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SCALING DOWN OF PETROLEUM DISTILLATION SIMULATION

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งานวิจัยนี้ได้ทำการจำลองการกลั่นปิโตรเลียม ซึ่งสมบัติทางด้านเทอร์โมไดนามิกส์ได้จากคำนวณโดยใช้สมการหลักอ้างอิงของ โซฟ-เรดลิช-กวอง เทคนิคการแก้สมการของแบบจำลองสามารถแก้สมการได้โดยใช้วิธีเมตริกซ์ วัตถุประสงค์ของงานวิจัยเพื่อทำการศึกษาวิธีในการลดเวลาที่ใช้ในการจำลองการกลั่นปิโตรเลียม ดังนั้นจึงได้ทำการพัฒนาเทคนิคที่ใช้องค์ประกอบเทียมรวม (combined pseudocomponent) หลักการของเทคนิคนี้ คือ จะมีการคำนวณค่าอุณหภูมิหอกลั่นเป็นลำดับแรก จากนั้นจึงคำนวณหาค่าของสัดส่วนโมลได้เป็นลำดับต่อไปนอกจากนี้ยังได้เสนออีกเทคนิคหนึ่งที่ใช้องค์ประกอบเทียมรวมเบาและองค์ประกอบเทียมรวมหนักในการคำนวณ

เวลาที่ใช้ในการจำลองการกลั่นโดยใช้เทคนิคที่พัฒนาขึ้นมานี้สามารถจำลองการกลั่นได้โดยใช้เวลาเพียง 11 เปอร์เซ็นต์ของเวลาที่ใช้ในการจำลองการกลั่นแบบปกติ งานวิจัยนี้แสดงให้เห็นว่า กฎการผสมของเค (Kay’s rules) สามารถนำมาใช้เพื่อคำนวณหาค่าคุณสมบัติขององค์ประกอบเทียมรวมได้

ภาควิชา วิศวกรรมเคมี

สาขาวิชา วิศวกรรมเคมี

ปีการศึกษา 2543

ลายมือชื่อนิสิต ....

ลายมือชื่ออาจารย์ที่ปรึกษา ....

ลายมือชื่ออาจารย์ที่ปรึกษาร่วม ....

4270452821 : MAJOR CHEMICAL ENGINEERING

KEY WORD: PETROLEUM FRACTION / DISTILLATION / SRK EQUATION / SIMULATION

PATCHAREE WONGJIRASAWAD : SCALING DOWN OF PETROLEUM DISTILLATION SIMULATION. THESIS ADVISOR : ASSOC. PROF. KROEKCHAI SUKANJANAJTEE, Ph.D., 119 pp. ISBN 974-13-0446-3.

Petroleum distillation simulation was performed in this work based on thermodynamic properties generated by Soave-Redlich-Kwong equation. The mathematic model of petroleum distillation was solved by tridiagonal matrix method. The objective of this work is to reduce the simulation time. It is accomplished by using combined pseudocomponents. The temperature profile of the distillation column is determined first, and then the product mole fractions are determined. In addition, another technique using light and heavy combined pseudocomponents is proposed.

The simulation time using the combined pseudocomponents technique is only about 11 percent that of normal technique. It was shown that the Kay's rules could be used for determining the properties of combined pseudocomponents.

Department………Chemical Engineering………… Student's signature ……………………………………..
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NOMENCLATURES

Latin Capital and Lowercase Letters

A, B	Parameters in Soave-Redlich-Kwong equation
B	Bottom flow rate
a, b	Constants in Soave-Redlich-Kwong equation
C	Number of component in a mixture
C_p	Molal specific heat
CP	Combined pseudocomponent
D	Distillate flow rate
F	Feed flow rate
H	Vapor enthalpy per mole
h	Liquid enthalpy per mole
K	Vapor-liquid equilibrium ratio, Watson Characterization Factor
k	A binary interaction parameter between each of components
L	Liquid flow rate
MW	Molecular weight
n	Number of mole, number of component
N	Number of stage
P	Pressure
Q	Heat transfer rate, intercooler or interheater sidestream
R	Universal gas constant
S	Sidestream flow rate
T	Temperature
U	Internal energy, liquid sidestream
V	Vapor flow rate, volume
v	Specific volume
W	Vapor sidestream
x	Mole fraction in liquid phase
y	Mole fraction in vapor phase

Z	Compressibility factor
z	Mole fraction

Greek Letters

ω	Acentric factor
ρ	Density
f	Fugacity
ϕ	Fugacity coefficient of a component in mixture

Subscripts

B	Boiling point
C	Critical point
D	Distillate
F	Feed
G	Gas
L	Liquid phase
V	Vapor phase
i, j	Particular component i in a stream leaving stage j
j	j^{th} stage
50	mid-volume boiling point

CHAPTER 1

INTRODUCTION

It is apparent that distillation is the most prominent separation process used particularly in the petroleum refining process. The refining of petroleum involved simple fractionation of the constituents already present in the crude oil. Simulation renders a convenient method for designing and studying the performance of a distillation solution.

In the petroleum industries operation of large entity, heat energy and material balances are of most importance in keeping a rigid control of all steps in the processing. Thus, computer simulation can help to solve manufacturing and material handing problems. Furthermore, by using mathematical methods to generate streams of pseudo-random numbers, it is possible to allow for the random variations that occur everywhere in real life because the ability to allow for randomness is one of the great strength of simulation. Thus, it is cheaper and safer to learn from mistakes made with a simulated system than to make them for real. Simulation can reduce cost, reduce risk, and improve your understanding of the system under study.

Soave-Redlich-Kwong equation can be used to generate thermodynamic properties of petroleum fractions for simulation. In the petroleum simulation, no less than 20 pseudocomponents are required for describing the petroleum mixture. Successive iterations are required in petroleum distillation calculation. Consequently, petroleum distillation simulation is relatively time consuming. It is desirable that simulation results can be obtained instantly. Therefore, the mission of this work is to scale down the calculating task so that simulation can be done in short time.

1.1 Objective of This Work

To develop method of petroleum distillation simulation that requires a short calculating time

1.2 Scope of This Work

1. Thermodynamic properties of petroleum fractions will be based on Soave-Redlich-Kwong Equation.
2. Study property of combined pseudocomponents.
3. Study different choice of component groupings for distillation simulation.
4. Develop a computer program for petroleum distillation simulation that fulfils the stated objective.

CHAPTER 2

DISTILLATION SIMULATION

2.1 Distillation

Distillation is the separation of substances that have different vapor pressure at any given temperature and based upon “ volatility “ which the process stream may be separated by distillation into a more volatile, “lighter component” and a less volatile,” heavier component”. Now, the operations have been almost entirely superseded by continuous distillation. The present system involves heating the crude by pumping it through tubes placed inside a furnace (tube still) and then allowing it to vaporize in a fractionating column, which is tapped at several point, allowing continuous side draw of the various boiling “ fraction”, or product. The residuum withdrawn from the bottom of the column may be subjected to a vacuum or steam distillation.

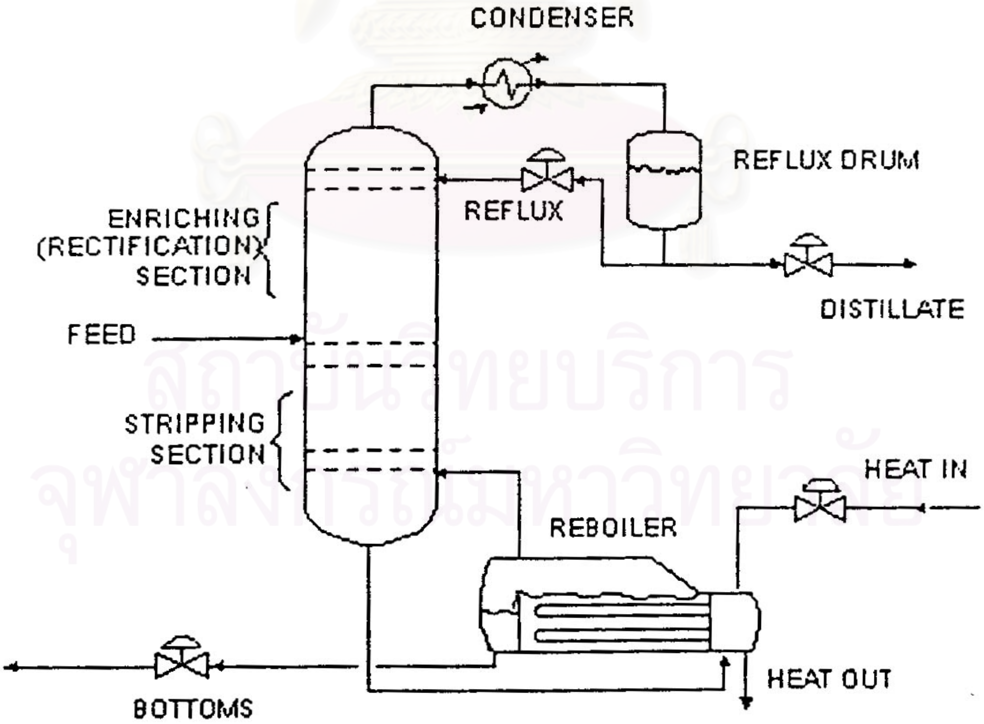


Figure 2.1 A Schematic of a Typical Distillation Unit

As indicated in Figure 2.2, the overhead vapor V_1, upon leaving the top plate enters the condenser where it is either partially or totally condensed. The liquid formed is collected in an accumulator from which the liquid stream L_0 (called reflux) and the top product stream D (called the distillated) are withdrawn. When the overhead vapor V_1 is totally condensed to the liquid state and the distillate D is withdrawn as a liquid, the condenser is called a total condenser. If V_1 is partially condensed to the liquid state to produce the reflux L_0 and the distillate D is withdrawn as a vapor, the condenser is called a partial condenser. The amount of liquid reflux is commonly expressed in terms of the reflux ratio, L_0/D. Although the internal liquid to vapor ratio, L/V, is sometimes referred to as the internal reflux ratio, the term reflux ratio will be reserved here in to mean L_0/D.

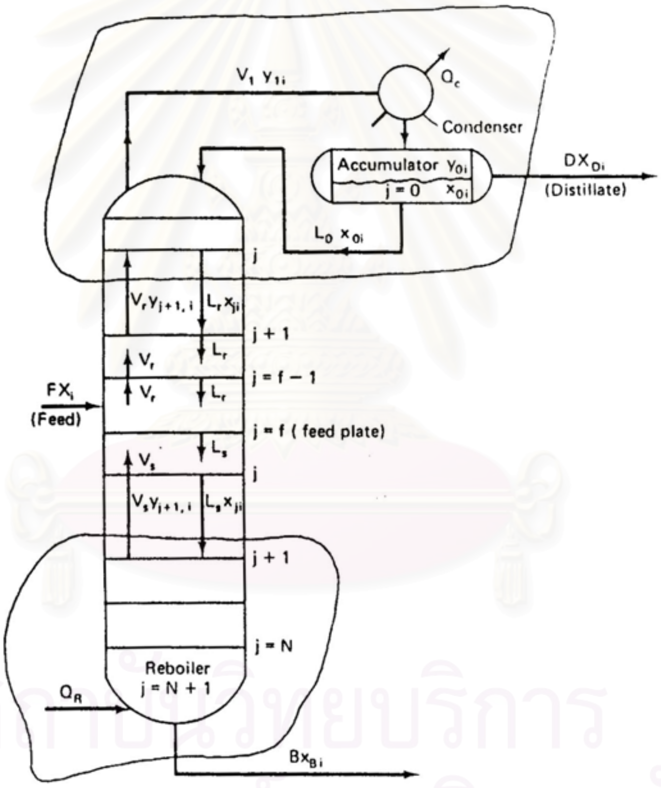


Figure 2.2 Sketch of a Conventional Column Distillation

The liquid that leaves the bottom plate of the column enters the reboiler, where it is partially vaporized. The vapor produced is allowed to flow back up through the column, and the liquid is withdrawn from the reboiler and called the bottom product B.

2.2 Distillation Model

The MESH Equations

To compute the composition of the top product D and the bottom product B which may be expected by use of a given distillation column operated at a given set of conditions, it is necessary to obtain a solution to the following equations:

- Equilibrium relationships
- Component-material balances
- Total-material balances
- Enthalpy balances

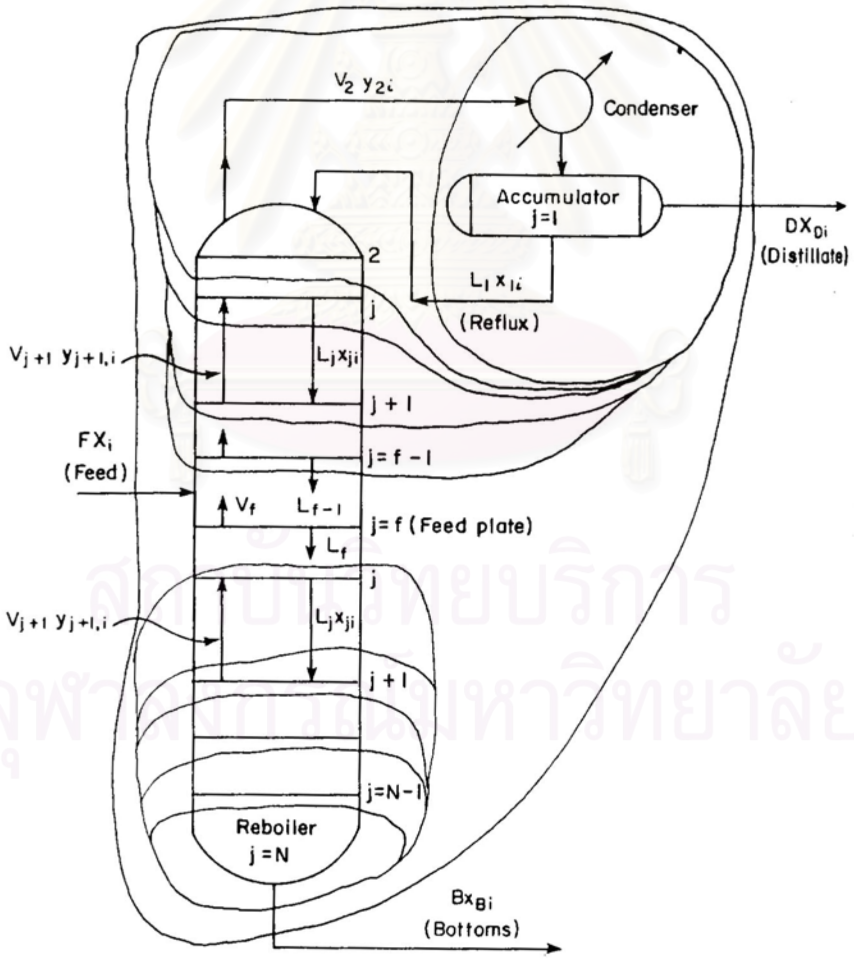


Figure 2.3 Representation of The Component-Material Balances

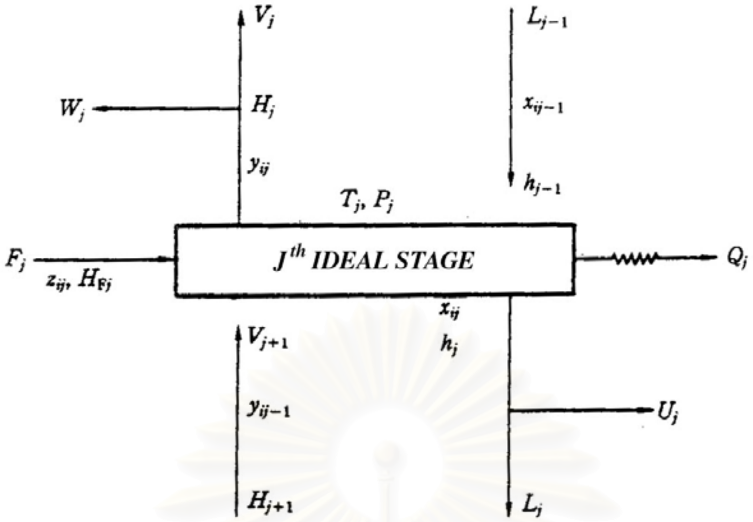


Figure 2.4 An Ideal Equilibrium Stage is Represented by The Mesh Equations

In the description of this process, the mole fraction of the most volatile component in the feed is represented by X, in the distillate by X_D, and in the bottoms by X_B. The subscript j is used as the counting integer for the number of the plates. Since the distillate is withdrawn from the accumulator (j=0) and the bottoms is withdrawn from the reboiler (j=N+1), the mole fractions in the distillate and bottoms have double representation, that is, $X_{Di} = x_{0i}$ (for a column having a total condenser) and $x_{Bi} = x_{N+1,i}$. When the column has a partial condenser (D is withdrawn as a vapor), $X_{Di} = y_{0i}$.

The rectifying section consists of the partial or total condenser and all plates down to the feed plate. The stripping section consists of the feed plate and all plates below it, including the reboiler. When the total flow rates do not vary from plate to plate within each section of the column, they are denoted by V_r (vapor) and L_r (liquid) in the rectifying section and by V_s and L_s in the stripping section. The feed rate (F), distillate rate (D), bottoms rate (B), and reflux rate (L_0) are all expressed in moles per unit time.

To find the compositions of the top and bottom products, the set of equations required to represent such a system is as follows:

Material balances (M-Equation)

$$V_{j+1}y_{j+1,i} = L_jX_{ji}+DX_{DI} \qquad ,1 \leq i \leq m,\ 0 \leq j \leq f\text{-}2 \tag{2-1}$$

$$V_fy_{fi}+V_Fy_{Fi} = L_{f-1}x_{f-1,i}+DX_{Di} \qquad ,1 \leq i \leq m \tag{2-2}$$

$$V_{j+1}y_{j+1,i} = L_jX_{ji}-BX_{BI} \qquad ,1 \leq i \leq m,\ f \leq j \leq N \tag{2-3}$$

$$FX_i = DX_{Di}+Bx_{Bi} \qquad ,1 \leq i \leq m \tag{2-4}$$

Equilibrium relationships (E-Equation)

$$y_{ji} = K_{ji}x_{ji} \qquad ,1 \leq i \leq m,\ \ 0 \leq j \leq N+1 \tag{2-5}$$

Component-material balances (S-Equation)

$$\sum_{i=1}^{m} y_{ji} = 1 \qquad ,0 \leq j \leq N+1 \tag{2-6}$$

$$\sum_{i=1}^{m} x_{ji} = 1 \qquad ,0 \leq j \leq N+1 \tag{2-7}$$

Enthalpy balances (H-Equation)

$$V_{j+1}H_{j+1} = L_jh_j+DH_D+Q_c \qquad ,0 \leq j \leq f\text{-}2 \tag{2-8}$$

$$V_fH_f+V_FH_F = L_{f-1}h_{f-1}+DH_D+Q_c \qquad ,f \leq j \leq N \tag{2-9}$$

$$V_{j+1}H_{j+1} = L_jh_j-Bh_B+Q_R \qquad ,f \leq j \leq N \tag{2-10}$$

$$FH = DH_D+Bh_B+Q_c-Q_R \qquad ,f \leq j \leq N \tag{2-11}$$

As in the case of the material balances for any one component, the number of independent energy balances is equal to the number of stages (j=0, 1, 2, … N, N+1). In this case the total number of independent equations is equal to (2m+3)(N+2). The enthalpy per mole of vapor and the enthalpy per mole of liquid leaving plate j are given by the following expressions (upper bar indicates a partial molar enthalpy).

$$H_j = \sum_{i=1}^{m} \overline{H}_{ji} y_{ji} \qquad \text{(vapor)} \qquad 2\text{-}12$$

$$h_j = \sum_{i=1}^{m} \overline{h}_{ji} x_{ji} \qquad \text{(liquid)} \qquad 2\text{-}13$$

where the enthalpy of each pure component i in the vapor and liquid streams leaving plate j are represented by H_{ji} and h_{ji}, respectively. These enthalpies are evaluated at the temperature and pressure of plate j. This meaning of H_D depends on the condenser used. For a total condenser (D is withdrawn from the accumulator as a liquid at its bubble point temperature T_0 at the column pressure, and $y_{ji}=x_{0i}=X_{Di}$),

$$H_D = \sum_{i=1}^{m} \overline{h}_{0i} X_{Di} = \sum_{i=1}^{m} \overline{h}_{0i} x_{0i} = h_o \qquad 2\text{-}14$$

For a partial condenser (D is withdrawn from the accumulator as a vapor at its dew point temperature T_0 at the column pressure, and $y_{0i}=X_{Di}$)

$$H_D = \sum_{i=1}^{m} \overline{H}_{0i} X_{Di} = \sum_{i=1}^{m} \overline{H}_{0i} y_{0i} = H_o \qquad 2\text{-}15$$

The enthalpy per mole of bottoms has double but equivalent representation, h_B and h_{N+1}, that is,

$$h_B = \sum_{i=1}^{m} \overline{h}_{Bi} x_{Bi} = \sum_{i=1}^{m} \overline{h}_{N+1,i} x_{N+1,i} = h_{N+1} \qquad 2\text{-}16$$

The symbols Q_c and Q_R are used to denote the condenser and reboiler duties, respectively. The condenser duty Q_c is equal to the net amount of heat removed per unit time by the condenser and the reboiler duty Q_R is equal to the net amount of heat introduced to the reboiler per unit time.

2.3 The Tridiagonal Matrix Method for Solving The MESH Equations [7]

Equilibrium relationships and material balances in distillation model are now combined and the L's are expressed as functions of V's by an overall material balance of all stages from the condenser through the j^{th} stage.

$$L_j = V_{j+1} + \sum_{k=2}^{j}(F_k - W_k - U_k) - D \qquad ,2 \le j \le n\text{-}1 \qquad 2\text{-}17$$

where,

$$D = V_1 + U_1 \qquad 2\text{-}18$$

The M-equation is then reduced to a tridiagonal matrix form,

$$B_1 x_{i1} + C_1 x_{i2} = D_1 \qquad 2\text{-}19$$

$$A_j x_{I,\,j\text{-}1} + B_j x_{ij} + C_j x_{I,\,j+1} = D_j \qquad ,2 \le j \le n\text{-}1 \qquad 2\text{-}20$$

$$A_n x_{I,\,n\text{-}1} + B_n x_{in} = D_n \qquad 2\text{-}21$$

or in matrix notation as,

$$\begin{bmatrix} B_1 & C_1 & & \\ A_2 & B_2 & C_2 & \\ & A_j & B_j & C_j \\ & A_{n-1} & B_{n-1} & C_{n-1} \\ & A_n & B_n & \end{bmatrix} \begin{bmatrix} X_{i1} \\ X_{i2} \\ X_{ij} \\ X_{i,\,n-1} \\ X_{in} \end{bmatrix} = \begin{bmatrix} D_1 \\ D_2 \\ D_j \\ D_{n-1} \\ D_n \end{bmatrix} \qquad 2\text{-}22$$

or simply,

$$[A_{Bc}]\{x_{ij}\} = \{D_j\} \qquad ,1 \le i \le m \qquad 2\text{-}23$$

where

$$B_1 = \text{-}(V_j K_{i1} + U_1) \ ; \ C_1 = V_2 K_{i2} \ ; \ D_1 = 0 \qquad 2\text{-}24$$

$$A_j = L_{j\text{-}1} = V_j + \sum_{k=2}^{j-1}(F_k - W_k - U_k) - D \qquad ,2 \le j \le n\text{-}1 \qquad 2\text{-}25$$

$$B_j = -[\,(V_j + W_j)K_{ij} + (L_j + U_j)\,]$$

$$= -[\,(V_j + W_j)K_{ij} + V_{j+1} + \sum_{k=2}^{j}(F_k - W_k - U_k) - D + U_j\,] \quad ,2 \leq j \leq n\text{-}1 \qquad 2\text{-}26$$

$$C_j = V_{j+1}K_{i,\,j+1} \qquad ,2 \leq j \leq n\text{-}1 \qquad 2\text{-}27$$

and

$$A_n = V_n + B \;;\; B_n = -(\,V_nK_{in} + B\,) \;;\; D_n = 0 \qquad 2\text{-}28$$

With the above manipulation of the M and E equations and further manipulations of the S and H equations, the MESH equations for multi-component separation at constant pressure in a complex column become,

$$M_{ij}(x_{ij},V_j,T_j) = [A_{Bc}]\,\{x_i\} - \{D\} = 0 \qquad ,1 \leq i \leq m,\ 1 \leq j \leq n \qquad 2\text{-}29$$

$$S_j(x_{ij},T_j) = \sum_{i=1}^{m} K_{ij}x_{ij} - 1.0 = 0 \qquad ,1 \leq j \leq n \qquad 2\text{-}30$$

$$H_j(x_{ij},V_j,T_j) = (H_{j+1} - h_j)V_{j+1} - (H_j - h_j)(\,V_j + W_j) - (h_j - h_{j-1})L_{j-1}$$

$$+ F_j(H_{Fj} - h_j) - Q = 0 \qquad ,1 \leq j \leq n \qquad 2\text{-}31$$

There are n(m+2) independent variables in these n(m+2) equations and therefore this system of equations has a unique solution. The problem now is to find a set of values of x_{ij}, V_j and T_j, to satisfy these MESH-equation. Because of their non-linear nature, a direct simultaneous solution is very difficult if not impossible. A simple and fast iterative procedure is presented in the following.

