63
22	301.91	0.8776	234.05	100	87.76	0.3750	2.5	2.48	2.60
23	306.39	0.8796	238.08	100	87.96	0.3694	2.5	2.48	2.56
24	311.96	0.8820	243.20	100	88.20	0.3627	2.5	2.49	2.52
25	318.83	0.8849	249.63	100	88.49	0.3545	2.5	2.50	2.46
26	327.19	0.8884	257.65	100	88.84	0.3448	2.5	2.51	2.39
27	337.25	0.8925	267.61	100	89.25	0.3335	2.5	2.52	2.31
28	349.22	0.8973	279.89	100	89.73	0.3206	2.5	2.53	2.22
29	363.30	0.9027	294.96	100	90.27	0.3060	2.5	2.55	2.12
30	379.70	0.9088	313.42	100	90.88	0.2900	2.5	2.56	2.01
31	398.64	0.9156	336.00	100	91.56	0.2725	2.5	2.58	1.89
32	420.32	0.9231	363.64	100	92.31	0.2539	2.5	2.60	1.76
33	444.97	0.9313	397.55	100	93.13	0.2343	2.5	2.63	1.63
34	472.79	0.9400	439.26	100	94.00	0.2140	2.5	2.65	1.49
35	504.02	0.9494	490.87	100	94.94	0.1934	2.5	2.68	1.34
36	538.86	0.9593	555.04	100	95.93	0.1728	2.5	2.71	1.20
37	577.56	0.9697	635.49	100	96.97	0.1526	2.5	2.74	1.06
38	620.31	0.9805	737.11	100	98.05	0.1330	2.5	2.77	0.92
39	667.38	0.9918	866.79	100	99.18	0.1144	2.5	2.80	0.79
40	718.96	1.0034	1033.93	100	100.34	0.0971	2.5	2.83	0.67
			Total	**4000**	**3544.15**	**14.41**	**100**	**100**	**100**

Table H-26 Material balance for petroleum stock No. 10

Cut	*TB*, °C	*Sp.gr*	*MW*	Volume, cm^3	Weight, g	Mole, gmol	*Zf*, vol.%	*Zf*, wt.%	*Zf*, mol.%
1	39.43	0.6480	72.18	100	64.80	0.8977	2.5	1.94	5.33
2	53.74	0.6716	78.93	100	67.16	0.8509	2.5	2.01	5.05
3	68.04	0.6916	85.64	100	69.16	0.8075	2.5	2.07	4.80
4	82.27	0.7088	92.42	100	70.88	0.7669	2.5	2.13	4.55
5	96.41	0.7240	99.33	100	72.40	0.7289	2.5	2.17	4.33
6	110.40	0.7375	106.38	100	73.75	0.6933	2.5	2.21	4.12
7	124.22	0.7498	113.59	100	74.98	0.6601	2.5	2.25	3.92
8	137.83	0.7609	120.96	100	76.09	0.6290	2.5	2.28	3.74
9	151.23	0.7710	128.50	100	77.10	0.6000	2.5	2.31	3.56
10	164.40	0.7804	136.20	100	78.04	0.5729	2.5	2.34	3.40
11	177.32	0.7890	144.06	100	78.90	0.5477	2.5	2.37	3.25
12	189.99	0.7970	152.07	100	79.70	0.5241	2.5	2.39	3.11
13	202.41	0.8045	160.24	100	80.45	0.5020	2.5	2.41	2.98
14	214.58	0.8114	168.56	100	81.14	0.4814	2.5	2.43	2.86
15	226.52	0.8180	177.03	100	81.80	0.4621	2.5	2.45	2.74
16	238.24	0.8242	185.66	100	82.42	0.4439	2.5	2.47	2.64
17	249.76	0.8300	194.47	100	83.00	0.4268	2.5	2.49	2.54
18	261.11	0.8356	203.47	100	83.56	0.4107	2.5	2.51	2.44
19	272.31	0.8409	212.68	100	84.09	0.3954	2.5	2.52	2.35
20	283.41	0.8459	222.14	100	84.59	0.3808	2.5	2.54	2.26
21	294.46	0.8508	231.89	100	85.08	0.3669	2.5	2.55	2.18
22	305.48	0.8556	241.97	100	85.56	0.3536	2.5	2.57	2.10
23	316.54	0.8602	252.46	100	86.02	0.3407	2.5	2.58	2.02
24	327.69	0.8648	263.42	100	86.48	0.3283	2.5	2.59	1.95
25	338.99	0.8693	274.94	100	86.93	0.3162	2.5	2.61	1.88
26	350.53	0.8737	287.14	100	87.37	0.3043	2.5	2.62	1.81
27	362.35	0.8781	300.13	100	87.81	0.2926	2.5	2.63	1.74
28	374.55	0.8826	314.07	100	88.26	0.2810	2.5	2.65	1.67
29	387.21	0.8871	329.12	100	88.71	0.2695	2.5	2.66	1.60
30	400.41	0.8917	345.49	100	89.17	0.2581	2.5	2.67	1.53
31	414.26	0.8964	363.44	100	89.64	0.2466	2.5	2.69	1.46
32	428.84	0.9012	383.23	100	90.12	0.2352	2.5	2.70	1.40
33	444.27	0.9061	405.20	100	90.61	0.2236	2.5	2.72	1.33
34	460.65	0.9112	429.79	100	91.12	0.2120	2.5	2.73	1.26
35	478.09	0.9164	457.44	100	91.64	0.2003	2.5	2.75	1.19
36	496.72	0.9219	488.76	100	92.19	0.1886	2.5	2.76	1.12
37	516.67	0.9275	524.46	100	92.75	0.1768	2.5	2.78	1.05
38	538.05	0.9334	565.39	100	93.34	0.1651	2.5	2.80	0.98
39	561.02	0.9394	612.65	100	93.94	0.1533	2.5	2.82	0.91
40	585.70	0.9458	667.51	100	94.58	0.1417	2.5	2.84	0.84
			Total	**4000**	**3335.30**	**16.84**	**100**	**100**	**100**

Table H-27 Material balance for petroleum stock No. 11

Cut	*TB*, °C	*Sp.gr*	*MW*	Volume, cm^3	Weight, g	Mole, gmol	*Zf*, vol.%	*Zf*, wt.%	*Zf*, mol.%
1	66.65	0.7096	85.06	100	70.96	0.8342	2.5	2.06	4.87
2	78.70	0.7250	90.56	100	72.50	0.8006	2.5	2.10	4.68
3	90.76	0.7388	96.17	100	73.88	0.7682	2.5	2.14	4.49
4	102.79	0.7514	101.92	100	75.14	0.7372	2.5	2.18	4.31
5	114.74	0.7629	107.80	100	76.29	0.7077	2.5	2.21	4.13
6	126.58	0.7734	113.81	100	77.34	0.6796	2.5	2.24	3.97
7	138.27	0.7832	119.94	100	78.32	0.6529	2.5	2.27	3.81
8	149.79	0.7922	126.19	100	79.22	0.6277	2.5	2.30	3.67
9	161.13	0.8005	132.56	100	80.05	0.6039	2.5	2.32	3.53
10	172.27	0.8083	139.03	100	80.83	0.5814	2.5	2.34	3.40
11	183.22	0.8156	145.61	100	81.56	0.5601	2.5	2.36	3.27
12	193.97	0.8225	152.29	100	82.25	0.5401	2.5	2.38	3.15
13	204.54	0.8289	159.09	100	82.89	0.5211	2.5	2.40	3.04
14	214.94	0.8350	166.00	100	83.50	0.5030	2.5	2.42	2.94
15	225.18	0.8408	173.03	100	84.08	0.4859	2.5	2.44	2.84
16	235.31	0.8464	180.22	100	84.64	0.4696	2.5	2.45	2.74
17	245.35	0.8517	187.58	100	85.17	0.4540	2.5	2.47	2.65
18	255.35	0.8568	195.14	100	85.68	0.4391	2.5	2.48	2.56
19	265.35	0.8617	202.96	100	86.17	0.4246	2.5	2.50	2.48
20	275.41	0.8666	211.09	100	86.66	0.4105	2.5	2.51	2.40
21	285.59	0.8713	219.59	100	87.13	0.3968	2.5	2.52	2.32
22	295.96	0.8761	228.54	100	87.61	0.3833	2.5	2.54	2.24
23	306.59	0.8807	238.02	100	88.07	0.3700	2.5	2.55	2.16
24	317.56	0.8855	248.17	100	88.55	0.3568	2.5	2.57	2.08
25	328.95	0.8902	259.11	100	89.02	0.3436	2.5	2.58	2.01
26	340.87	0.8951	270.99	100	89.51	0.3303	2.5	2.59	1.93
27	353.40	0.9000	283.99	100	90.00	0.3169	2.5	2.61	1.85
28	366.66	0.9051	298.35	100	90.51	0.3034	2.5	2.62	1.77
29	380.77	0.9103	314.31	100	91.03	0.2896	2.5	2.64	1.69
30	395.82	0.9158	332.19	100	91.58	0.2757	2.5	2.65	1.61
31	411.97	0.9214	352.37	100	92.14	0.2615	2.5	2.67	1.53
32	429.32	0.9273	375.29	100	92.73	0.2471	2.5	2.69	1.44
33	448.03	0.9334	401.51	100	93.34	0.2325	2.5	2.70	1.36
34	468.23	0.9398	431.70	100	93.98	0.2177	2.5	2.72	1.27
35	490.09	0.9465	466.68	100	94.65	0.2028	2.5	2.74	1.18
36	513.75	0.9534	507.51	100	95.34	0.1879	2.5	2.76	1.10
37	539.39	0.9606	555.47	100	96.06	0.1729	2.5	2.78	1.01
38	567.16	0.9682	612.21	100	96.82	0.1581	2.5	2.81	0.92
39	597.26	0.9760	679.83	100	97.60	0.1436	2.5	2.83	0.84
40	629.86	0.9841	761.03	100	98.41	0.1293	2.5	2.85	0.76
			Total	**4000**	**3451.22**	**17.12**	**100**	**100**	**100**

Table H-28 Material balance for petroleum stock No. 12

Cut	*TB*, °C	*Sp.gr*	*MW*	Volume, cm^3	Weight, g	Mole, gmol	*Zf*, vol.%	*Zf*, wt.%	*Zf*, mol.%
1	70.32	0.7035	86.77	100	70.35	0.8108	2.5	2.06	4.97
2	82.20	0.7179	92.34	100	71.79	0.7775	2.5	2.10	4.77
3	94.32	0.7312	98.15	100	73.12	0.7450	2.5	2.14	4.57
4	106.58	0.7435	104.19	100	74.35	0.7136	2.5	2.18	4.38
5	118.95	0.7549	110.46	100	75.49	0.6834	2.5	2.21	4.19
6	131.36	0.7655	116.97	100	76.55	0.6544	2.5	2.24	4.02
7	143.76	0.7754	123.71	100	77.54	0.6268	2.5	2.27	3.85
8	156.10	0.7846	130.66	100	78.46	0.6005	2.5	2.30	3.68
9	168.36	0.7932	137.82	100	79.32	0.5756	2.5	2.32	3.53
10	180.50	0.8013	145.17	100	80.13	0.5520	2.5	2.35	3.39
11	192.49	0.8089	152.72	100	80.89	0.5297	2.5	2.37	3.25
12	204.32	0.8160	160.44	100	81.60	0.5086	2.5	2.39	3.12
13	215.97	0.8227	168.33	100	82.27	0.4888	2.5	2.41	3.00
14	227.45	0.8291	176.39	100	82.91	0.4700	2.5	2.43	2.88
15	238.74	0.8351	184.62	100	83.51	0.4523	2.5	2.45	2.78
16	249.85	0.8408	193.02	100	84.08	0.4356	2.5	2.46	2.67
17	260.80	0.8462	201.58	100	84.62	0.4198	2.5	2.48	2.58
18	271.60	0.8514	210.33	100	85.14	0.4048	2.5	2.50	2.48
19	282.28	0.8564	219.29	100	85.64	0.3905	2.5	2.51	2.40
20	292.87	0.8612	228.49	100	86.12	0.3769	2.5	2.52	2.31
21	303.40	0.8658	237.95	100	86.58	0.3639	2.5	2.54	2.23
22	313.92	0.8703	247.73	100	87.03	0.3513	2.5	2.55	2.16
23	324.48	0.8747	257.88	100	87.47	0.3392	2.5	2.56	2.08
24	335.13	0.8790	268.49	100	87.90	0.3274	2.5	2.58	2.01
25	345.93	0.8832	279.63	100	88.32	0.3159	2.5	2.59	1.94
26	356.95	0.8875	291.41	100	88.75	0.3046	2.5	2.60	1.87
27	368.27	0.8917	303.94	100	89.17	0.2934	2.5	2.61	1.80
28	379.96	0.8960	317.39	100	89.60	0.2823	2.5	2.63	1.73
29	392.11	0.9003	331.93	100	90.03	0.2712	2.5	2.64	1.66
30	404.81	0.9048	347.75	100	90.48	0.2602	2.5	2.65	1.60
31	418.16	0.9093	365.10	100	90.93	0.2491	2.5	2.67	1.53
32	432.27	0.9140	384.27	100	91.40	0.2378	2.5	2.68	1.46
33	447.24	0.9188	405.62	100	91.88	0.2265	2.5	2.69	1.39
34	463.19	0.9238	429.53	100	92.38	0.2151	2.5	2.71	1.32
35	480.25	0.9289	456.52	100	92.89	0.2035	2.5	2.72	1.25
36	498.54	0.9343	487.18	100	93.43	0.1918	2.5	2.74	1.18
37	518.20	0.9399	522.24	100	93.99	0.1800	2.5	2.76	1.10
38	539.36	0.9458	562.59	100	94.58	0.1681	2.5	2.77	1.03
39	562.18	0.9519	609.35	100	95.19	0.1562	2.5	2.79	0.96
40	586.82	0.9583	663.88	100	95.83	0.1443	2.5	2.81	0.89
			Total	**4000**	**3411.69**	**16.30**	**100**	**100**	**100**

Table H-29 Material balance for petroleum stock No. 13

Cut	*TB*, °C	*Sp.gr*	*MW*	Volume, cm^3	Weight, g	Mole, gmol	*Zf*, vol.%	*Zf*, wt.%	*Zf*, mol.%
1	37.99	0.6465	71.55	100	64.65	0.9037	2.5	2.05	4.13
2	47.44	0.6630	76.01	100	66.30	0.8722	2.5	2.10	3.99
3	56.91	0.6776	80.44	100	67.76	0.8423	2.5	2.15	3.85
4	66.37	0.6907	84.87	100	69.07	0.8138	2.5	2.19	3.72
5	75.78	0.7025	89.32	100	70.25	0.7866	2.5	2.23	3.60
6	85.12	0.7133	93.79	100	71.33	0.7606	2.5	2.26	3.48
7	94.36	0.7233	98.30	100	72.33	0.7358	2.5	2.29	3.36
8	103.47	0.7324	102.83	100	73.24	0.7122	2.5	2.32	3.26
9	112.45	0.7408	107.40	100	74.08	0.6898	2.5	2.35	3.15
10	121.27	0.7487	111.98	100	74.87	0.6685	2.5	2.37	3.06
11	129.92	0.7560	116.59	100	75.60	0.6484	2.5	2.39	2.96
12	138.38	0.7627	121.19	100	76.27	0.6294	2.5	2.42	2.88
13	146.63	0.7691	125.80	100	76.91	0.6113	2.5	2.44	2.80
14	154.68	0.7750	130.40	100	77.50	0.5943	2.5	2.46	2.72
15	162.51	0.7805	134.98	100	78.05	0.5783	2.5	2.47	2.64
16	170.12	0.7857	139.54	100	78.57	0.5631	2.5	2.49	2.57
17	177.51	0.7906	144.06	100	79.06	0.5488	2.5	2.50	2.51
18	184.68	0.7952	148.55	100	79.52	0.5353	2.5	2.52	2.45
19	191.63	0.7995	153.00	100	79.95	0.5226	2.5	2.53	2.39
20	198.36	0.8036	157.40	100	80.36	0.5106	2.5	2.55	2.33
21	204.88	0.8074	161.75	100	80.74	0.4992	2.5	2.56	2.28
22	211.20	0.8111	166.05	100	81.11	0.4884	2.5	2.57	2.23
23	217.34	0.8145	170.31	100	81.45	0.4782	2.5	2.58	2.19
24	223.30	0.8178	174.53	100	81.78	0.4686	2.5	2.59	2.14
25	229.11	0.8209	178.72	100	82.09	0.4593	2.5	2.60	2.10
26	234.77	0.8239	182.88	100	82.39	0.4505	2.5	2.61	2.06
27	240.32	0.8268	187.02	100	82.68	0.4421	2.5	2.62	2.02
28	245.77	0.8296	191.17	100	82.96	0.4339	2.5	2.63	1.98
29	251.15	0.8323	195.33	100	83.23	0.4261	2.5	2.64	1.95
30	256.48	0.8349	199.54	100	83.49	0.4184	2.5	2.64	1.91
31	261.80	0.8375	203.80	100	83.75	0.4109	2.5	2.65	1.88
32	267.15	0.8400	208.15	100	84.00	0.4036	2.5	2.66	1.85
33	272.54	0.8426	212.62	100	84.26	0.3963	2.5	2.67	1.81
34	278.02	0.8451	217.25	100	84.51	0.3890	2.5	2.68	1.78
35	283.64	0.8476	222.07	100	84.76	0.3817	2.5	2.69	1.75
36	289.42	0.8502	227.12	100	85.02	0.3744	2.5	2.69	1.71
37	295.41	0.8529	232.47	100	85.29	0.3669	2.5	2.70	1.68
38	301.67	0.8556	238.15	100	85.56	0.3593	2.5	2.71	1.64
39	308.23	0.8584	244.24	100	85.84	0.3514	2.5	2.72	1.61
40	315.15	0.8613	250.80	100	86.13	0.3434	2.5	2.73	1.57
			Total	**4000**	**3156.72**	**21.87**	**100**	**100**	**100**