When the flow rates and compositions of feed streams are given, and the amounts of all the product streams are specified, F_j, z_{ij}, W_j, U_j, D, and B are all constants. If an initial set of V_1 and T_j is assumed, $[A_{BC}]$and $\{D\}$ are also constant, provided that the equilibrium ratios, K_{ij}'s, can be expressed as function of T_j,s. Then the M-equation, Equation 2-29, is a linear system. By taking advantage of the tridiagonal form of the matrix $[A_{BC}]$and by grouping the vector $\{D\}$ with $[A_{BC}]$as,

$$\begin{bmatrix} B_1 & C_1 & & & D_1 \\ A_2 & B_2 & C_2 & & D_2 \\ & A_j & B_j & C_j & D_j \\ & A_{n-1} & B_{n-1} & C_{n-1} & D_{n-1} \\ & A_n & B_n & & D_n \end{bmatrix} \qquad ,1 \leq i \leq m \qquad 2\text{-}32$$

the solution of equation 2-29 for $[x_{ij}]$ can be easily obtained by use of a simple algorithm derived from the Gauss elimination method. In this algorithm, two auxiliary quantities, p_j and q_j are calculated by first evaluating p_j and q_j and advancing forward with j increasing, that is

$$p_1 = C_1/B_1 \; ; \; q_1 = D_1/B_1 \qquad 2\text{-}33$$

$$p_j = C_j/(B_j - A_j p_{j-1}) \qquad ,2 \leq j \leq n\text{-}1 \qquad 2\text{-}34$$

$$q_j = (D_j - A_j q_{j-1})/(B_j - A_j p_{j-1}) \qquad ,2 \leq j \leq n \qquad 2\text{-}35$$

Then, values of x_{ij}'s are calculated by first evaluating x_{in} and receding backward with j decreasing until x_{i1} is reached. Thus,

$$X_{in} = q_n \qquad 2\text{-}36$$

$$X_{ij} = q_j - p_j x_{i,j+1} \qquad ,1 \leq j \leq n\text{-}1 \qquad 2\text{-}37$$

When the x's obtained from the above algorithm are substituted into the S-equation, Equation 2-30 and if K_{ij}'s could be expressed as function of T_j such as

$$K_{ij} = \hat{\phi}_{ij}^{L}(P, T, x_i) / \hat{\phi}_{ij}^{V}(P, T, y_i) \qquad ,1 \leq i \leq m \qquad 2\text{-}38$$

the S-equation is a function of T only, that is,

$$S_j(T_j) = \sum_{i=1}^{m} \left(\hat{\phi}_{ij}^{L}(P, T, x_i) / \hat{\phi}_{ij}^{V}(P, T, y_i) \right) x_{ij} - 1.0 = 0 \qquad ,1 \leq j \leq n \qquad 2\text{-}39$$

For the solution of this equation, either the Muller's method or the Newton-Raphson may be used. The process is repeated until

$$S_{ik} = S_j(T_{ik}) \leq \varepsilon \qquad \text{(on the } k^{th} \text{ iterative)} \qquad 2\text{-}40$$

When x_{ij}'s are obtained from the M-equation and new T_j's are calculated from the S-equation by Newton-Raphson method, new values of V_j can be calculated directly from the H-equation, Equation 2-31

The enthalpies of the internal streams are calculated by equation 2-41

$$\frac{H - H^*}{RT} = Z - 1 - \frac{A}{B}\left[1 - \frac{T}{a}\left(\frac{da}{dT}\right)\right]\ln\left(1 + \frac{B}{Z}\right) \qquad ,1 \leq j \leq n \qquad 2\text{-}41$$

together with isobaric enthalpy change at ideal gas state;

$$\Delta H = \int_{T1}^{T1} Cp^* dT \qquad 2\text{-}42$$

where c_p^* is the ideal gas state heat capacity

2.4 Petroleum Distillation Simulation

To apply the MESH equations for petroleum distillation simulation, petroleum feed is broken down into a number of fractions of narrow boiling point range. Each fraction is regarded as one component and is called “pseudocomponent”. Figure 2.5 illustrates the formation of 11 fractions or pseudo components on the ASTM boiling point curve.

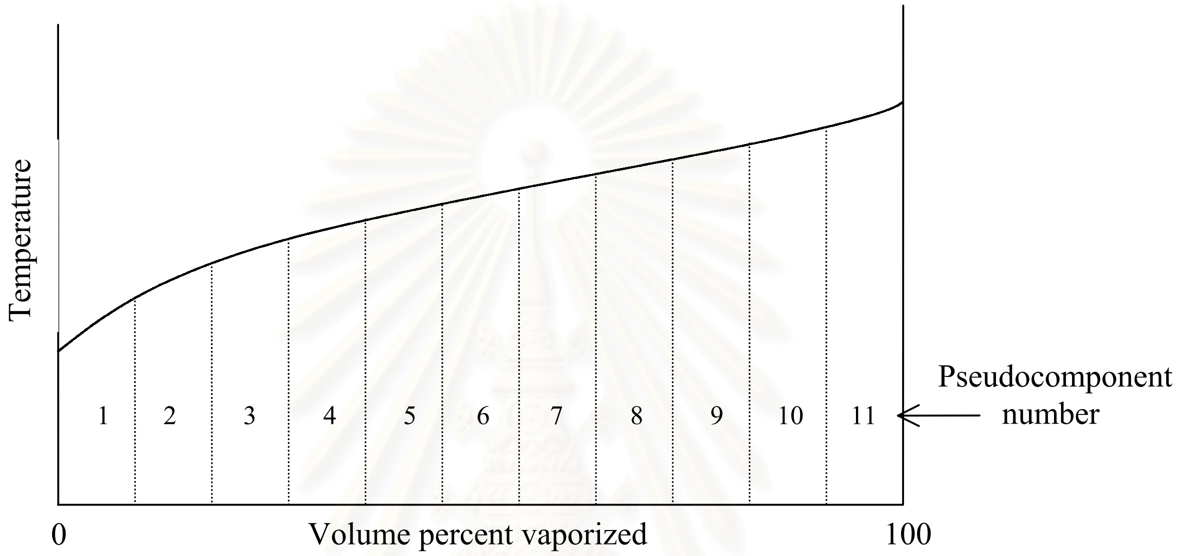


Figure 2.5 Formation of Pseudocomponent

2.5 Newton-Raphson Method

Slope Methods for Finding Roots

If $f(x)$, $f'(x)$, and $f''(x)$ are continuous near a root p, then this extra information regarding the nature of $f(x)$ can be used to develop algorithms that will produce sequences $\{p_k)$ that converge faster to p than either the bisection or false position method. The Newton-Raphson (or simply Newton's) method is one of the most useful and best known algorithms that relies on the continuity of $f'(x)$ and $f''(x)$. We shall introduce it graphically and then give a more rigorous treatment based on the Taylor polynomial.

Assume that the initial approximation p_0 is near the root p. Then the graph of $y = f(x)$ intersects the x-axis at the point $(p,0)$, and the point $(p_0, f(p_0))$ lies on the curve near the point $(p,0)$ (see Figure 2.6). Define p_1 to be the point of intersection of the x-axis and the line tangent to the curve at the point $(p_0, f(p_0))$. Then Figure 2.6 shows that p_1 will be closer to p than p_0 in this case. An equation relating p_1 and p_0 can be found if we write down two versions for the slope of the tangent line L:

$$m = \frac{0 - f(p_0)}{p_1 - p_0} \qquad 2\text{-}43$$

which is the slope of the line through $(p_1, 0)$ and $(p_0, f(p_0))$, and

$$m = f'(p_0), \qquad 2\text{-}44$$

which is the slope at the point $(p_0, f(p_0))$. Equating the values of the slope m in equation (43) and (44) and the solving for p_1 result in

$$p_1 = p_0 - \frac{f(p_0)}{f'(p_0)} \qquad 2\text{-}45$$

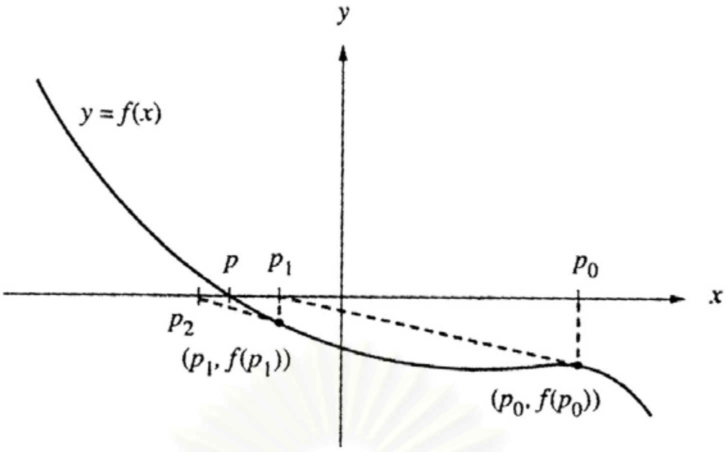


Figure 2.6 The Geometric Construction of p_1 and p_2 for The Newton-Raphson Method.

The process above can be repeated to obtain a sequence $\{p_k\}$ that converge to *p*. Assume that $f \in C^2[a,b]$ and there exists a number $p \in C^2[a,b]$, where $f(p) = 0$. If $f'(p) \neq 0$, then there exists a $\delta > 0$ such that the sequence $\{p_k\}_{k=0}^{\infty}$ defined by the iteration

$$p_k = g(p_{k-1}) = p_{k-1} - \frac{f(p_{k-1})}{f'(p_{k-1})} \quad \text{for } k = 1,2, \ldots \qquad 2\text{-}46$$

will converge to *p* for any initial approximation $p_0 \in [p - \delta, p + \delta]$.

CHAPTER 3

PETROLEUM

3.1 Petroleum Fractions Characterisation

General Characteristic of Petroleum

Crude petroleum or crude oil as product from the field is a relatively low-value meterial since, in its native state, it is rarely usable directly. Thus it is usually refined and further processed into a number of products whose total value is many times that of the original oil. The first step in any oil refinery is the separation of the crude oil into various fractions by the process of distillation. These fractions may be products in their own right or may be feedstock for refining or processing units. Usually, properties of a petroleum fraction are characterised as follows.

ASTM Distillation

The ASTM D86 and D1160 tests are reasonably rapid batch laboratory distillations involving the equivalent of approximately one equilibrium stage and no reflux except for that caused due to heat losses. Apparatus typical of the D86 test is shown in Fig 3.1. It consists of a heated 100 ml or 125 ml Engler flask containing a calibrated thermometer of suitable range to measure the temperature of the vapor at the inlet to the condensing tube, an inclined brass condenser in a cooling bath using a suitable coolant, and a graduated cylinder for collecting the distillate. A stem correction is not applied to the temperature reading. Related tests using similar apparatus are the D216 test for natural gasoline and the Engler distillation.

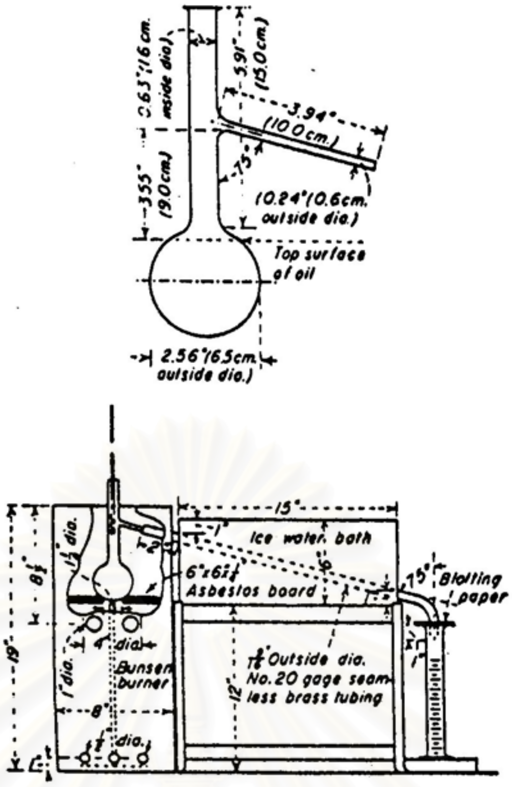


Figure 3.1 ASTM Distillation Apparatus

In the widely used ASTM D86 test, 100 ml of sample is charged to the flask and heated at a sufficient rate to produce the first drop of distillate from the lower end of the condenser tube in from 5 to 15 min, depending on the nature of the sample. The temperature of the vapor at that instant is recorded as the initial boiling point (IBP). Heating is continued at a rate such that the time from the IBP to 5 volume percent recovered of the sample in the cylinder is 60 to 75 sec. Again, vapor temperature is recorded. Then, successive vapor temperature are recorded for from 10 to 90 percent recovered in intervals of 10, and at 95 percent recovered, with the heating rate adjusted so that 4 to 5 ml are collected per minute. At 95 percent recovered, the burner flame is increased if necessary to achieve a maximum vapor temperature referred to as the end point (EP) in from 3 to 5 additional min. The percent recovery is reported as the maximum percent recovered in the cylinder.

As discussed by Nelson, virtually no fractionation occurs in an ASTM distillation. Thus, components in the mixture do distill one by one in the order of their boiling points but as mixtures of successively higher boiling points. The IBP, EP, and intermediate points have little theoretical significance, and in fact, components boiling below the IBP and above EP are present in the sample. Nevertheless, because ASTM distillations are quickly conducted, have been successfully automated, require only a small sample, and are quite reproducible, they are widely used for comparison and as a basis for specifications on a large number of petroleum intermediates and products, including many solvents and fuels.

Typical ASTM curves for several such products are shown in Figure 3.2

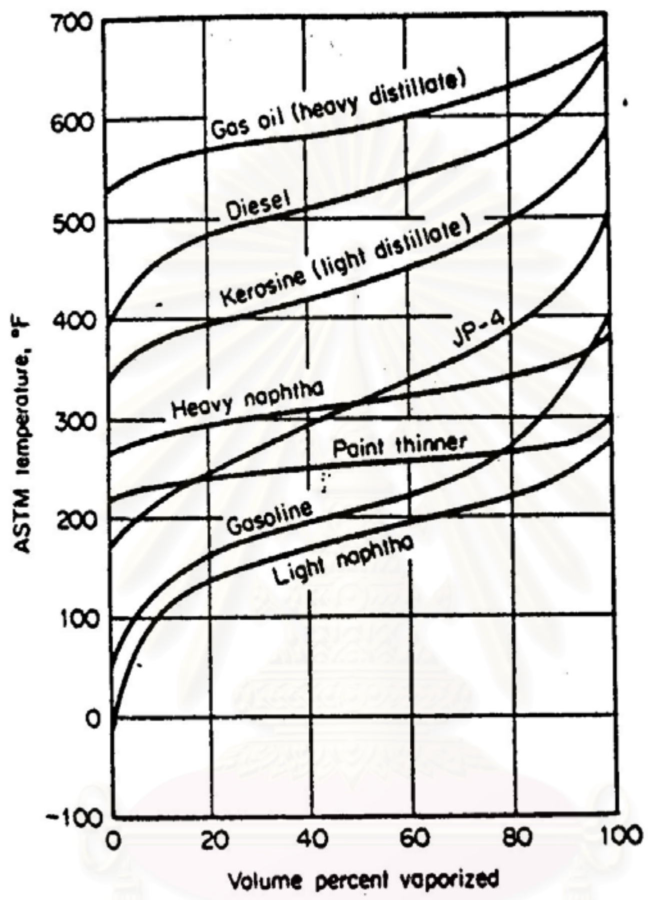


Figure 3.2 Representative ASTM D86 Distillation Curves.

TBP Distillation

True-boiling-point (TBP) distillations are normally run on crude oils and not on petroleum fraction. This method is basically a batch distillation using a large number of stages and a high reflux-to-distillate ratio so that the temperature at any point on the temperature-volumetric yield curve represents the actual boiling point of the hydrocarbon material present at that volume percentage point. Thus, data from a TBP distillation test provides a much better theoretical basis for characterization. If the sample contains compounds that have moderate differences in boiling points such as in a light gasoline containing light hydrocarbons (e.g. iso-butane, n-butane, isopentane etc.), a plot of overhead-vapor-distillate temperature versus percent distilled in a TBP test would appear in the form of steps as in Figure 3.3. However, if the sample has a higher average boiling range in which the number of close-boiling isomers increases, the steps become indistinct and a TBP curve such as that in Figure 3.4 results. Because the degree of separation for a TBP distillation tests in much higher than for an ASTM distillation test, the IBP is lower and the EP is higher for the TBP method when compared with the ASTM method, an shown in Figure 3.4

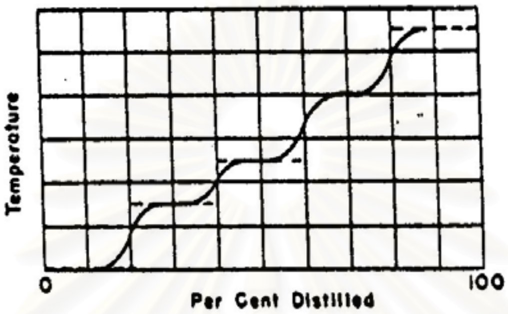


Figure 3.3 Variation of Boiling Temperature with Percent Distilled in TBP Distillation of Light Hydrocarbon

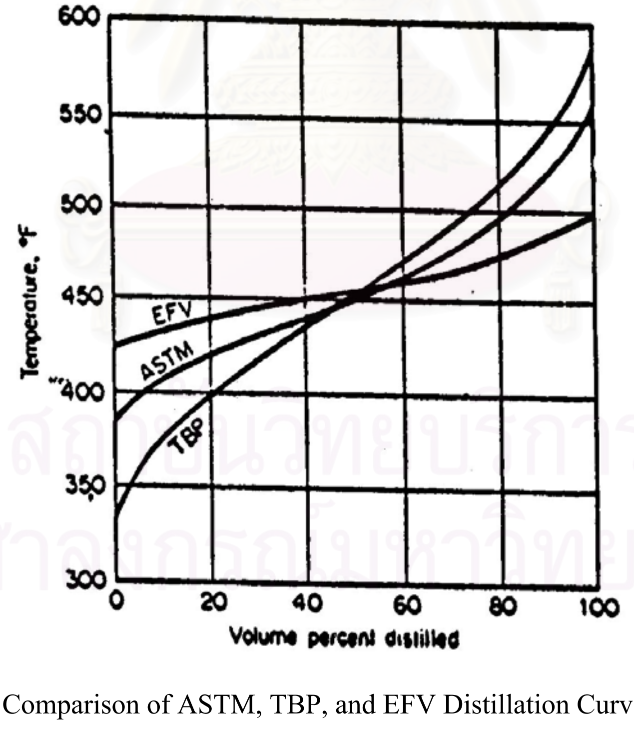


Figure 3.4 Comparison of ASTM, TBP, and EFV Distillation Curves for Kerosene.

A standard TBP laboratory-distillation-test method has not been well accepted. Instead, as discussed by Nelson, batch distillation equipment that can achieve a good degree of fractionation is usually considered suitable. In general, TBP distillations are conducted in columns with 15 to

100 theoretical stages at reflux of 5 or greater. Thus, the new ASTM D2892 test method, which involves a column with 14 to 17 theoretical stages and a reflux ration of 5, essentially meets the minimum requirements. Distillate may be collected at a constant or a variable rate. Operation may be at 101.3 kPa pressure or at a vacuum at the top of the column as low as 0.067 kPa for high-boiling fractions, with 1.3 kPa being common. Results from vacuum operation are extrapolated to 101.3 kPa by the vapor-pressure correlation of Maxwell and Bonnel, and in the ASTM D2892 test method, it involves a correlation for the nature of the sample in terms of the UOP characterization factor.

EFV Distillations

A third fundamental type of laboratory distillation, which is the most tedious to perform of the three types of the laboratory distillations, is equilibrium-flash-distillation(EFV), for which no standard test exists. The sample is heated in such a manner that the total vapor produced remains in contact with the total remaining liquid until the desired temperature is reached at a set pressure. The volume percent vaporized at these conditions is recorded. To determine the complete flash curve, a series of run at a fixed pressure is conducted over a range of temperature sufficient to cover a range of vaporization from 0 to 100 percent. As seen in Figure 3.4, the component separation achieved by an EFV distillation is much less than by the ASTM or TBP distillation tests. The initial and final EFV points are the bubble point and the dew point respectively of the sample. If desired, EFV curves can be established at a series of pressures.

ASTM-TBP-EFV Relationships

Because of the time and expense involved in conducting laboratory distillation tests of all basic types, it has become increasingly common to use empirical correlations to estimate the other two distillation curves when either the ASTM, TBP, or EFV curve is avaible. Preferred correlations given in the following are based on the work of Edmister and Maxwell as shown in Figure 3.5 to 3.6.

For the interconversion between ASTM and TBP distillation of topping column sidestream products, it is helpful to have an empirical expression for the correlation. Nelson found that the preceding types of distillation, a sigmoidal-shaped curve results whenever values of the dependent variables, y (or temperature, deg.F) are plotted against the independent variable, x cumulative-percent-less than, (CPLT) , (or volume percent distilled), on arithmetic coordinate graph paper. This sigmoidal-shaped curve can be transformed into a straight line when value of x are plotted on a probability scale. This method is called Nelson’s method for extrapolating crude oil TBP curves into the high boiling range.

Values of x on the linear abscissa scale are quickly transformed into value of x on the probability 3-1 to 3-3.

$$q = x/100 \quad \text{(when } x< 50\%\text{)}$$

$$q = 1- x/100 \quad \text{(when } x>50\%\text{)} \qquad 3\text{-}1$$

$$n = \ln (1/q^2) \qquad 3\text{-}2$$

$$x^* = n-(a_0+a_1n)/(1+a_2n+a_3n^2) \qquad 3\text{-}3$$

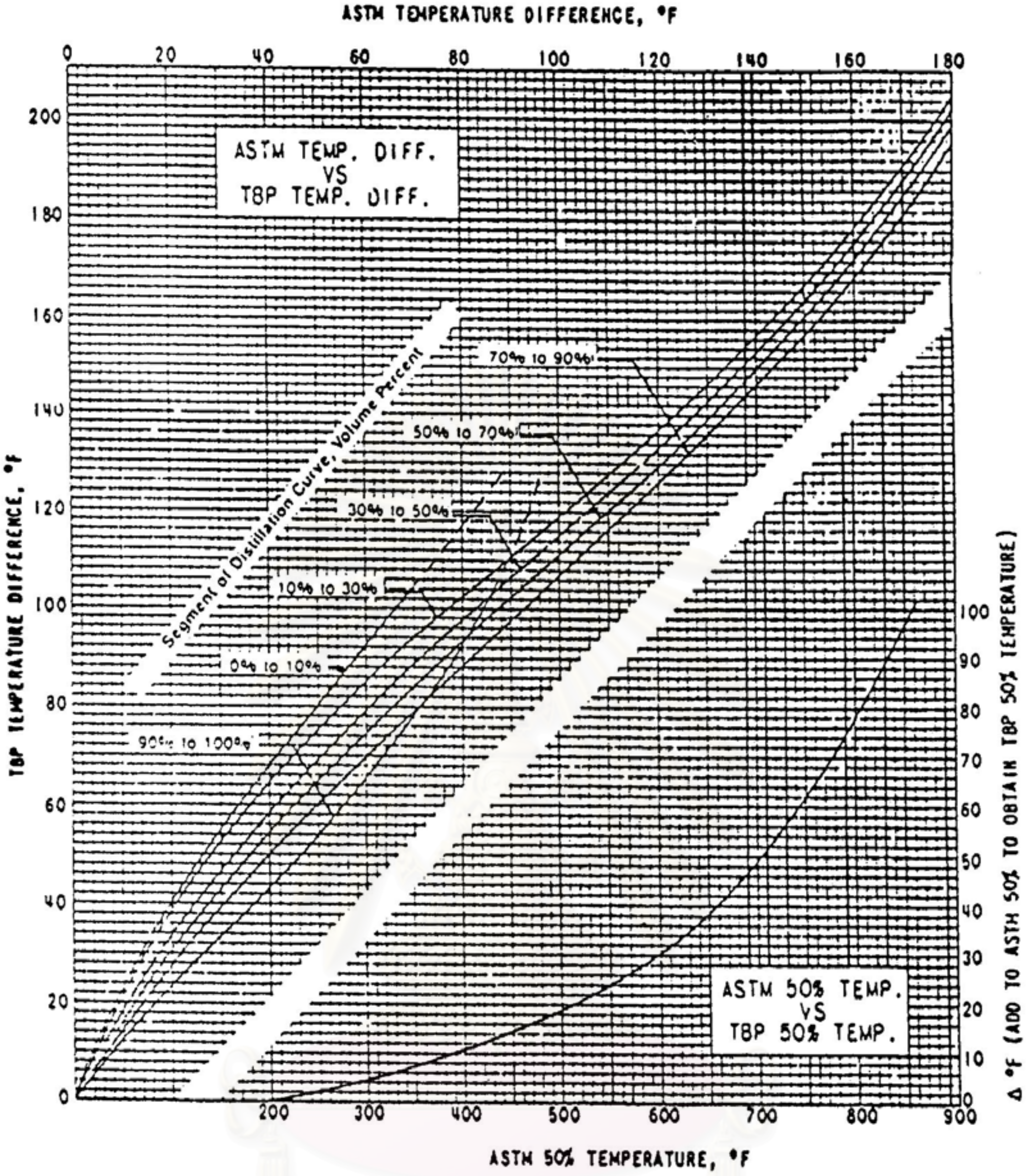


Figure 3.5 (lower right). ASTM 50% Temperature vs. TBP 50% Temperature

Figure 3.6 (top left). ASTM Temperature Difference vs. TBP 50% Temperature Difference [6]

where, a_0 = 2.30753
a_1 = 0.27061
a_2 = 0.99229
a_3 = 0.04481

For values of x that are less than 50% the sign x^* is changed from positive to negative. The transformations which linearizes the y versus CPLT curve uses the method of least squares fit a best straight line through the transformed data points and the equation of the line is expressed as

$$y = mx + b \tag{3-4}$$

where

m = slope of the least squares fit line through the probability paper plotted data points

b = y-intercept of that line

API Gravity

Gravity of a crude oil or petroleum fraction is generally measured by the ASTM D287 test or the equivalent ASTM D1298 test and may be reported as specific gravity (Sp.Gr) 60/60 °F and referred to water at 60 °F or, commonly, as API gravity which is defined as

$$\text{API gravity} = \frac{141.5}{\text{Sg.Gr}(60/60\text{F})} - 131.5 \tag{3-5}$$

Water, thus, has an API gravity of 10 and most crude oils and petroleum fractions have values of API gravity in the range of 10-80.

3.2 Correlation for Characteristic of The Heavy Fraction

To use an equation of state like the Soave-Redlich-Kwong equations on a petroleum mixture, the critical temperature, T_c, critical pressure, P_c, and the acentric factor, ω, are needed for each component. For petroleum fractions, these properties can be evaluated from the following correlations.

Cavett (1964) Relations

$$T_c = 768.071+1.7134T_{50}-0.10834*10^{-2}\,T_{50}^{2}+0.3889*10^{-6}\,T_{50}^{3}-0.89213-10^{-2}\,T_{50}API \\ +0.53095*10^{-6}\,T_{50}^{2}API+0.32712*10^{-7}\,T_{50}^{2}API^{2} \qquad 3\text{-}6$$

$$\log P_c = 2.829+0.9412*10^{-3}\,T_{50-0.30475*10}{}^{-5}\,T_{50}^{2}+0.15141*10^{-8}\,T_{50}^{3}-0.20876*10^{-4}\,T_{50}API \\ +0.11048*10^{-7}\,T_{50}^{2}API+0.1395*10^{-9}\,T_{50}^{2}API^{2}-0.4827*10^{-7}\,T_{50}API^{2} \qquad 3\text{-}7$$

where $$API = 141.5/SG - 131.5 \qquad 3\text{-}8$$

The critical temperature, T_c, and the mid-volume boiling point of the fraction, T_{50}, are given in °F, P_c in psia, and SG in 60/60 °F

Lee-Kesler Correlations (1976)

$$\omega = \frac{(\ln P_{Br}-5.92714+6.09648/T_{Br}+1.28862\ln T_{Br}-0.169347T_{Br}^{6})}{(15.2518-15.6875/T_{Br}-13.4721\ln T_{Br}+0.43577\,T_{Br}^{6})} \quad \text{for } T_{Br} < 0.8 \qquad 3\text{-}9$$

$$\omega = -7.904+0.1352K-0.007465K^{2}+8.359\,T_{Br}+(1.408-0.01063K)/\,T_{Br} \quad \text{for } T_{Br} > 0.8 \qquad 3\text{-}10$$

$$
\begin{aligned}
MW \quad = \quad & -12272.6+9486.4SG+(4.6523-3.3287SG)\ T_{Br}+(1-0.77084SG-0.02058SG^{2}* \\
& (1.3437-720.79/\ T_{Br})*10^{7}/\ T_{Br}+(1-0.80882SG+0.02226SG^{2})* \\
& (1.8828-181.98/\ T_{Br})*10^{12}/\ T_{Br}^{\ 3}
\end{aligned}
\qquad 3\text{-}11
$$

The boiling point, T_B, and the critical temperature, T_c, are in degree Rankine and the specific gravity, SG, in $60^{\circ}F/60^{\circ}F$. The critical pressure, P_c, in psia. $T_{Br=}\ T_B/T_c$ and $P_{Br} = P_B/P_c$ where P_B is the pressure where T_B has been measured. K is the Watson characterization factor which equals $T_B^{\ 1/3}/\ SG$. MW is the molecular weight.

Ideal Gas C_p's for Petroleum Fractions

For petroleum fractions, the following empirical equation by Kesler and Lee [6] is sufficiently accurate for engineering applications

$$C_p^{\ *} \quad = \quad A+BT+CT^{2}+CF(A'+B'T+C'T^{2}) \qquad 3\text{-}12$$

where

$A \quad = \quad -0.32646+0.02678K$

$B \quad = \quad -(1.3892+1.2122K+0.03803K^{2})10^{-4}$

$C \quad = \quad -1.5393*10^{-7}$

$A' \quad = \quad -0.0084773+0.080809SG$

$B' \quad = \quad (201773-2.0826SG)10^{-4}$

$C' \quad = \quad -(0.78649-0.70423SG)10^{-7}$

$CF \quad = \quad \{(12.8/K-1)(10/K-1)*100\}^{2}$

$K \quad = \quad (T_B)^{1/3}/SG$

$T_B \quad = \quad$ mean average boiling point, $^{o}R = (^{o}F+ 460)$

CHAPTER 4

Thermodynamic Properties

4.1 Soave-Redlich-Kwong Equation

An equation relating the pressure to the temperature and volume is called “equation of state”. It provides a most efficient and versatile means of expressing various thermodynamic functions in terms of P-V-T data. The Soave-Redlich-Kwong equation of state is ;

$$P = \frac{RT}{V-b} - \frac{a}{V(V+b)} \tag{4-1}$$

As the derivative, it expresses the parameter a as a product of a temperature –independent parameter, a', and a temperature dependent term, f(T), as follows:

$$a = a' f(T) \tag{4-2}$$

In the original Soave-Redlich-Kwong equation $f(T) = T^{-1/2}$

Expressing equation 4-1 in cubic form in terms of molar volume, V, gives

$$V^3 - \left(\frac{RT}{P}\right)V^2 + \left(\frac{a}{P} - \frac{bRT}{P} - b^2\right)V - \frac{ab}{P} = 0 \tag{4-3}$$

at the critical point: $$a_c = a' f(T_c) \tag{4-4}$$

from equation 4-2 and 4-4

$$a = a_c \frac{f(T)}{f(T_c)} \tag{4-5}$$

From this point on the ratio, $\frac{f(T)}{f(T_c)}$ will be denoted by α following the Soave notation. Thus, the above equation becomes

$$a = a_c\alpha \qquad 4\text{-}6$$

As obvious from $\frac{f(T)}{f(T_c)}$, α must be unity at $T = T_c$

and

$$a_c = 0.42748(RT_c^{2})/P_c \qquad 4\text{-}7$$

$$\alpha = T_r^{-0.5} \qquad 4\text{-}8$$

$$b = 0.08664RT_c/P_c \qquad 4\text{-}9$$

Replacing V in Equation 4-1 with ZRT/P and rearranging gives

$$Z^3-Z^2+(A-B-B^2)Z-AB = 0 \qquad 4\text{-}10$$

where

$$A = \frac{aP}{(RT)^2} \qquad 4\text{-}11$$

$$B = \frac{bP}{RT} \qquad 4\text{-}12$$

Combining Equation 4-11 with 4-6 and 4-7, and Equation 4-12 with 4-9 gives parameter of pure state

$$A = 0.42748\frac{P_r}{T_r^{\,2}}\alpha \qquad 4\text{-}13$$

$$B = 0.08664\frac{P_r}{T_r} \qquad 4\text{-}14$$

For mixture or solution, the van der Waal's mixing rules are usually used:

$$B = \sum_i^m \sum_j^m x_i x_j B_{ij} \qquad 4\text{-}15$$

where

$$b = \sum_i^m x_i b_i \qquad 4\text{-}16$$

$$b_i = 0.08664\frac{RT_{ci}}{P_{ci}} \qquad 4\text{-}17$$

$$a = \sum_{i}^{m}\sum_{j}^{m} x_i x_j (a_i a_j)^{0.5}(1-k_{ij}) \tag{4-18}$$

$$a_i = a_{ci}\alpha_i \tag{4-19}$$

$$a_{ci} = 0.42748\frac{(RT_{ci})^2}{P_{ci}} \tag{4-20}$$

$$\alpha_i^{0.5} = 1+m_i(1-T_{ri}^{0.5}) \tag{4-21}$$

$$m_i = 0.48+1.574\omega_i-0.176\omega_i^2 \tag{4-22}$$

4.2 Fugacity Coefficient

Two auxiliary functions which are of particular use in the thermodynamic treatment of solutions are the fugacity "f" and the fugacity coefficient "ϕ". Their definitions for the case of component in solution is:

$$d\overline{G}_i \quad = \quad RT\,d(\ln \hat{f}_i) \quad = \quad \overline{V}_i dP \qquad \text{const. T} \qquad 4\text{-}23$$

$$\lim_{P\rightarrow 0}(\hat{f}_i / x_i P) \quad = \quad 1 \qquad 4\text{-}24$$

$$\hat{\phi}_i \quad = \quad \hat{f}_i / x_i P \qquad 4\text{-}25$$

The fugacity coefficient expression based on the Soave-Redlich-Kwong is as follows.

$$\ln \hat{\phi}_i \quad = \quad \frac{1}{RT}\int_{\infty}^{v}\left[\frac{RT}{V_t} - \left(\frac{\partial P}{\partial n_i}\right)_{T,Vi,nj}\right] dV_t - \ln Z \qquad 4\text{-}26$$

The derivative in this equation can be obtained from equation 4-1 written in terms of total volume, V_t.

$$P \quad = \quad \frac{nRT}{V_t - nb} - \frac{n^2 a}{V_t(V_t + nb)} \qquad 4\text{-}27$$

Differentiating P in this equation with respect to n_i, at constant T, V_t, and n_j, gives

$$\left(\frac{\partial P}{\partial n_i}\right)_{T,Vt,nj} \quad = \quad \frac{RT}{V_t - nb} - \left[\frac{nRT}{(V_t - nb)^2} + \frac{n^2 a}{V_t(V_t - nb)}\right]\left(\frac{\partial (nb)}{\partial n_i}\right)_{nj}$$
$$+ \frac{1}{V_t(V_t - nb)}\frac{\partial}{\partial n_i}\left(n^2 a\right)_{T,nj} \qquad 4\text{-}28$$

Combing Equation 4-26 and 4-28 and making the integration give

$$\ln \hat{\phi}_i \quad = \quad -\ln\left(Z - \frac{Pb}{RT}\right) + (Z-1)B'_i$$
$$- \frac{a}{bRT}(A'_i - B'_i)\ln\left(1 + \frac{b}{V}\right) \qquad 4\text{-}29$$

Using the notations of A and B instead of a and b gives

$$\ln \hat{\phi}_i = -\ln(Z-B)+(Z-1)B'_i - \frac{A}{B}(A'_i - B'_i)\ln\left(1+\frac{B}{V}\right) \qquad 4\text{-}30$$

where

$$A'_i = \frac{1}{a}\left[2a_i^{0.5}\sum_{j}^{m} x_j a_j^{0.5}(1-k_{ij})\right] \qquad 4\text{-}31$$

$$B'_i = \frac{b_i}{b} \qquad 4\text{-}32$$

4.3 Phase Equilibrium Constant (K_i)

In practical design, the equilibrium ratio K_i is used, which may be related to the fugacity coefficients through equation 4-33,

$$K_i = y_i/x_i = \hat{\phi}_i^{\ L}/\hat{\phi}_i^{\ V} \tag{4-33}$$

Fugacity coefficients of Soave-Redlich-Kwong expression

$$\ln \hat{\phi}_i = -\ln\left[Z - \frac{Pb}{RT}\right] + (Z-1)B_i' - \frac{a}{bRT}(A_i' - B_i')\ln\left[1 + \frac{Pb}{RTZ}\right] \tag{4-34}$$

Thus, liquid fugacity coefficients

$$\ln \hat{\phi}_i^{\ L} = -\ln\left[Z^L - \frac{Pb^L}{RT}\right] + \left(Z^L - 1\right)B_i'^L - \frac{a^L}{b^L RT}\left(A_i'^L - B_i'^L\right)\ln\left[1 + \frac{Pb^L}{RTZ^L}\right] \tag{4-35}$$

and, vapor fugacity coefficients

$$\ln \hat{\phi}_i^{\ V} = -\ln\left[Z^V - \frac{Pb^V}{RT}\right] + \left(Z^V - 1\right)B_i'^V - \frac{a^V}{b^V RT}\left(A_i'^V - B_i'^V\right)\ln\left[1 + \frac{Pb^V}{RTZ^V}\right] \tag{4-36}$$

Then, divide equation 4-35 by 4-36

$$\begin{aligned}\ln\left(\frac{\hat{\phi}_i'^L}{\hat{\phi}_i'^V}\right) = {} & -\ln\left[\frac{Z^L - (Pb^L/RT)}{Z^V - (Pb^V/RT)}\right] + \left[\left(Z^L - 1\right)B_i'^L - \left(Z^V - 1\right)B_i'^V\right] \\ & - \frac{1}{RT}\left[\frac{a^L}{b^L}\left(A_i'^L - B_i'^L\right)\ln\left[1 + \frac{Pb^L}{RTZ^L}\right] - \frac{a^V}{b^V}\left(A_i'^V - B_i'^V\right)\ln\left[1 + \frac{Pb^V}{RTZ^V}\right]\right] = U\end{aligned} \tag{4-37}$$

Let

$$\ln\left(\frac{\hat{\phi}_i'^L}{\hat{\phi}_i'^V}\right) = U \tag{4-38}$$

comparing equation 4-33 and 4-38

$$K_i \quad = \quad \left(\frac{\hat{\phi}_i{}'^{L}}{\hat{\phi}_i{}'^{V}}\right) \quad = \quad \exp(U) \qquad 4\text{-}39$$

4.4 Enthalpy Departure

Expressions for enthalpy departure for the Soave-Redlich-Kwong is as follows.

$$\frac{H-H^*}{RT} = \quad Z-1+\frac{1}{RT}\int_{\infty}^{V}\left[T\left(\frac{\partial P}{\partial T}\right)_V - P\right]dV \qquad 4\text{-}40$$

Equation of state provide the P-V-T relation required to evaluate the right side of the above equation.

Differentiating equation 4-1 with respect to T, at constant V, and multiplying by T, give

$$T\left(\frac{\partial P}{\partial T}\right)_V = \quad \frac{RT}{V-b}-\frac{T}{V(V+b)}\left(\frac{da}{dT}\right) \qquad 4\text{-}41$$

The integrand in equation 4-40 then becomes

$$T\left(\frac{\partial P}{\partial T}\right)_V - P = \frac{T}{V(V+b)}\left[a-T\left(\frac{da}{dT}\right)\right] \qquad 4\text{-}42$$

Combining equation 4-40 with 4-42 and then integrating gives

$$\frac{H-H^*}{RT} = \quad Z-1-\frac{1}{bRT}\left[a-T\left(\frac{da}{dT}\right)\right]\ln\left(1+\frac{b}{V}\right) \qquad 4\text{-}43$$

Making use of (a = b/RT) = (A/B) and (b/V) = (B/Z) gives

$$\frac{H-H^*}{RT} = \quad Z-1-\frac{A}{B}\left[1-\frac{T}{a}\left(\frac{da}{dT}\right)\right]\ln\left(1+\frac{B}{Z}\right) \qquad 4\text{-}44$$

where

$$T\left(\frac{da}{dT}\right) = \quad -\sum_{i}^{m}\sum_{j}^{m} x_i x_j m_j (a_i a_{c_j} T_{r_j})^{0.5}(1-k_{ij}) \qquad 4\text{-}45$$

CHAPTER 5

ALGORITHM OF MODEL SOLUTION

5.1 Set of Equations Used in Distillation Simulation

5.1.1 Equations for distillation process :

Equations 2-17, 2-18, 2-24, 2-25, 2-26, 2-27, 2-28, 2-30, 2-31, 2-33, 2-34, 2-35, 2-36 and 2-37.

5.1.2 Properties equations based on SRK :

Equation 4-10 for compressibility factor.

Equation 4-30 for fugacity coefficient.

Equations 4-37, 4-39 for vapor-liquid equilibrium.

Equations 2-41, 2-42 and 2-44 for enthalpy.

5.1.3 Correlation equations for petroleum fractions

Equations 3-5, 3-6, 3-7, 3-9, 3-10, 3-11 and 3-12.

5.1.4 Equation for convergence

Equation 2-45.

5.2 Computational Procedure

Step 1. Specified feed and operating condition.

Step 2. Assume an initial vapor flow rate profile $(V_j)_0$ by means of constant molal overflow and initialize liquid concentration profile $(x_{ij})_0$.

Step 3. Assume initial temperature T_0.

Step 4. Set initial vapor concentration equal liquid concentration, $y_{ij} = x_{ij}$.

Step 5. Calculate thermodynamics properties of each component and each stage.

Step 6. Calculate initial K_i from $K_i = \dfrac{\phi_{ij}^{L} x_{ij}}{\phi_{ij}^{V}}$, and then calculate the elements of the matrix $[A_{BC}]$, using Equation (2-24) to (2-28).

Step 7. Solve the M-equation, Equation (2-29), for x_{ij} 's, using the tridiagonal matrix algorithm from Gauss elimination.

Step 8. Normalize x_{ij}.

Step 9. Calculate y_{ij} by Equation (2-5).

Step 10. Calculate temperature profile (T_j) of each stage by Newton-Raphson method

Step 11 Recalculate thermodynamics properties and K_i

Step 12. Calculate the enthalpies of the internal vapor and liquid stream by Equation (4-43) and (4-44).

Step 13. Solve Equation (2-31) for a new set of $(V_j)_{k.}$

Step 14. Repeat step (7) through (13) until $\sum \left[(T_j)_k - (T_j)_{k-1}\right]^2 \leq \varepsilon_T$, where ε_T is a predescribed tolerance.

The flow chart diagram of such a computational routine is shown in Figure 5.1

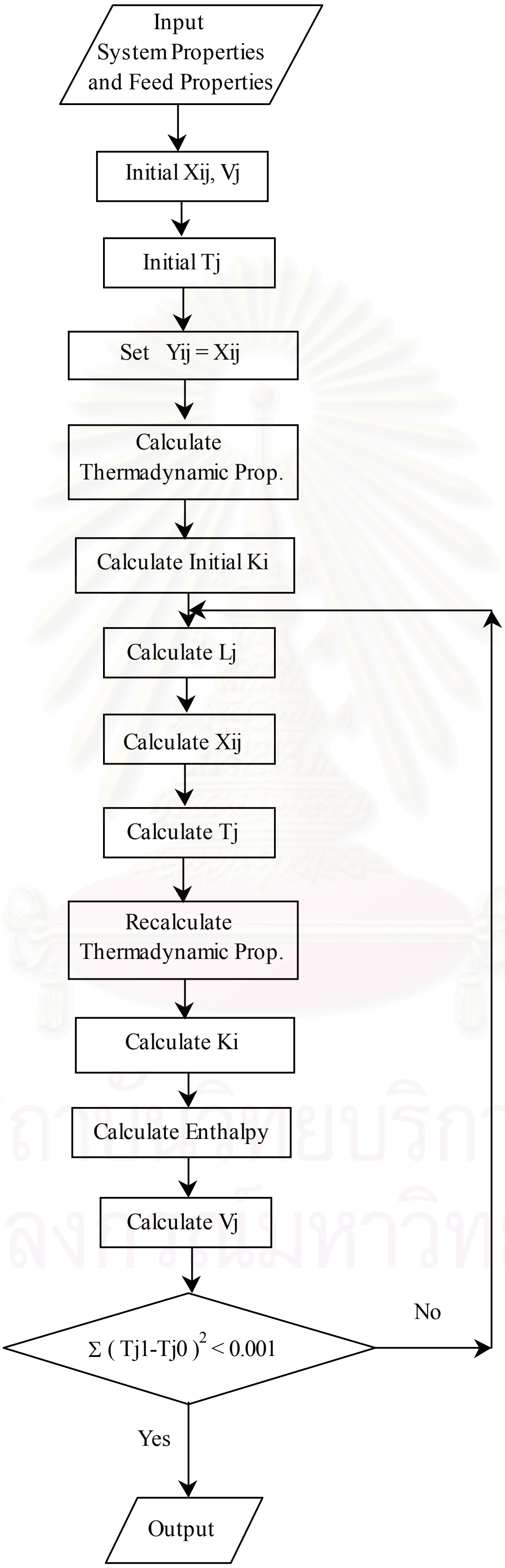


Figure 5.1 Flow Chart of The Distillation Simulation

CHAPTER 6

RESULT AND DISCUSSION

6.1 Petroleum Distillation Simulation Based on SRK Equation

At present petroleum fraction fractional distillation design and simulation is conveniently accomplished due to availability of modern powerful computers. The Soave-Redlish-Kwong equation of state (SRK) can be used to generate required properties of petroleum fraction for petroleum distillation simulation [9]. Furthermore, it was shown that at least 20 pseudocomponents should be used to represent a petroleum fraction mixture in order to obtain accurate result.

There are many cubic equations of state in the literature. The SRK was chosen for this work since it can generate relatively accurate saturated pressure of hydrocarbon. Table 6.1 presents comparison of saturated pressure derived from the SRK and Peng Robinson equation of states (PR) by this work.