Table H-30 Material balance for petroleum stock No. 14

Cut	*TB*, °C	*Sp.gr*	*MW*	Volume, cm^3	Weight, g	Mole, gmol	*Zf*, vol.%	*Zf*, wt.%	*Zf*, mol.%
1	203.20	0.7951	161.66	100	79.51	0.4918	2.5	2.37	3.35
2	202.77	0.7949	161.37	100	79.49	0.4926	2.5	2.37	3.36
3	204.31	0.7958	162.42	100	79.58	0.4899	2.5	2.37	3.34
4	207.44	0.7975	164.57	100	79.75	0.4846	2.5	2.37	3.31
5	211.82	0.8000	167.60	100	80.00	0.4773	2.5	2.38	3.26
6	217.12	0.8029	171.34	100	80.29	0.4686	2.5	2.39	3.20
7	223.06	0.8062	175.60	100	80.62	0.4591	2.5	2.40	3.13
8	229.37	0.8095	180.21	100	80.95	0.4492	2.5	2.41	3.06
9	235.82	0.8129	185.03	100	81.29	0.4393	2.5	2.42	3.00
10	242.22	0.8161	189.90	100	81.61	0.4298	2.5	2.43	2.93
11	248.39	0.8192	194.69	100	81.92	0.4208	2.5	2.44	2.87
12	254.18	0.8221	199.27	100	82.21	0.4125	2.5	2.45	2.81
13	259.49	0.8246	203.55	100	82.46	0.4051	2.5	2.45	2.76
14	264.23	0.8269	207.42	100	82.69	0.3986	2.5	2.46	2.72
15	268.34	0.8288	210.84	100	82.88	0.3931	2.5	2.47	2.68
16	271.81	0.8304	213.75	100	83.04	0.3885	2.5	2.47	2.65
17	274.63	0.8317	216.15	100	83.17	0.3848	2.5	2.48	2.62
18	276.85	0.8327	218.05	100	83.27	0.3819	2.5	2.48	2.60
19	278.52	0.8334	219.48	100	83.34	0.3797	2.5	2.48	2.59
20	279.74	0.8340	220.54	100	83.40	0.3782	2.5	2.48	2.58
21	280.63	0.8344	221.31	100	83.44	0.3770	2.5	2.48	2.57
22	281.34	0.8347	221.94	100	83.47	0.3761	2.5	2.48	2.57
23	282.06	0.8350	222.56	100	83.50	0.3752	2.5	2.49	2.56
24	283.00	0.8355	223.39	100	83.55	0.3740	2.5	2.49	2.55
25	284.40	0.8361	224.61	100	83.61	0.3722	2.5	2.49	2.54
26	286.53	0.8370	226.49	100	83.70	0.3696	2.5	2.49	2.52
27	289.68	0.8384	229.30	100	83.84	0.3656	2.5	2.50	2.49
28	294.20	0.8404	233.37	100	84.04	0.3601	2.5	2.50	2.46
29	300.43	0.8430	239.08	100	84.30	0.3526	2.5	2.51	2.41
30	308.77	0.8465	246.91	100	84.65	0.3429	2.5	2.52	2.34
31	319.62	0.8510	257.42	100	85.10	0.3306	2.5	2.53	2.25
32	333.46	0.8565	271.36	100	85.65	0.3156	2.5	2.55	2.15
33	350.74	0.8631	289.67	100	86.31	0.2980	2.5	2.57	2.03
34	371.97	0.8709	313.61	100	87.09	0.2777	2.5	2.59	1.89
35	397.70	0.8799	344.90	100	87.99	0.2551	2.5	2.62	1.74
36	428.48	0.8901	385.93	100	89.01	0.2306	2.5	2.65	1.57
37	464.91	0.9013	440.08	100	90.13	0.2048	2.5	2.68	1.40
38	507.62	0.9137	512.23	100	91.37	0.1784	2.5	2.72	1.22
39	557.25	0.9270	609.60	100	92.70	0.1521	2.5	2.76	1.04
40	614.49	0.9413	743.12	100	94.13	0.1267	2.5	2.80	0.86
			Total	**4000**	**3359.05**	**14.66**	**100**	**100**	**100**

Table H-31 Material balance for petroleum stock No. 15

Cut	*TB*, °C	*Sp.gr*	*MW*	Volume, cm^3	Weight, g	Mole, gmol	*Zf*, vol.%	*Zf*, wt.%	*Zf*, mol.%
1	39.45	0.6557	72.48	100	65.57	0.9047	2.5	1.95	5.18
2	52.16	0.6771	78.37	100	67.71	0.8640	2.5	2.01	4.94
3	64.76	0.6954	84.18	100	69.54	0.8260	2.5	2.07	4.73
4	77.23	0.7113	90.00	100	71.13	0.7903	2.5	2.11	4.52
5	89.59	0.7254	95.88	100	72.54	0.7566	2.5	2.16	4.33
6	101.86	0.7381	101.86	100	73.81	0.7246	2.5	2.19	4.15
7	114.04	0.7496	107.97	100	74.96	0.6943	2.5	2.23	3.97
8	126.14	0.7603	114.25	100	76.03	0.6655	2.5	2.26	3.81
9	138.18	0.7702	120.70	100	77.02	0.6381	2.5	2.29	3.65
10	150.17	0.7794	127.34	100	77.94	0.6120	2.5	2.32	3.50
11	162.13	0.7880	134.21	100	78.80	0.5872	2.5	2.34	3.36
12	174.06	0.7962	141.31	100	79.62	0.5634	2.5	2.37	3.22
13	185.99	0.8039	148.68	100	80.39	0.5407	2.5	2.39	3.09
14	197.94	0.8113	156.33	100	81.13	0.5190	2.5	2.41	2.97
15	209.92	0.8184	164.30	100	81.84	0.4981	2.5	2.43	2.85
16	221.96	0.8252	172.61	100	82.52	0.4781	2.5	2.45	2.74
17	234.06	0.8317	181.30	100	83.17	0.4588	2.5	2.47	2.62
18	246.27	0.8381	190.41	100	83.81	0.4401	2.5	2.49	2.52
19	258.59	0.8442	199.97	100	84.42	0.4222	2.5	2.51	2.42
20	271.05	0.8502	210.04	100	85.02	0.4048	2.5	2.53	2.32
21	283.69	0.8561	220.66	100	85.61	0.3880	2.5	2.55	2.22
22	296.51	0.8618	231.90	100	86.18	0.3716	2.5	2.56	2.13
23	309.56	0.8675	243.83	100	86.75	0.3558	2.5	2.58	2.04
24	322.86	0.8730	256.51	100	87.30	0.3404	2.5	2.60	1.95
25	336.43	0.8785	270.03	100	87.85	0.3253	2.5	2.61	1.86
26	350.32	0.8840	284.50	100	88.40	0.3107	2.5	2.63	1.78
27	364.54	0.8894	300.01	100	88.94	0.2964	2.5	2.64	1.70
28	379.13	0.8947	316.69	100	89.47	0.2825	2.5	2.66	1.62
29	394.13	0.9001	334.68	100	90.01	0.2689	2.5	2.68	1.54
30	409.57	0.9054	354.15	100	90.54	0.2557	2.5	2.69	1.46
31	425.48	0.9107	375.26	100	91.07	0.2427	2.5	2.71	1.39
32	441.91	0.9161	398.24	100	91.61	0.2300	2.5	2.72	1.32
33	458.89	0.9214	423.32	100	92.14	0.2177	2.5	2.74	1.25
34	476.45	0.9268	450.76	100	92.68	0.2056	2.5	2.76	1.18
35	494.64	0.9322	480.90	100	93.22	0.1938	2.5	2.77	1.11
36	513.50	0.9376	514.09	100	93.76	0.1824	2.5	2.79	1.04
37	533.06	0.9431	550.76	100	94.31	0.1712	2.5	2.80	0.98
38	553.38	0.9486	591.39	100	94.86	0.1604	2.5	2.82	0.92
39	574.49	0.9541	636.58	100	95.41	0.1499	2.5	2.84	0.86
40	596.45	0.9597	686.99	100	95.97	0.1397	2.5	2.85	0.80
			Total	**4000**	**3363.04**	**17.48**	**100**	**100**	**100**

Table H-32 Material balance for petroleum stock No. 16

Cut	*TB*, °C	*Sp.gr*	*MW*	Volume, cm^3	Weight, g	Mole, gmol	*Zf*, vol.%	*Zf*, wt.%	*Zf*, mol.%
1	38.57	0.5772	66.90	100	57.72	0.8628	2.5	1.72	5.62
2	57.31	0.6755	80.57	100	67.55	0.8384	2.5	2.01	5.46
3	75.47	0.7089	89.17	100	70.89	0.7950	2.5	2.11	5.18
4	93.07	0.7315	97.51	100	73.15	0.7502	2.5	2.18	4.89
5	110.10	0.7487	105.89	100	74.87	0.7071	2.5	2.23	4.61
6	126.60	0.7628	114.39	100	76.28	0.6668	2.5	2.27	4.34
7	142.57	0.7746	123.04	100	77.46	0.6296	2.5	2.31	4.10
8	158.04	0.7850	131.84	100	78.50	0.5954	2.5	2.34	3.88
9	173.03	0.7941	140.80	100	79.41	0.5640	2.5	2.37	3.67
10	187.58	0.8023	149.92	100	80.23	0.5351	2.5	2.39	3.49
11	201.70	0.8097	159.19	100	80.97	0.5087	2.5	2.41	3.31
12	215.42	0.8166	168.63	100	81.66	0.4842	2.5	2.44	3.15
13	228.80	0.8229	178.24	100	82.29	0.4617	2.5	2.45	3.01
14	241.84	0.8288	188.02	100	82.88	0.4408	2.5	2.47	2.87
15	254.61	0.8343	198.01	100	83.43	0.4213	2.5	2.49	2.74
16	267.13	0.8394	208.23	100	83.94	0.4031	2.5	2.50	2.63
17	279.46	0.8443	218.72	100	84.43	0.3860	2.5	2.52	2.51
18	291.64	0.8489	229.50	100	84.89	0.3699	2.5	2.53	2.41
19	303.72	0.8532	240.64	100	85.32	0.3546	2.5	2.54	2.31
20	315.75	0.8574	252.18	100	85.74	0.3400	2.5	2.56	2.21
21	327.79	0.8614	264.22	100	86.14	0.3260	2.5	2.57	2.12
22	339.89	0.8651	276.82	100	86.51	0.3125	2.5	2.58	2.04
23	352.12	0.8688	290.09	100	86.88	0.2995	2.5	2.59	1.95
24	364.53	0.8723	304.13	100	87.23	0.2868	2.5	2.60	1.87
25	377.20	0.8756	319.09	100	87.56	0.2744	2.5	2.61	1.79
26	390.18	0.8789	335.10	100	87.89	0.2623	2.5	2.62	1.71
27	403.55	0.8820	352.36	100	88.20	0.2503	2.5	2.63	1.63
28	417.39	0.8850	371.05	100	88.50	0.2385	2.5	2.64	1.55
29	431.76	0.8880	391.42	100	88.80	0.2269	2.5	2.65	1.48
30	446.75	0.8908	413.75	100	89.08	0.2153	2.5	2.66	1.40
31	462.43	0.8935	438.34	100	89.35	0.2038	2.5	2.66	1.33
32	478.90	0.8962	465.57	100	89.62	0.1925	2.5	2.67	1.25
33	496.23	0.8988	495.90	100	89.88	0.1812	2.5	2.68	1.18
34	514.52	0.9013	529.81	100	90.13	0.1701	2.5	2.69	1.11
35	533.85	0.9038	567.94	100	90.38	0.1591	2.5	2.70	1.04
36	554.32	0.9061	611.01	100	90.61	0.1483	2.5	2.70	0.97
37	576.02	0.9085	659.88	100	90.85	0.1377	2.5	2.71	0.90
38	599.06	0.9107	715.62	100	91.07	0.1273	2.5	2.72	0.83
39	623.54	0.9130	779.47	100	91.30	0.1171	2.5	2.72	0.76
40	649.56	0.9151	852.98	100	91.51	0.1073	2.5	2.73	0.70
			Total	**4000**	**3353.08**	**15.35**	**100**	**100**	**100**

Table H-33 Material balance for petroleum stock No. 17

Cut	*TB*, °C	*Sp.gr*	*MW*	Volume, cm^3	Weight, g	Mole, gmol	*Zf*, vol.%	*Zf*, wt.%	*Zf*, mol.%
1	176.38	0.7145	145.75	100	71.45	0.4902	2.5	1.91	4.37
2	196.98	0.8041	156.37	100	80.41	0.5142	2.5	2.16	4.59
3	216.59	0.8314	167.72	100	83.14	0.4957	2.5	2.23	4.42
4	235.18	0.8496	179.61	100	84.96	0.4730	2.5	2.28	4.22
5	252.76	0.8635	191.78	100	86.35	0.4502	2.5	2.31	4.01
6	269.30	0.8747	204.04	100	87.47	0.4287	2.5	2.34	3.82
7	284.83	0.8841	216.25	100	88.41	0.4088	2.5	2.37	3.65
8	299.37	0.8922	228.31	100	89.22	0.3908	2.5	2.39	3.48
9	312.94	0.8994	240.11	100	89.94	0.3746	2.5	2.41	3.34
10	325.56	0.9058	251.57	100	90.58	0.3601	2.5	2.43	3.21
11	337.30	0.9116	262.65	100	91.16	0.3471	2.5	2.44	3.09
12	348.19	0.9169	273.29	100	91.69	0.3355	2.5	2.46	2.99
13	358.29	0.9218	283.47	100	92.18	0.3252	2.5	2.47	2.90
14	367.67	0.9264	293.21	100	92.64	0.3159	2.5	2.48	2.82
15	376.40	0.9306	302.50	100	93.06	0.3076	2.5	2.49	2.74
16	384.57	0.9346	311.41	100	93.46	0.3001	2.5	2.50	2.68
17	392.25	0.9383	320.00	100	93.83	0.2932	2.5	2.51	2.61
18	399.57	0.9419	328.35	100	94.19	0.2869	2.5	2.52	2.56
19	406.61	0.9452	336.59	100	94.52	0.2808	2.5	2.53	2.50
20	413.49	0.9484	344.84	100	94.84	0.2750	2.5	2.54	2.45
21	420.34	0.9514	353.27	100	95.14	0.2693	2.5	2.55	2.40
22	427.28	0.9544	362.07	100	95.44	0.2636	2.5	2.56	2.35
23	434.46	0.9571	371.45	100	95.71	0.2577	2.5	2.57	2.30
24	442.03	0.9598	381.67	100	95.98	0.2515	2.5	2.57	2.24
25	450.13	0.9624	393.02	100	96.24	0.2449	2.5	2.58	2.18
26	458.92	0.9648	405.82	100	96.48	0.2377	2.5	2.59	2.12
27	468.59	0.9672	420.46	100	96.72	0.2300	2.5	2.59	2.05
28	479.31	0.9695	437.38	100	96.95	0.2217	2.5	2.60	1.98
29	491.27	0.9717	457.15	100	97.17	0.2126	2.5	2.60	1.90
30	504.65	0.9738	480.37	100	97.38	0.2027	2.5	2.61	1.81
31	519.68	0.9759	507.85	100	97.59	0.1922	2.5	2.62	1.71
32	536.55	0.9779	540.54	100	97.79	0.1809	2.5	2.62	1.61
33	555.49	0.9799	579.63	100	97.99	0.1691	2.5	2.63	1.51
34	576.72	0.9818	626.61	100	98.18	0.1567	2.5	2.63	1.40
35	600.49	0.9836	683.38	100	98.36	0.1439	2.5	2.64	1.28
36	627.02	0.9854	752.34	100	98.54	0.1310	2.5	2.64	1.17
37	656.59	0.9872	836.69	100	98.72	0.1180	2.5	2.65	1.05
38	689.45	0.9889	940.54	100	98.89	0.1051	2.5	2.65	0.94
39	725.86	0.9906	1069.36	100	99.06	0.0926	2.5	2.65	0.83
40	766.08	0.9922	1230.40	100	99.22	0.0806	2.5	2.66	0.72
			Total	**4000**	**3731.05**	**11.22**	**100**	**100**	**100**

Table H-34 Material balance for petroleum stock No. 18

Cut	*TB*, °C	*Sp.gr*	*MW*	Volume, cm^3	Weight, g	Mole, gmol	*Zf*, vol.%	*Zf*, wt.%	*Zf*, mol.%
1	72.13	0.6185	84.09	100	61.85	0.7355	2.5	1.90	4.74
2	88.40	0.6984	95.37	100	69.84	0.7324	2.5	2.14	4.72
3	103.70	0.7230	103.10	100	72.30	0.7013	2.5	2.22	4.52
4	118.10	0.7395	110.51	100	73.95	0.6692	2.5	2.27	4.31
5	131.65	0.7519	117.73	100	75.19	0.6387	2.5	2.31	4.11
6	144.40	0.7620	124.81	100	76.20	0.6105	2.5	2.34	3.93
7	156.42	0.7705	131.75	100	77.05	0.5849	2.5	2.36	3.77
8	167.77	0.7779	138.54	100	77.79	0.5615	2.5	2.39	3.62
9	178.52	0.7844	145.21	100	78.44	0.5402	2.5	2.41	3.48
10	188.71	0.7902	151.75	100	79.02	0.5207	2.5	2.42	3.35
11	198.43	0.7954	158.19	100	79.54	0.5028	2.5	2.44	3.24
12	207.73	0.8002	164.54	100	80.02	0.4863	2.5	2.46	3.13
13	216.69	0.8047	170.84	100	80.47	0.4710	2.5	2.47	3.03
14	225.37	0.8088	177.13	100	80.88	0.4566	2.5	2.48	2.94
15	233.84	0.8126	183.45	100	81.26	0.4430	2.5	2.49	2.85
16	242.17	0.8162	189.85	100	81.62	0.4299	2.5	2.50	2.77
17	250.45	0.8196	196.39	100	81.96	0.4173	2.5	2.52	2.69
18	258.75	0.8228	203.13	100	82.28	0.4051	2.5	2.53	2.61
19	267.14	0.8258	210.15	100	82.58	0.3930	2.5	2.53	2.53
20	275.69	0.8287	217.54	100	82.87	0.3810	2.5	2.54	2.45
21	284.50	0.8315	225.38	100	83.15	0.3689	2.5	2.55	2.38
22	293.64	0.8341	233.78	100	83.41	0.3568	2.5	2.56	2.30
23	303.19	0.8366	242.86	100	83.66	0.3445	2.5	2.57	2.22
24	313.24	0.8390	252.75	100	83.90	0.3320	2.5	2.57	2.14
25	323.86	0.8413	263.60	100	84.13	0.3192	2.5	2.58	2.06
26	335.17	0.8436	275.58	100	84.36	0.3061	2.5	2.59	1.97
27	347.22	0.8457	288.90	100	84.57	0.2927	2.5	2.60	1.89
28	360.13	0.8478	303.76	100	84.78	0.2791	2.5	2.60	1.80
29	373.97	0.8498	320.46	100	84.98	0.2652	2.5	2.61	1.71
30	388.85	0.8517	339.26	100	85.17	0.2511	2.5	2.61	1.62
31	404.85	0.8536	360.55	100	85.36	0.2368	2.5	2.62	1.52
32	422.07	0.8554	384.73	100	85.54	0.2223	2.5	2.63	1.43
33	440.61	0.8572	412.32	100	85.72	0.2079	2.5	2.63	1.34
34	460.56	0.8589	443.90	100	85.89	0.1935	2.5	2.64	1.25
35	482.03	0.8606	480.20	100	86.06	0.1792	2.5	2.64	1.15
36	505.12	0.8622	522.06	100	86.22	0.1652	2.5	2.65	1.06
37	529.92	0.8638	570.51	100	86.38	0.1514	2.5	2.65	0.98
38	556.55	0.8654	626.85	100	86.54	0.1381	2.5	2.66	0.89
39	585.11	0.8669	692.63	100	86.69	0.1252	2.5	2.66	0.81
40	615.70	0.8684	769.75	100	86.84	0.1128	2.5	2.66	0.73
			Total	**4000**	**3258.49**	**15.53**	**100**	**100**	**100**