Table 6.1 Vapor Pressure of Some Hydrocarbons

Methane	**Temperature 130 K**			**Temperature 140 K**			**Temperature 150 K**			**Temperature 160 K**		
	Standard	**PR**	**SRK**	**Standard**	**PR**	**SRK**	**Standard**	**PR**	**SRK**	**Standard**	**PR**	**SRK**
Vapor Pressure	3.71	3.69	3.64	6.52	6.44	6.41	10.60	10.46	10.47	16.18	16.03	16.10
% Deviation		*-0.76%*	*-2.13%*		*-1.23%*	*-1.67%*		*-1.31%*	*-1.17%*		*-0.94%*	*-0.50%*

Butane	**Temperature 330 K**			**Temperature 340 K**			**Temperature 350 K**			**Temperature 360 K**		
	Standard	**PR**	**SRK**	**Standard**	**PR**	**SRK**	**Standard**	**PR**	**SRK**	**Standard**	**PR**	**SRK**
Vapor Pressure	6.00	5.95	6.01	7.65	7.57	7.67	9.60	9.51	9.63	11.90	11.80	11.95
% Deviation		*-0.84%*	*0.28%*		*-0.96%*	*0.27%*		*-0.96%*	*0.30%*		*-0.85%*	*0.40%*

Pentane	**Temperature 350 K**			**Temperature 360 K**			**Temperature 370 K**			**Temperature 380 K**		
	Standard	**PR**	**SRK**	**Standard**	**PR**	**SRK**	**Standard**	**PR**	**SRK**	**Standard**	**PR**	**SRK**
Vapor Pressure	3.42	3.39	3.43	4.40	4.36	4.41	5.58	5.52	5.59	6.97	6.90	7.00
% Deviation		*-0.90%*	*0.17%*		*-0.98%*	*0.24%*		*-0.99%*	*0.34%*		*-0.92%*	*0.47%*

Table 6.1 Vapor Pressure of Some Hydrocarbons (continued)

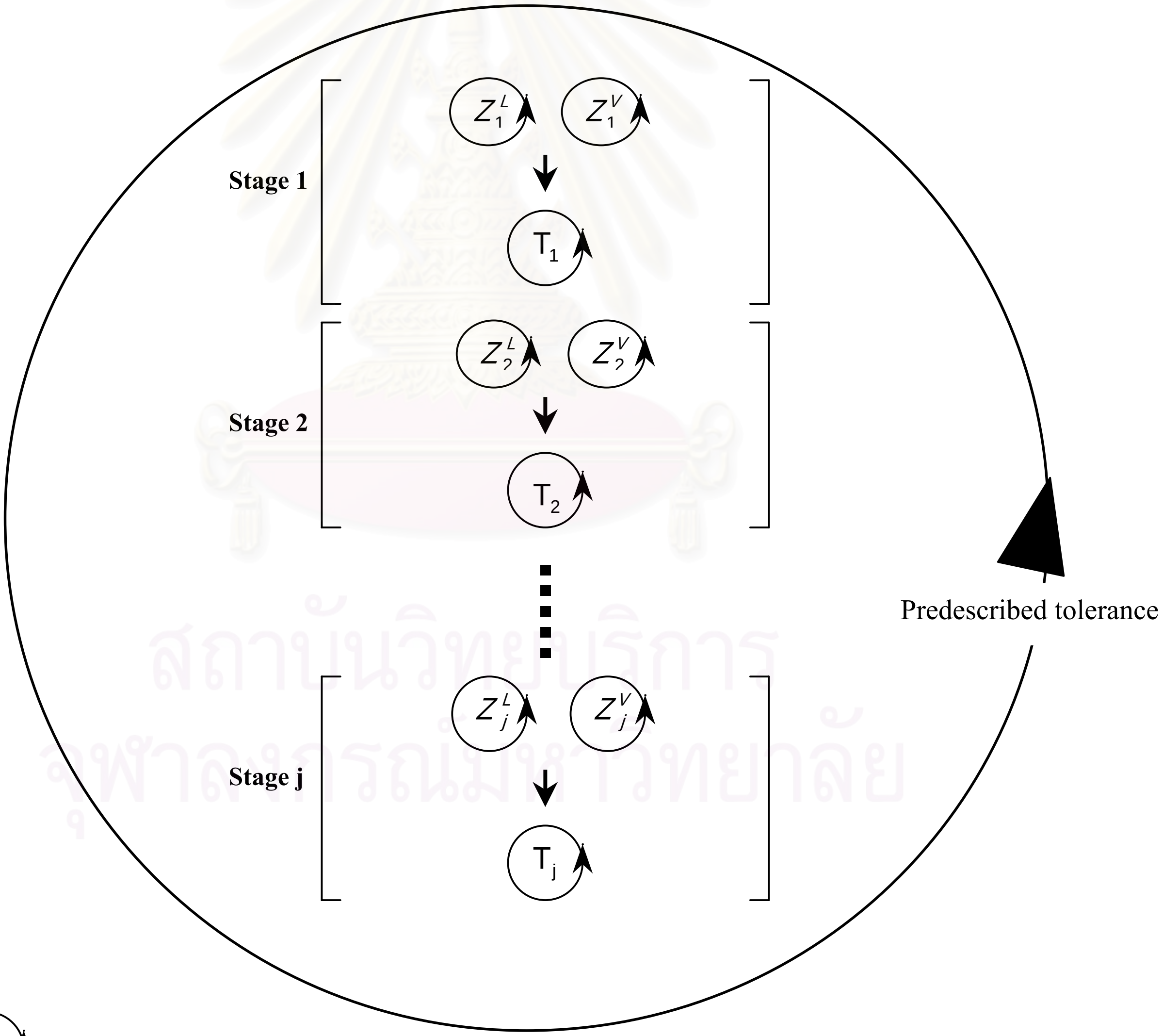
Hexane	**Temperature 390 K**			**Temperature 400 K**			**Temperature 410 K**			**Temperature 420 K**		
	Standard	**PR**	**SRK**	**Standard**	**PR**	**SRK**	**Standard**	**PR**	**SRK**	**Standard**	**PR**	**SRK**
Vapor Pressure	3.73	3.67	3.71	4.68	4.61	4.67	5.81	5.72	5.80	7.12	7.02	7.13
% Deviation		*-1.68%*	*-0.38%*		*-1.64%*	*-0.23%*		*-1.54%*	*-0.07%*		*-1.37%*	*0.12%*

Octane	**Temperature 450 K**			**Temperature 460 K**			**Temperature 470 K**			**Temperature 480 K**		
	Standard	**PR**	**SRK**	**Standard**	**PR**	**SRK**	**Standard**	**PR**	**SRK**	**Standard**	**PR**	**SRK**
Vapor Pressure	3.53	3.48	3.53	4.34	4.28	4.34	5.29	5.21	5.29	6.38	6.28	6.38
% Deviation		*-1.36%*	*0.02%*		*-1.47%*	*-0.02%*		*-1.53%*	*-0.04%*		*-1.53%*	*-0.04%*

Note : Standard value is by Antoine Equation.

6.2 Characteristic of Petroleum Fractional Distillation Calculation

Petroleum fractional distillation calculation is a length process requiring rigorous iterative procedure as shown pictorially in Figure 6.1. The time for calculation increased as the number of stages and the number of pseudocomponents increase. For each trial of the iterative loop for determining the temperature profile of the distillation column by energy balance, the compressibility factor iterative loops for both liquid and vapor phases in each stage of the column is required. Compressibility factor is a function of temperature, pressure and composition of petroleum fraction. In this latter iterative loops, the roots (Z_i) of the cubic equation is determined with the aid of Newton Raphson's convergence method.



Remark ↻ : Trial and Error Step

Figure 6.1 Iteration Procedure of The Distillation Simulation

6.3 Validity of Combining Pseudocomponents

6.3.1 Definition of a Combined Pseudocomponent

A combined pseudocomponent (CP) is defined in this work as a component representing a mixture of pseudocomponents. Thus, for validity, a CP must have the same properties as those of the pseudocomponent mixture. Logically, properties of a CP should be obtained from those of pseudocomponents with the aid of a mixing rule.

6.3.2 Mixing Rules for CP

There are many mixing rules in the literature. However, in practice, a simple mixing rule is used if it can provide property values of sufficient accuracy. Since a petroleum fraction contains hydrocarbon mixture in which properties of all components are similar, the Kay's rules, a linear mixing rule in composition, is tested in this work for accuracy.

To use the SRK equation of state, the critical temperature and critical pressure of the material system are required. Therefore, the Kay's rules are as follows.

$$T_{c,m} = \sum_{1}^{m} x_i T_{c,i} \qquad 6\text{-}1$$

$$P_{c,m} = \sum_{1}^{m} x_i P_{c,i} \qquad 6\text{-}2$$

Fugacity coefficient and enthalpy are the two properties tested, since these two properties are used in distillation simulation. The results, as shown in Tables 6.2 and 6.3, indicate that the Kay's rules are suitable for petroleum fraction grouping.

Table 6.2 Fugacity Coefficient of Hydrocarbon and Mixture

Component	**Mole Fraction**	**Fugacity Coefficient**			
		T = 160 ^{o}F	T = 180 ^{o}F	T = 200 ^{o}F	T = 220 ^{o}F
Pure Component					
Ethane	0.03	1.0296	1.0262	1.0232	1.0207
Propane	0.20	1.0163	1.0158	1.0152	1.0147
n-Butane	0.37	0.9990	1.0007	1.0021	1.0034
n-Pentane	0.35	0.9825	0.9864	0.9897	0.9926
n-Hexane	0.05	0.9662	0.9722	0.9774	0.9820
Mixture					
$\exp(\Sigma\, x_i \ln\phi_i)$ *		0.9959	0.9979	0.9997	1.0013
ϕ_m **		0.9974	0.9993	1.0010	1.0024

* by equation $\ln \phi_m = \Sigma x_i \ln \phi_i$

** by equation 4-30 together with equations 6-1 and 6-2

Enthalpy calculating used the same components and mole fraction in Table 6.2, as follow.

Table 6.3 Enthalpy of Hydrocarbon Mixture

Mixture	**Enthalpy**			
	T = 160 ^{o}F	T = 180 ^{o}F	T = 200 ^{o}F	T = 220 ^{o}F
$\Sigma\, x_i(H_i-H_i^*)$ *	-383.767	-330.874	-280.644	-232.765
$(H-H^*)$ **	-370.053	-324.436	-281.396	-240.639

* by equation $H_m = \Sigma x_i H_i$

** by equation 4-44 together with equations 6-1 and 6-2

6.4 Specification of Distillation Column and Petroleum Feed

Specification of distillation column, feed plate and petroleum feed used in this work are the same as those used by Ruangridth [9] which in turn are based on the illustration problem by Holland [4]. Also the initial guess values of x_{ij}, T_j and V_j by Ruangridth were used.

A crude oil having the characteristics in Table 6.4 and Figure 6.2 is to be topped to produce a jet fuel in a fractionating tower with no side streams, but with a reboiler. Stream is introduced at the bottom of the column so that the effective distillation pressure can be considered as 760 mm Hg., 560 deg.F. The fractionating tower contain a total of 18 equilibrium stages. Thus, the feed is introduced on the 17th stage.

Table 6.4 Crude Oil TBP Distillation at 760 mm Hg. [1]

% Volume Distilled	Temperature ^{o}F	Density g/cm^3	API gravity
0	105		
5	230	0.725	63.5
10	300	0.796	46.7
20	392	0.830	39
30	458	0.852	34.5
40	505	0.865	32
50	542	0.875	30.8
60	585	0.890	27.5
70	640	0.912	23.5
80	720	0.930	20.4
90	880	0.980	13.1
99	1090		

From the specifications the 0 to 55 vol % portion of the crude oil will satisfy the boiling range requirement of jet fuel. The design data of this distillation is given in Table 6.5 to 6.7.

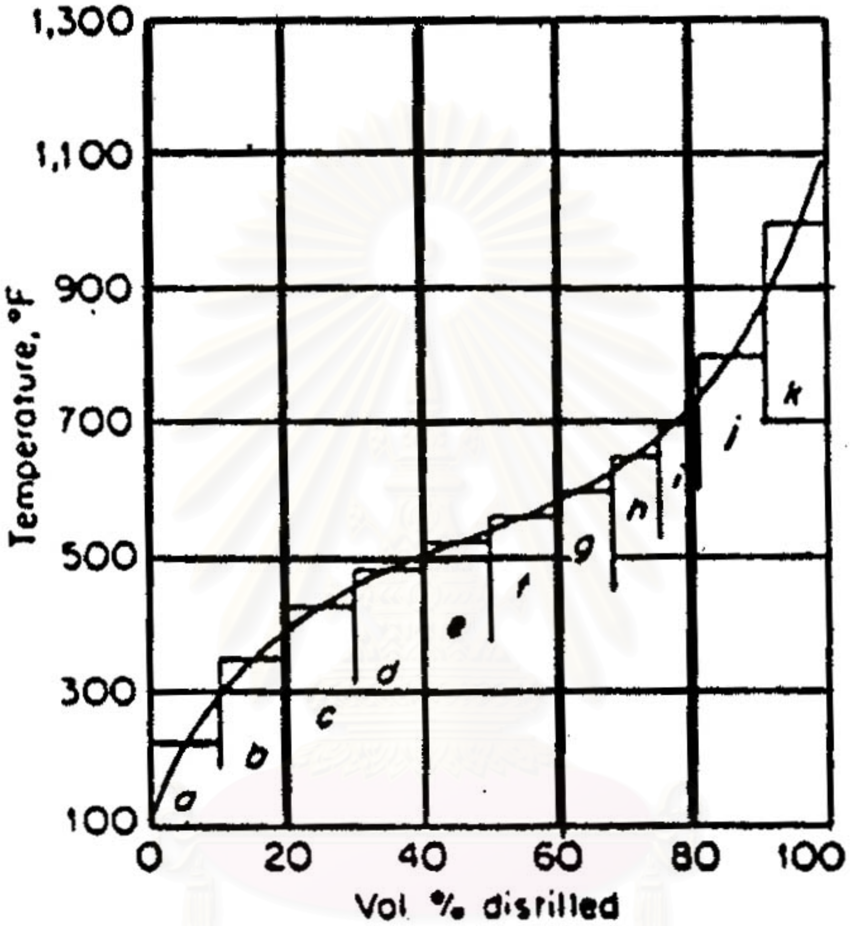


Figure 6.2 TBP Curve of Feed and Component Designation.

Table 6.5 The Properties of Crude Oil (11 pseudocomponents)

Comp.	Vol %	TBP % deg.F.	ρ g/cu.cm.	API	ρ lb/cu.ft.	lb/100cu.ft. mixture	Mol. weight	Moles/100 cu.ft. mixture	Mol. Frac.
1	10	225	0.745	58.5	46.50	465.0	102	4.56	0.1720
2	10	350	0.815	42.0	50.91	509.1	141	3.61	0.1362
3	10	430	0.842	36.5	52.58	525.8	165	3.19	0.1202
4	10	485	0.860	33.0	53.70	537.0	192	2.80	0.1055
5	10	528	0.870	31.0	54.36	543.6	210	2.59	0.0977
6	10	565	0.880	29.3	54.94	549.4	227	2.42	0.0913
7	8	600	0.896	26.5	55.91	447.3	242	1.85	0.0697
8	7	650	0.913	23.5	57.00	399.0	270	1.48	0.0558
9	6	700	0.930	22.3	57.45	344.7	300	1.15	0.0434
10	10	800	0.955	16.8	59.00	590.0	353	1.67	0.0631
11	9	1000	1.030	6.0	64.25	578.3	485	1.19	0.0450

Table 6.6 Composition of The Distillate and Bottoms

Component	Feed		Distillate		Bottoms	
	mole	x_F	mole	x_D	mole	x_B
1	0.1730	0.1730	0.1730	0.2200		
2	0.1370	0.1370	0.1370	0.1740		
3	0.1215	0.1215	0.1215	0.1540		
4	0.0990	0.0990	0.0990	0.1255		
5	0.0987	0.0987	0.0987	0.1251		
6	0.0920	0.0920	0.0900	0.1140	0.0020	0.0095
7	0.0705	0.0705	0.0635	0.0806	0.0070	0.0330
8	0.0562	0.0562	0.0057	0.0072	0.0505	0.2380
9	0.0434	0.0434			0.0434	0.2045
10	0.0641	0.0641			0.0641	0.3025
11	0.0450	0.0450			0.0450	0.2120
		1.0000	0.7884	1.0000	0.2120	1.0000

Theoretical plates (N) = 18

Reflux ratio = 1.83

V = 2.228, L = 1.44, D = 0.788

Table 6.7 Feed Concentration

Component	Flowrate (lbmole/hr)	Mole Fraction, z(i,j)
1	4.55	0.1729
2	3.61	0.1372
3	3.19	0.1212
4	2.6	0.0988
5	2.59	0.0984
6	2.42	0.0919
7	1.85	0.0703
8	1.48	0.0562
9	1.15	0.0437
10	1.69	0.0642
11	1.19	0.0452
	26.32	1.0000

6.5 Simulation Time of Various Numbers of Pseudocomponents

Based on specification in section 6.4, several simulations were performed with each simulation using different number of pseudocomponents. The numbers of pseudocomponent used were 11, 20, 30 and 40. The result of simulation shows that computing time increases with increase in number of components, and tends to be exponential (increase rapidly) when the number of pseudocomponents exceed 30 as shown in Figure 6.3.

Simulations were repeated using computers of various speeds. The effect of number of components on computing times is similar for all computers as shown in Table 6.8 and Figure 6.3.

Table 6.8 Comparison of Running Time

CASE	Computing Time (msec)				Percentage *			
	P 75	P 166	PII 350	K6-2 500	P 75	P 166	PII 350	K6-2 500
11 components	3570	1370	500	440	100.0%	100.0%	100.0%	100.0%
20 components	7530	3020	1100	930	210.9%	220.4%	220.0%	211.4%
30 components	12140	5110	1760	1540	340.1%	373.0%	352.0%	350.0%
40 components	23350	9720	3350	3020	654.1%	709.5%	670.0%	686.4%

Computer Specification

P 75 : Intel Pentium 75 Mhz., Ram 24 MB.

P 166 : Intel Pentium 166 Mhz., Ram 64 MB.

PII 350 : Intel Pentium II 350 Mhz., Ram 64 MB.

K6-2 500 : AMD K6-2 500 MHz., Ram 128 MB.

$$* \quad \text{Percentage} = \frac{\text{Computing time}}{\text{Computing time of 11 pseudocomponents}} \times 100$$

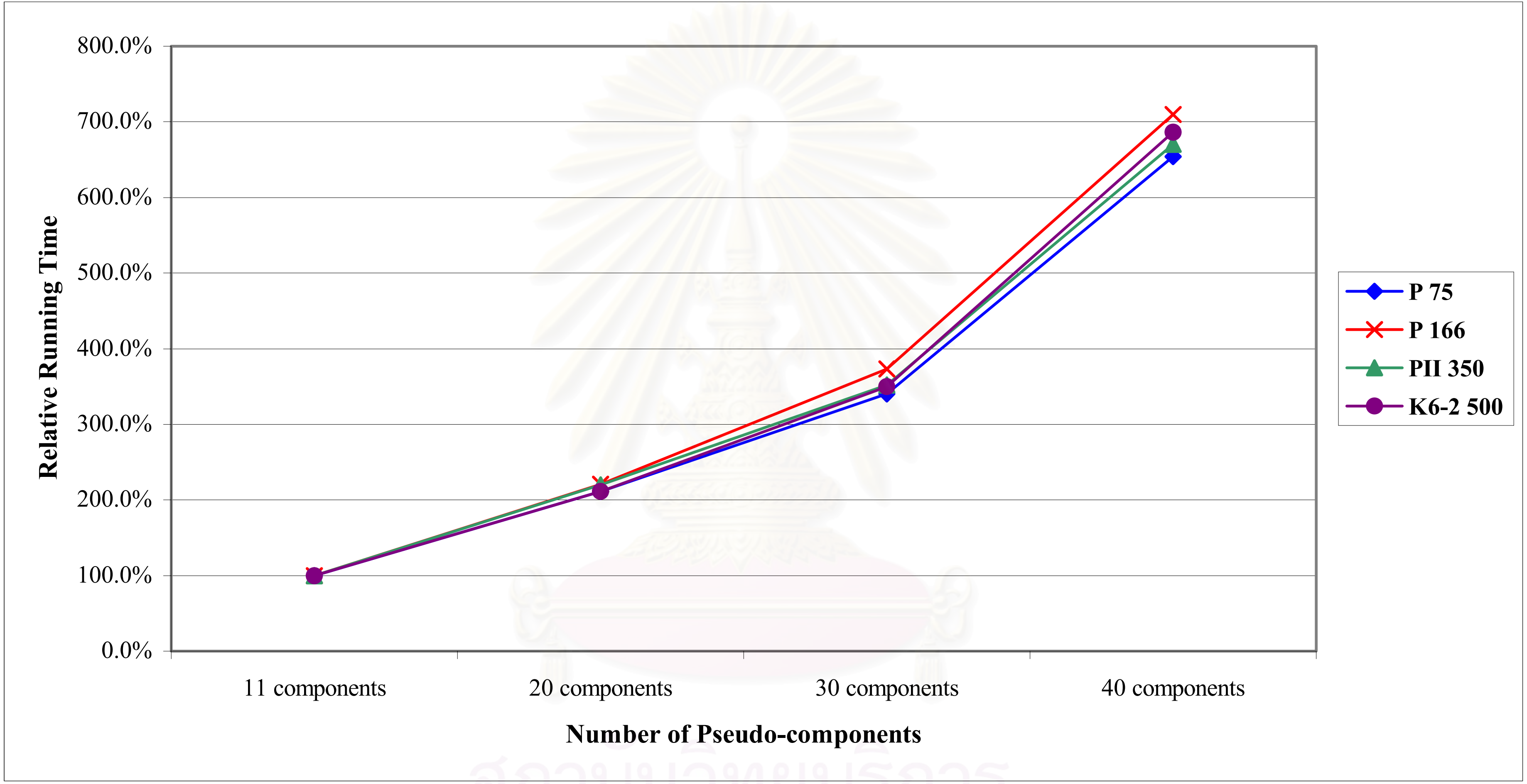


Figure6.3 Comparison of Running Time in Percentage

6.6 Simulation Times of Various Techniques

In this work, the petroleum fraction feed is assumed to consist of 20 pseudocomponents, since according to Ruangridth [9], the smallest number of pseudocomponents that give accurate simulation result is 20.

The normal simulation technique is presented in 6.6.1. Various simulations were tried using different pseudocomponents grouping. The two best techniques chosen are described in 6.6.2 and 6.6.3.

6.6.1 : Normal Simulation Technique (20 pseudocomponents)

The feed characteristics for 11 pseudocomponents are in Table 6.4 and Figure 6.2. In the case of 20 pseudocomponents, the feed characteristics are in Table 6.9. The simulation result is presented in Figures 6.5 to 6.9 and Table A1 to A3 in Appendix.

Solution

Table 6.9 The Properties of Crude Oil (20 pseudocomponents) Feed.

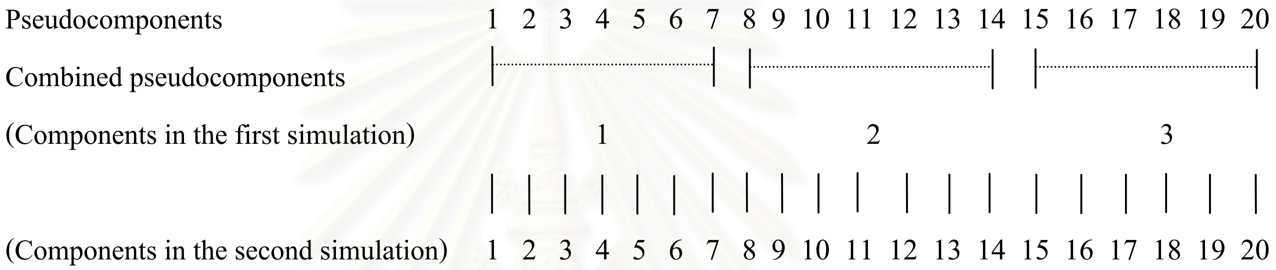
Comp.	Vol %	TBP.50% deg.F.	API	Moles/100 cu.ft. mixture	Mol. Frac.
1	5	140	69.8	2.30	0.0874
2	5	225	58.5	2.25	0.0855
3	5	294	47.8	1.77	0.0673
4	5	350	42.0	1.84	0.0699
5	5	395	38.8	1.59	0.0604
6	5	430	36.5	1.60	0.0608
7	5	458	34.8	1.30	0.0494
8	5	485	33.0	1.30	0.0494
9	5	507	31.8	1.30	0.0494
10	5	528	31.0	1.29	0.0490
11	5	548	30.2	1.26	0.0479
12	5	565	29.3	1.16	0.04407
13	5	585	27.8	1.14	0.04331
14	5	612	25.5	1.08	0.04103
15	5	650	23.5	1.11	0.04217
16	5	690	22.5	0.93	0.03533
17	5	735	21	0.92	0.03495
18	5	790	17.5	0.78	0.02964
19	5	875	12.2	0.78	0.02964
20	5	1000	6	0.62	0.02356
				26.32	1.0000

6.6.2 : Temperature Profile by CP Technique

In this simulation technique, the temperature profile of the distillation column is determined first by using CP’s in order to reduce the task of calculation.

After the temperature profile has been obtained, simulation is repeated with the petroleum fractional of feed and input data of 6.6.1 are used.

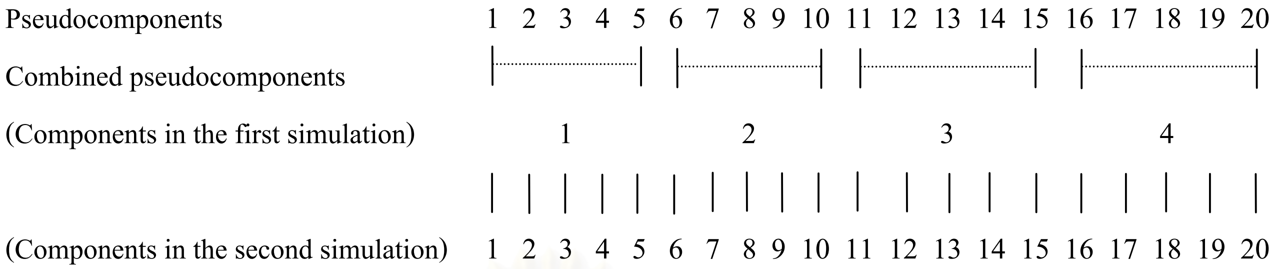
6.6.2.1 : 3 combined pseudocomponents from 20 pseudocomponents grouping



The above outlines the procedure of simulation. First, the simulation is done using 3 CP. Then the simulation is repeated using 20 pseudocomponents together with the temperature profile obtained in the first simulation. This latter simulation required only one iterative temperature loop to give the final temperature, vapor flow rates and product compositions.

The result of this simulation is presented in Table A4 in Appendix.

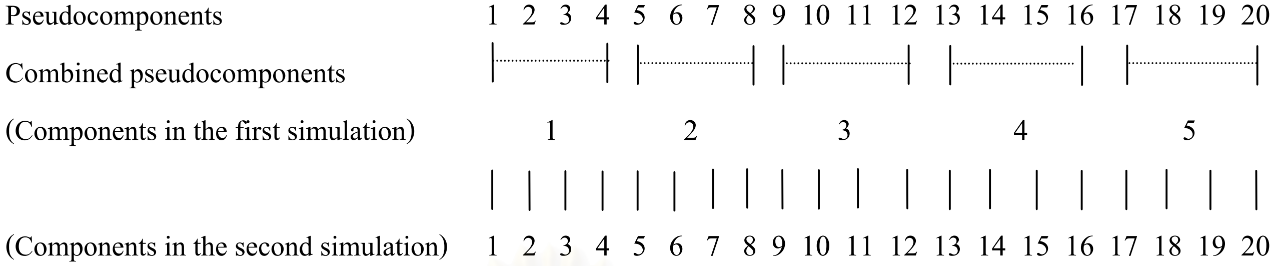
6.6.2.2 : 4 combined pseudocomponents from 20 pseudocomponents grouping



The above outlines the procedure of simulation. First, the simulation is done using 4 CP. Then the simulation is repeated using 20 pseudocomponents together with the temperature profile obtained in the first simulation. This latter simulation required only one iterative temperature loop to give the final temperature, vapor flow rates and product compositions.

The result of this simulation is presented in Figure 6.5-6.9 and Table A5 in Appendix.

6.6.2.3 : 5 combined pseudocomponents from 20 pseudocomponents grouping



The above outlines the procedure of simulation. First, the simulation is done using 5 CP. Then the simulation is repeated using 20 pseudocomponents together with the temperature profile obtained in the first simulation. This latter simulation required only one iterative temperature loop to give the final temperature, vapor flow rates and product compositions.

The result of this simulation is presented in Table A6 in Appendix.

6.6.2.4 : 7 combined pseudocomponents from 20 pseudocomponents grouping

Pseudocomponents	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
Combined pseudocomponents (Components in the first simulation)		1			2			3			4			5			6		7	
(Components in the second simulation)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20

The above outlines the procedure of simulation. First, the simulation is done using 7 CP. Then the simulation is repeated using 20 pseudocomponents together with the temperature profile obtained in the first simulation. This latter simulation required only one iterative temperature loop to give the final temperature, vapor flow rates and product compositions.

The result of this simulation is presented in Table A7 in Appendix.

6.6.3 : Light and Heavy CP's Technique

Another method to reduce the number of components is as follows. All pseudocomponents that are not expected to appear in the bottom product may be grouped into one component called light CP. Similarly, all pseudocomponents that are not expected to appear in the distillate product may be grouped into one component called heavy CP. Thus, the component grouping is shown as follows.

Pseudocomponents	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
2 Combined pseudocomponents	|⋯	⋯	⋯|	|	|	|	|	|	|	|	|	|	|	|	|	|⋯	⋯	⋯	⋯	⋯|
14 components used in simulation		1		2	3	4	5	6	7	8	9	10	11	12	13			14		

Simulation is done by normal simulation technique with 14 components. The result is presented in Figure 6.5-6.9 and Table A8 in Appendix.

6.6.4 : %Deviation of Temperature Profiles (T_j) Compared with Normal Simulation Technique

The temperature profiles of the distillation column as simulated by various techniques are similar as shown in Figure 6.4. As shown in Table 6.18, the deviation of temperature from that of normal techniques is very small, not exceed 2% for all CP techniques, except for the case of 3 CP techniques, the deviation is less than 4%.

<u>Table 6.10</u> %Deviation of Temperature Profiles (T_j) Compared with Normal Simulation Technique

Stage	**3 Combined Pseudocomponents**	**4 Combined Pseudocomponents**	**5 Combined Pseudocomponents**	**7 Combined Pseudocomponents**	**14 Combined Pseudocomponents**
1	1.11%	0.85%	0.09%	0.05%	0.34%
2	-0.28%	0.28%	-0.70%	-0.45%	0.12%
3	-0.61%	0.28%	-0.88%	-0.53%	0.17%
4	-1.01%	0.35%	-0.98%	-0.55%	0.20%
5	-1.48%	0.43%	-1.02%	-0.54%	0.18%
6	-1.97%	0.49%	-1.02%	-0.49%	0.12%
7	-2.43%	0.51%	-0.97%	-0.42%	0.02%
8	-2.83%	0.48%	-0.90%	-0.35%	-0.12%
9	-3.17%	0.39%	-0.81%	-0.28%	-0.30%
10	-3.44%	0.22%	-0.71%	-0.24%	-0.52%
11	-3.65%	-0.03%	-0.62%	-0.23%	-0.78%
12	-3.80%	-0.35%	-0.56%	-0.25%	-1.05%
13	-3.88%	-0.72%	-0.57%	-0.31%	-1.34%
14	-3.89%	-1.13%	-0.65%	-0.39%	-1.63%
15	-3.83%	-1.52%	-0.82%	-0.47%	-1.87%
16	-3.61%	-1.80%	-1.04%	-0.49%	-1.99%
17	-2.98%	-1.71%	-1.12%	-0.45%	-1.73%
18	-1.09%	-0.18%	-0.77%	-0.56%	-0.05%

$$\%\ \text{Deviation} = \left(\frac{T_{\text{combined}} - T_{\text{20 pseudo}}}{T_{\text{20 pseudo}}}\right) * 100$$

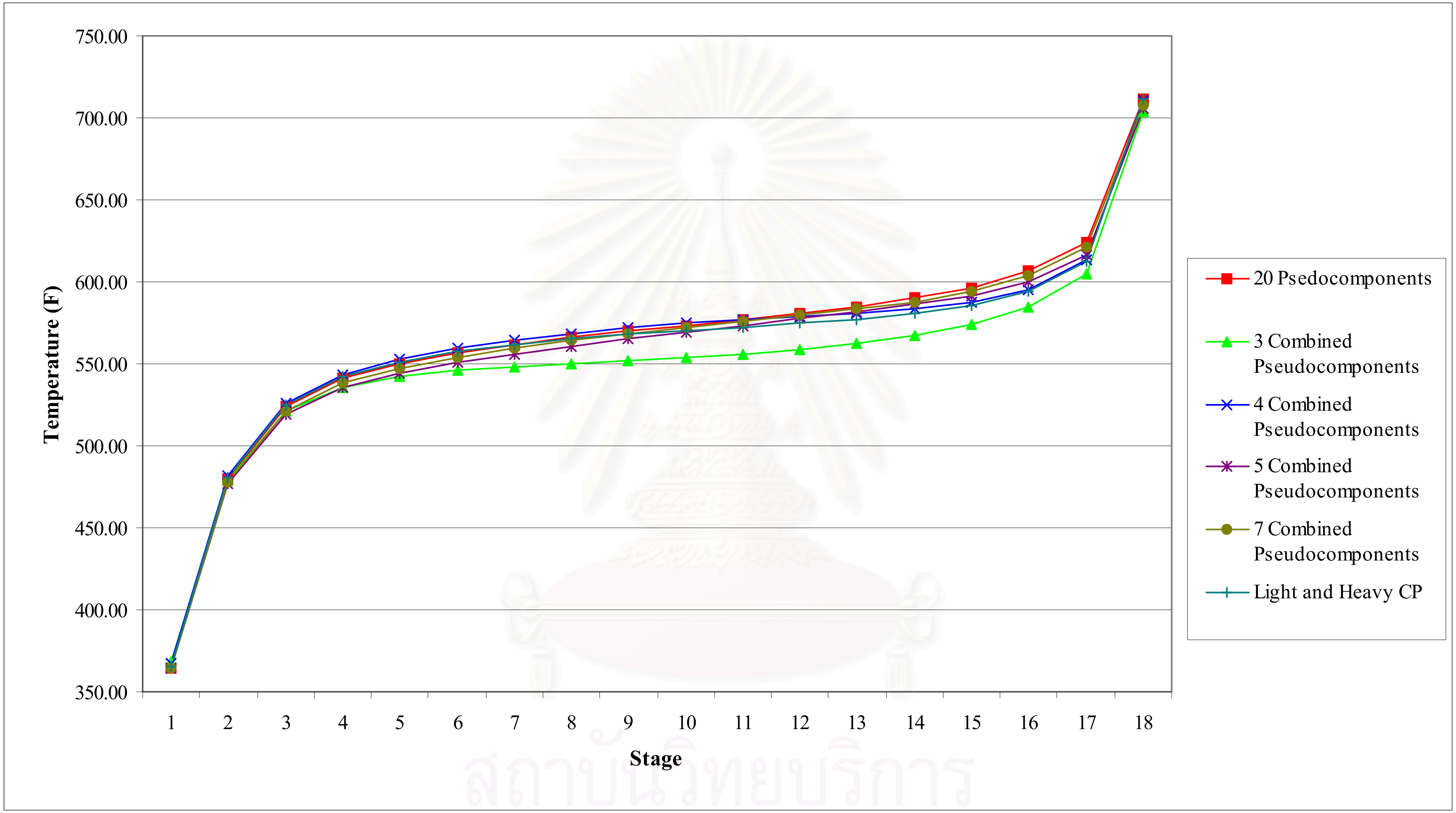


Figure6.4 Comparison of Temperature Profiles

6.6.5 : Running Time of 20 Pseudocomponents and Combined Pseudocomponents

Running time is the total time of program execution. Initial properties of system and initial data of various techniques are the same and setted in code program to start at the same status. Time count starts when program is executed and stops at the end of calculation. In this running time, the display results is not included.

The calculation running times on the K6-2 500 computer for various techniques are presented on Table 6.19. It is evident that the shortest running time is obtained by the "Temperature Profile by CP Technique" using 4 CP. This running time is about 10% that of normal technique.

Table 6.11 Running Time of 20 Pseudocomponents and Combined Pseudocomponents

Case	Computing Time (msec.)
Normal Technique	
20 pseudocomponents	990
Temperature Profile by CP Technique	
3 Combined pseudocomponents	160
4 Combined pseudocomponents	110
5 Combined pseudocomponents	280
7 Combined pseudocomponents	320
Light and Heavy CP's Technique	
14 Components	660

6.6.6 : Comparison of Simulation Results

The results of petroleum fraction distillation by using CP technique are agreeable to that of normal technique. Figure 6.4 compares the temperature profiles, Figure 6.5 compares the liquid mole fraction profiles of distillate, Figure 6.6 compares the liquid mole fraction profiles of bottom, Figure 6.7 compares the vapor mole fraction profiles of distillate, Figure 6.8 compares the vapor mole fraction profiles of bottom, and Figure 6.9 compares the vapor flow rate profiles.

In Figure 6.8, deviation of y_i by light and heavy CP technique for that of normal technique is largest for pseudocomponent number 15. This may be caused by the deviation of phase equilibrium constant K_i of heavy CP from average K_i value of pseudocomponents 16-20. The value of K_i of heavy CP is 0.6595 while the average K_i of pseudocomponents 16-20 is 0.6787. Note that the bottom stage containing mostly pseudocomponent number 15-20.