Table H-35 Physical properties for Basrah crude oil

Cut	TB, °C	$Sp.gr$	MW	Tc, °C	Pc, kPa	ω	$V^{L(15)}$, cm^3/mol	$\delta^{(25)}$, J/cm^3
1	31.18	0.5541	61.82	171.09	2479.58	0.2930	111.57	28.04
2	53.19	0.6667	78.56	220.68	3265.90	0.2531	117.83	28.65
3	73.96	0.7074	88.46	250.40	3268.76	0.2656	125.05	28.94
4	93.56	0.7352	97.68	275.82	3168.77	0.2835	132.86	29.08
5	112.06	0.7565	106.64	298.54	3040.78	0.3030	140.95	29.12
6	129.52	0.7740	115.45	319.22	2909.34	0.3227	149.16	29.10
7	146.01	0.7888	124.15	338.24	2783.46	0.3423	157.39	29.04
8	161.61	0.8018	132.76	355.85	2666.35	0.3614	165.58	28.96
9	176.40	0.8132	141.28	372.25	2558.74	0.3800	173.72	28.87
10	190.45	0.8236	149.70	387.60	2460.48	0.3980	181.77	28.76
11	203.82	0.8330	158.06	402.05	2370.67	0.4155	189.75	28.64
12	216.63	0.8416	166.37	415.71	2288.23	0.4324	197.67	28.52
13	228.93	0.8496	174.66	428.71	2212.19	0.4490	205.57	28.39
14	240.82	0.8571	182.98	441.14	2141.52	0.4653	213.49	28.26
15	252.39	0.8641	191.37	453.11	2075.17	0.4814	221.48	28.12
16	263.73	0.8706	199.91	464.72	2012.25	0.4975	229.62	27.98
17	274.93	0.8768	208.66	476.06	1951.93	0.5137	237.97	27.83
18	286.08	0.8827	217.71	487.23	1893.44	0.5302	246.65	27.67
19	297.28	0.8883	227.17	498.30	1836.08	0.5472	255.74	27.50
20	308.63	0.8936	237.15	509.37	1779.17	0.5649	265.40	27.32
21	320.24	0.8987	247.80	520.52	1722.22	0.5835	275.74	27.12
22	332.20	0.9035	259.26	531.84	1664.71	0.6034	286.94	26.91
23	344.62	0.9082	271.72	529.19	1642.65	0.7751	299.18	26.67
24	357.61	0.9127	285.38	540.29	1574.43	0.8067	312.68	26.42
25	371.29	0.9170	300.49	551.77	1504.03	0.8411	327.68	26.14
26	385.75	0.9212	317.32	563.68	1431.38	0.8786	344.47	25.83
27	401.13	0.9252	336.22	576.11	1356.37	0.9196	363.40	25.50
28	417.52	0.9291	357.56	589.12	1279.12	0.9609	384.84	25.13
29	435.06	0.9329	381.81	602.79	1199.77	1.0063	409.28	24.74
30	453.87	0.9365	409.55	617.19	1118.56	1.0550	437.30	24.31
31	474.06	0.9401	441.41	632.38	1035.94	1.1073	469.54	23.84
32	495.77	0.9435	478.22	648.43	952.36	1.1632	506.84	23.34
33	519.12	0.9469	520.97	665.41	868.39	1.2230	550.19	22.80
34	544.25	0.9501	570.88	683.39	784.70	1.2869	600.84	22.22
35	571.28	0.9533	629.46	702.42	702.01	1.3549	660.28	21.61
36	600.35	0.9564	698.59	722.58	621.10	1.4272	730.43	20.95
37	631.60	0.9594	780.63	743.93	542.76	1.5037	813.63	20.27
38	665.15	0.9624	878.50	766.53	467.85	1.5844	912.84	19.55
39	701.17	0.9653	996.07	790.47	397.09	1.6695	1031.93	18.79
40	739.79	0.9681	1138.15	815.80	331.24	1.7586	1175.69	18.01

Table H-36 Physical properties for Jambur crude oil

Cut	*TB*, °C	*Sp.gr*	*MW*	*Tc*, °C	*Pc*, kPa	ω	$V^{L(15)}$, cm^3/mol	$\delta^{(25)}$, J/cm^3
1	33.56	0.5143	57.41	161.70	2029.57	0.3384	111.64	28.11
2	54.63	0.6262	77.26	212.19	2820.25	0.2841	123.37	28.04
3	74.72	0.6677	88.16	241.62	2873.08	0.2936	132.03	28.18
4	93.86	0.6962	98.05	266.69	2812.29	0.3103	140.83	28.23
5	112.10	0.7181	107.58	289.14	2714.04	0.3294	149.80	28.22
6	129.48	0.7361	116.95	309.66	2604.74	0.3494	158.88	28.17
7	146.05	0.7514	126.24	328.63	2495.48	0.3697	168.00	28.09
8	161.86	0.7648	135.48	346.30	2390.83	0.3898	177.15	27.99
9	176.96	0.7767	144.68	362.83	2292.70	0.4097	186.28	27.88
10	191.40	0.7874	153.84	378.39	2201.57	0.4293	195.39	27.75
11	205.24	0.7971	162.98	393.07	2117.40	0.4485	204.47	27.62
12	218.54	0.8061	172.12	407.00	2039.63	0.4673	213.53	27.49
13	231.35	0.8144	181.26	420.26	1967.59	0.4858	222.58	27.35
14	243.74	0.8221	190.44	432.93	1900.67	0.5040	231.64	27.21
15	255.76	0.8294	199.68	445.11	1838.15	0.5220	240.76	27.06
16	267.50	0.8362	209.03	456.87	1779.29	0.5399	249.98	26.91
17	279.01	0.8427	218.54	468.28	1723.53	0.5579	259.35	26.76
18	290.35	0.8488	228.27	479.42	1670.27	0.5760	268.93	26.60
19	301.62	0.8546	238.28	490.34	1618.92	0.5944	278.82	26.44
20	312.87	0.8601	248.67	501.13	1569.00	0.6132	289.10	26.27
21	324.18	0.8655	259.51	511.84	1520.09	0.6327	299.86	26.10
22	335.65	0.8705	270.93	522.54	1471.69	0.6530	311.23	25.91
23	347.33	0.8754	283.06	519.32	1442.58	0.8317	323.34	25.71
24	359.32	0.8801	296.02	529.61	1388.19	0.8617	336.35	25.50
25	371.70	0.8846	310.00	540.07	1332.94	0.8936	350.43	25.27
26	384.56	0.8890	325.18	550.75	1276.64	0.9275	365.79	25.03
27	397.97	0.8932	341.77	561.73	1219.18	0.9604	382.64	24.77
28	412.05	0.8973	360.04	573.05	1160.40	0.9964	401.26	24.49
29	426.87	0.9012	380.29	584.79	1100.26	1.0344	421.97	24.18
30	442.54	0.9050	402.85	596.99	1038.84	1.0746	445.11	23.86
31	459.14	0.9088	428.12	609.71	976.21	1.1172	471.11	23.51
32	476.79	0.9124	456.62	623.02	912.50	1.1624	500.47	23.13
33	495.58	0.9159	488.88	636.97	848.02	1.2105	533.77	22.73
34	515.61	0.9193	525.59	651.61	783.03	1.2615	571.72	22.30
35	536.98	0.9226	567.57	667.01	717.90	1.3156	615.16	21.84
36	559.81	0.9259	615.81	683.21	653.03	1.3730	665.11	21.35
37	584.21	0.9290	671.51	700.28	588.90	1.4338	722.80	20.83
38	610.28	0.9321	736.14	718.27	526.00	1.4980	789.73	20.28
39	638.15	0.9352	811.48	737.25	464.87	1.5657	867.75	19.70
40	667.91	0.9381	899.78	757.26	406.05	1.6369	959.14	19.09

Table H-37 Physical properties for Bai – Hassan crude oil

Cut	TB, °C	$Sp.gr$	MW	Tc, °C	Pc, kPa	ω	$V^{L(15)}$, cm^3/mol	$\delta^{(25)}$, J/cm^3
1	35.84	0.5041	56.58	160.58	1898.18	0.3559	112.23	28.15
2	50.58	0.6256	75.55	208.20	2887.76	0.2764	120.76	28.12
3	64.69	0.6723	83.75	233.18	3099.44	0.2711	124.57	28.48
4	78.21	0.7046	90.47	253.87	3161.96	0.2751	128.41	28.78
5	91.19	0.7296	96.60	272.24	3159.88	0.2828	132.41	29.01
6	103.70	0.7501	102.45	289.06	3125.53	0.2922	136.57	29.18
7	115.80	0.7677	108.14	304.74	3074.01	0.3025	140.87	29.31
8	127.54	0.7830	113.76	319.52	3013.39	0.3134	145.29	29.40
9	138.99	0.7967	119.37	333.60	2947.76	0.3247	149.83	29.46
10	150.20	0.8090	125.01	347.10	2879.52	0.3362	154.52	29.50
11	161.24	0.8202	130.73	360.16	2809.83	0.3480	159.38	29.52
12	172.18	0.8306	136.58	372.87	2739.33	0.3602	164.44	29.51
13	183.07	0.8402	142.61	385.33	2668.37	0.3726	169.73	29.48
14	193.99	0.8492	148.89	397.61	2596.80	0.3855	175.32	29.43
15	205.02	0.8576	155.46	409.81	2524.62	0.3989	181.26	29.36
16	216.20	0.8656	162.40	421.99	2451.65	0.4129	187.62	29.27
17	227.62	0.8731	169.78	434.23	2377.66	0.4276	194.47	29.16
18	239.35	0.8802	177.71	446.59	2302.51	0.4432	201.90	29.02
19	251.47	0.8870	186.27	459.15	2225.95	0.4597	210.01	28.86
20	264.03	0.8934	195.58	471.96	2147.97	0.4775	218.91	28.67
21	277.14	0.8996	205.78	485.08	2068.39	0.4966	228.74	28.46
22	290.85	0.9056	217.01	498.58	1987.27	0.5172	239.64	28.22
23	305.25	0.9113	229.44	512.49	1904.60	0.5397	251.79	27.96
24	320.43	0.9167	243.29	526.89	1820.43	0.5642	265.39	27.66
25	336.44	0.9220	258.78	541.81	1735.00	0.5910	280.66	27.33
26	353.39	0.9271	276.19	542.47	1684.67	0.7724	297.90	26.96
27	371.36	0.9321	295.85	557.38	1583.91	0.8175	317.41	26.56
28	390.42	0.9368	318.14	572.90	1481.83	0.8670	339.58	26.13
29	410.67	0.9415	343.53	589.06	1378.90	0.9214	364.88	25.66
30	432.19	0.9460	372.56	605.91	1275.67	0.9760	393.84	25.16
31	455.07	0.9503	405.91	623.50	1172.72	1.0351	427.12	24.62
32	479.41	0.9546	444.38	641.87	1070.69	1.0975	465.52	24.05
33	505.28	0.9587	488.94	661.06	970.22	1.1634	510.01	23.44
34	532.79	0.9627	540.80	681.12	872.02	1.2328	561.75	22.80
35	562.03	0.9666	601.43	702.09	776.76	1.3057	622.19	22.12
36	593.09	0.9705	672.65	724.02	685.13	1.3820	693.13	21.41
37	626.07	0.9742	756.73	746.96	597.80	1.4618	776.79	20.67
38	661.07	0.9778	856.50	770.94	515.37	1.5449	875.92	19.91
39	698.18	0.9814	975.50	796.03	438.45	1.6312	994.02	19.12
40	737.50	0.9849	1118.26	822.26	367.52	1.7206	1135.45	18.31

Table H-38 Material balance for Basrah crude oil

Cut	*TB*, °C	*Sp.gr*	*MW*	Volume, cm^3	Weight, g	Mole, gmol	*Zf*, vol.%	*Zf*, wt.%	*Zf*, mol.%
1	31.18	0.5541	61.82	100	55.41	0.8963	2.5	1.59	5.62
2	53.19	0.6667	78.56	100	66.67	0.8487	2.5	1.92	5.32
3	73.96	0.7074	88.46	100	70.74	0.7997	2.5	2.03	5.02
4	93.56	0.7352	97.68	100	73.52	0.7527	2.5	2.11	4.72
5	112.06	0.7565	106.64	100	75.65	0.7095	2.5	2.17	4.45
6	129.52	0.7740	115.45	100	77.40	0.6704	2.5	2.22	4.21
7	146.01	0.7888	124.15	100	78.88	0.6354	2.5	2.27	3.99
8	161.61	0.8018	132.76	100	80.18	0.6039	2.5	2.30	3.79
9	176.40	0.8132	141.28	100	81.32	0.5756	2.5	2.34	3.61
10	190.45	0.8236	149.70	100	82.36	0.5501	2.5	2.37	3.45
11	203.82	0.8330	158.06	100	83.30	0.5270	2.5	2.39	3.31
12	216.63	0.8416	166.37	100	84.16	0.5059	2.5	2.42	3.17
13	228.93	0.8496	174.66	100	84.96	0.4864	2.5	2.44	3.05
14	240.82	0.8571	182.98	100	85.71	0.4684	2.5	2.46	2.94
15	252.39	0.8641	191.37	100	86.41	0.4515	2.5	2.48	2.83
16	263.73	0.8706	199.91	100	87.06	0.4355	2.5	2.50	2.73
17	274.93	0.8768	208.66	100	87.68	0.4202	2.5	2.52	2.64
18	286.08	0.8827	217.71	100	88.27	0.4054	2.5	2.54	2.54
19	297.28	0.8883	227.17	100	88.83	0.3910	2.5	2.55	2.45
20	308.63	0.8936	237.15	100	89.36	0.3768	2.5	2.57	2.36
21	320.24	0.8987	247.80	100	89.87	0.3627	2.5	2.58	2.28
22	332.20	0.9035	259.26	100	90.35	0.3485	2.5	2.60	2.19
23	344.62	0.9082	271.72	100	90.82	0.3342	2.5	2.61	2.10
24	357.61	0.9127	285.38	100	91.27	0.3198	2.5	2.62	2.01
25	371.29	0.9170	300.49	100	91.70	0.3052	2.5	2.63	1.91
26	385.75	0.9212	317.32	100	92.12	0.2903	2.5	2.65	1.82
27	401.13	0.9252	336.22	100	92.52	0.2752	2.5	2.66	1.73
28	417.52	0.9291	357.56	100	92.91	0.2598	2.5	2.67	1.63
29	435.06	0.9329	381.81	100	93.29	0.2443	2.5	2.68	1.53
30	453.87	0.9365	409.55	100	93.65	0.2287	2.5	2.69	1.43
31	474.06	0.9401	441.41	100	94.01	0.2130	2.5	2.70	1.34
32	495.77	0.9435	478.22	100	94.35	0.1973	2.5	2.71	1.24
33	519.12	0.9469	520.97	100	94.69	0.1818	2.5	2.72	1.14
34	544.25	0.9501	570.88	100	95.01	0.1664	2.5	2.73	1.04
35	571.28	0.9533	629.46	100	95.33	0.1514	2.5	2.74	0.95
36	600.35	0.9564	698.59	100	95.64	0.1369	2.5	2.75	0.86
37	631.60	0.9594	780.63	100	95.94	0.1229	2.5	2.76	0.77
38	665.15	0.9624	878.50	100	96.24	0.1095	2.5	2.76	0.69
39	701.17	0.9653	996.07	100	96.53	0.0969	2.5	2.77	0.61
40	739.79	0.9681	1138.15	100	96.81	0.0851	2.5	2.78	0.53
			Total	**4000**	**3480.94**	**15.94**	**100**	**100**	**100**