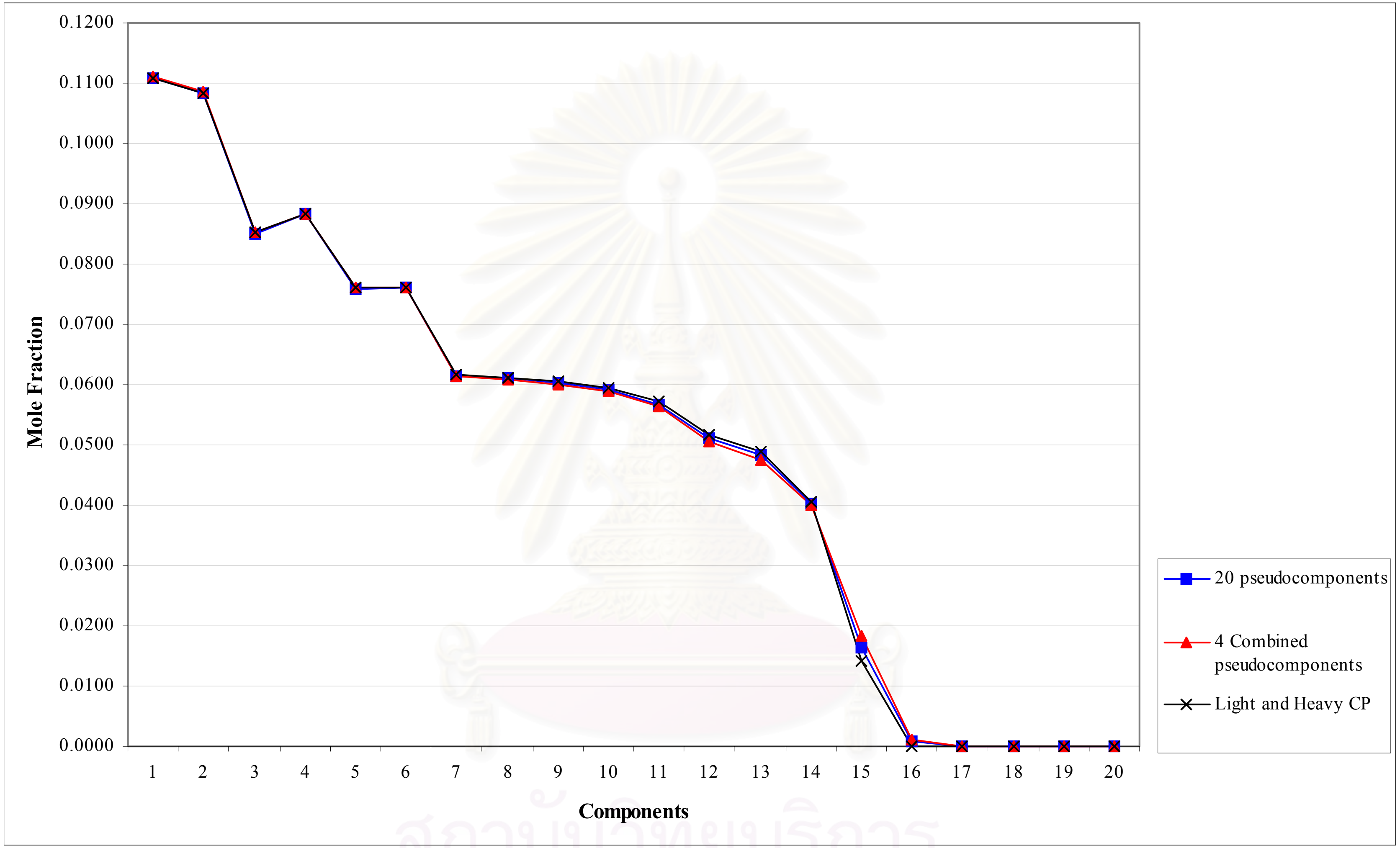


Figure 6.5 Comparison of Liquid Mole Fraction Profiles in Distillate

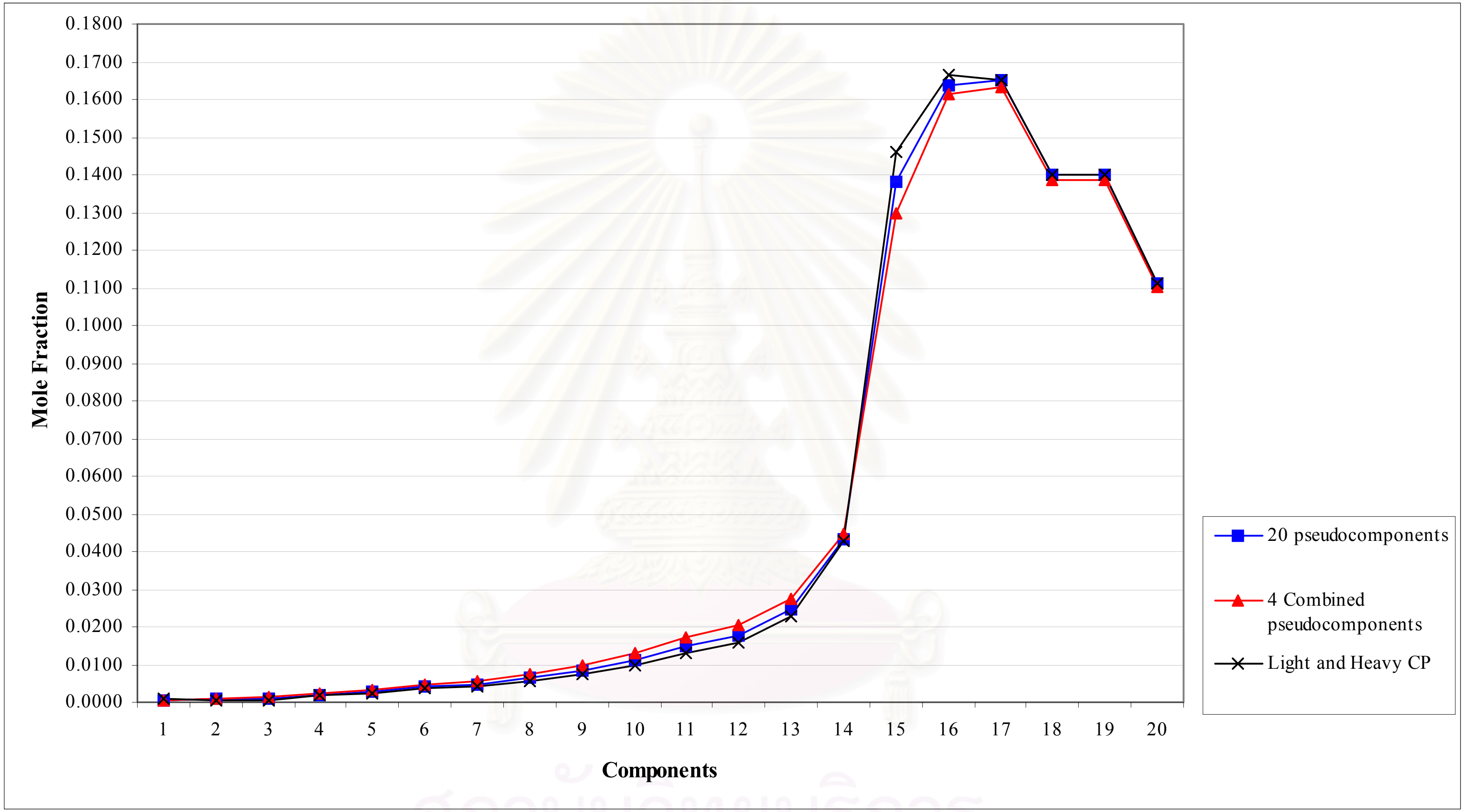


Figure 6.6 Comparison of Liquid Mole Fraction Profiles in Bottom

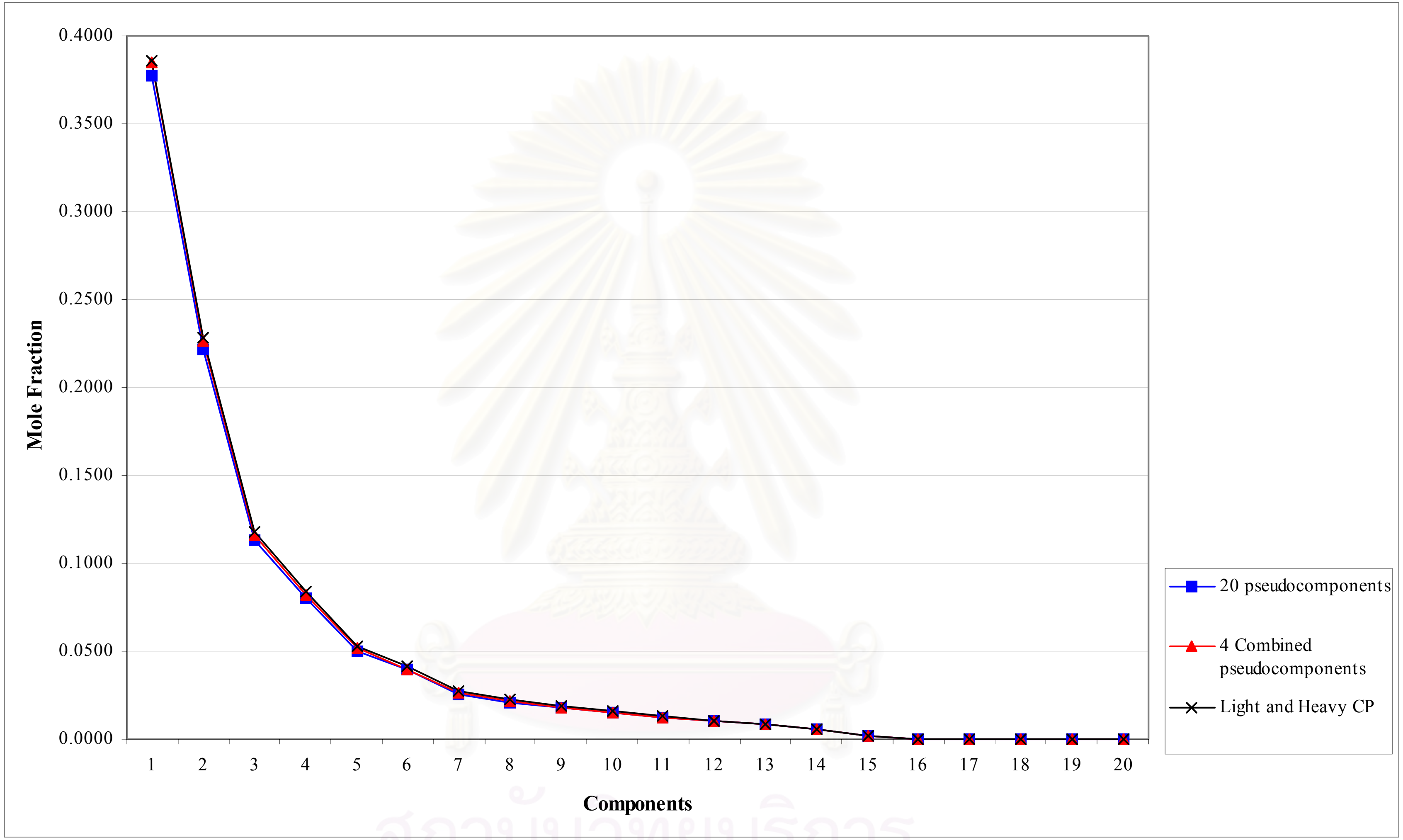


Figure 6.7 Comparison of Vapor Mole Fraction Profiles in Distillate

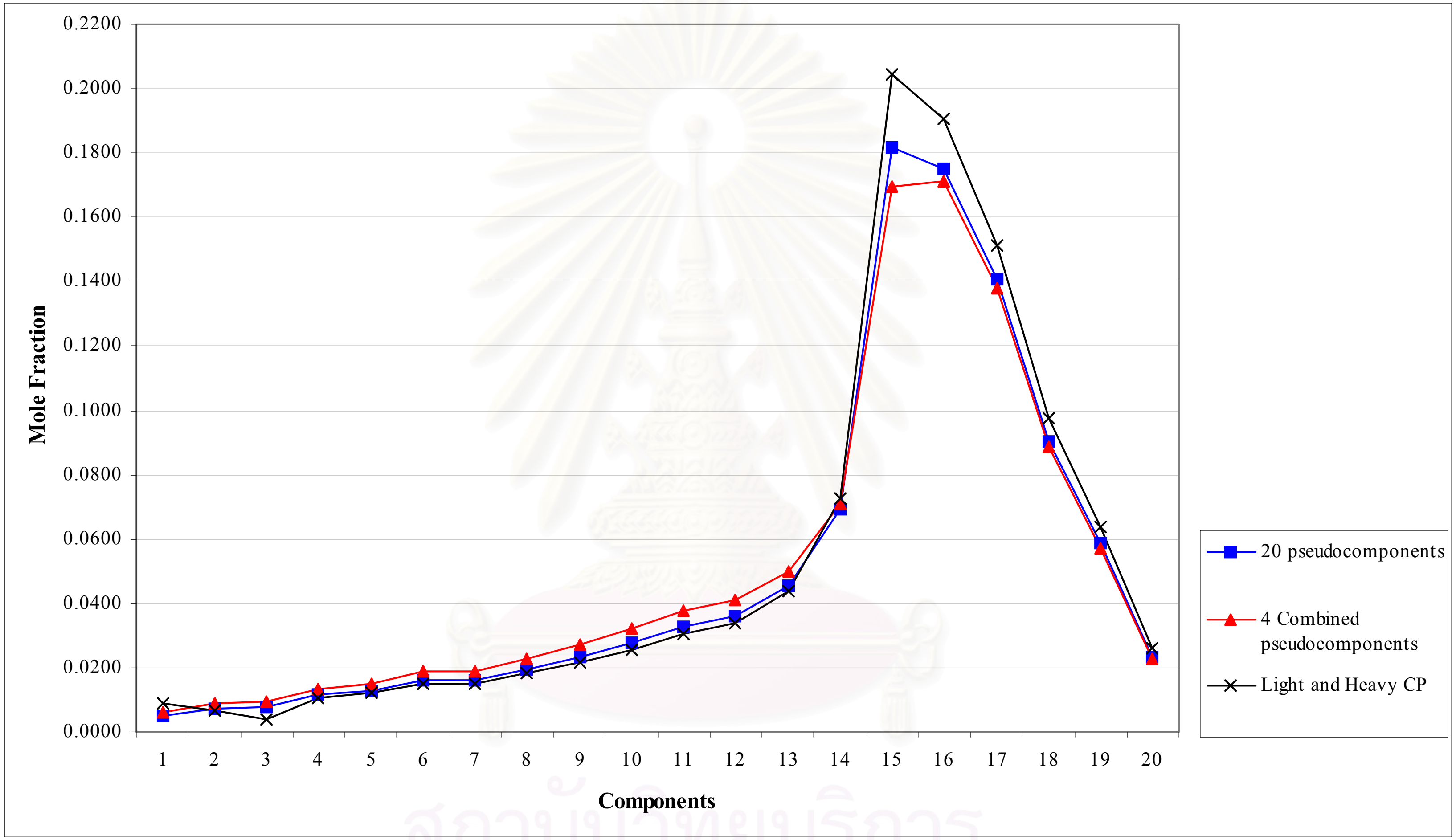


Figure 6.8 Comparison of Vapor Mole Fraction Profiles in Bottom

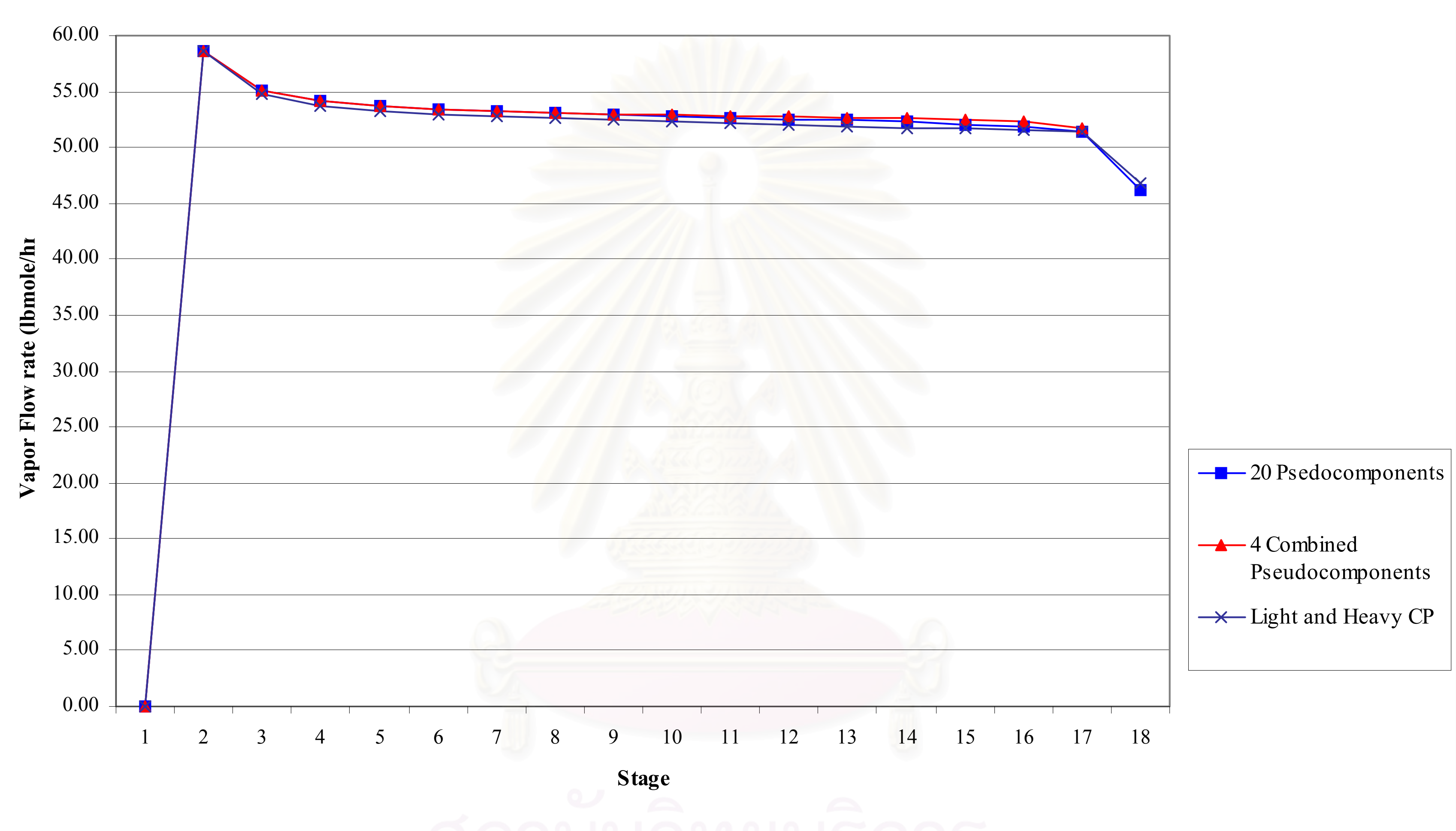


Figure 6.9 Comparison of Vapor Flow Rate Profiles

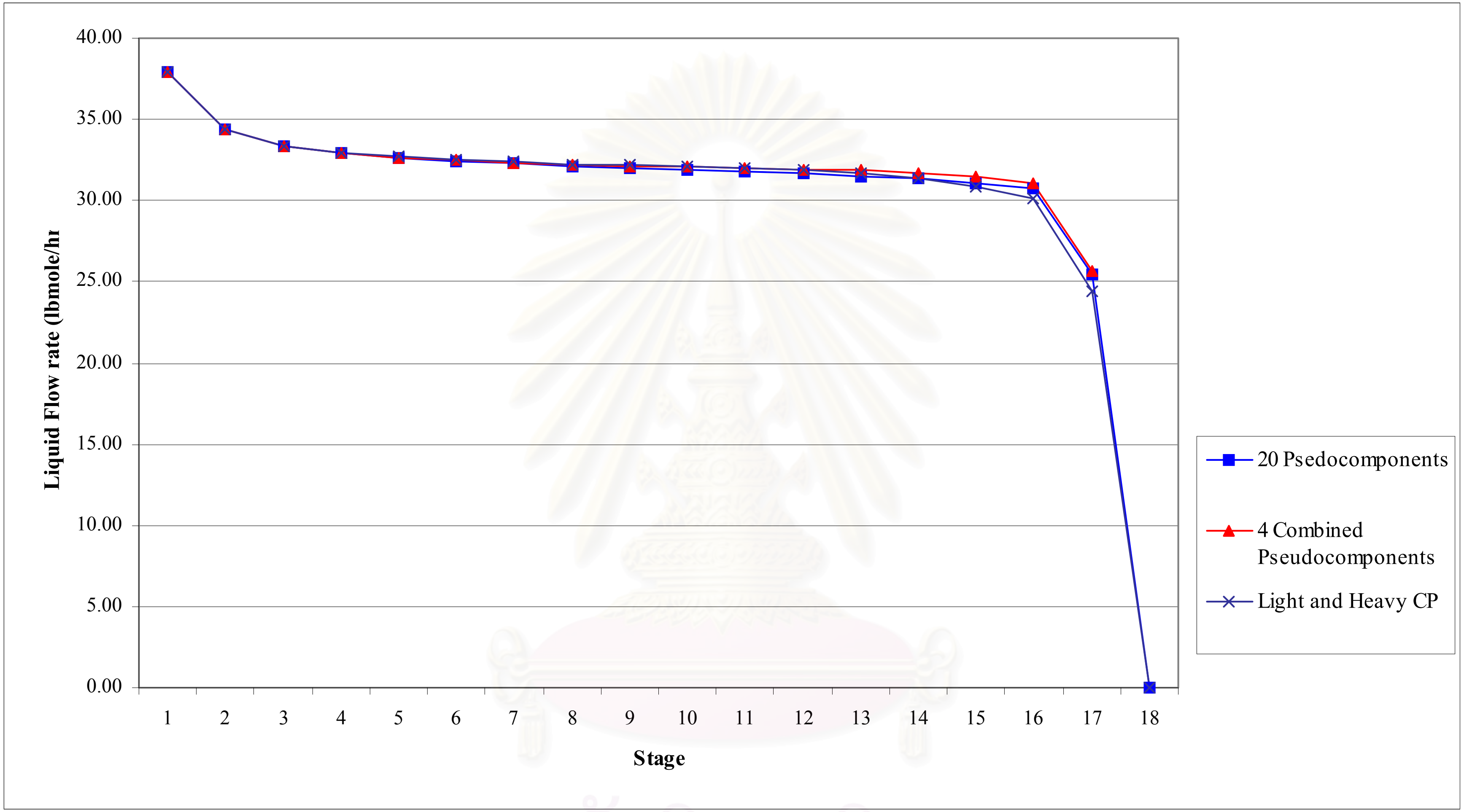


Figure 6.10 Comparison of Liquid Flow Rate Profiles

CHAPTER 7

CONCLUSION

In this work, techniques for reducing petroleum distillation developed. The petroleum distillation simulation was based on the properties generated by SRK equation. The distillation model was solved by tridiagonal matrix method. The results of this work can be concluded as follow.

1. The Kay's rule can be used in determining properties of combined pseudocomponents.
2. In general, for petroleum fraction distillation simulation, the "Temperature profile by CP technique" using 4 CP, may be employed. The running time of this technique is only about 11% that of normal simulation technique.
3. The "Temperature profile by CP technique" using 4 CP yields less than 2% deviation in temperature profile from that of normal technique.
4. Running time of normal simulation technique can be reduced with the aid of light and heavy combined pseudocomponents. The light combined pseudocomponent is the mixture of light pseudocomponents that will not go to the bottom products and the heavy combined pseudocomponent is the mixture of heavy pseudocomponents that will not go to the overhead product.

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APPENDIX

APPENDIX A

Data and Results

Input Data

N (No. of stage)	= 18	Feed Stage	= 17
B (lbmole/hr)	= 5.58	m (No. of component)	= 20

A1 Initial Operating Conditions Set (18 stages, 20 pseudocomponents)

Stage	P(psia)	W(lbmole/hr)	U(lbmole/hr)	Q(Btu/hr)	V(lbmole/hr)	T (deg. F)
1	14.696	0	20.75	0	0.00	257.12
2	14.696	0	0	0	58.64	368.23
3	14.696	0	0	0	55.00	433.97
4	14.696	0	0	0	55.00	451.34
5	14.696	0	0	0	55.00	457.05
6	14.696	0	0	0	55.00	459.42
7	14.696	0	0	0	55.00	461.53
8	14.696	0	0	0	55.00	462.04
9	14.696	0	0	0	55.00	463.02
10	14.696	0	0	0	55.00	463.74
11	14.696	0	0	0	55.00	464.40
12	14.696	0	0	0	55.00	465.12
13	14.696	0	0	0	55.00	465.80
14	14.696	0	0	0	55.00	466.54
15	14.696	0	0	0	55.00	467.38
16	14.696	0	0	0	55.00	468.23
17	14.696	0	0	0	55.00	469.26
18	14.696	0	0	0	55.00	620.96

A2 Initial Liquid Concentration, x_{ij} (18 stages, 20 pseudocomponents)

i Stage	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	0.4196	0.2026	0.1151	0.0725	0.0479	0.0335	0.0238	0.0191	0.0158	0.0136	0.0114	0.0092	0.0102	0.0052	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.1098	0.1035	0.0865	0.0840	0.0742	0.0692	0.0617	0.0591	0.0573	0.0573	0.0558	0.0506	0.0724	0.0525	0.0060	0.0001	0.0000	0.0000	0.0000	0.0000
3	0.0513	0.0549	0.0508	0.0564	0.0558	0.0590	0.0589	0.0618	0.0656	0.0718	0.0766	0.0749	0.1268	0.1181	0.0170	0.0004	0.0000	0.0000	0.0000	0.0000
4	0.0462	0.0466	0.0417	0.0450	0.0442	0.0472	0.0485	0.0524	0.0580	0.0666	0.0751	0.0773	0.1484	0.1710	0.0390	0.0009	0.0000	0.0000	0.0000	0.0000
5	0.0460	0.0456	0.0399	0.0417	0.0400	0.0416	0.0420	0.0452	0.0503	0.0586	0.0678	0.0718	0.1510	0.2095	0.0471	0.0018	0.0000	0.0000	0.0000	0.0000
6	0.0462	0.0455	0.0396	0.0408	0.0385	0.0392	0.0388	0.0410	0.0451	0.0522	0.0606	0.0649	0.1442	0.2349	0.0655	0.0032	0.0001	0.0000	0.0000	0.0000
7	0.0463	0.0455	0.0395	0.0405	0.0379	0.0381	0.0371	0.0338	0.0419	0.0477	0.0549	0.0586	0.1336	0.2485	0.0856	0.0053	0.0002	0.0000	0.0000	0.0000
8	0.0464	0.0455	0.0394	0.0403	0.0376	0.0376	0.0363	0.0375	0.0400	0.0449	0.0508	0.0537	0.1221	0.2522	0.1069	0.0086	0.0004	0.0000	0.0000	0.0000
9	0.0464	0.0455	0.0394	0.0402	0.0374	0.0372	0.0357	0.0367	0.0387	0.0429	0.0478	0.0499	0.1115	0.2478	0.1286	0.0133	0.0009	0.0000	0.0000	0.0000
10	0.0465	0.0455	0.0394	0.0401	0.0373	0.0370	0.0353	0.0361	0.0379	0.0416	0.0457	0.0471	0.1021	0.2371	0.1496	0.0200	0.0018	0.0000	0.0000	0.0000
11	0.0466	0.0456	0.0394	0.0401	0.0371	0.0367	0.0350	0.0356	0.0372	0.0406	0.0441	0.0449	0.0941	0.2218	0.1686	0.0292	0.0034	0.0000	0.0000	0.0000
12	0.0467	0.0456	0.0394	0.0400	0.0370	0.0365	0.0347	0.0352	0.0366	0.0397	0.0429	0.0431	0.0873	0.2033	0.1843	0.0413	0.0062	0.0000	0.0000	0.0000
13	0.0468	0.0457	0.0394	0.0399	0.0369	0.0363	0.0343	0.0348	0.0361	0.0390	0.0417	0.0417	0.0815	0.1829	0.1950	0.0566	0.0112	0.0002	0.0000	0.0000
14	0.0469	0.0457	0.0394	0.0399	0.0368	0.0361	0.0342	0.0345	0.0356	0.0382	0.0407	0.0403	0.0765	0.1617	0.1990	0.0748	0.0193	0.0005	0.0000	0.0000
15	0.0470	0.0458	0.0394	0.0398	0.0366	0.0359	0.0339	0.0341	0.0351	0.0375	0.0397	0.0390	0.0720	0.1405	0.1952	0.0949	0.0320	0.0016	0.0001	0.0001
16	0.0472	0.0459	0.0394	0.0398	0.0365	0.0357	0.0336	0.0336	0.0345	0.0367	0.0386	0.0377	0.0677	0.1201	0.1824	0.1145	0.0505	0.0045	0.0005	0.0005
17	0.0474	0.0460	0.0395	0.0397	0.0364	0.0355	0.0332	0.0332	0.0339	0.0359	0.0375	0.0364	0.0635	0.1007	0.1602	0.1295	0.0745	0.0123	0.0024	0.0023
18	0.0044	0.0066	0.0072	0.0094	0.0104	0.0122	0.0134	0.0151	0.0173	0.0204	0.0237	0.0250	0.0523	0.1069	0.2183	0.2244	0.1629	0.0443	0.0136	0.0120

A3 Output of Results

- Running Time on K6-2 500 MHz of 20 pseudocomponents is 990 msec.

A3-a Liquid Concentration, x_{ij} (18 stages, 20 pseudocomponents)

Stage \ i	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	0.1108	0.1083	0.0850	0.0882	0.0759	0.0760	0.0614	0.0610	0.0604	0.0592	0.0568	0.0512	0.0483	0.0404	0.0164	0.0008	0.0000	0.0000	0.0000	0.0000
2	0.0186	0.0279	0.0312	0.0445	0.0502	0.0625	0.0602	0.0708	0.0807	0.0902	0.0981	0.0982	0.1053	0.1048	0.0536	0.0032	0.0001	0.0000	0.0000	0.0000
3	0.0075	0.0123	0.0151	0.0241	0.0306	0.0424	0.0449	0.0585	0.0727	0.0887	0.1051	0.1136	0.1335	0.1512	0.0930	0.0066	0.0002	0.0000	0.0000	0.0000
4	0.0062	0.0096	0.0114	0.0176	0.0223	0.0314	0.0343	0.0466	0.0608	0.0784	0.0988	0.1131	0.1432	0.1815	0.1326	0.0114	0.0005	0.0000	0.0000	0.0000
5	0.0060	0.0090	0.0104	0.0155	0.0191	0.0263	0.0284	0.0388	0.0513	0.0680	0.0889	0.1060	0.1425	0.1995	0.1717	0.0177	0.0009	0.0000	0.0000	0.0000
6	0.0059	0.0088	0.0099	0.0147	0.0176	0.0238	0.0253	0.0339	0.0446	0.0594	0.0791	0.0968	0.1361	0.2074	0.2090	0.0260	0.0017	0.0000	0.0000	0.0000
7	0.0058	0.0086	0.0097	0.0142	0.0168	0.0224	0.0234	0.0309	0.0401	0.0530	0.0707	0.0875	0.1268	0.2075	0.2431	0.0365	0.0029	0.0001	0.0000	0.0000
8	0.0057	0.0085	0.0095	0.0138	0.0163	0.0215	0.0222	0.0289	0.0370	0.0482	0.0638	0.0791	0.1164	0.2017	0.2727	0.0495	0.0050	0.0002	0.0000	0.0000
9	0.0056	0.0083	0.0093	0.0135	0.0159	0.0208	0.0214	0.0275	0.0348	0.0447	0.0583	0.0718	0.1062	0.1917	0.2965	0.0651	0.0082	0.0005	0.0000	0.0000
10	0.0056	0.0082	0.0091	0.0132	0.0155	0.0202	0.0207	0.0264	0.0330	0.0419	0.0539	0.0657	0.0965	0.1789	0.3136	0.0833	0.0132	0.0011	0.0000	0.0000
11	0.0055	0.0081	0.0090	0.0130	0.0151	0.0197	0.0200	0.0254	0.0316	0.0397	0.0504	0.0604	0.0877	0.1644	0.3230	0.1038	0.0207	0.0023	0.0001	0.0000
12	0.0054	0.0080	0.0088	0.0127	0.0148	0.0192	0.0194	0.0245	0.0303	0.0378	0.0473	0.0560	0.0797	0.1491	0.3240	0.1261	0.0318	0.0047	0.0003	0.0000
13	0.0054	0.0079	0.0087	0.0124	0.0144	0.0186	0.0188	0.0237	0.0291	0.0359	0.0445	0.0519	0.0725	0.1334	0.3160	0.1488	0.0474	0.0095	0.0010	0.0000
14	0.0053	0.0077	0.0085	0.0121	0.0140	0.0180	0.0181	0.0227	0.0278	0.0341	0.0418	0.0481	0.0657	0.1177	0.2984	0.1697	0.0685	0.0186	0.0031	0.0002
15	0.0052	0.0075	0.0082	0.0117	0.0135	0.0173	0.0173	0.0216	0.0262	0.0320	0.0389	0.0442	0.0590	0.1017	0.2702	0.1854	0.0948	0.0348	0.0095	0.0010
16	0.0051	0.0073	0.0079	0.0111	0.0127	0.0163	0.0162	0.0201	0.0243	0.0294	0.0354	0.0398	0.0518	0.0850	0.2304	0.1900	0.1232	0.0611	0.0268	0.0062
17	0.0048	0.0069	0.0074	0.0103	0.0117	0.0148	0.0146	0.0179	0.0215	0.0258	0.0307	0.0340	0.0431	0.0665	0.1770	0.1740	0.1432	0.0958	0.0673	0.0330
18	0.0004	0.0008	0.0011	0.0020	0.0027	0.0041	0.0046	0.0064	0.0085	0.0113	0.0148	0.0177	0.0247	0.0433	0.1381	0.1638	0.1649	0.1399	0.1399	0.1112

A3-b Vapor Concentration, y_{ij} (18 stages, 20 pseudocomponents)

Stage \ i	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	0.3771	0.2217	0.1131	0.0804	0.0504	0.0392	0.0259	0.0211	0.0178	0.0151	0.0126	0.0101	0.0082	0.0056	0.0018	0.0001	0.0000	0.0000	0.0000	0.0000
2	0.1109	0.1083	0.0849	0.0882	0.0759	0.0761	0.0615	0.0610	0.0604	0.0592	0.0568	0.0511	0.0483	0.0404	0.0164	0.0008	0.0000	0.0000	0.0000	0.0000
3	0.0531	0.0582	0.0514	0.0609	0.0599	0.0676	0.0606	0.0672	0.0731	0.0785	0.0825	0.0805	0.0839	0.0806	0.0396	0.0023	0.0001	0.0000	0.0000	0.0000
4	0.0467	0.0488	0.0420	0.0486	0.0479	0.0552	0.0512	0.0594	0.0680	0.0773	0.0866	0.0897	0.1008	0.1087	0.0636	0.0044	0.0002	0.0000	0.0000	0.0000
5	0.0467	0.0476	0.0400	0.0448	0.0431	0.0487	0.0447	0.0522	0.0607	0.0710	0.0826	0.0891	0.1065	0.1270	0.0877	0.0073	0.0003	0.0000	0.0000	0.0000
6	0.0470	0.0477	0.0392	0.0439	0.0411	0.0457	0.0413	0.0474	0.0548	0.0645	0.0764	0.0847	0.1059	0.1376	0.1113	0.0111	0.0006	0.0000	0.0000	0.0000
7	0.0470	0.0476	0.0393	0.0435	0.0403	0.0442	0.0393	0.0445	0.0508	0.0593	0.0704	0.0790	0.1019	0.1423	0.1339	0.0162	0.0010	0.0000	0.0000	0.0000
8	0.0469	0.0478	0.0393	0.0431	0.0400	0.0434	0.0382	0.0426	0.0481	0.0554	0.0652	0.0733	0.0960	0.1421	0.1544	0.0225	0.0018	0.0001	0.0000	0.0000
9	0.0467	0.0474	0.0391	0.0430	0.0398	0.0429	0.0377	0.0415	0.0462	0.0525	0.0610	0.0681	0.0898	0.1384	0.1721	0.0304	0.0030	0.0001	0.0000	0.0000
10	0.0472	0.0475	0.0389	0.0428	0.0395	0.0425	0.0372	0.0407	0.0448	0.0503	0.0577	0.0637	0.0834	0.1322	0.1864	0.0398	0.0050	0.0003	0.0000	0.0000
11	0.0470	0.0476	0.0391	0.0429	0.0392	0.0422	0.0366	0.0400	0.0438	0.0487	0.0551	0.0599	0.0775	0.1243	0.1965	0.0508	0.0080	0.0007	0.0000	0.0000
12	0.0467	0.0477	0.0389	0.0427	0.0392	0.0420	0.0363	0.0394	0.0429	0.0474	0.0529	0.0568	0.0721	0.1154	0.2019	0.0631	0.0126	0.0014	0.0001	0.0000
13	0.0474	0.0479	0.0391	0.0425	0.0390	0.0416	0.0360	0.0390	0.0423	0.0462	0.0510	0.0540	0.0673	0.1060	0.2022	0.0765	0.0192	0.0028	0.0002	0.0000
14	0.0472	0.0476	0.0391	0.0425	0.0389	0.0414	0.0357	0.0385	0.0416	0.0452	0.0494	0.0516	0.0629	0.0965	0.1971	0.0900	0.0286	0.0057	0.0006	0.0000
15	0.0473	0.0475	0.0388	0.0424	0.0388	0.0412	0.0353	0.0380	0.0407	0.0441	0.0478	0.0493	0.0588	0.0869	0.1860	0.1024	0.0412	0.0112	0.0019	0.0001
16	0.0479	0.0480	0.0390	0.0421	0.0383	0.0409	0.0349	0.0373	0.0399	0.0428	0.0461	0.0470	0.0547	0.0772	0.1686	0.1115	0.0569	0.0209	0.0057	0.0006
17	0.0475	0.0483	0.0392	0.0423	0.0384	0.0405	0.0344	0.0365	0.0389	0.0414	0.0441	0.0444	0.0504	0.0670	0.1441	0.1137	0.0735	0.0365	0.0160	0.0037
18	0.0049	0.0073	0.0078	0.0114	0.0126	0.0162	0.0159	0.0194	0.0231	0.0276	0.0327	0.0358	0.0452	0.0693	0.1817	0.1752	0.1406	0.0905	0.0586	0.0235

A3-c Temperature and Vapor Flow Rate Profiles (18 stages, 20 pseudocomponents)

Stage	T (deg. F)	V (lbmole/hr)
1	364.42	0.00
2	480.10	58.64
3	524.12	55.11
4	541.14	54.12
5	550.34	53.68
6	556.69	53.40
7	561.69	53.20
8	565.96	53.04
9	569.80	52.90
10	573.43	52.77
11	577.04	52.65
12	580.80	52.53
13	585.00	52.41
14	590.01	52.27
15	596.58	52.09
16	606.36	51.85
17	623.72	51.45
18	711.50	46.16

A4 Output of Results of Case 6.6.2.1

- Running Time on K6-2 500 MHz of 3 combined pseudocomponents is 160 msec.