Table H-39 Material balance for Jambur crude oil

Cut	*TB*, °C	*Sp.gr*	*MW*	Volume, cm^3	Weight, g	Mole, gmol	*Zf*, vol.%	*Zf*, wt.%	*Zf*, mol.%
1	33.56	0.5143	57.41	100	51.43	0.8958	2.5	1.54	5.91
2	54.63	0.6262	77.26	100	62.62	0.8106	2.5	1.87	5.35
3	74.72	0.6677	88.16	100	66.77	0.7574	2.5	2.00	5.00
4	93.86	0.6962	98.05	100	69.62	0.7101	2.5	2.08	4.68
5	112.10	0.7181	107.58	100	71.81	0.6676	2.5	2.15	4.40
6	129.48	0.7361	116.95	100	73.61	0.6294	2.5	2.20	4.15
7	146.05	0.7514	126.24	100	75.14	0.5952	2.5	2.25	3.93
8	161.86	0.7648	135.48	100	76.48	0.5645	2.5	2.29	3.72
9	176.96	0.7767	144.68	100	77.67	0.5368	2.5	2.32	3.54
10	191.40	0.7874	153.84	100	78.74	0.5118	2.5	2.35	3.38
11	205.24	0.7971	162.98	100	79.71	0.4891	2.5	2.38	3.23
12	218.54	0.8061	172.12	100	80.61	0.4683	2.5	2.41	3.09
13	231.35	0.8144	181.26	100	81.44	0.4493	2.5	2.43	2.96
14	243.74	0.8221	190.44	100	82.21	0.4317	2.5	2.46	2.85
15	255.76	0.8294	199.68	100	82.94	0.4154	2.5	2.48	2.74
16	267.50	0.8362	209.03	100	83.62	0.4000	2.5	2.50	2.64
17	279.01	0.8427	218.54	100	84.27	0.3856	2.5	2.52	2.54
18	290.35	0.8488	228.27	100	84.88	0.3718	2.5	2.54	2.45
19	301.62	0.8546	238.28	100	85.46	0.3587	2.5	2.55	2.37
20	312.87	0.8601	248.67	100	86.01	0.3459	2.5	2.57	2.28
21	324.18	0.8655	259.51	100	86.55	0.3335	2.5	2.59	2.20
22	335.65	0.8705	270.93	100	87.05	0.3213	2.5	2.60	2.12
23	347.33	0.8754	283.06	100	87.54	0.3093	2.5	2.62	2.04
24	359.32	0.8801	296.02	100	88.01	0.2973	2.5	2.63	1.96
25	371.70	0.8846	310.00	100	88.46	0.2854	2.5	2.64	1.88
26	384.56	0.8890	325.18	100	88.90	0.2734	2.5	2.66	1.80
27	397.97	0.8932	341.77	100	89.32	0.2613	2.5	2.67	1.72
28	412.05	0.8973	360.04	100	89.73	0.2492	2.5	2.68	1.64
29	426.87	0.9012	380.29	100	90.12	0.2370	2.5	2.69	1.56
30	442.54	0.9050	402.85	100	90.50	0.2247	2.5	2.71	1.48
31	459.14	0.9088	428.12	100	90.88	0.2123	2.5	2.72	1.40
32	476.79	0.9124	456.62	100	91.24	0.1998	2.5	2.73	1.32
33	495.58	0.9159	488.88	100	91.59	0.1873	2.5	2.74	1.24
34	515.61	0.9193	525.59	100	91.93	0.1749	2.5	2.75	1.15
35	536.98	0.9226	567.57	100	92.26	0.1626	2.5	2.76	1.07
36	559.81	0.9259	615.81	100	92.59	0.1504	2.5	2.77	0.99
37	584.21	0.9290	671.51	100	92.90	0.1384	2.5	2.78	0.91
38	610.28	0.9321	736.14	100	93.21	0.1266	2.5	2.79	0.84
39	638.15	0.9352	811.48	100	93.52	0.1152	2.5	2.80	0.76
40	667.91	0.9381	899.78	100	93.81	0.1043	2.5	2.80	0.69
			Total	**4000**	**3345.15**	**15.16**	**100**	**100**	**100**

Table H-40 Material balance for Bai – Hassan crude oil

Cut	*TB*, °C	*Sp.gr*	*MW*	Volume, cm^3	Weight, g	Mole, gmol	*Zf*, vol.%	*Zf*, wt.%	*Zf*, mol.%
1	35.84	0.5041	56.58	100	50.41	0.8910	2.5	1.45	4.97
2	50.58	0.6256	75.55	100	62.56	0.8281	2.5	1.81	4.62
3	64.69	0.6723	83.75	100	67.23	0.8028	2.5	1.94	4.47
4	78.21	0.7046	90.47	100	70.46	0.7788	2.5	2.03	4.34
5	91.19	0.7296	96.60	100	72.96	0.7552	2.5	2.10	4.21
6	103.70	0.7501	102.45	100	75.01	0.7322	2.5	2.16	4.08
7	115.80	0.7677	108.14	100	76.77	0.7099	2.5	2.21	3.96
8	127.54	0.7830	113.76	100	78.30	0.6883	2.5	2.26	3.84
9	138.99	0.7967	119.37	100	79.67	0.6674	2.5	2.30	3.72
10	150.20	0.8090	125.01	100	80.90	0.6472	2.5	2.33	3.61
11	161.24	0.8202	130.73	100	82.02	0.6274	2.5	2.37	3.50
12	172.18	0.8306	136.58	100	83.06	0.6081	2.5	2.40	3.39
13	183.07	0.8402	142.61	100	84.02	0.5892	2.5	2.42	3.28
14	193.99	0.8492	148.89	100	84.92	0.5704	2.5	2.45	3.18
15	205.02	0.8576	155.46	100	85.76	0.5517	2.5	2.47	3.08
16	216.20	0.8656	162.40	100	86.56	0.5330	2.5	2.50	2.97
17	227.62	0.8731	169.78	100	87.31	0.5142	2.5	2.52	2.87
18	239.35	0.8802	177.71	100	88.02	0.4953	2.5	2.54	2.76
19	251.47	0.8870	186.27	100	88.70	0.4762	2.5	2.56	2.65
20	264.03	0.8934	195.58	100	89.34	0.4568	2.5	2.58	2.55
21	277.14	0.8996	205.78	100	89.96	0.4372	2.5	2.60	2.44
22	290.85	0.9056	217.01	100	90.56	0.4173	2.5	2.61	2.33
23	305.25	0.9113	229.44	100	91.13	0.3972	2.5	2.63	2.21
24	320.43	0.9167	243.29	100	91.67	0.3768	2.5	2.64	2.10
25	336.44	0.9220	258.78	100	92.20	0.3563	2.5	2.66	1.99
26	353.39	0.9271	276.19	100	92.71	0.3357	2.5	2.67	1.87
27	371.36	0.9321	295.85	100	93.21	0.3151	2.5	2.69	1.76
28	390.42	0.9368	318.14	100	93.68	0.2945	2.5	2.70	1.64
29	410.67	0.9415	343.53	100	94.15	0.2741	2.5	2.72	1.53
30	432.19	0.9460	372.56	100	94.60	0.2539	2.5	2.73	1.42
31	455.07	0.9503	405.91	100	95.03	0.2341	2.5	2.74	1.30
32	479.41	0.9546	444.38	100	95.46	0.2148	2.5	2.75	1.20
33	505.28	0.9587	488.94	100	95.87	0.1961	2.5	2.77	1.09
34	532.79	0.9627	540.80	100	96.27	0.1780	2.5	2.78	0.99
35	562.03	0.9666	601.43	100	96.66	0.1607	2.5	2.79	0.90
36	593.09	0.9705	672.65	100	97.05	0.1443	2.5	2.80	0.80
37	626.07	0.9742	756.73	100	97.42	0.1287	2.5	2.81	0.72
38	661.07	0.9778	856.50	100	97.78	0.1142	2.5	2.82	0.64
39	698.18	0.9814	975.50	100	98.14	0.1006	2.5	2.83	0.56
40	737.50	0.9849	1118.26	100	98.49	0.0881	2.5	2.84	0.49
			Total	**4000**	**3466.01**	**17.94**	**100**	**100**	**100**

Appendix I

Predicted flash volumes and error analysis for part one of present work

Table I-1 Predicted flash volumes for 106 flash data points
(18 petroleum stocks) using unmodified models mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	Predicted flash volumes, vol.%					
				SRK	SRK + Van	PR	PR + Van	Ideal *K*	RD graph
1 API=32.4	5	251	121.7	0	0	0	0	0	8.55
	10	290	143.3	2.91	2.79	2.93	2.71	2.85	10.76
	20	364	184.4	17.62	17.37	17.54	17.3	17.43	20.57
	50	565	296.1	49.79	46.51	52.72	46.47	52.16	53.2
	70	698	370.0	70.39	67.35	73.06	67.34	73.94	64.49
2 API=36.5	5	260	126.7	0	0	0	0	0	7.86
	10	282	138.9	3.96	3.87	3.77	3.94	3.93	9.16
	20	330	165.6	20.95	20.71	20.85	20.63	20.73	16.51
	50	467	241.7	55.49	56	56.17	55.96	55.93	46.96
	70	556	291.1	68.2	68.59	72.18	68.56	71.75	66.38
3 API=27.2	5	290	143.3	0	0	0	0	0	6.3
	10	334	167.8	6.48	6.39	6.61	6.31	6.45	10.38
	20	417	213.9	17.98	17.73	17.99	18.23	17.79	22.36
	50	648	342.2	48.77	43.87	51.98	43.83	50.94	53.71
	70	795	423.9	70.48	66.36	75.44	66.35	73.88	64.8
4 API=37.3	5	285	140.6	3.87	3.75	3.93	3.66	3.83	0.62
	10	308	153.3	8.93	8.79	8.98	8.71	8.86	6.72
	20	353	178.3	18.81	18.58	18.79	18.5	18.63	19.94
	50	499	259.4	46.25	45.44	48.6	46.39	48.2	53.71
	70	630	332.2	67.61	65.33	71.36	65.31	70.55	67.72
5 API=34.9	5	379	192.8	4.01	3.95	4.14	3.84	4.05	0
	10	421	216.1	10.01	9.97	10.21	9.87	10.06	4.22
	20	456	235.6	19.79	19.69	20.02	19.59	19.72	26.63
	50	563	295.0	47.09	47.29	49.72	47.72	48.88	50.75
	70	635	335.0	61.52	61.56	65.41	65.41	64.29	71.75
6 API=40.9	5	260	126.7	0	0	0	0	0	3.62
	10	278	136.7	5.79	5.65	5.75	5.55	5.73	6.37
	20	313	156.1	17.42	17.2	17.36	17.12	17.27	18.62
	50	404	206.7	43.2	44.87	45.02	44.81	44.83	58.19
	70	462	238.9	58.6	60.35	61.58	60.31	61.34	80.48

Continue, **Table I-1** Predicted flash volumes for 106 flash data points (18 petroleum stocks) using unmodified models mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	Predicted flash volumes, vol.%					
				SRK	SRK + Van	PR	PR + Van	Ideal *K*	RD graph
7 API=40.8	5	250	121.1	0	0	0	0	0	3.47
	10	269	131.7	5.78	5.66	5.82	5.56	5.74	7.68
	20	307	152.8	17.2	17	17.2	16.92	17.04	19.23
	50	442	227.8	47.04	47.79	49.29	47.74	49.05	58.52
	70	544	284.4	63.34	62.97	67.13	62.94	67.7	82.25
8 API=37.1	5	265	129.4	3.79	3.67	3.85	3.58	3.73	0
	10	296	146.7	11.21	11.07	11.26	10.99	11.12	3.35
	20	357	180.6	24.1	23.7	23.91	23.63	23.74	13.37
	50	541	282.8	52.42	49.24	55.47	49.2	55.04	48.5
	70	665	351.7	70.44	67.17	75.15	67.16	74.19	71.6
9 API=28.2	5	450	232.2	0	0	0	0	0	0
	10	460	237.8	2.67	2.57	2.7	2.44	2.71	11.61
	20	483	250.6	9.36	9.34	9.53	9.22	9.44	38.54
	50	558	292.2	40.03	40.82	40.96	40.8	40.72	49.4
	70	599	315.0	56.7	59.11	59.65	59.05	59	72.66
10 API=38.2	5	247	119.4	2.52	2.31	2.52	2.22	2.9	4.29
	10	275	135.0	7.84	7.84	8.05	7.76	7.91	8.31
	20	351	177.2	21.9	21.9	22.12	21.63	22	18.34
	50	536	280.0	47.79	47.9	54.66	47.75	54.25	50.34
	70	653	345.0	67.35	67.35	75.34	67.33	74.3	66.19
11 API=32.5	5	299	148.3	3.99	3.86	4	3.77	3.93	1.83
	10	326	163.3	10.82	10.69	10.84	10.6	10.76	5.52
	20	382	194.4	24.62	24.26	24.43	24.91	24.28	15.51
	50	533	278.3	52.44	51.42	55.3	51.38	54.93	48.46
	70	627	330.6	67.04	65.4	71.29	65.38	70.57	68.66
12 API=34.4	10	322	161.1	7.5	7.38	7.51	7.29	7.3	7.67
	20	378	192.2	20.06	19.8	19.69	19.72	19.84	18.27
	50	548	286.7	50.32	48.77	53.19	48.72	52.71	51.28
	70	665	351.7	70.62	68.01	75.14	67.99	74.3	66.11
13 API=47.8	10	214	101.1	0	0	0	0	0	12.81
	20	262	127.8	13.32	12.97	13.19	12.87	13.09	21.51
	25	285	140.6	21.32	20.87	21.1	20.77	20.97	26.89
	30	295	146.1	24.95	24.42	24.67	24.34	24.53	33.14
	35	312	155.6	31.5	30.78	31.05	30.69	30.69	39.69
	50	352	177.8	41.87	43.33	43.61	43.27	43.27	59.54
	70	399	203.9	60.85	62.03	63.96	61.99	61.99	75.3
14 API=37.0	10	475	246.1	0	0	0	0	0	5.79
	30	501	260.6	26.81	27.02	27.06	26.86	26.74	48.48
	50	516	268.9	44.89	44.4	44.57	44.39	44.51	49.97
	70	532	277.8	50.75	52.73	52.94	52.64	52.36	59.82

Continue, **Table I-1** Predicted flash volumes for 106 flash data points (18 petroleum stocks) using unmodified models mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	Predicted flash volumes, vol.%					
				SRK	SRK + Van	PR	PR + Van	Ideal *K*	RD graph
15 API=38.6	0.00001	200	93.3	0	0	0	0	0	2.11
	10	273	133.9	10.38	10.18	10.4	10.1	10.24	7.54
	30	392	200.0	32.59	33.09	33.21	33.06	33.1	27.44
	50	506	263.3	49.37	47.19	52.04	47.06	51.76	51.81
	66.6	600	315.6	62.32	59	66.38	58.97	65.74	65.93
	70	659	348.3	67.57	64.76	72.19	64.74	71.29	68.46
16 API=37.3	10	283	139.4	6.74	6.29	6.85	6.2	6.38	9.25
	15	317	158.3	11.9	11.51	12.03	11.48	11.59	15.65
	20	350	176.7	17.01	16.59	17.1	16.51	16.66	21.83
	25	383	195.0	22.33	19.21	22.33	19.15	21.91	28.16
	30	425	218.3	29.58	26.67	29.36	26.62	28.89	34.77
	35	458	236.7	31.86	30.64	33.28	30.58	32.85	40.45
	40	484	251.1	35.76	33.5	37.5	33.45	37.01	46.59
	50	566	296.7	48.18	43.48	51.16	43.44	50.34	53.76
	60	617	325.0	55.88	51.89	59.72	51.86	58.6	64.62
	70	700	371.1	68.02	64.09	73	64.07	71.57	70.97
17 API=20.2	10	583	306.1	8.31	7.57	8.39	7.42	7.73	0
	15	600	315.6	11.69	11.01	11.88	10.86	11.2	9.7
	20	625	329.4	17.13	16.45	17.5	16.32	16.58	18.73
	25	642	338.9	21.28	20.52	21.77	20.39	20.62	27.39
	30	667	352.8	28.21	23.93	28.9	23.81	27.35	37.22
	35	700	371.1	37.01	34.86	37.52	34.73	36.57	42.92
	40	733	389.4	43.28	39.54	46.49	39.45	44.12	49.57
	50	758	403.3	50.18	47.71	54.03	47.64	51.37	57.88
	60	808	431.1	62.43	60.81	67.22	60.76	64.42	70.27
	70	866	463.3	73.17	72.06	78.51	72.03	75.93	83.38
18 API=42.2	10	300	148.9	0	0	0	0	0	13.22
	15	325	162.8	4.16	3.71	4.28	3.59	3.82	20.01
	20	350	176.7	10.2	9.8	10.4	9.69	9.89	25.52
	25	371	188.3	15.53	15.12	15.76	15.02	15.19	30.78
	30	400	204.4	23.45	22.91	23.64	22.82	22.94	37.81
	35	417	213.9	28.42	27.71	28.56	27.66	27.74	40.33
	40	442	227.8	34.94	32.61	34.88	32.54	34.45	44.59
	50	500	260.0	45.73	45.84	48.32	45.78	47.32	52.42
	60	533	278.3	52.67	52.32	55.91	52.27	54.79	60.65
	70	583	306.1	61.82	60.91	65.94	60.88	64.64	74.09

Table I-2 *ADD%* values for 106 flash data points
(18 petroleum stocks) using unmodified models mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	*AAD%*					
				SRK	SRK + Van	PR	PR + Van	Ideal *K*	RD graph
1 API=32.4	5	251	121.7	100.00	100.00	100.00	100.00	100.00	71.00
	10	290	143.3	70.90	72.10	70.70	72.90	71.50	7.60
	20	364	184.4	11.90	13.15	12.30	13.50	12.85	2.85
	50	565	296.1	0.42	6.98	5.44	7.06	4.32	6.40
	70	698	370.0	0.56	3.79	4.37	3.80	5.63	7.87
2 API=36.5	5	260	126.7	100.00	100.00	100.00	100.00	100.00	57.20
	10	282	138.9	60.40	61.30	62.30	60.60	60.70	8.40
	20	330	165.6	4.75	3.55	4.25	3.15	3.65	17.45
	50	467	241.7	10.98	12.00	12.34	11.92	11.86	6.08
	70	556	291.1	2.57	2.01	3.11	2.06	2.50	5.17
3 API=27.2	5	290	143.3	100.00	100.00	100.00	100.00	100.00	26.00
	10	334	167.8	35.20	36.10	33.90	36.90	35.50	3.80
	20	417	213.9	10.10	11.35	10.05	8.85	11.05	11.80
	50	648	342.2	2.46	12.26	3.96	12.34	1.88	7.42
	70	795	423.9	0.69	5.20	7.77	5.21	5.54	7.43
4 API=37.3	5	285	140.6	22.60	25.00	21.40	26.80	23.40	87.60
	10	308	153.3	10.70	12.10	10.20	12.90	11.40	32.80
	20	353	178.3	5.95	7.10	6.05	7.50	6.85	0.30
	50	499	259.4	7.50	9.12	2.80	7.22	3.60	7.42
	70	630	332.2	3.41	6.67	1.94	6.70	0.79	3.26
5 API=34.9	5	379	192.8	19.80	21.00	17.20	23.20	19.00	100.00
	10	421	216.1	0.10	0.30	2.10	1.30	0.60	57.80
	20	456	235.6	1.05	1.55	0.10	2.05	1.40	33.15
	50	563	295.0	5.82	5.42	0.56	4.56	2.24	1.50
	70	635	335.0	12.11	12.06	6.56	6.56	8.16	2.50
6 API=40.9	5	260	126.7	100.00	100.00	100.00	100.00	100.00	27.60
	10	278	136.7	42.10	43.50	42.50	44.50	42.70	36.30
	20	313	156.1	12.90	14.00	13.20	14.40	13.65	6.90
	50	404	206.7	13.60	10.26	9.96	10.38	10.34	16.38
	70	462	238.9	16.29	13.79	12.03	13.84	12.37	14.97
7 API=40.8	5	250	121.1	100.00	100.00	100.00	100.00	100.00	30.60
	10	269	131.7	42.20	43.40	41.80	44.40	42.60	23.20
	20	307	152.8	14.00	15.00	14.00	15.40	14.80	3.85
	50	442	227.8	5.92	4.42	1.42	4.52	1.90	17.04
	70	544	284.4	9.51	10.04	4.10	10.09	3.29	17.50
8 API=37.1	5	265	129.4	24.20	26.60	23.00	28.40	25.40	100.00
	10	296	146.7	12.10	10.70	12.60	9.90	11.20	66.50
	20	357	180.6	20.50	18.50	19.55	18.15	18.70	33.15
	50	541	282.8	4.84	1.52	10.94	1.60	10.08	3.00
	70	665	351.7	0.63	4.04	7.36	4.06	5.99	2.29