A4-a Liquid Concentration, x_{ij} (18 stages, 3 combined pseudocomponents)

i Stage	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	0.1123	0.1097	0.0861	0.0892	0.0767	0.0767	0.0618	0.0611	0.0602	0.0587	0.0558	0.0498	0.0463	0.0378	0.0167	0.0010	0.0000	0.0000	0.0000	0.0000
2	0.0190	0.0285	0.0319	0.0454	0.0512	0.0636	0.0611	0.0717	0.0814	0.0905	0.0976	0.0969	0.1023	0.0992	0.0553	0.0042	0.0001	0.0000	0.0000	0.0000
3	0.0081	0.0131	0.0160	0.0253	0.0318	0.0438	0.0462	0.0597	0.0737	0.0893	0.1048	0.1120	0.1294	0.1424	0.0953	0.0087	0.0003	0.0000	0.0000	0.0000
4	0.0072	0.0109	0.0127	0.0194	0.0242	0.0337	0.0363	0.0486	0.0625	0.0796	0.0987	0.1113	0.1379	0.1687	0.1331	0.0145	0.0007	0.0000	0.0000	0.0000
5	0.0072	0.0108	0.0122	0.0181	0.0218	0.0295	0.0314	0.0418	0.0541	0.0702	0.0897	0.1045	0.1363	0.1821	0.1672	0.0218	0.0012	0.0000	0.0000	0.0000
6	0.0074	0.0110	0.0123	0.0179	0.0212	0.0281	0.0292	0.0382	0.0489	0.0632	0.0814	0.0964	0.1298	0.1859	0.1964	0.0306	0.0021	0.0001	0.0000	0.0000
7	0.0076	0.0112	0.0124	0.0180	0.0210	0.0276	0.0283	0.0363	0.0459	0.0585	0.0748	0.0889	0.1217	0.1834	0.2201	0.0408	0.0035	0.0001	0.0000	0.0000
8	0.0077	0.0113	0.0125	0.0180	0.0210	0.0274	0.0279	0.0354	0.0440	0.0554	0.0700	0.0826	0.1134	0.1768	0.2381	0.0525	0.0056	0.0003	0.0000	0.0000
9	0.0077	0.0113	0.0125	0.0180	0.0210	0.0272	0.0275	0.0347	0.0428	0.0533	0.0664	0.0776	0.1059	0.1682	0.2508	0.0657	0.0088	0.0005	0.0000	0.0000
10	0.0077	0.0113	0.0125	0.0179	0.0208	0.0269	0.0272	0.0341	0.0419	0.0516	0.0636	0.0735	0.0992	0.1585	0.2583	0.0803	0.0134	0.0011	0.0000	0.0000
11	0.0077	0.0112	0.0124	0.0178	0.0206	0.0266	0.0268	0.0335	0.0409	0.0501	0.0612	0.0700	0.0933	0.1485	0.2609	0.0962	0.0201	0.0022	0.0001	0.0000
12	0.0076	0.0111	0.0122	0.0175	0.0202	0.0261	0.0262	0.0327	0.0398	0.0486	0.0589	0.0668	0.0879	0.1383	0.2588	0.1129	0.0296	0.0045	0.0003	0.0000
13	0.0074	0.0109	0.0120	0.0171	0.0197	0.0254	0.0255	0.0318	0.0386	0.0469	0.0565	0.0636	0.0826	0.1279	0.2517	0.1299	0.0428	0.0087	0.0009	0.0000
14	0.0072	0.0106	0.0116	0.0165	0.0191	0.0245	0.0246	0.0305	0.0370	0.0448	0.0538	0.0602	0.0772	0.1172	0.2393	0.1458	0.0604	0.0165	0.0028	0.0001
15	0.0070	0.0102	0.0111	0.0158	0.0182	0.0233	0.0233	0.0289	0.0350	0.0422	0.0505	0.0561	0.0712	0.1057	0.2207	0.1584	0.0827	0.0305	0.0084	0.0009
16	0.0066	0.0095	0.0104	0.0147	0.0169	0.0216	0.0216	0.0267	0.0321	0.0386	0.0460	0.0508	0.0638	0.0923	0.1943	0.1636	0.1076	0.0536	0.0237	0.0055
17	0.0059	0.0085	0.0092	0.0130	0.0148	0.0189	0.0188	0.0231	0.0277	0.0332	0.0393	0.0432	0.0535	0.0753	0.1567	0.1540	0.1278	0.0858	0.0609	0.0305
18	0.0005	0.0010	0.0014	0.0026	0.0036	0.0054	0.0062	0.0086	0.0115	0.0154	0.0201	0.0240	0.0328	0.0524	0.1311	0.1550	0.1567	0.1330	0.1330	0.1057

A4-b Vapor Concentration, y_{ij} (18 stages, 3 combined pseudocomponents)

Stage \ i	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	0.3914	0.2300	0.1174	0.0834	0.0521	0.0405	0.0266	0.0216	0.0182	0.0153	0.0126	0.0100	0.0081	0.0054	0.0018	0.0001	0.0000	0.0000	0.0000	0.0000
2	0.1127	0.1100	0.0863	0.0894	0.0768	0.0768	0.0619	0.0612	0.0603	0.0587	0.0559	0.0499	0.0464	0.0378	0.0167	0.0010	0.0000	0.0000	0.0000	0.0000
3	0.0564	0.0609	0.0534	0.0626	0.0611	0.0685	0.0611	0.0672	0.0726	0.0774	0.0806	0.0778	0.0797	0.0743	0.0397	0.0029	0.0001	0.0000	0.0000	0.0000
4	0.0526	0.0541	0.0455	0.0520	0.0505	0.0573	0.0524	0.0598	0.0676	0.0759	0.0836	0.0852	0.0937	0.0975	0.0616	0.0054	0.0002	0.0000	0.0000	0.0000
5	0.0544	0.0550	0.0451	0.0500	0.0470	0.0522	0.0471	0.0536	0.0609	0.0697	0.0791	0.0835	0.0967	0.1100	0.0810	0.0085	0.0004	0.0000	0.0000	0.0000
6	0.0564	0.0566	0.0461	0.0504	0.0465	0.0505	0.0448	0.0500	0.0563	0.0642	0.0735	0.0788	0.0943	0.1150	0.0975	0.0122	0.0007	0.0000	0.0000	0.0000
7	0.0579	0.0580	0.0471	0.0512	0.0468	0.0503	0.0439	0.0483	0.0535	0.0603	0.0686	0.0737	0.0897	0.1152	0.1109	0.0165	0.0011	0.0000	0.0000	0.0000
8	0.0591	0.0591	0.0479	0.0519	0.0473	0.0505	0.0437	0.0475	0.0520	0.0578	0.0649	0.0693	0.0846	0.1124	0.1215	0.0215	0.0018	0.0001	0.0000	0.0000
9	0.0598	0.0598	0.0484	0.0524	0.0476	0.0507	0.0437	0.0471	0.0511	0.0561	0.0623	0.0659	0.0799	0.1082	0.1295	0.0272	0.0029	0.0001	0.0000	0.0000
10	0.0602	0.0602	0.0487	0.0527	0.0478	0.0508	0.0437	0.0469	0.0506	0.0551	0.0604	0.0632	0.0759	0.1033	0.1351	0.0337	0.0044	0.0003	0.0000	0.0000
11	0.0604	0.0604	0.0488	0.0528	0.0479	0.0508	0.0436	0.0467	0.0501	0.0542	0.0589	0.0610	0.0724	0.0982	0.1385	0.0410	0.0068	0.0006	0.0000	0.0000
12	0.0603	0.0603	0.0488	0.0527	0.0478	0.0506	0.0434	0.0464	0.0497	0.0535	0.0578	0.0593	0.0694	0.0932	0.1399	0.0490	0.0101	0.0011	0.0000	0.0000
13	0.0601	0.0600	0.0486	0.0525	0.0476	0.0504	0.0431	0.0460	0.0492	0.0528	0.0567	0.0578	0.0668	0.0882	0.1393	0.0577	0.0150	0.0022	0.0001	0.0000
14	0.0595	0.0596	0.0482	0.0521	0.0472	0.0499	0.0427	0.0455	0.0485	0.0520	0.0555	0.0563	0.0643	0.0833	0.1365	0.0667	0.0217	0.0044	0.0005	0.0000
15	0.0588	0.0589	0.0477	0.0515	0.0467	0.0493	0.0422	0.0449	0.0478	0.0510	0.0543	0.0547	0.0618	0.0784	0.1315	0.0756	0.0310	0.0084	0.0014	0.0001
16	0.0575	0.0577	0.0469	0.0507	0.0459	0.0485	0.0415	0.0440	0.0468	0.0498	0.0528	0.0529	0.0592	0.0734	0.1240	0.0836	0.0431	0.0158	0.0043	0.0005
17	0.0552	0.0557	0.0454	0.0493	0.0447	0.0473	0.0404	0.0429	0.0455	0.0483	0.0510	0.0508	0.0563	0.0680	0.1139	0.0895	0.0582	0.0288	0.0127	0.0029
18	0.0063	0.0092	0.0101	0.0143	0.0164	0.0209	0.0207	0.0255	0.0305	0.0364	0.0429	0.0469	0.0579	0.0808	0.1656	0.1587	0.1275	0.0817	0.0526	0.0209

A4-c Temperature and Vapor Flow Rate Profiles (18 stages, 3 combined pseudocomponents)

Stage	T (deg. F)	V (lbmole/hr)
1	368.48	0.00
2	478.75	58.64
3	520.90	53.14
4	535.67	51.89
5	542.18	51.42
6	545.75	51.15
7	548.07	50.98
8	549.92	50.85
9	551.73	50.77
10	553.68	50.70
11	555.96	50.64
12	558.76	50.58
13	562.32	50.53
14	567.04	50.46
15	573.74	50.37
16	584.45	50.26
17	605.14	50.11
18	703.75	45.96

A5 Output of Results of Case 6.6.2.2

- Running Time on K6-2 500 MHz. of 4 combined pseudocomponents is 110 msec.

A5-a Liquid Concentration, x_{ij} (18 stages, 4 combined pseudocomponents)

Stage \ i	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	0.1111	0.1085	0.0852	0.0883	0.0760	0.0760	0.0614	0.0608	0.0601	0.0588	0.0563	0.0506	0.0476	0.0400	0.0183	0.0010	0.0000	0.0000	0.0000	0.0000
2	0.0185	0.0278	0.0311	0.0444	0.0501	0.0623	0.0600	0.0705	0.0802	0.0895	0.0970	0.0970	0.1037	0.1037	0.0599	0.0041	0.0001	0.0000	0.0000	0.0000
3	0.0074	0.0122	0.0150	0.0239	0.0304	0.0421	0.0446	0.0579	0.0719	0.0876	0.1035	0.1116	0.1308	0.1489	0.1034	0.0086	0.0003	0.0000	0.0000	0.0000
4	0.0062	0.0095	0.0112	0.0174	0.0220	0.0310	0.0338	0.0459	0.0598	0.0770	0.0967	0.1104	0.1395	0.1778	0.1466	0.0146	0.0006	0.0000	0.0000	0.0000
5	0.0059	0.0089	0.0102	0.0153	0.0187	0.0258	0.0279	0.0379	0.0501	0.0663	0.0864	0.1028	0.1379	0.1939	0.1884	0.0225	0.0012	0.0000	0.0000	0.0000
6	0.0058	0.0086	0.0097	0.0143	0.0172	0.0232	0.0246	0.0330	0.0433	0.0576	0.0764	0.0932	0.1307	0.2001	0.2274	0.0327	0.0022	0.0001	0.0000	0.0000
7	0.0057	0.0084	0.0095	0.0139	0.0164	0.0218	0.0228	0.0299	0.0388	0.0511	0.0678	0.0837	0.1208	0.1984	0.2618	0.0454	0.0037	0.0001	0.0000	0.0000
8	0.0056	0.0084	0.0093	0.0136	0.0160	0.0210	0.0216	0.0280	0.0357	0.0464	0.0610	0.0752	0.1101	0.1909	0.2900	0.0606	0.0063	0.0003	0.0000	0.0000
9	0.0056	0.0083	0.0093	0.0134	0.0157	0.0205	0.0209	0.0268	0.0337	0.0430	0.0557	0.0681	0.0998	0.1795	0.3107	0.0784	0.0102	0.0006	0.0000	0.0000
10	0.0057	0.0084	0.0093	0.0133	0.0155	0.0201	0.0205	0.0260	0.0323	0.0406	0.0518	0.0623	0.0904	0.1657	0.3226	0.0982	0.0160	0.0013	0.0000	0.0000
11	0.0058	0.0084	0.0093	0.0133	0.0155	0.0200	0.0202	0.0254	0.0314	0.0390	0.0488	0.0578	0.0822	0.1509	0.3253	0.1194	0.0245	0.0027	0.0001	0.0000
12	0.0059	0.0086	0.0094	0.0134	0.0155	0.0200	0.0201	0.0251	0.0307	0.0378	0.0466	0.0543	0.0753	0.1359	0.3185	0.1406	0.0364	0.0055	0.0004	0.0000
13	0.0060	0.0087	0.0095	0.0135	0.0156	0.0200	0.0200	0.0249	0.0303	0.0369	0.0449	0.0514	0.0695	0.1215	0.3028	0.1604	0.0523	0.0107	0.0011	0.0000
14	0.0061	0.0088	0.0096	0.0136	0.0156	0.0199	0.0199	0.0246	0.0298	0.0360	0.0434	0.0489	0.0644	0.1079	0.2787	0.1763	0.0726	0.0199	0.0034	0.0002
15	0.0061	0.0089	0.0096	0.0136	0.0155	0.0197	0.0196	0.0242	0.0291	0.0349	0.0417	0.0464	0.0596	0.0949	0.2472	0.1858	0.0966	0.0357	0.0099	0.0011
16	0.0060	0.0087	0.0094	0.0132	0.0150	0.0190	0.0188	0.0231	0.0277	0.0331	0.0392	0.0431	0.0542	0.0818	0.2085	0.1847	0.1213	0.0604	0.0267	0.0062
17	0.0056	0.0080	0.0086	0.0121	0.0137	0.0173	0.0171	0.0208	0.0248	0.0295	0.0347	0.0378	0.0466	0.0667	0.1613	0.1666	0.1382	0.0926	0.0655	0.0325
18	0.0005	0.0010	0.0013	0.0023	0.0032	0.0048	0.0054	0.0075	0.0100	0.0132	0.0171	0.0203	0.0275	0.0447	0.1297	0.1613	0.1632	0.1385	0.1385	0.1101

<u>A5-b</u> Vapor Concentration, y_{ij} (18 stages, 4 combined pseudocomponents)

i Stage	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	0.3852	0.2265	0.1157	0.0822	0.0514	0.0400	0.0263	0.0214	0.0181	0.0152	0.0127	0.0101	0.0083	0.0057	0.0020	0.0001	0.0000	0.0000	0.0000	0.0000
2	0.1109	0.1086	0.0855	0.0887	0.0764	0.0765	0.0618	0.0612	0.0606	0.0592	0.0566	0.0509	0.0480	0.0403	0.0185	0.0010	0.0000	0.0000	0.0000	0.0000
3	0.0531	0.0580	0.0515	0.0610	0.0600	0.0677	0.0607	0.0671	0.0729	0.0782	0.0820	0.0798	0.0829	0.0801	0.0444	0.0030	0.0001	0.0000	0.0000	0.0000
4	0.0468	0.0488	0.0418	0.0485	0.0478	0.0551	0.0511	0.0592	0.0676	0.0768	0.0858	0.0886	0.0994	0.1078	0.0712	0.0057	0.0002	0.0000	0.0000	0.0000
5	0.0463	0.0475	0.0396	0.0447	0.0428	0.0484	0.0445	0.0518	0.0601	0.0702	0.0815	0.0877	0.1046	0.1253	0.0977	0.0094	0.0004	0.0000	0.0000	0.0000
6	0.0463	0.0472	0.0391	0.0434	0.0408	0.0452	0.0409	0.0468	0.0541	0.0636	0.0750	0.0829	0.1034	0.1351	0.1233	0.0142	0.0007	0.0000	0.0000	0.0000
7	0.0465	0.0473	0.0390	0.0430	0.0400	0.0437	0.0389	0.0438	0.0499	0.0582	0.0688	0.0769	0.0988	0.1385	0.1469	0.0205	0.0013	0.0000	0.0000	0.0000
8	0.0469	0.0475	0.0391	0.0429	0.0397	0.0430	0.0379	0.0420	0.0471	0.0541	0.0634	0.0709	0.0924	0.1369	0.1671	0.0281	0.0023	0.0001	0.0000	0.0000
9	0.0474	0.0480	0.0393	0.0431	0.0396	0.0427	0.0373	0.0409	0.0453	0.0512	0.0591	0.0655	0.0855	0.1315	0.1830	0.0371	0.0038	0.0002	0.0000	0.0000
10	0.0482	0.0486	0.0397	0.0434	0.0398	0.0426	0.0370	0.0403	0.0441	0.0492	0.0558	0.0610	0.0788	0.1235	0.1934	0.0473	0.0061	0.0004	0.0000	0.0000
11	0.0492	0.0495	0.0404	0.0439	0.0401	0.0428	0.0370	0.0400	0.0434	0.0478	0.0533	0.0573	0.0726	0.1140	0.1978	0.0583	0.0094	0.0008	0.0000	0.0000
12	0.0504	0.0506	0.0411	0.0446	0.0406	0.0432	0.0372	0.0399	0.0431	0.0469	0.0516	0.0544	0.0674	0.1040	0.1961	0.0696	0.0142	0.0016	0.0001	0.0000
13	0.0517	0.0518	0.0420	0.0454	0.0412	0.0437	0.0375	0.0400	0.0429	0.0463	0.0503	0.0522	0.0629	0.0942	0.1888	0.0803	0.0207	0.0031	0.0002	0.0000
14	0.0530	0.0531	0.0429	0.0463	0.0419	0.0443	0.0378	0.0403	0.0429	0.0460	0.0494	0.0505	0.0593	0.0850	0.1767	0.0897	0.0291	0.0059	0.0006	0.0000
15	0.0541	0.0541	0.0437	0.0471	0.0425	0.0448	0.0382	0.0405	0.0429	0.0457	0.0486	0.0491	0.0563	0.0768	0.1610	0.0970	0.0397	0.0108	0.0019	0.0001
16	0.0546	0.0546	0.0442	0.0476	0.0429	0.0451	0.0384	0.0405	0.0428	0.0454	0.0479	0.0479	0.0538	0.0696	0.1428	0.1013	0.0523	0.0192	0.0053	0.0006
17	0.0539	0.0541	0.0439	0.0474	0.0428	0.0450	0.0382	0.0403	0.0425	0.0448	0.0470	0.0466	0.0514	0.0632	0.1232	0.1019	0.0663	0.0329	0.0144	0.0033
18	0.0061	0.0088	0.0095	0.0133	0.0151	0.0190	0.0188	0.0228	0.0271	0.0321	0.0376	0.0408	0.0501	0.0711	0.1694	0.1711	0.1377	0.0884	0.0571	0.0228

5-c Temperature and Vapor Flow Rate Profiles (18 stages, 4 combined pseudocomponents)

Stage	T (deg. F)	V (lbmole/hr)
1	367.53	0.00
2	481.43	58.64
3	525.58	54.16
4	543.05	53.10
5	552.73	52.62
6	559.43	52.35
7	564.57	52.13
8	568.68	51.93
9	572.00	51.75
10	574.68	51.58
11	576.87	51.42
12	578.79	51.26
13	580.76	51.11
14	583.33	50.96
15	587.49	50.82
16	595.42	50.68
17	613.08	50.52
18	710.23	46.10

A6 Output of Results of Case 6.6.2.3

- Running Time on K6-2 500 MHz. of 5 combined pseudocomponents is 280 msec.