Continue, **Table I-2** *ADD%* values for 106 flash data points
(18 petroleum stocks) using unmodified models mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	*AAD%*					
				SRK	SRK + Van	PR	PR + Van	Ideal *K*	RD graph
9 API=28.2	5	450	232.2	100.00	100.00	100.00	100.00	100.00	100.00
	10	460	237.8	73.30	74.30	73.00	75.60	72.90	16.10
	20	483	250.6	53.20	53.30	52.35	53.90	52.80	92.70
	50	558	292.2	19.94	18.36	18.08	18.40	18.56	1.20
	70	599	315.0	19.00	15.56	14.79	15.64	15.71	3.80
10 API=38.2	5	247	119.4	49.60	53.80	49.60	55.60	42.00	14.20
	10	275	135.0	21.60	21.60	19.50	22.40	20.90	16.90
	20	351	177.2	9.50	9.50	10.60	8.15	10.00	8.30
	50	536	280.0	4.42	4.20	9.32	4.50	8.50	0.68
	70	653	345.0	3.79	3.79	7.63	3.81	6.14	5.44
11 API=32.5	5	299	148.3	20.20	22.80	20.00	24.60	21.40	63.40
	10	326	163.3	8.20	6.90	8.40	6.00	7.60	44.80
	20	382	194.4	23.10	21.30	22.15	24.55	21.40	22.45
	50	533	278.3	4.88	2.84	10.60	2.76	9.86	3.08
	70	627	330.6	4.23	6.57	1.84	6.60	0.81	1.91
12 API=43.5	10	322	161.1	25.00	26.20	24.90	27.10	27.00	23.30
	20	378	192.2	0.30	1.00	1.55	1.40	0.80	8.65
	50	548	286.7	0.64	2.46	6.38	2.56	5.42	2.56
	70	665	351.7	0.89	2.84	7.34	2.87	6.14	5.56
13 API=47.8	10	214	101.1	100.00	100.00	100.00	100.00	100.00	28.10
	20	262	127.8	33.40	35.15	34.05	35.65	34.55	7.55
	25	285	140.6	14.72	16.52	15.60	16.92	16.12	7.56
	30	295	146.1	16.83	18.60	17.77	18.87	18.23	10.47
	35	312	155.6	10.00	12.06	11.29	12.31	12.31	13.40
	50	352	177.8	16.26	13.34	12.78	13.46	13.46	19.08
	70	399	203.9	13.07	11.39	8.63	11.44	11.44	7.57
14 API=37.0	10	475	246.1	100.00	100.00	100.00	100.00	100.00	42.10
	30	501	260.6	10.63	9.93	9.80	10.47	10.87	61.60
	50	516	268.9	10.22	11.20	10.86	11.22	10.98	0.06
	70	532	277.8	27.50	24.67	24.37	24.80	25.20	14.54
15 API=38.6	0.00001	273	133.9	100.00	100.00	100.00	100.00	100.00	100.00
	10	300	148.9	3.80	1.80	4.00	1.00	2.40	24.60
	30	392	200.0	8.63	10.30	10.70	10.20	10.33	8.53
	50	400	204.4	1.26	5.62	4.08	5.88	3.52	3.62
	66.6	506	263.3	6.43	11.41	0.33	11.46	1.29	1.01
	70	600	315.6	3.47	7.49	3.13	7.51	1.84	2.20
16 API=37.3	10	283	139.4	32.60	37.10	31.50	38.00	36.20	7.50
	15	317	158.3	20.67	23.27	19.80	23.47	22.73	4.33
	20	350	176.7	14.95	17.05	14.50	17.45	16.70	9.15
	25	383	195.0	10.68	23.16	10.68	23.40	12.36	12.64

Continue, **Table I-2** *ADD%* values for 106 flash data points
(18 petroleum stocks) using unmodified models mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	*AAD%*					
				SRK	SRK + Van	PR	PR + Van	Ideal *K*	RD graph
16 API=37.3	30	425	218.3	1.40	11.10	2.13	11.27	3.70	15.90
	35	458	236.7	8.97	12.46	4.91	12.63	6.14	15.57
	40	484	251.1	10.60	16.25	6.25	16.38	7.48	16.48
	50	566	296.7	3.64	13.04	2.32	13.12	0.68	7.52
	60	617	325.0	6.87	13.52	0.47	13.57	2.33	7.70
	70	700	371.1	2.83	8.44	4.29	8.47	2.24	1.39
17 API=20.2	10	583	306.1	16.90	24.30	16.10	25.80	22.70	100.00
	15	600	315.6	22.07	26.60	20.80	27.60	25.33	35.33
	20	625	329.4	14.35	17.75	12.50	18.40	17.10	6.35
	25	642	338.9	14.88	17.92	12.92	18.44	17.52	9.56
	30	667	352.8	5.97	20.23	3.67	20.63	8.83	24.07
	35	700	371.1	5.74	0.40	7.20	0.77	4.49	22.63
	40	733	389.4	8.20	1.15	16.23	1.38	10.30	23.93
	50	758	403.3	0.36	4.58	8.06	4.72	2.74	15.76
	60	808	431.1	4.05	1.35	12.03	1.27	7.37	17.12
	70	866	463.3	4.53	2.94	12.16	2.90	8.47	19.11
18 API=42.2	10	300	148.9	100.00	100.00	100.00	100.00	100.00	32.20
	15	325	162.8	72.27	75.27	71.47	76.07	74.53	33.40
	20	350	176.7	49.00	51.00	48.00	51.55	50.55	27.60
	25	371	188.3	37.88	39.52	36.96	39.92	39.24	23.12
	30	400	204.4	21.83	23.63	21.20	23.93	23.53	26.03
	35	417	213.9	18.80	20.83	18.40	20.97	20.74	15.23
	40	442	227.8	12.65	18.48	12.80	18.65	13.88	11.48
	50	500	260.0	8.54	8.32	3.36	8.44	5.36	4.84
	60	533	278.3	12.22	12.80	6.82	12.88	8.68	1.08
	70	583	306.1	11.69	12.99	5.80	13.03	7.66	5.84
No. of points (106)			**Average**	**23.51**	**24.98**	**23.40**	**25.18**	**23.75**	**21.81**

Table I-3 *AD%* for 106 flash data points
(18 petroleum stocks) using unmodified models mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	*AD%*					
				SRK	SRK + Van	PR	PR + Van	Ideal *K*	RD graph
1 API=32.4	5	251	121.7	100.00	100.00	100.00	100.00	100.00	-71.00
	10	290	143.3	70.90	72.10	70.70	72.90	71.50	-7.60
	20	364	184.4	11.90	13.15	12.30	13.50	12.85	-2.85
	50	565	296.1	0.42	6.98	-5.44	7.06	-4.32	-6.40
	70	698	370.0	-0.56	3.79	-4.37	3.80	-5.63	7.87
2 API=36.5	5	260	126.7	100.00	100.00	100.00	100.00	100.00	-57.20
	10	282	138.9	60.40	61.30	62.30	60.60	60.70	8.40
	20	330	165.6	-4.75	-3.55	-4.25	-3.15	-3.65	17.45
	50	467	241.7	-10.98	-12.00	-12.34	-11.92	-11.86	6.08
	70	556	291.1	2.57	2.01	-3.11	2.06	-2.50	5.17
3 API=27.2	5	290	143.3	100.00	100.00	100.00	100.00	100.00	-26.00
	10	334	167.8	35.20	36.10	33.90	36.90	35.50	-3.80
	20	417	213.9	10.10	11.35	10.05	8.85	11.05	-11.80
	50	648	342.2	2.46	12.26	-3.96	12.34	-1.88	-7.42
	70	795	423.9	-0.69	5.20	-7.77	5.21	-5.54	7.43
4 API=37.3	5	285	140.6	22.60	25.00	21.40	26.80	23.40	87.60
	10	308	153.3	10.70	12.10	10.20	12.90	11.40	32.80
	20	353	178.3	5.95	7.10	6.05	7.50	6.85	0.30
	50	499	259.4	7.50	9.12	2.80	7.22	3.60	-7.42
	70	630	332.2	3.41	6.67	-1.94	6.70	-0.79	3.26
5 API=34.9	5	379	192.8	19.80	21.00	17.20	23.20	19.00	100.00
	10	421	216.1	-0.10	0.30	-2.10	1.30	-0.60	57.80
	20	456	235.6	1.05	1.55	-0.10	2.05	1.40	-33.15
	50	563	295.0	5.82	5.42	0.56	4.56	2.24	-1.50
	70	635	335.0	12.11	12.06	6.56	6.56	8.16	-2.50
6 API=40.9	5	260	126.7	100.00	100.00	100.00	100.00	100.00	27.60
	10	278	136.7	42.10	43.50	42.50	44.50	42.70	36.30
	20	313	156.1	12.90	14.00	13.20	14.40	13.65	6.90
	50	404	206.7	13.60	10.26	9.96	10.38	10.34	-16.38
	70	462	238.9	16.29	13.79	12.03	13.84	12.37	-14.97
7 API=40.8	5	250	121.1	100.00	100.00	100.00	100.00	100.00	30.60
	10	269	131.7	42.20	43.40	41.80	44.40	42.60	23.20
	20	307	152.8	14.00	15.00	14.00	15.40	14.80	3.85
	50	442	227.8	5.92	4.42	1.42	4.52	1.90	-17.04
	70	544	284.4	9.51	10.04	4.10	10.09	3.29	-17.50
8 API=37.1	5	265	129.4	24.20	26.60	23.00	28.40	25.40	100.00
	10	296	146.7	-12.10	-10.70	-12.60	-9.90	-11.20	66.50
	20	357	180.6	-20.50	-18.50	-19.55	-18.15	-18.70	33.15
	50	541	282.8	-4.84	1.52	-10.94	1.60	-10.08	3.00
	70	665	351.7	-0.63	4.04	-7.36	4.06	-5.99	-2.29

Continue, **Table I-3** *AD%* for 106 flash data points
(18 petroleum stocks) using unmodified models mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	*AD%*					
				SRK	SRK + Van	PR	PR + Van	Ideal *K*	RD graph
9 API=28.2	5	450	232.2	100.00	100.00	100.00	100.00	100.00	100.00
	10	460	237.8	73.30	74.30	73.00	75.60	72.90	-16.10
	20	483	250.6	53.20	53.30	52.35	53.90	52.80	-92.70
	50	558	292.2	19.94	18.36	18.08	18.40	18.56	1.20
	70	599	315.0	19.00	15.56	14.79	15.64	15.71	-3.80
10 API=38.2	5	247	119.4	49.60	53.80	49.60	55.60	42.00	14.20
	10	275	135.0	21.60	21.60	19.50	22.40	20.90	16.90
	20	351	177.2	-9.50	-9.50	-10.60	-8.15	-10.00	8.30
	50	536	280.0	4.42	4.20	-9.32	4.50	-8.50	-0.68
	70	653	345.0	3.79	3.79	-7.63	3.81	-6.14	5.44
11 API=32.5	5	299	148.3	20.20	22.80	20.00	24.60	21.40	63.40
	10	326	163.3	-8.20	-6.90	-8.40	-6.00	-7.60	44.80
	20	382	194.4	-23.10	-21.30	-22.15	-24.55	-21.40	22.45
	50	533	278.3	-4.88	-2.84	-10.60	-2.76	-9.86	3.08
	70	627	330.6	4.23	6.57	-1.84	6.60	-0.81	1.91
12 API=43.5	10	322	161.1	25.00	26.20	24.90	27.10	27.00	23.30
	20	378	192.2	-0.30	1.00	1.55	1.40	0.80	8.65
	50	548	286.7	-0.64	2.46	-6.38	2.56	-5.42	-2.56
	70	665	351.7	-0.89	2.84	-7.34	2.87	-6.14	5.56
13 API=47.8	10	214	101.1	100.00	100.00	100.00	100.00	100.00	-28.10
	20	262	127.8	33.40	35.15	34.05	35.65	34.55	-7.55
	25	285	140.6	14.72	16.52	15.60	16.92	16.12	-7.56
	30	295	146.1	16.83	18.60	17.77	18.87	18.23	-10.47
	35	312	155.6	10.00	12.06	11.29	12.31	12.31	-13.40
	50	352	177.8	16.26	13.34	12.78	13.46	13.46	-19.08
	70	399	203.9	13.07	11.39	8.63	11.44	11.44	-7.57
14 API=37.0	10	475	246.1	100.00	100.00	100.00	100.00	100.00	42.10
	30	501	260.6	10.63	9.93	9.80	10.47	10.87	-61.60
	50	516	268.9	10.22	11.20	10.86	11.22	10.98	0.06
	70	532	277.8	27.50	24.67	24.37	24.80	25.20	14.54
15 API=38.6	0.00001	273	133.9	100.00	100.00	100.00	100.00	100.00	100.00
	10	300	148.9	-3.80	-1.80	-4.00	-1.00	-2.40	24.60
	30	392	200.0	-8.63	-10.30	-10.70	-10.20	-10.33	8.53
	50	400	204.4	1.26	5.62	-4.08	5.88	-3.52	-3.62
	66.6	506	263.3	6.43	11.41	0.33	11.46	1.29	1.01
	70	600	315.6	3.47	7.49	-3.13	7.51	-1.84	2.20
16 API=37.3	10	283	139.4	32.60	37.10	31.50	38.00	36.20	7.50
	15	317	158.3	20.67	23.27	19.80	23.47	22.73	-4.33
	20	350	176.7	14.95	17.05	14.50	17.45	16.70	-9.15
	25	383	195.0	10.68	23.16	10.68	23.40	12.36	-12.64

Continue, **Table I-3** *AD%* for 106 flash data points
(18 petroleum stocks) using unmodified models mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	*AD%*					
				SRK	SRK + Van	PR	PR + Van	Ideal *K*	RD graph
16 API=37.3	30	425	218.3	1.40	11.10	2.13	11.27	3.70	-15.90
	35	458	236.7	8.97	12.46	4.91	12.63	6.14	-15.57
	40	484	251.1	10.60	16.25	6.25	16.38	7.48	-16.48
	50	566	296.7	3.64	13.04	-2.32	13.12	-0.68	-7.52
	60	617	325.0	6.87	13.52	0.47	13.57	2.33	-7.70
	70	700	371.1	2.83	8.44	-4.29	8.47	-2.24	-1.39
17 API=20.2	10	583	306.1	16.90	24.30	16.10	25.80	22.70	100.00
	15	600	315.6	22.07	26.60	20.80	27.60	25.33	35.33
	20	625	329.4	14.35	17.75	12.50	18.40	17.10	6.35
	25	642	338.9	14.88	17.92	12.92	18.44	17.52	-9.56
	30	667	352.8	5.97	20.23	3.67	20.63	8.83	-24.07
	35	700	371.1	-5.74	0.40	-7.20	0.77	-4.49	-22.63
	40	733	389.4	-8.20	1.15	-16.23	1.38	-10.30	-23.93
	50	758	403.3	-0.36	4.58	-8.06	4.72	-2.74	-15.76
	60	808	431.1	-4.05	-1.35	-12.03	-1.27	-7.37	-17.12
	70	866	463.3	-4.53	-2.94	-12.16	-2.90	-8.47	-19.11
18 API=42.2	10	300	148.9	100.00	100.00	100.00	100.00	100.00	-32.20
	15	325	162.8	72.27	75.27	71.47	76.07	74.53	-33.40
	20	350	176.7	49.00	51.00	48.00	51.55	50.55	-27.60
	25	371	188.3	37.88	39.52	36.96	39.92	39.24	-23.12
	30	400	204.4	21.83	23.63	21.20	23.93	23.53	-26.03
	35	417	213.9	18.80	20.83	18.40	20.97	20.74	-15.23
	40	442	227.8	12.65	18.48	12.80	18.65	13.88	-11.48
	50	500	260.0	8.54	8.32	3.36	8.44	5.36	-4.84
	60	533	278.3	12.22	12.80	6.82	12.88	8.68	-1.08
	70	583	306.1	11.69	12.99	5.80	13.03	7.66	-5.84
No. of points(106)			**Average**	**20.91**	**23.06**	**18.42**	**23.30**	**19.73**	**3.22**

Table I-4 Predicted flash volumes for 45 flash data points
(5 petroleum stocks) using modified models No. 1 mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	Predicted flash volumes, vol.%		
				SRK	SRK +Van	Ideal K
3 API=27.2	5	290	143.3	0	0	0
	10	334	167.8	7.57	6.41	6.46
	20	417	213.9	19.22	17.73	17.8
	50	648	342.2	50.7	43.88	50.92
	70	795	423.9	72.17	66.37	73.85
4 API=37.3	5	285	140.6	8.24	3.84	3.9
	10	308	153.3	13.34	8.88	8.98
	20	353	178.3	24.2	18.6	18.69
	50	499	259.4	50.87	45.49	48.29
	70	630	332.2	70.63	65.36	70.54
9 API=28.2	5	450	232.2	5.81	0.23	0.35
	10	460	237.8	8.98	2.66	2.79
	20	483	250.6	18.21	9.56	9.52
	50	558	292.2	48.99	40.83	40.73
	70	599	315.0	62.65	59.15	58.83
16 API=37.3	10	283	139.4	8.82	6.34	6.42
	15	317	158.3	14.14	11.56	11.63
	20	350	176.7	19.44	16.63	16.69
	25	383	195.0	25.01	19.25	21.94
	30	425	218.3	30.76	26.71	28.91
	35	458	236.7	34.41	30.67	32.86
	40	484	251.1	38.38	33.54	37.02
	50	566	296.7	50.93	43.51	50.34
	60	617	325.0	58.65	51.91	58.58
	70	700	371.1	70.73	64.1	71.34
18 API=42.2	10	300	148.9	0	0	0
	15	325	162.8	8.73	3.81	3.89
	20	350	176.7	15.18	9.89	9.96
	25	371	188.3	20.95	15.2	15.25
	30	400	204.4	29.55	22.99	22.99
	35	417	213.9	34.86	27.81	27.78
	40	442	227.8	37.21	32.67	34.46
	50	500	260.0	50.43	45.89	47.34
	60	533	278.3	56.91	52.36	54.79
	70	583	306.1	65.45	60.9	64.63

Table I-5 *ADD%* values for 45 flash data points
(5 petroleum stocks) using modified models No. 1 mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	*AAD%*		
				SRK	SRK +Van	Ideal K
3 API=27.2	5	290	143.3	100.00	100.00	100.00
	10	334	167.8	24.30	35.90	35.40
	20	417	213.9	3.90	11.35	11.00
	50	648	342.2	1.40	12.24	1.84
	70	795	423.9	3.10	5.19	5.50
4 API=37.3	5	285	140.6	64.80	23.20	22.00
	10	308	153.3	33.40	11.20	10.20
	20	353	178.3	21.00	7.00	6.55
	50	499	259.4	1.74	9.02	3.42
	70	630	332.2	0.90	6.63	0.77
9 API=28.2	5	450	232.2	16.20	95.40	93.00
	10	460	237.8	10.20	73.40	72.10
	20	483	250.6	8.95	52.20	52.40
	50	558	292.2	2.02	18.34	18.54
	70	599	315.0	10.50	15.50	15.96
16 API=37.3	10	283	139.4	11.80	36.60	35.80
	15	317	158.3	5.73	22.93	22.47
	20	350	176.7	2.80	16.85	16.55
	25	383	195.0	0.04	23.00	12.24
	30	425	218.3	2.53	10.97	3.63
	35	458	236.7	1.69	12.37	6.11
	40	484	251.1	4.05	16.15	7.45
	50	566	296.7	1.86	12.98	0.68
	60	617	325.0	2.25	13.48	2.37
	70	700	371.1	1.04	8.43	1.91
18 API=42.2	10	300	148.9	100.00	100.00	100.00
	15	325	162.8	41.80	74.60	74.07
	20	350	176.7	24.10	50.55	50.20
	25	371	188.3	16.20	39.20	39.00
	30	400	204.4	1.50	23.37	23.37
	35	417	213.9	0.40	20.54	20.63
	40	442	227.8	6.98	18.33	13.85
	50	500	260.0	0.86	8.22	5.32
	60	533	278.3	5.15	12.73	8.68
	70	583	306.1	6.50	13.00	7.67
No. of points(45)			**Average**	**15.42**	**28.88**	**25.73**

Table I-6 *AD%* values for 45 flash data points
(5 petroleum stocks) using modified models No. 1 mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	*AD%*		
				SRK	SRK +Van	Ideal K
3 API=27.2	5	290	143.3	100.00	100.00	100.00
	10	334	167.8	24.30	35.90	35.40
	20	417	213.9	3.90	11.35	11.00
	50	648	342.2	-1.40	12.24	-1.84
	70	795	423.9	-3.10	5.19	-5.50
4 API=37.3	5	285	140.6	-64.80	23.20	22.00
	10	308	153.3	-33.40	11.20	10.20
	20	353	178.3	-21.00	7.00	6.55
	50	499	259.4	-1.74	9.02	3.42
	70	630	332.2	-0.90	6.63	-0.77
9 API=28.2	5	450	232.2	-16.20	95.40	93.00
	10	460	237.8	10.20	73.40	72.10
	20	483	250.6	8.95	52.20	52.40
	50	558	292.2	2.02	18.34	18.54
	70	599	315.0	10.50	15.50	15.96
16 API=37.3	10	283	139.4	11.80	36.60	35.80
	15	317	158.3	5.73	22.93	22.47
	20	350	176.7	2.80	16.85	16.55
	25	383	195.0	-0.04	23.00	12.24
	30	425	218.3	-2.53	10.97	3.63
	35	458	236.7	1.69	12.37	6.11
	40	484	251.1	4.05	16.15	7.45
	50	566	296.7	-1.86	12.98	-0.68
	60	617	325.0	2.25	13.48	2.37
	70	700	371.1	-1.04	8.43	-1.91
18 API=42.2	10	300	148.9	100.00	100.00	100.00
	15	325	162.8	41.80	74.60	74.07
	20	350	176.7	24.10	50.55	50.20
	25	371	188.3	16.20	39.20	39.00
	30	400	204.4	1.50	23.37	23.37
	35	417	213.9	0.40	20.54	20.63
	40	442	227.8	6.98	18.33	13.85
	50	500	260.0	-0.86	8.22	5.32
	60	533	278.3	5.15	12.73	8.68
	70	583	306.1	6.50	13.00	7.67
No. of points(45)			**Average**	**6.91**	**28.88**	**25.12**

Table I-7 Predicted flash volumes for 106 flash data points
(18 petroleum stocks) using modified models No. 1 mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	Predicted flash volumes, vol.%	
				PR	PR + Van
1 API=32.4	5	251	121.7	0	0
	10	290	143.3	3.02	3.44
	20	364	184.4	17.54	17.91
	50	565	296.1	52.06	47.24
	70	698	370.0	73.78	68.14
2 API=36.5	5	260	126.7	0	0
	10	282	138.9	4.04	4.77
	20	330	165.6	20.88	21.45
	50	467	241.7	55.91	56.52
	70	556	291.1	71.61	69
3 API=27.2	5	290	143.3	0	0
	10	334	167.8	6.63	6.89
	20	417	213.9	17.92	18.23
	50	648	342.2	50.82	44.52
	70	795	423.9	73.56	66.89
4 API=37.3	5	285	140.6	4.01	4.42
	10	308	153.3	9.03	9.44
	20	353	178.3	18.77	19.21
	50	499	259.4	48.22	46.07
	70	630	332.2	70.29	65.83
5 API=34.9	5	379	192.8	4.15	4.82
	10	421	216.1	10.15	10.85
	20	456	235.6	19.82	20.61
	50	563	295.0	48.92	48.12
	70	635	335.0	64.27	62.17
6 API=40.9	5	260	126.7	0	0
	10	278	136.7	5.87	6.5
	20	313	156.1	17.2	17.98
	50	404	206.7	44.86	45.55
	70	462	238.9	61.29	60.29
7 API=40.8	5	250	121.1	0	0
	10	269	131.7	5.92	6.44
	20	307	152.8	17.22	17.71
	50	442	227.8	49.06	48.35
	70	544	284.4	66.52	63.43
8 API=37.1	5	265	129.4	3.94	4.36
	10	296	146.7	11.31	11.68
	20	357	180.6	23.87	24.26
	50	541	282.8	54.89	49.8
	70	665	351.7	73.82	67.64

Continue, **Table I-7** Predicted flash volumes for 106 flash data points (18 petroleum stocks) using modified models No. 1 mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	Predicted flash volumes, vol.%	
				PR	PR + Van
9 API=28.2	5	450	232.2	0.27	1.06
	10	460	237.8	2.72	3.55
	20	483	250.6	9.44	10.44
	50	558	292.2	40.71	41.58
	70	599	315.0	58.82	59.85
10 API=38.2	5	247	119.4	2.61	2.92
	10	275	135.0	8.12	8.42
	20	351	177.2	22.1	22.46
	50	536	280.0	54.06	48.59
	70	653	345.0	73.89	67.87
11 API=32.5	5	299	148.3	4.1	4.58
	10	326	163.3	10.9	11.36
	20	382	194.4	24.39	24.89
	50	533	278.3	54.78	51.94
	70	627	330.6	70.28	65.81
12 API=43.5	10	322	161.1	7.99	8.45
	20	378	192.2	20.11	20.57
	50	548	286.7	50.63	47.51
	70	665	351.7	69.73	64.1
13 API=47.8	10	214	101.1	0	0
	20	262	127.8	13.26	13.78
	25	285	140.6	21.13	21.66
	30	295	146.1	24.67	25.21
	35	312	155.6	30.99	31.57
	50	352	177.8	43.47	44.09
	70	399	203.9	63.62	62.83
14 API=37.0	10	475	246.1	0	0
	30	501	260.6	18.43	22.29
	50	516	268.9	39.33	42.97
	70	532	277.8	47.28	49.79
15 API=38.6	0.00001	200	93.3	0	0
	10	273	133.9	10.46	10.77
	30	392	200.0	33.15	33.37
	50	506	263.3	51.66	47.62
	66.6	600	315.6	65.47	59.47
	70	659	348.3	70.94	65.22
16 API=37.3	10	283	139.4	6.86	6.87
	15	317	158.3	11.99	12.07
	20	350	176.7	17.02	17.16
	25	383	195.0	22.2	19.76

Continue, **Table I-7** Predicted flash volumes for 106 flash data points (18 petroleum stocks) using modified models No. 1 mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	Predicted flash volumes, vol.%	
				PR	PR + Van
16 API=37.3	30	425	218.3	29.14	27.24
	35	458	236.7	33	31.11
	40	484	251.1	37.17	34.1
	50	566	296.7	50.35	44.07
	60	617	325.0	58.52	52.47
	70	700	371.1	71.18	64.63
17 API=20.2	10	583	306.1	8.24	8.66
	15	600	315.6	11.58	12.1
	20	625	329.4	16.93	17.58
	25	642	338.9	20.96	21.7
	30	667	352.8	27.62	25.09
	35	700	371.1	36.69	36.09
	40	733	389.4	44.4	40.68
	50	758	403.3	51.67	48.81
	60	808	431.1	64.65	61.73
	70	866	463.3	75.93	72.76
18 API=42.2	10	300	148.9	0	0
	15	325	162.8	4.31	4.54
	20	350	176.7	10.36	10.61
	25	371	188.3	15.65	15.92
	30	400	204.4	23.43	23.72
	35	417	213.9	28.25	28.56
	40	442	227.8	34.67	33.46
	50	500	260.0	47.68	46.56
	60	533	278.3	55.07	52.99
	70	583	306.1	64.78	61.5

Table I-8 *AAD%* for 106 flash data points
(18 petroleum stocks) using modified models No. 1 mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	*AAD%*	
				PR	PR + Van
1 API=32.4	5	251	121.7	100.00	100.00
	10	290	143.3	69.80	65.60
	20	364	184.4	12.30	10.45
	50	565	296.1	4.12	5.52
	70	698	370.0	5.40	2.66
2 API=36.5	5	260	126.7	100.00	100.00
	10	282	138.9	59.60	52.30
	20	330	165.6	4.40	7.25
	50	467	241.7	11.82	13.04
	70	556	291.1	2.30	1.43
3 API=27.2	5	290	143.3	100.00	100.00
	10	334	167.8	33.70	31.10
	20	417	213.9	10.40	8.85
	50	648	342.2	1.64	10.96
	70	795	423.9	5.09	4.44
4 API=37.3	5	285	140.6	19.80	11.60
	10	308	153.3	9.70	5.60
	20	353	178.3	6.15	3.95
	50	499	259.4	3.56	7.86
	70	630	332.2	0.41	5.96
5 API=34.9	5	379	192.8	17.00	3.60
	10	421	216.1	1.50	8.50
	20	456	235.6	0.90	3.05
	50	563	295.0	2.16	3.76
	70	635	335.0	8.19	11.19
6 API=40.9	5	260	126.7	100.00	100.00
	10	278	136.7	41.30	35.00
	20	313	156.1	14.00	10.10
	50	404	206.7	10.28	8.90
	70	462	238.9	12.44	13.87
7 API=40.8	5	250	121.1	100.00	100.00
	10	269	131.7	40.80	35.60
	20	307	152.8	13.90	11.45
	50	442	227.8	1.88	3.30
	70	544	284.4	4.97	9.39
8 API=37.1	5	265	129.4	21.20	12.80
	10	296	146.7	13.10	16.80
	20	357	180.6	19.35	21.30
	50	541	282.8	9.78	0.40
	70	665	351.7	5.46	3.37

Continue, **Table I-8** *AAD%* for 106 flash data points
(18 petroleum stocks) using modified models No. 1 mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	*AAD%*	
				PR	PR + Van
9 API=28.2	5	450	232.2	94.60	78.80
	10	460	237.8	72.80	64.50
	20	483	250.6	52.80	47.80
	50	558	292.2	18.58	16.84
	70	599	315.0	15.97	14.50
10 API=38.2	5	247	119.4	47.80	41.60
	10	275	135.0	18.80	15.80
	20	351	177.2	10.50	12.30
	50	536	280.0	8.12	2.82
	70	653	345.0	5.56	3.04
11 API=32.5	5	299	148.3	18.00	8.40
	10	326	163.3	9.00	13.60
	20	382	194.4	21.95	24.45
	50	533	278.3	9.56	3.88
	70	627	330.6	0.40	5.99
12 API=43.5	10	322	161.1	20.10	15.50
	20	378	192.2	0.55	2.85
	50	548	286.7	1.26	4.98
	70	665	351.7	0.39	8.43
13 API=47.8	10	214	101.1	100.00	100.00
	20	262	127.8	33.70	31.10
	25	285	140.6	15.48	13.36
	30	295	146.1	17.77	15.97
	35	312	155.6	11.46	9.80
	50	352	177.8	13.06	11.82
	70	399	203.9	9.11	10.24
14 API=37.0	10	475	246.1	100.00	100.00
	30	501	260.6	38.57	25.70
	50	516	268.9	21.34	14.06
	70	532	277.8	32.46	28.87
15 API=38.6	0.00001	273	133.9	100.00	100.00
	10	300	148.9	4.60	7.70
	30	392	200.0	10.50	11.23
	50	400	204.4	3.32	4.76
	66.6	506	263.3	1.70	10.71
	70	600	315.6	1.34	6.83
16 API=37.3	10	283	139.4	31.40	31.30
	15	317	158.3	20.07	19.53
	20	350	176.7	14.90	14.20
	25	383	195.0	11.20	20.96

Continue, **Table I-8** *AAD%* for 106 flash data points
(18 petroleum stocks) using modified models No. 1 mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	*AAD%*	
				PR	PR + Van
16 API=37.3	30	425	218.3	2.87	9.20
	35	458	236.7	5.71	11.11
	40	484	251.1	7.08	14.75
	50	566	296.7	0.70	11.86
	60	617	325.0	2.47	12.55
	70	700	371.1	1.69	7.67
17 API=20.2	10	583	306.1	17.60	13.40
	15	600	315.6	22.80	19.33
	20	625	329.4	15.35	12.10
	25	642	338.9	16.16	13.20
	30	667	352.8	7.93	16.37
	35	700	371.1	4.83	3.11
	40	733	389.4	11.00	1.70
	50	758	403.3	3.34	2.38
	60	808	431.1	7.75	2.88
	70	866	463.3	8.47	3.94
18 API=42.2	10	300	148.9	100.00	100.00
	15	325	162.8	71.27	69.73
	20	350	176.7	48.20	46.95
	25	371	188.3	37.40	36.32
	30	400	204.4	21.90	20.93
	35	417	213.9	19.29	18.40
	40	442	227.8	13.33	16.35
	50	500	260.0	4.64	6.88
	60	533	278.3	8.22	11.68
	70	583	306.1	7.46	12.14
No. of points (106)		**Average**		**23.40**	**24.90**

Table I-9 *AD%* for 106 flash data points
(18 petroleum stocks) using modified models No. 1 mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	*AD%*	
				PR	PR + Van
1 API=32.4	5	251	121.7	100.00	100.00
	10	290	143.3	69.80	65.60
	20	364	184.4	12.30	10.45
	50	565	296.1	-4.12	5.52
	70	698	370.0	-5.40	2.66
2 API=36.5	5	260	126.7	100.00	100.00
	10	282	138.9	59.60	52.30
	20	330	165.6	-4.40	-7.25
	50	467	241.7	-11.82	-13.04
	70	556	291.1	-2.30	1.43
3 API=27.2	5	290	143.3	100.00	100.00
	10	334	167.8	33.70	31.10
	20	417	213.9	10.40	8.85
	50	648	342.2	-1.64	10.96
	70	795	423.9	-5.09	4.44
4 API=37.3	5	285	140.6	19.80	11.60
	10	308	153.3	9.70	5.60
	20	353	178.3	6.15	3.95
	50	499	259.4	3.56	7.86
	70	630	332.2	-0.41	5.96
5 API=34.9	5	379	192.8	17.00	3.60
	10	421	216.1	-1.50	-8.50
	20	456	235.6	0.90	-3.05
	50	563	295.0	2.16	3.76
	70	635	335.0	8.19	11.19
6 API=40.9	5	260	126.7	100.00	100.00
	10	278	136.7	41.30	35.00
	20	313	156.1	14.00	10.10
	50	404	206.7	10.28	8.90
	70	462	238.9	12.44	13.87
7 API=40.8	5	250	121.1	100.00	100.00
	10	269	131.7	40.80	35.60
	20	307	152.8	13.90	11.45
	50	442	227.8	1.88	3.30
	70	544	284.4	4.97	9.39
8 API=37.1	5	265	129.4	21.20	12.80
	10	296	146.7	-13.10	-16.80
	20	357	180.6	-19.35	-21.30
	50	541	282.8	-9.78	0.40
	70	665	351.7	-5.46	3.37

Continue, **Table I-9** *AD%* for 106 flash data points
(18 petroleum stocks) using modified models No. 1 mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	*AD%*	
				PR	PR + Van
9 API=28.2	5	450	232.2	94.60	78.80
	10	460	237.8	72.80	64.50
	20	483	250.6	52.80	47.80
	50	558	292.2	18.58	16.84
	70	599	315.0	15.97	14.50
10 API=38.2	5	247	119.4	47.80	41.60
	10	275	135.0	18.80	15.80
	20	351	177.2	-10.50	-12.30
	50	536	280.0	-8.12	2.82
	70	653	345.0	-5.56	3.04
11 API=32.5	5	299	148.3	18.00	8.40
	10	326	163.3	-9.00	-13.60
	20	382	194.4	-21.95	-24.45
	50	533	278.3	-9.56	-3.88
	70	627	330.6	-0.40	5.99
12 API=43.5	10	322	161.1	20.10	15.50
	20	378	192.2	-0.55	-2.85
	50	548	286.7	-1.26	4.98
	70	665	351.7	0.39	8.43
13 API=47.8	10	214	101.1	100.00	100.00
	20	262	127.8	33.70	31.10
	25	285	140.6	15.48	13.36
	30	295	146.1	17.77	15.97
	35	312	155.6	11.46	9.80
	50	352	177.8	13.06	11.82
	70	399	203.9	9.11	10.24
14 API=37.0	10	475	246.1	100.00	100.00
	30	501	260.6	38.57	25.70
	50	516	268.9	21.34	14.06
	70	532	277.8	32.46	28.87
15 API=38.6	0.00001	273	133.9	100.00	100.00
	10	300	148.9	-4.60	-7.70
	30	392	200.0	-10.50	-11.23
	50	400	204.4	-3.32	4.76
	66.6	506	263.3	1.70	10.71
	70	600	315.6	-1.34	6.83
16 API=37.3	10	283	139.4	31.40	31.30
	15	317	158.3	20.07	19.53
	20	350	176.7	14.90	14.20
	25	383	195.0	11.20	20.96

Continue, **Table I-9** *AD%* for 106 flash data points
(18 petroleum stocks) using modified models No. 1 mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	*AD%*	
				PR	PR + Van
16 API=37.3	30	425	218.3	2.87	9.20
	35	458	236.7	5.71	11.11
	40	484	251.1	7.08	14.75
	50	566	296.7	-0.70	11.86
	60	617	325.0	2.47	12.55
	70	700	371.1	-1.69	7.67
17 API=20.2	10	583	306.1	17.60	13.40
	15	600	315.6	22.80	19.33
	20	625	329.4	15.35	12.10
	25	642	338.9	16.16	13.20
	30	667	352.8	7.93	16.37
	35	700	371.1	-4.83	-3.11
	40	733	389.4	-11.00	-1.70
	50	758	403.3	-3.34	2.38
	60	808	431.1	-7.75	-2.88
	70	866	463.3	-8.47	-3.94
18 API=42.2	10	300	148.9	100.00	100.00
	15	325	162.8	71.27	69.73
	20	350	176.7	48.20	46.95
	25	371	188.3	37.40	36.32
	30	400	204.4	21.90	20.93
	35	417	213.9	19.29	18.40
	40	442	227.8	13.33	16.35
	50	500	260.0	4.64	6.88
	60	533	278.3	8.22	11.68
	70	583	306.1	7.46	12.14
No. of points(106)		**Average**		**19.50**	**23.10**

Table I-10 Predicted flash volumes for 61 flash data points (10 petroleum stocks) using modified models No. 2 mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	Predicted flash volumes, vol.%				
				SRK	SRK + Van	PR	PR + Van	Ideal *K*
1 API=32.4	5	251	121.7	0	0	0	0	0
	10	290	143.3	5.63	6.69	5.61	6.6	6.77
	20	364	184.4	19.33	19.9	19.16	19.84	19.85
	50	565	296.1	49.98	48.46	52.91	48.41	53.63
	70	698	370.0	69.8	68.95	74.48	68.92	74.73
2 API=36.5	5	260	126.7	0.28	1.4	0.22	1.29	1.5
	10	282	138.9	8.69	9.55	8.66	9.45	9.62
	20	330	165.6	24.52	24.54	24.28	24.46	24.59
	50	467	241.7	54.42	57.37	57.13	57.31	72.6
	70	556	291.1	68.31	69.78	72.28	69.69	72.65
3 API=27.2	5	290	143.3	1.58	2.67	1.65	2.6	2.76
	10	334	167.8	8.03	8.88	8.09	8.81	8.98
	20	417	213.9	19.03	19.32	18.95	19.49	19.59
	50	648	342.2	48.48	45.89	51.14	45.49	52.2
	70	795	423.9	69.21	67.17	74.24	67.35	73.9
6 API=40.9	5	260	126.7	3.68	4.82	3.62	4.71	4.91
	10	278	136.7	9.69	10.55	9.64	10.45	10.64
	20	313	156.1	20.88	21.09	20.74	21	21.18
	50	404	206.7	45.21	47.23	47.11	47.17	47.29
	70	462	238.9	59.56	61.99	62.58	62.02	63.02
7 API=40.8	5	250	121.1	3.48	4.53	3.47	4.43	4.62
	10	269	131.7	9.26	10.1	9.27	10	10.1
	20	307	152.8	20.2	20.56	20.1	20.48	20.63
	50	442	227.8	47.94	49.45	50.22	49.4	50.66
	70	544	284.4	63.46	64.24	67.24	64.27	67.66
9 API=28.2	5	450	232.2	2.03	4.46	1.99	4.33	4.67
	10	460	237.8	4.5	6.98	4.5	6.85	7.19
	20	483	250.6	11.39	14.74	11.51	14.67	14.4
	50	558	292.2	40.35	46.39	42.1	46.31	46.11
	70	599	315.0	57.11	62.78	60.02	62.78	62.64
13 API=47.8	10	214	101.1	0.96	1.79	0.84	1.67	1.92
	20	262	127.8	17.25	17.22	17.1	17.12	17.36
	25	285	140.6	25.27	24.64	24.97	24.55	24.79
	30	295	146.1	28.95	28.17	28.55	28.11	28.16
	35	312	155.6	35.62	34.31	34.98	34.26	34.2
	50	352	177.8	44.96	45.92	46.89	45.71	45.99
	70	399	203.9	63.63	63.9	66.85	63.86	65.44
14 API=37.0	10	475	246.1	0.89	11.01	0.54	10.82	11.07
	30	501	260.6	32.51	42.95	32.49	42.82	42.36
	50	516	268.9	44.9	49.62	45.12	49.52	49.33
	70	532	277.8	52.92	61.34	55.13	61.26	61.04

Continue, **Table I-10** Predicted flash volumes for 61 flash data points (10 petroleum stocks) using modified models No. 2 mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	Predicted flash volumes, vol.%				
				SRK	SRK + Van	PR	PR + Van	Ideal *K*
16 API=37.3	10	283	139.4	8.31	9.03	8.39	8.32	8.8
	15	317	158.3	13.38	13.52	13.45	13.44	13.76
	20	350	176.7	18.38	18.35	18.39	18.27	18.63
	25	383	195.0	23.58	21.13	23.49	21.33	23.72
	30	425	218.3	30.58	28.37	30.05	28.29	30.08
	35	458	236.7	32.57	31.74	33.99	31.71	34.42
	40	484	251.1	36.35	35.37	38.09	35.31	38.56
	50	566	296.7	48.46	45.62	51.45	45.72	51.95
	60	617	325.0	55.99	53.98	59.89	54.06	60.01
	70	700	371.1	67.74	65.98	72.71	65.87	72.47
18 API=42.2	10	300	148.9	0.43	1.71	0.45	1.59	1.87
	15	325	162.8	6.29	7.44	6.41	7.33	7.59
	20	350	176.7	12.26	13.63	12.44	13.59	13.42
	25	371	188.3	17.53	18.77	17.71	18.65	18.55
	30	400	204.4	25.3	25.81	25.41	25.71	26.1
	35	417	213.9	30.15	30.82	30.16	30.75	30.78
	40	442	227.8	35.01	34.89	35.43	34.87	35.6
	50	500	260.0	46.26	48.26	48.85	48.07	49.6
	60	533	278.3	52.94	54.59	56.18	54.53	56.82
	70	583	306.1	61.81	62.87	65.92	62.83	66.23

Table I-11 *ADD%* for 61 flash data points
(10 petroleum stocks) using modified models No. 2 mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	*AAD%*				
				SRK	SRK + Van	PR	PR + Van	Ideal *K*
1 API=32.4	5	251	121.7	100.00	100.00	100.00	100.00	100.00
	10	290	143.3	43.70	33.10	43.90	34.00	32.30
	20	364	184.4	3.35	0.50	4.20	0.80	0.75
	50	565	296.1	0.04	3.08	5.82	3.18	7.26
	70	698	370.0	0.29	1.50	6.40	1.54	6.76
2 API=36.5	5	260	126.7	94.40	72.00	95.60	74.20	70.00
	10	282	138.9	13.10	4.50	13.40	5.50	3.80
	20	330	165.6	22.60	22.70	21.40	22.30	22.95
	50	467	241.7	8.84	14.74	14.26	14.62	45.20
	70	556	291.1	2.41	0.31	3.26	0.44	3.79
3 API=27.2	5	290	143.3	68.40	46.60	67.00	48.00	44.80
	10	334	167.8	19.70	11.20	19.10	11.90	10.20
	20	417	213.9	4.85	3.40	5.25	2.55	2.05
	50	648	342.2	3.04	8.22	2.28	9.02	4.40
	70	795	423.9	1.13	4.04	6.06	3.79	5.57
6 API=40.9	5	260	126.7	26.40	3.60	27.60	5.80	1.80
	10	278	136.7	3.10	5.50	3.60	4.50	6.40
	20	313	156.1	4.40	5.45	3.70	5.00	5.90
	50	404	206.7	9.58	5.54	5.78	5.66	5.42
	70	462	238.9	14.91	11.44	10.60	11.40	9.97
7 API=40.8	5	250	121.1	30.40	9.40	30.60	11.40	7.60
	10	269	131.7	7.40	1.00	7.30	0.00	1.00
	20	307	152.8	1.00	2.80	0.50	2.40	3.15
	50	442	227.8	4.12	1.10	0.44	1.20	1.32
	70	544	284.4	9.34	8.23	3.94	8.19	3.34
9 API=28.2	5	450	232.2	59.40	10.80	60.20	13.40	6.60
	10	460	237.8	55.00	30.20	55.00	31.50	28.10
	20	483	250.6	43.05	26.30	42.45	26.65	28.00
	50	558	292.2	19.30	7.22	15.80	7.38	7.78
	70	599	315.0	18.41	10.31	14.26	10.31	10.51
13 API=47.8	10	214	101.1	90.40	82.10	91.60	83.30	80.80
	20	262	127.8	13.75	13.90	14.50	14.40	13.20
	25	285	140.6	1.08	1.44	0.12	1.80	0.84
	30	295	146.1	3.50	6.10	4.83	6.30	6.13
	35	312	155.6	1.77	1.97	0.06	2.11	2.29
	50	352	177.8	10.08	8.16	6.22	8.58	8.02
	70	399	203.9	9.10	8.71	4.50	8.77	6.51
14 API=37.0	10	475	246.1	91.10	10.10	94.60	8.20	10.70
	30	501	260.6	8.37	43.17	8.30	42.73	41.20
	50	516	268.9	10.20	0.76	9.76	0.96	1.34
	70	532	277.8	24.40	12.37	21.24	12.49	12.80

Continue, **Table I-11** *ADD%* for 61 flash data points
(10 petroleum stocks) using modified models No. 2 mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	*AAD%*				
				SRK	SRK + Van	PR	PR + Van	Ideal *K*
16 API=37.3	10	283	139.4	16.90	9.70	16.10	16.80	12.00
	15	317	158.3	10.80	9.87	10.33	10.40	8.27
	20	350	176.7	8.10	8.25	8.05	8.65	6.85
	25	383	195.0	5.68	15.48	6.04	14.68	5.12
	30	425	218.3	1.93	5.43	0.17	5.70	0.27
	35	458	236.7	6.94	9.31	2.89	9.40	1.66
	40	484	251.1	9.13	11.58	4.78	11.73	3.60
	50	566	296.7	3.08	8.76	2.90	8.56	3.90
	60	617	325.0	6.68	10.03	0.18	9.90	0.02
	70	700	371.1	3.23	5.74	3.87	5.90	3.53
18 API=42.2	10	300	148.9	95.70	82.90	95.50	84.10	81.30
	15	325	162.8	58.07	50.40	57.27	51.13	49.40
	20	350	176.7	38.70	31.85	37.80	32.05	32.90
	25	371	188.3	29.88	24.92	29.16	25.40	25.80
	30	400	204.4	15.67	13.97	15.30	14.30	13.00
	35	417	213.9	13.86	11.94	13.83	12.14	12.06
	40	442	227.8	12.48	12.78	11.43	12.83	11.00
	50	500	260.0	7.48	3.48	2.30	3.86	0.80
	60	533	278.3	11.77	9.02	6.37	9.12	5.30
	70	583	306.1	11.70	10.19	5.83	10.24	5.39
No. of points(61)			**Average**	**21.69**	**16.379**	**20.9**	**16.77**	**15.61**

Table I-12 *AD%* for 61 flash data points
(10 petroleum stocks) using modified models No. 2 mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	*AD%*				
				SRK	SRK + Van	PR	PR + Van	Ideal *K*
1 API=32.4	5	251	121.7	100.00	100.00	100.00	100.00	100.00
	10	290	143.3	33.10	33.10	43.90	34.00	32.30
	20	364	184.4	0.50	0.50	4.20	0.80	0.75
	50	565	296.1	3.08	3.08	-5.82	3.18	-7.26
	70	698	370.0	1.50	1.50	-6.40	1.54	-6.76
2 API=36.5	5	260	126.7	94.40	72.00	95.60	74.20	70.00
	10	282	138.9	13.10	4.50	13.40	5.50	3.80
	20	330	165.6	-22.60	-22.70	-21.40	-22.30	-22.95
	50	467	241.7	-8.84	-14.74	-14.26	-14.62	-45.20
	70	556	291.1	2.41	0.31	-3.26	0.44	-3.79
3 API=27.2	5	290	143.3	68.40	46.60	67.00	48.00	44.80
	10	334	167.8	19.70	11.20	19.10	11.90	10.20
	20	417	213.9	4.85	3.40	5.25	2.55	2.05
	50	648	342.2	3.04	8.22	-2.28	9.02	-4.40
	70	795	423.9	1.13	4.04	-6.06	3.79	-5.57
6 API=40.9	5	260	126.7	26.40	3.60	27.60	5.80	1.80
	10	278	136.7	3.10	-5.50	3.60	-4.50	-6.40
	20	313	156.1	-4.40	-5.45	-3.70	-5.00	-5.90
	50	404	206.7	9.58	5.54	5.78	5.66	5.42
	70	462	238.9	14.91	11.44	10.60	11.40	9.97
7 API=40.8	5	250	121.1	30.40	9.40	30.60	11.40	7.60
	10	269	131.7	7.40	-1.00	7.30	0.00	-1.00
	20	307	152.8	-1.00	-2.80	-0.50	-2.40	-3.15
	50	442	227.8	4.12	1.10	-0.44	1.20	-1.32
	70	544	284.4	9.34	8.23	3.94	8.19	3.34
9 API=28.2	5	450	232.2	59.40	10.80	60.20	13.40	6.60
	10	460	237.8	55.00	30.20	55.00	31.50	28.10
	20	483	250.6	43.05	26.30	42.45	26.65	28.00
	50	558	292.2	19.30	7.22	15.80	7.38	7.78
	70	599	315.0	18.41	10.31	14.26	10.31	10.51
13 API=47.8	10	214	101.1	90.40	82.10	91.60	83.30	80.80
	20	262	127.8	13.75	13.90	14.50	14.40	13.20
	25	285	140.6	-1.08	1.44	0.12	1.80	0.84
	30	295	146.1	3.50	6.10	4.83	6.30	6.13
	35	312	155.6	-1.77	1.97	0.06	2.11	2.29
	50	352	177.8	10.08	8.16	6.22	8.58	8.02
	70	399	203.9	9.10	8.71	4.50	8.77	6.51
14 API=37.0	10	475	246.1	91.10	-10.10	94.60	-8.20	-10.70
	30	501	260.6	-8.37	-43.17	-8.30	-42.73	-41.20
	50	516	268.9	10.20	0.76	9.76	0.96	1.34
	70	532	277.8	24.40	12.37	21.24	12.49	12.80

Continue, **Table I-12** *AD%* for 61 flash data points
(10 petroleum stocks) using modified models No. 2 mode flash methods

Petroleum stock No.	Exp. Flash vol.%	Exp. Flash temp., °F	Exp. Flash temp., °C	*AD%*				
				SRK	SRK + Van	PR	PR + Van	Ideal *K*
16 API=37.3	10	283	139.4	16.90	9.70	16.10	16.80	12.00
	15	317	158.3	10.80	9.87	10.33	10.40	8.27
	20	350	176.7	8.10	8.25	8.05	8.65	6.85
	25	383	195.0	5.68	15.48	6.04	14.68	5.12
	30	425	218.3	-1.93	5.43	-0.17	5.70	-0.27
	35	458	236.7	6.94	9.31	2.89	9.40	1.66
	40	484	251.1	9.13	11.58	4.78	11.73	3.60
	50	566	296.7	3.08	8.76	-2.90	8.56	-3.90
	60	617	325.0	6.68	10.03	0.18	9.90	-0.02
	70	700	371.1	3.23	5.74	-3.87	5.90	-3.53
18 API=42.2	10	300	148.9	95.70	82.90	95.50	84.10	81.30
	15	325	162.8	58.07	50.40	57.27	51.13	49.40
	20	350	176.7	38.70	31.85	37.80	32.05	32.90
	25	371	188.3	29.88	24.92	29.16	25.40	25.80
	30	400	204.4	15.67	13.97	15.30	14.30	13.00
	35	417	213.9	13.86	11.94	13.83	12.14	12.06
	40	442	227.8	12.48	12.78	11.43	12.83	11.00
	50	500	260.0	7.48	3.48	2.30	3.86	0.80
	60	533	278.3	11.77	9.02	6.37	9.12	5.30
	70	583	306.1	11.70	10.19	5.83	10.24	5.39
No. of points(61)			**Average**	**19.90**	**19.90**	**12.92**	**18.31**	**13.50**

Appendix J

Comparison between modified and unmodified acentric factors

Table J-1 Acentric factor Comparison for petroleum stoke No. 2

Cut	*TB*, °C	Lee – Kasler ω	Modified ω
1	160.50	0.2583	0.1669
2	171.08	0.2643	0.1737
3	183.43	0.2716	0.1821
4	197.23	0.2800	0.1918
5	212.18	0.2894	0.2027
6	228.02	0.2996	0.2147
7	244.50	0.3104	0.2275
8	261.42	0.3218	0.2411
9	278.58	0.3337	0.2553
10	295.82	0.3458	0.2700
11	313.01	0.3581	0.2849
12	330.05	0.3705	0.3001
13	346.84	0.3830	0.3155
14	363.36	0.3954	0.3309
15	379.56	0.4078	0.3463
16	395.44	0.4201	0.3618
17	411.04	0.4324	0.3772
18	426.41	0.4446	0.3927
19	441.63	0.4569	0.4084
20	456.81	0.4694	0.4243
21	472.08	0.4821	0.4406
22	487.60	0.4951	0.4574
23	503.58	0.5088	0.4751
24	520.21	0.5232	0.4938
25	537.75	0.5386	0.5139
26	556.46	0.5554	0.5357
27	576.64	0.5738	0.5598
28	598.61	0.5942	0.5866
29	622.71	0.6171	0.6168
30	649.35	0.6430	0.6509
31	678.90	0.8358	0.8263
32	711.82	0.8814	0.8779
33	748.54	0.9334	0.9369
34	789.56	0.9871	1.0044
35	835.38	1.0481	1.0819
36	886.53	1.1154	1.1707
37	943.60	1.1892	1.2725
38	1007.18	1.2698	1.3891
39	1077.88	1.3574	1.5221
40	1156.35	1.4522	1.6728

Table J-2 Acentric factor Comparison for petroleum stoke No. 3

Cut	*TB*, °C	Lee – Kasler *ω*	Modified *ω*
1	150.39	0.2507	0.1576
2	180.69	0.2679	0.1772
3	211.98	0.2870	0.1994
4	243.92	0.3077	0.2238
5	276.23	0.3295	0.2499
6	308.62	0.3523	0.2775
7	340.87	0.3757	0.3062
8	372.75	0.3995	0.3358
9	404.09	0.4236	0.3661
10	434.72	0.4479	0.3968
11	464.52	0.4721	0.4278
12	493.38	0.4961	0.4588
13	521.25	0.5199	0.4897
14	548.07	0.5434	0.5204
15	573.84	0.5665	0.5507
16	598.57	0.5892	0.5806
17	622.29	0.6115	0.6100
18	645.10	0.6333	0.6389
19	667.08	0.8132	0.8016
20	688.36	0.8421	0.8345
21	709.11	0.8706	0.8670
22	729.52	0.8991	0.8994
23	749.79	0.9278	0.9320
24	770.17	0.9538	0.9652
25	790.92	0.9816	0.9995
26	812.37	1.0102	1.0354
27	834.82	1.0399	1.0735
28	858.65	1.0712	1.1144
29	884.24	1.1046	1.1590
30	911.98	1.1406	1.2079
31	942.36	1.1796	1.2623
32	975.82	1.2221	1.3232
33	1012.86	1.2686	1.3915
34	1054.02	1.3196	1.4686
35	1099.86	1.3756	1.5557
36	1150.96	1.4370	1.6541
37	1207.94	1.5041	1.7649
38	1271.44	1.5772	1.8890
39	1342.14	1.6566	2.0269
40	1420.73	1.7424	2.1779

Table J-3 Acentric factor Comparison for petroleum stoke No. 6

Cut	*TB*, °C	Lee – Kasler ω	Modified ω
1	143.66	0.2563	0.1668
2	156.28	0.2633	0.1747
3	170.77	0.2717	0.1842
4	186.72	0.2813	0.1952
5	203.75	0.2920	0.2076
6	221.52	0.3035	0.2210
7	239.72	0.3157	0.2353
8	258.09	0.3283	0.2503
9	276.36	0.3411	0.2656
10	294.36	0.3541	0.2812
11	311.91	0.3670	0.2968
12	328.87	0.3797	0.3123
13	345.15	0.3920	0.3275
14	360.67	0.4040	0.3423
15	375.41	0.4156	0.3566
16	389.38	0.4267	0.3704
17	402.61	0.4374	0.3838
18	415.17	0.4476	0.3967
19	427.18	0.4575	0.4091
20	438.77	0.4672	0.4214
21	450.12	0.4768	0.4335
22	461.44	0.4864	0.4458
23	472.98	0.4964	0.4585
24	485.02	0.5069	0.4719
25	497.87	0.5182	0.4865
26	511.89	0.5307	0.5026
27	527.46	0.5448	0.5208
28	544.99	0.5610	0.5416
29	564.94	0.5797	0.5659
30	587.80	0.6016	0.5943
31	614.09	0.6274	0.6279
32	644.37	0.6581	0.6677
33	679.23	0.8593	0.8490
34	719.28	0.9165	0.9129
35	765.22	0.9791	0.9882
36	817.71	1.0504	1.0769
37	877.48	1.1303	1.1809
38	945.33	1.2192	1.3027
39	1022.00	1.3173	1.4445
40	1108.40	1.4247	1.6085

Table J-4 Acentric factor Comparison for petroleum stoke No. 7

Cut	*TB*, °C	Lee – Kasler *ω*	Modified *ω*
1	129.35	0.2530	0.1644
2	147.77	0.2627	0.1752
3	166.25	0.2733	0.1872
4	184.74	0.2845	0.2000
5	203.15	0.2962	0.2134
6	221.44	0.3082	0.2274
7	239.56	0.3205	0.2418
8	257.48	0.3329	0.2566
9	275.19	0.3455	0.2716
10	292.67	0.3583	0.2869
11	309.93	0.3711	0.3024
12	326.99	0.3840	0.3181
13	343.88	0.3971	0.3340
14	360.64	0.4102	0.3502
15	377.31	0.4235	0.3667
16	393.97	0.4371	0.3835
17	410.69	0.4509	0.4007
18	427.56	0.4650	0.4185
19	444.68	0.4796	0.4369
20	462.17	0.4948	0.4561
21	480.14	0.5106	0.4763
22	498.73	0.5273	0.4976
23	518.10	0.5451	0.5203
24	538.40	0.5640	0.5447
25	559.79	0.5844	0.5710
26	582.48	0.6066	0.5995
27	606.64	0.6308	0.6307
28	632.51	0.6574	0.6650
29	660.27	0.8452	0.8314
30	690.18	0.8879	0.8787
31	722.46	0.9335	0.9308
32	757.39	0.9820	0.9884
33	795.24	1.0341	1.0521
34	836.27	1.0899	1.1227
35	880.77	1.1496	1.2009
36	929.05	1.2134	1.2877
37	981.42	1.2815	1.3838
38	1038.20	1.3539	1.4900
39	1099.75	1.4308	1.6070
40	1166.42	1.5122	1.7351

Table J-5 Acentric factor Comparison for petroleum stoke No. 9

Cut	*TB*, °C	Lee – Kasler ω	Modified ω
1	267.92	0.3240	0.2434
2	310.60	0.3539	0.2795
3	348.62	0.3816	0.3136
4	382.22	0.4070	0.3452
5	411.70	0.4299	0.3740
6	437.35	0.4503	0.3999
7	459.47	0.4682	0.4229
8	478.33	0.4838	0.4429
9	494.26	0.4972	0.4602
10	507.53	0.5085	0.4748
11	518.47	0.5179	0.4870
12	527.37	0.5256	0.4971
13	534.55	0.5319	0.5053
14	540.34	0.5369	0.5119
15	545.04	0.5411	0.5174
16	548.99	0.5446	0.5219
17	552.51	0.5477	0.5260
18	555.94	0.5508	0.5300
19	559.60	0.5541	0.5343
20	563.84	0.5579	0.5393
21	569.01	0.5625	0.5454
22	575.45	0.5684	0.5531
23	583.50	0.5757	0.5628
24	593.53	0.5849	0.5749
25	605.89	0.5964	0.5901
26	620.94	0.6106	0.6088
27	639.05	0.6279	0.6317
28	660.60	0.8050	0.7922
29	685.94	0.8393	0.8312
30	715.46	0.8800	0.8776
31	749.55	0.9281	0.9322
32	788.57	0.9791	0.9962
33	832.94	1.0380	1.0709
34	883.02	1.1037	1.1575
35	939.23	1.1762	1.2574
36	1001.94	1.2556	1.3719
37	1071.60	1.3419	1.5025
38	1148.56	1.4348	1.6501
39	1233.28	1.5342	1.8151
40	1326.13	1.6396	1.9965

Table J-6 Acentric factor Comparison for petroleum stoke No. 13

Cut	*TB*, °C	Lee – Kasler ω	Modified ω
1	100.38	0.2375	0.1471
2	117.40	0.2448	0.1547
3	134.44	0.2531	0.1638
4	151.47	0.2623	0.1740
5	168.40	0.2720	0.1850
6	185.21	0.2822	0.1966
7	201.84	0.2926	0.2087
8	218.25	0.3032	0.2211
9	234.42	0.3140	0.2338
10	250.29	0.3249	0.2466
11	265.86	0.3358	0.2595
12	281.08	0.3466	0.2725
13	295.94	0.3574	0.2855
14	310.42	0.3681	0.2985
15	324.52	0.3787	0.3113
16	338.22	0.3891	0.3241
17	351.52	0.3994	0.3367
18	364.42	0.4095	0.3491
19	376.93	0.4194	0.3614
20	389.04	0.4291	0.3735
21	400.78	0.4386	0.3854
22	412.17	0.4480	0.3971
23	423.21	0.4571	0.4086
24	433.94	0.4661	0.4199
25	444.39	0.4749	0.4311
26	454.59	0.4836	0.4422
27	464.57	0.4922	0.4531
28	474.38	0.5008	0.4640
29	484.06	0.5093	0.4749
30	493.67	0.5178	0.4858
31	503.25	0.5264	0.4968
32	512.87	0.5351	0.5079
33	522.58	0.5439	0.5193
34	532.45	0.5530	0.5310
35	542.55	0.5624	0.5432
36	552.96	0.5722	0.5558
37	563.75	0.5825	0.5690
38	575.01	0.5933	0.5830
39	586.82	0.6048	0.5979
40	599.27	0.6170	0.6138

Table J-7 Acentric factor Comparison for petroleum stoke No. 14

Cut	*TB*, °C	Lee – Kasler *ω*	Modified *ω*
1	397.76	0.4461	0.3948
2	396.98	0.4455	0.3940
3	399.76	0.4478	0.3969
4	405.39	0.4525	0.4028
5	413.27	0.4592	0.4111
6	422.82	0.4673	0.4213
7	433.50	0.4765	0.4328
8	444.86	0.4864	0.4452
9	456.48	0.4966	0.4581
10	468.00	0.5069	0.4711
11	479.10	0.5168	0.4838
12	489.53	0.5263	0.4958
13	499.08	0.5351	0.5070
14	507.61	0.5430	0.5171
15	515.01	0.5500	0.5259
16	521.26	0.5559	0.5334
17	526.34	0.5607	0.5396
18	530.33	0.5645	0.5444
19	533.33	0.5673	0.5481
20	535.53	0.5694	0.5508
21	537.13	0.5710	0.5528
22	538.42	0.5722	0.5543
23	539.72	0.5735	0.5559
24	541.41	0.5751	0.5580
25	543.92	0.5775	0.5611
26	547.75	0.5813	0.5659
27	553.43	0.5868	0.5730
28	561.56	0.5948	0.5832
29	572.77	0.6059	0.5975
30	587.78	0.6210	0.6168
31	607.32	0.6411	0.6425
32	632.22	0.6673	0.6761
33	663.33	0.8603	0.8464
34	701.55	0.9158	0.9075
35	747.86	0.9805	0.9836
36	803.27	1.0572	1.0773
37	868.84	1.1464	1.1918
38	945.71	1.2486	1.3305
39	1035.05	1.3640	1.4966
40	1138.09	1.4925	1.6929

Table J-8 Acentric factor Comparison for petroleum stoke No. 16

Cut	*TB*, °C	Lee – Kasler *ω*	Modified *ω*
1	101.43	0.2894	0.2160
2	135.15	0.2552	0.1666
3	167.82	0.2674	0.1787
4	199.46	0.2849	0.1984
5	230.07	0.3044	0.2212
6	259.71	0.3248	0.2454
7	288.41	0.3457	0.2706
8	316.19	0.3667	0.2962
9	343.10	0.3878	0.3220
10	369.19	0.4088	0.3481
11	394.50	0.4298	0.3743
12	419.10	0.4507	0.4005
13	443.04	0.4716	0.4269
14	466.41	0.4924	0.4534
15	489.24	0.5133	0.4800
16	511.64	0.5343	0.5069
17	533.68	0.5555	0.5340
18	555.43	0.5769	0.5616
19	576.99	0.5987	0.5896
20	598.46	0.6210	0.6182
21	619.93	0.6439	0.6477
22	641.50	0.6677	0.6781
23	663.29	0.8519	0.8384
24	685.40	0.8852	0.8750
25	707.95	0.9198	0.9130
26	731.07	0.9536	0.9526
27	754.88	0.9891	0.9942
28	779.51	1.0257	1.0379
29	805.10	1.0637	1.0841
30	831.80	1.1032	1.1332
31	859.73	1.1445	1.1853
32	889.05	1.1877	1.2409
33	919.94	1.2330	1.3003
34	952.52	1.2805	1.3637
35	986.97	1.3305	1.4315
36	1023.47	1.3829	1.5040
37	1062.18	1.4381	1.5813
38	1103.28	1.4960	1.6637
39	1146.96	1.5568	1.7509
40	1193.42	1.6206	1.8428

Table J-9 Acentric factor Comparison for petroleum stoke No. 18

Cut	*TB*, °C	Lee – Kasler ω	Modified ω
1	161.84	0.3272	0.2575
2	191.11	0.2982	0.2178
3	218.66	0.3100	0.2302
4	244.58	0.3254	0.2479
5	268.96	0.3419	0.2673
6	291.92	0.3584	0.2872
7	313.56	0.3748	0.3070
8	333.99	0.3908	0.3265
9	353.34	0.4064	0.3456
10	371.69	0.4216	0.3643
11	389.18	0.4363	0.3826
12	405.92	0.4507	0.4005
13	422.04	0.4648	0.4182
14	437.66	0.4788	0.4357
15	452.90	0.4927	0.4532
16	467.91	0.5067	0.4709
17	482.82	0.5209	0.4889
18	497.75	0.5355	0.5073
19	512.84	0.5506	0.5265
20	528.25	0.5665	0.5466
21	544.10	0.5833	0.5678
22	560.55	0.6013	0.5906
23	577.73	0.6207	0.6150
24	595.82	0.6419	0.6415
25	614.96	0.6651	0.6705
26	635.30	0.6908	0.7023
27	657.00	0.8744	0.8583
28	680.23	0.9130	0.8992
29	705.15	0.9532	0.9439
30	731.93	0.9964	0.9927
31	760.73	1.0428	1.0461
32	791.72	1.0925	1.1044
33	825.09	1.1457	1.1681
34	861.01	1.2025	1.2375
35	899.66	1.2631	1.3129
36	941.21	1.3276	1.3947
37	985.85	1.3959	1.4828
38	1033.78	1.4682	1.5772
39	1085.19	1.5444	1.6775
40	1140.27	1.6245	1.7829

الخلاصة

تعتبر حسابات حاله الاتزان للبخار و السائل للمقاطع النفطية مهمة جدا لعمليات التصميم و التشغيل للمعدات النفطية. و من أهم هذه الحسابات هو استنباط منحني التقطير ألاتزاني (Flash vaporization curve) من منحني درجات الغليان الحقيقية للنفط الخام (True boiling point curve) و ذلك بواسطة طريقتين: الأولى و هي الطرق التخطيطية (Graphical methods) و الثانية و هي تقسم النفط الخام إلى مركبات كاذبة أو الطريقة ألحاسوبيه (Pseudo – components (computer) methods).

تم تقسيم الغرض من الدراسة المقدمة إلى قسمين: القسم الأول و يتضمن جزئين حيث تم في الجزء الأول اختيار و فحص طريقه تخطيطية واحده و عدد من طرق تقسيم النفط الخام إلى مركبات كاذبة أو الطرق ألحاسوبيه لمعرفه أيهم ذات أداء أفضل بينما يتضمن الجزء الثاني دراسة تطبيق عدد من الطرق لغرض تحسين دقه الطرق المختارة في استنباط منحني التقطير ألاتزاني. لقد تم في القسم الأول لهذه الدراسة اختيار الطريقة التخطيطية لـ Raizi – Daubert (RD graph) و خمسه من طرق تقسيم النفوط الخام إلى مركبات كاذبة و تشمل هذه الطرق استخدام طريقه معادله الحالة لـ Soave – Redlich – Kowng (SRK) و طريقه معادله الحالة لـ Peng – Robinson (PR) و كذلك طرق استخدام معامل الفعالية و المتضمن استخدام معادلتي الحالة لـ (SRK) و (PR) لطور البخار، بينما تم استخدام نموذج (van – Laar) لطور السائل (PR + Van و SRK + Van)، و أخيرا تم استخدام طريقه المحاليل المثالية لثابت التوازن (Ideal K). و لغرض إنجاز القسم الأول من الدراسة تم تجميع البيانات اللازمة لـ 18 نفط خام من المصادر العلمية و تشمل هذه البيانات على كلا من منحنيات درجات الحرارة الحقيقية و منحنيات التقطير ألاتزاني و منحنيات الكثافة النوعية (Specific gravity) لهذه النفوط المستخدمة. لقد دلت نتائج القسم الأول من هذا البحث على إن معادله المحاليل المثالية (Ideal K) المطورة اعتمادا على النموذج الجديد و المقترح في هذا

البحث لحساب الضغط البخاري (Vapor pressure) هو أفضل طريقه لاحتساب منحنى التقطير ألاتزاني للنفوط المستخدمة حيث أخذت معادله الضغط البخاري الشكل الآتي:

$$ln\,P^{s} = ln\,P^{sA} + \left(Sp.gr - Sp.gr^{A}\right)F_{1}F_{2} + \left(1 - \frac{0.85}{TBr}\right)$$

و كان معدل الانحراف المطلق ($AAD\%$) لمعادله المحاليل المثالية المطورة يساوي 15.62% مقارنه بقيم معدل الانحراف المطلق للطرق غير المعدلة و البالغة 23.51% و 24.98% و 23.40% و 25.18% و 23.73% و 21.81% لكل من طريقه SRK و SRK + Van و PR و PR + Van و Ideal K و RD graph و حسب الترتيب.

إن استخدام معادله (Ideal K) المطورة أدى إلى تحسين معدل الانحراف المطلق لعشره من النفوط المستخدمة و بواقع أكثر من 30%. إن التحسينات في أداء هذه الطريقة مرتبط إلى حد كبير بعدم دقه النتائج ألمختبريه (قياس منحني درجات الغليان الحقيقية) و كذلك عدم دقه احتساب الخواص الفيزياويه مثل درجه الحرارة الحرجة و الضغط الحرج و ω ... الخ للمقاطع النفطية.

يتضمن القسم الثاني من الدراسة المقدمة استخدام معادله (Ideal K) المطورة لاحتساب منحنيات التقطير ألاتزاني و درجات حرارة التبخير (Flash zone temperatures) لأربعه أنواع نفط عراقية و هي كركوك و البصرة و جمبور و باي حسن حيث تم الحصول على منحنى درجات الغليان الحقيقية و منحنى الكثافة النوعية لهذه الأنواع تجريبيا مستخدما منظومة التقطير ألمختبريه في مصفى الدورة. لقد كانت نتائج درجات حرارة التبخير لهذه النفوط كالتالي 318 °م و 327 °م و 335 °م و 290 °م لنفط كركوك و البصرة و جمبور و باي حسن على الترتيب. إن قيم هذه الدرجات الحرارية أعلاه تعتبر أوليه حيث يجب تعديلها وفقا لدرجه حرارة و ضغط و كميه بخار الماء (Stripping steam) المستخدم عاده في برج تقطير النفط الخام.

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عدي عامر فاضل

دراسة اتزان بخار – سائل للمقاطع النفطية

أطروحة
مقدمة إلى كلية الهندسة في جامعة النهرين
و هي جزء من متطلبات نيل درجة دكتوراه فلسفة
في الهندسة الكيمياوية

من قبل
عدي عامر فاضل الزبيدي
بكالوريوس 1995
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