A6-a Liquid Concentration, x_{ij} (18 stages, 5 combined pseudocomponents)

Stage \ i	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	0.1124	0.1098	0.0862	0.0894	0.0769	0.0770	0.0621	0.0616	0.0609	0.0595	0.0569	0.0510	0.0476	0.0377	0.0106	0.0004	0.0000	0.0000	0.0000	0.0000
2	0.0192	0.0289	0.0324	0.0462	0.0521	0.0648	0.0624	0.0733	0.0833	0.0929	0.1006	0.1003	0.1063	0.1001	0.0355	0.0017	0.0000	0.0000	0.0000	0.0000
3	0.0079	0.0129	0.0159	0.0255	0.0324	0.0448	0.0475	0.0618	0.0767	0.0934	0.1103	0.1185	0.1377	0.1478	0.0631	0.0036	0.0001	0.0000	0.0000	0.0000
4	0.0066	0.0102	0.0120	0.0187	0.0238	0.0336	0.0368	0.0501	0.0653	0.0842	0.1058	0.1206	0.1513	0.1820	0.0923	0.0063	0.0003	0.0000	0.0000	0.0000
5	0.0063	0.0095	0.0109	0.0165	0.0204	0.0282	0.0307	0.0420	0.0558	0.0741	0.0970	0.1155	0.1541	0.2054	0.1231	0.0102	0.0005	0.0000	0.0000	0.0000
6	0.0061	0.0092	0.0104	0.0155	0.0187	0.0255	0.0272	0.0368	0.0488	0.0654	0.0875	0.1073	0.1505	0.2197	0.1549	0.0155	0.0010	0.0000	0.0000	0.0000
7	0.0059	0.0089	0.0101	0.0148	0.0178	0.0238	0.0251	0.0334	0.0438	0.0585	0.0788	0.0983	0.1431	0.2263	0.1869	0.0226	0.0018	0.0001	0.0000	0.0000
8	0.0058	0.0087	0.0098	0.0143	0.0170	0.0227	0.0236	0.0310	0.0402	0.0531	0.0713	0.0896	0.1335	0.2262	0.2180	0.0319	0.0032	0.0001	0.0000	0.0000
9	0.0057	0.0084	0.0095	0.0139	0.0164	0.0217	0.0225	0.0292	0.0374	0.0488	0.0649	0.0814	0.1230	0.2206	0.2468	0.0438	0.0055	0.0003	0.0000	0.0000
10	0.0056	0.0083	0.0093	0.0135	0.0159	0.0209	0.0215	0.0278	0.0352	0.0453	0.0595	0.0741	0.1123	0.2104	0.2718	0.0587	0.0093	0.0008	0.0000	0.0000
11	0.0055	0.0081	0.0090	0.0131	0.0154	0.0202	0.0207	0.0265	0.0333	0.0424	0.0549	0.0676	0.1019	0.1966	0.2911	0.0766	0.0153	0.0017	0.0001	0.0000
12	0.0054	0.0080	0.0089	0.0128	0.0150	0.0195	0.0199	0.0254	0.0316	0.0399	0.0510	0.0619	0.0920	0.1801	0.3030	0.0973	0.0244	0.0037	0.0002	0.0000
13	0.0054	0.0079	0.0087	0.0125	0.0146	0.0190	0.0193	0.0244	0.0302	0.0377	0.0475	0.0567	0.0827	0.1617	0.3056	0.1197	0.0380	0.0077	0.0008	0.0000
14	0.0053	0.0078	0.0086	0.0123	0.0143	0.0184	0.0186	0.0234	0.0288	0.0357	0.0443	0.0521	0.0739	0.1421	0.2970	0.1419	0.0570	0.0156	0.0027	0.0001
15	0.0054	0.0078	0.0085	0.0121	0.0139	0.0179	0.0180	0.0225	0.0274	0.0336	0.0412	0.0476	0.0657	0.1217	0.2754	0.1604	0.0817	0.0301	0.0083	0.0009
16	0.0053	0.0077	0.0083	0.0118	0.0135	0.0172	0.0172	0.0213	0.0258	0.0313	0.0378	0.0429	0.0573	0.1004	0.2394	0.1696	0.1094	0.0544	0.0240	0.0056
17	0.0051	0.0073	0.0079	0.0110	0.0125	0.0158	0.0157	0.0193	0.0232	0.0278	0.0331	0.0369	0.0476	0.0776	0.1873	0.1604	0.1311	0.0878	0.0620	0.0306
18	0.0005	0.0009	0.0012	0.0022	0.0030	0.0045	0.0051	0.0071	0.0094	0.0126	0.0165	0.0200	0.0283	0.0525	0.1519	0.1568	0.1565	0.1328	0.1328	0.1055

A6-b Vapor Concentration, y_{ij} (18 stages, 5 combined pseudocomponents)

i Stage	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	0.3836	0.2252	0.1148	0.0815	0.0510	0.0396	0.0261	0.0212	0.0179	0.0151	0.0125	0.0100	0.0081	0.0052	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.1130	0.1103	0.0866	0.0897	0.0771	0.0771	0.0622	0.0616	0.0609	0.0595	0.0568	0.0509	0.0475	0.0376	0.0106	0.0004	0.0000	0.0000	0.0000	0.0000
3	0.0548	0.0598	0.0530	0.0627	0.0617	0.0695	0.0624	0.0689	0.0748	0.0802	0.0840	0.0815	0.0839	0.0763	0.0260	0.0012	0.0000	0.0000	0.0000	0.0000
4	0.0485	0.0505	0.0433	0.0503	0.0497	0.0574	0.0533	0.0618	0.0707	0.0803	0.0897	0.0924	0.1028	0.1052	0.0427	0.0024	0.0001	0.0000	0.0000	0.0000
5	0.0479	0.0491	0.0410	0.0464	0.0446	0.0506	0.0468	0.0547	0.0637	0.0747	0.0869	0.0936	0.1110	0.1259	0.0605	0.0040	0.0002	0.0000	0.0000	0.0000
6	0.0476	0.0486	0.0403	0.0450	0.0425	0.0473	0.0430	0.0498	0.0579	0.0686	0.0816	0.0906	0.1129	0.1404	0.0794	0.0064	0.0003	0.0000	0.0000	0.0000
7	0.0472	0.0482	0.0399	0.0442	0.0414	0.0456	0.0409	0.0466	0.0537	0.0633	0.0759	0.0858	0.1110	0.1496	0.0992	0.0096	0.0006	0.0000	0.0000	0.0000
8	0.0469	0.0478	0.0395	0.0437	0.0407	0.0445	0.0395	0.0444	0.0506	0.0591	0.0706	0.0804	0.1067	0.1542	0.1193	0.0140	0.0011	0.0000	0.0000	0.0000
9	0.0466	0.0475	0.0392	0.0433	0.0402	0.0437	0.0386	0.0429	0.0483	0.0558	0.0660	0.0751	0.1010	0.1546	0.1390	0.0199	0.0020	0.0001	0.0000	0.0000
10	0.0464	0.0472	0.0389	0.0429	0.0397	0.0430	0.0378	0.0418	0.0466	0.0531	0.0621	0.0701	0.0946	0.1514	0.1572	0.0273	0.0034	0.0002	0.0000	0.0000
11	0.0462	0.0470	0.0387	0.0425	0.0393	0.0425	0.0372	0.0408	0.0452	0.0510	0.0588	0.0656	0.0881	0.1452	0.1729	0.0366	0.0057	0.0005	0.0000	0.0000
12	0.0462	0.0469	0.0386	0.0423	0.0390	0.0420	0.0366	0.0400	0.0440	0.0491	0.0559	0.0615	0.0815	0.1365	0.1848	0.0477	0.0094	0.0010	0.0000	0.0000
13	0.0465	0.0471	0.0386	0.0423	0.0388	0.0417	0.0362	0.0394	0.0430	0.0476	0.0534	0.0579	0.0752	0.1259	0.1914	0.0602	0.0151	0.0023	0.0001	0.0000
14	0.0471	0.0476	0.0389	0.0424	0.0388	0.0415	0.0359	0.0388	0.0421	0.0462	0.0512	0.0546	0.0691	0.1138	0.1914	0.0735	0.0233	0.0047	0.0005	0.0000
15	0.0479	0.0483	0.0394	0.0428	0.0390	0.0416	0.0358	0.0385	0.0414	0.0450	0.0492	0.0516	0.0635	0.1009	0.1839	0.0860	0.0344	0.0094	0.0016	0.0001
16	0.0490	0.0492	0.0400	0.0434	0.0394	0.0417	0.0358	0.0382	0.0409	0.0440	0.0475	0.0489	0.0583	0.0878	0.1686	0.0957	0.0485	0.0179	0.0049	0.0005
17	0.0496	0.0499	0.0405	0.0439	0.0397	0.0419	0.0358	0.0380	0.0403	0.0430	0.0458	0.0464	0.0535	0.0750	0.1462	0.1003	0.0644	0.0319	0.0140	0.0032
18	0.0056	0.0080	0.0087	0.0121	0.0137	0.0174	0.0172	0.0210	0.0251	0.0300	0.0356	0.0395	0.0506	0.0818	0.1944	0.1629	0.1293	0.0830	0.0536	0.0214

A6-c Temperature and Vapor Flow Rate Profiles (18 stages, 5 combined pseudocomponents)

Stage	T (deg. F)	V (lbmole/hr)
1	364.74	0.00
2	476.73	58.64
3	519.52	54.54
4	535.86	53.57
5	544.71	53.16
6	551.00	52.94
7	556.22	52.77
8	560.86	52.64
9	565.21	52.51
10	569.39	52.38
11	573.48	52.25
12	577.54	52.11
13	581.68	51.94
14	586.16	51.75
15	591.67	51.53
16	600.05	51.27
17	616.74	50.96
18	705.99	46.25

A7 Output of Results of Case 6.6.2.4

- Running Time on K6-2 500 MHz. of 7 combined pseudocomponents is 320 msec.

A7-a Liquid Concentration, x_{ij} (18 stages, 7 combined pseudocomponents)

Stage \ i	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	0.1118	0.1092	0.0858	0.0889	0.0765	0.0766	0.0619	0.0614	0.0607	0.0594	0.0569	0.0511	0.0479	0.0389	0.0125	0.0005	0.0000	0.0000	0.0000	0.0000
2	0.0190	0.0286	0.0320	0.0456	0.0515	0.0640	0.0616	0.0724	0.0824	0.0920	0.0997	0.0996	0.1060	0.1021	0.0413	0.0021	0.0001	0.0000	0.0000	0.0000
3	0.0077	0.0126	0.0156	0.0249	0.0317	0.0440	0.0466	0.0606	0.0753	0.0918	0.1085	0.1169	0.1365	0.1497	0.0728	0.0045	0.0001	0.0000	0.0000	0.0000
4	0.0064	0.0099	0.0117	0.0182	0.0232	0.0327	0.0358	0.0488	0.0637	0.0822	0.1034	0.1181	0.1488	0.1830	0.1058	0.0078	0.0003	0.0000	0.0000	0.0000
5	0.0061	0.0092	0.0106	0.0160	0.0197	0.0273	0.0297	0.0407	0.0540	0.0718	0.0941	0.1123	0.1505	0.2050	0.1401	0.0124	0.0006	0.0000	0.0000	0.0000
6	0.0059	0.0089	0.0101	0.0149	0.0181	0.0245	0.0262	0.0354	0.0470	0.0630	0.0843	0.1036	0.1459	0.2175	0.1748	0.0187	0.0012	0.0000	0.0000	0.0000
7	0.0057	0.0086	0.0097	0.0143	0.0171	0.0229	0.0241	0.0321	0.0420	0.0561	0.0755	0.0943	0.1376	0.2220	0.2088	0.0269	0.0022	0.0001	0.0000	0.0000
8	0.0056	0.0084	0.0095	0.0138	0.0164	0.0218	0.0227	0.0297	0.0384	0.0507	0.0680	0.0854	0.1275	0.2198	0.2407	0.0376	0.0038	0.0002	0.0000	0.0000
9	0.0055	0.0082	0.0092	0.0134	0.0159	0.0209	0.0216	0.0281	0.0358	0.0466	0.0618	0.0773	0.1167	0.2121	0.2689	0.0510	0.0064	0.0004	0.0000	0.0000
10	0.0055	0.0081	0.0090	0.0131	0.0154	0.0203	0.0208	0.0267	0.0338	0.0434	0.0567	0.0703	0.1060	0.2003	0.2918	0.0673	0.0107	0.0009	0.0000	0.0000
11	0.0054	0.0080	0.0089	0.0129	0.0151	0.0197	0.0201	0.0257	0.0321	0.0408	0.0525	0.0642	0.0959	0.1855	0.3077	0.0863	0.0173	0.0019	0.0001	0.0000
12	0.0054	0.0079	0.0088	0.0127	0.0148	0.0192	0.0195	0.0248	0.0308	0.0386	0.0490	0.0589	0.0866	0.1687	0.3153	0.1076	0.0272	0.0041	0.0003	0.0000
13	0.0054	0.0079	0.0087	0.0125	0.0145	0.0188	0.0190	0.0239	0.0295	0.0367	0.0459	0.0544	0.0781	0.1508	0.3131	0.1300	0.0415	0.0084	0.0009	0.0000
14	0.0053	0.0078	0.0086	0.0122	0.0142	0.0183	0.0184	0.0231	0.0283	0.0349	0.0431	0.0503	0.0703	0.1324	0.3002	0.1516	0.0611	0.0167	0.0029	0.0001
15	0.0053	0.0077	0.0084	0.0119	0.0138	0.0177	0.0178	0.0221	0.0270	0.0330	0.0403	0.0462	0.0628	0.1137	0.2757	0.1690	0.0863	0.0318	0.0087	0.0009
16	0.0052	0.0074	0.0081	0.0114	0.0131	0.0168	0.0167	0.0208	0.0251	0.0305	0.0368	0.0416	0.0550	0.0944	0.2383	0.1768	0.1143	0.0569	0.0251	0.0058
17	0.0049	0.0070	0.0075	0.0106	0.0120	0.0152	0.0151	0.0185	0.0223	0.0267	0.0319	0.0355	0.0456	0.0732	0.1856	0.1659	0.1359	0.0910	0.0642	0.0316
18	0.0004	0.0009	0.0012	0.0021	0.0029	0.0043	0.0048	0.0067	0.0090	0.0120	0.0157	0.0190	0.0268	0.0488	0.1481	0.1595	0.1596	0.1354	0.1354	0.1076

<u>A7-b</u> Vapor Concentration, y_{ij} (18 stages, 7 combined pseudocomponents)

Stage \ i	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	0.3811	0.2239	0.1142	0.0811	0.0507	0.0395	0.0260	0.0212	0.0179	0.0151	0.0126	0.0100	0.0081	0.0054	0.0013	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.1124	0.1098	0.0862	0.0893	0.0768	0.0768	0.0620	0.0614	0.0607	0.0594	0.0568	0.0510	0.0478	0.0387	0.0124	0.0005	0.0000	0.0000	0.0000	0.0000
3	0.0541	0.0591	0.0524	0.0621	0.0611	0.0689	0.0618	0.0684	0.0743	0.0798	0.0836	0.0813	0.0841	0.0782	0.0304	0.0015	0.0000	0.0000	0.0000	0.0000
4	0.0476	0.0497	0.0426	0.0495	0.0490	0.0566	0.0526	0.0610	0.0699	0.0795	0.0889	0.0918	0.1027	0.1074	0.0497	0.0029	0.0001	0.0000	0.0000	0.0000
5	0.0469	0.0481	0.0402	0.0455	0.0438	0.0497	0.0460	0.0538	0.0627	0.0736	0.0858	0.0926	0.1103	0.1279	0.0701	0.0050	0.0002	0.0000	0.0000	0.0000
6	0.0465	0.0475	0.0395	0.0440	0.0416	0.0464	0.0422	0.0487	0.0568	0.0673	0.0801	0.0891	0.1115	0.1418	0.0914	0.0078	0.0004	0.0000	0.0000	0.0000
7	0.0463	0.0472	0.0390	0.0433	0.0405	0.0446	0.0400	0.0455	0.0524	0.0618	0.0741	0.0838	0.1089	0.1498	0.1131	0.0117	0.0007	0.0000	0.0000	0.0000
8	0.0461	0.0469	0.0387	0.0428	0.0399	0.0435	0.0386	0.0434	0.0493	0.0576	0.0687	0.0781	0.1038	0.1528	0.1344	0.0169	0.0013	0.0000	0.0000	0.0000
9	0.0460	0.0468	0.0385	0.0425	0.0394	0.0428	0.0377	0.0419	0.0471	0.0542	0.0640	0.0726	0.0976	0.1516	0.1544	0.0236	0.0023	0.0001	0.0000	0.0000
10	0.0460	0.0467	0.0384	0.0423	0.0391	0.0423	0.0371	0.0409	0.0454	0.0516	0.0601	0.0676	0.0908	0.1467	0.1718	0.0319	0.0040	0.0002	0.0000	0.0000
11	0.0461	0.0468	0.0384	0.0422	0.0389	0.0419	0.0366	0.0401	0.0442	0.0496	0.0569	0.0631	0.0841	0.1390	0.1855	0.0419	0.0066	0.0005	0.0000	0.0000
12	0.0464	0.0470	0.0386	0.0422	0.0388	0.0417	0.0363	0.0395	0.0432	0.0480	0.0543	0.0593	0.0776	0.1294	0.1946	0.0534	0.0106	0.0012	0.0000	0.0000
13	0.0468	0.0474	0.0388	0.0424	0.0388	0.0416	0.0360	0.0390	0.0424	0.0467	0.0521	0.0560	0.0717	0.1185	0.1980	0.0661	0.0166	0.0025	0.0002	0.0000
14	0.0473	0.0478	0.0390	0.0426	0.0389	0.0415	0.0359	0.0387	0.0418	0.0457	0.0503	0.0532	0.0664	0.1070	0.1954	0.0792	0.0252	0.0051	0.0005	0.0000
15	0.0478	0.0482	0.0393	0.0428	0.0390	0.0415	0.0357	0.0383	0.0412	0.0447	0.0487	0.0507	0.0615	0.0955	0.1865	0.0917	0.0369	0.0101	0.0017	0.0001
16	0.0480	0.0484	0.0395	0.0429	0.0390	0.0414	0.0355	0.0379	0.0406	0.0437	0.0470	0.0483	0.0571	0.0841	0.1712	0.1019	0.0518	0.0190	0.0052	0.0006
17	0.0483	0.0486	0.0395	0.0428	0.0388	0.0411	0.0351	0.0373	0.0396	0.0423	0.0451	0.0456	0.0524	0.0725	0.1485	0.1064	0.0685	0.0340	0.0149	0.0034
18	0.0055	0.0078	0.0084	0.0117	0.0132	0.0167	0.0165	0.0201	0.0241	0.0287	0.0341	0.0377	0.0481	0.0766	0.1910	0.1671	0.1331	0.0855	0.0553	0.0221

A7-c Temperature and Vapor Flow Rate Profiles (18 stages, 7 combined pseudocomponents)

Stage	T (deg. F)	V (lbmole/hr)
1	364.60	0.00
2	477.95	58.64
3	521.33	54.85
4	538.14	53.89
5	547.39	53.46
6	553.98	53.23
7	559.33	53.05
8	563.99	52.88
9	568.19	52.73
10	572.06	52.59
11	575.72	52.44
12	579.35	52.29
13	583.18	52.14
14	587.70	51.98
15	593.80	51.81
16	603.38	51.60
17	620.91	51.25
18	707.48	46.14

A8 Output of Results of Case 6.6.3

- Running Time on K6-2 500 MHz. of 14 combined pseudocomponents is 660 msec.

A8-a Liquid Concentration, x_{ij} (18 stages, 14 combined pseudocomponents)

Stage \ i	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	0.1107	0.1083	0.0852	0.0882	0.0760	0.0762	0.0616	0.0612	0.0607	0.0595	0.0572	0.0516	0.0489	0.0406	0.0143	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.0268	0.0262	0.0206	0.0449	0.0507	0.0632	0.0609	0.0717	0.0818	0.0917	0.0999	0.1003	0.1077	0.1063	0.0472	0.0000	0.0000	0.0000	0.0000	0.0000
3	0.0116	0.0114	0.0090	0.0244	0.0311	0.0431	0.0457	0.0596	0.0742	0.0907	0.1078	0.1167	0.1375	0.1546	0.0826	0.0000	0.0000	0.0000	0.0000	0.0000
4	0.0092	0.0090	0.0071	0.0179	0.0227	0.0321	0.0351	0.0478	0.0625	0.0809	0.1022	0.1173	0.1490	0.1877	0.1193	0.0000	0.0000	0.0000	0.0000	0.0000
5	0.0087	0.0085	0.0067	0.0158	0.0195	0.0270	0.0293	0.0400	0.0531	0.0707	0.0929	0.1113	0.1502	0.2093	0.1569	0.0000	0.0000	0.0000	0.0000	0.0000
6	0.0085	0.0083	0.0065	0.0150	0.0181	0.0245	0.0261	0.0352	0.0466	0.0624	0.0836	0.1029	0.1456	0.2215	0.1950	0.0000	0.0000	0.0000	0.0000	0.0000
7	0.0083	0.0082	0.0064	0.0145	0.0173	0.0232	0.0243	0.0323	0.0422	0.0562	0.0756	0.0944	0.1380	0.2264	0.2325	0.0000	0.0000	0.0000	0.0000	0.0000
8	0.0082	0.0081	0.0063	0.0142	0.0169	0.0224	0.0233	0.0304	0.0392	0.0516	0.0690	0.0865	0.1291	0.2255	0.2688	0.0001	0.0001	0.0001	0.0001	0.0001
9	0.0081	0.0080	0.0063	0.0140	0.0165	0.0218	0.0225	0.0292	0.0372	0.0483	0.0638	0.0797	0.1201	0.2204	0.3030	0.0003	0.0003	0.0002	0.0002	0.0002
10	0.0081	0.0079	0.0062	0.0138	0.0162	0.0213	0.0219	0.0282	0.0357	0.0458	0.0598	0.0740	0.1115	0.2123	0.3344	0.0007	0.0007	0.0006	0.0006	0.0005
11	0.0080	0.0078	0.0062	0.0136	0.0160	0.0209	0.0215	0.0275	0.0345	0.0438	0.0566	0.0692	0.1035	0.2019	0.3619	0.0017	0.0016	0.0014	0.0014	0.0011
12	0.0079	0.0077	0.0061	0.0134	0.0157	0.0205	0.0210	0.0268	0.0334	0.0421	0.0538	0.0650	0.0961	0.1897	0.3836	0.0040	0.0039	0.0033	0.0033	0.0026
13	0.0078	0.0076	0.0060	0.0131	0.0153	0.0200	0.0204	0.0259	0.0322	0.0403	0.0510	0.0609	0.0886	0.1751	0.3957	0.0092	0.0091	0.0078	0.0078	0.0062
14	0.0076	0.0074	0.0059	0.0127	0.0148	0.0192	0.0195	0.0246	0.0305	0.0379	0.0475	0.0561	0.0801	0.1564	0.3905	0.0206	0.0204	0.0173	0.0173	0.0138
15	0.0073	0.0071	0.0056	0.0119	0.0138	0.0178	0.0180	0.0226	0.0278	0.0344	0.0425	0.0496	0.0691	0.1315	0.3564	0.0425	0.0421	0.0357	0.0357	0.0284
16	0.0068	0.0067	0.0053	0.0109	0.0125	0.0159	0.0159	0.0198	0.0241	0.0294	0.0359	0.0410	0.0555	0.1005	0.2872	0.0767	0.0759	0.0644	0.0644	0.0512
17	0.0063	0.0062	0.0049	0.0097	0.0110	0.0138	0.0137	0.0167	0.0200	0.0241	0.0287	0.0321	0.0416	0.0695	0.1982	0.1162	0.1149	0.0975	0.0975	0.0775
18	0.0007	0.0007	0.0005	0.0018	0.0025	0.0036	0.0041	0.0057	0.0075	0.0100	0.0131	0.0159	0.0226	0.0428	0.1459	0.1667	0.1649	0.1399	0.1399	0.1112

A8-b Vapor Concentration, y_{ij} (18 stages, 14 combined pseudocomponents)

Stage \ i	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	0.3858	0.2287	0.1177	0.0839	0.0528	0.0413	0.0274	0.0224	0.0190	0.0161	0.0135	0.0108	0.0089	0.0061	0.0017	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.1576	0.1005	0.0555	0.0879	0.0758	0.0761	0.0616	0.0612	0.0607	0.0596	0.0574	0.0518	0.0491	0.0408	0.0144	0.0000	0.0000	0.0000	0.0000	0.0000
3	0.0814	0.0533	0.0301	0.0610	0.0601	0.0679	0.0611	0.0677	0.0738	0.0796	0.0839	0.0821	0.0857	0.0818	0.0350	0.0000	0.0000	0.0000	0.0000	0.0000
4	0.0686	0.0453	0.0258	0.0487	0.0482	0.0556	0.0517	0.0601	0.0690	0.0788	0.0884	0.0918	0.1036	0.1111	0.0566	0.0000	0.0000	0.0000	0.0000	0.0000
5	0.0667	0.0442	0.0253	0.0449	0.0432	0.0490	0.0453	0.0529	0.0618	0.0726	0.0848	0.0920	0.1104	0.1311	0.0789	0.0000	0.0000	0.0000	0.0000	0.0000
6	0.0663	0.0441	0.0253	0.0438	0.0413	0.0460	0.0417	0.0482	0.0560	0.0664	0.0791	0.0882	0.1110	0.1440	0.1018	0.0000	0.0000	0.0000	0.0000	0.0000
7	0.0662	0.0441	0.0254	0.0433	0.0405	0.0445	0.0399	0.0453	0.0520	0.0613	0.0733	0.0830	0.1080	0.1513	0.1249	0.0000	0.0000	0.0000	0.0000	0.0000
8	0.0661	0.0441	0.0255	0.0431	0.0401	0.0438	0.0388	0.0435	0.0494	0.0575	0.0684	0.0777	0.1033	0.1540	0.1477	0.0000	0.0000	0.0000	0.0000	0.0000
9	0.0660	0.0442	0.0255	0.0430	0.0399	0.0433	0.0382	0.0424	0.0476	0.0547	0.0644	0.0729	0.0978	0.1533	0.1696	0.0001	0.0001	0.0001	0.0000	0.0000
10	0.0659	0.0442	0.0256	0.0429	0.0397	0.0430	0.0377	0.0416	0.0463	0.0527	0.0612	0.0687	0.0922	0.1501	0.1903	0.0003	0.0002	0.0002	0.0001	0.0000
11	0.0659	0.0442	0.0256	0.0428	0.0396	0.0427	0.0374	0.0411	0.0454	0.0511	0.0588	0.0652	0.0869	0.1450	0.2092	0.0008	0.0006	0.0004	0.0002	0.0001
12	0.0658	0.0442	0.0256	0.0428	0.0394	0.0425	0.0372	0.0406	0.0447	0.0500	0.0568	0.0623	0.0821	0.1386	0.2257	0.0019	0.0015	0.0009	0.0006	0.0002
13	0.0657	0.0442	0.0257	0.0427	0.0393	0.0423	0.0369	0.0402	0.0441	0.0489	0.0551	0.0598	0.0775	0.1311	0.2386	0.0045	0.0035	0.0022	0.0014	0.0005
14	0.0655	0.0443	0.0258	0.0426	0.0392	0.0421	0.0366	0.0398	0.0434	0.0479	0.0534	0.0572	0.0729	0.1220	0.2454	0.0104	0.0081	0.0051	0.0032	0.0012
15	0.0651	0.0443	0.0261	0.0425	0.0389	0.0417	0.0361	0.0391	0.0424	0.0465	0.0513	0.0543	0.0677	0.1105	0.2414	0.0232	0.0181	0.0113	0.0071	0.0026
16	0.0646	0.0445	0.0264	0.0422	0.0385	0.0411	0.0354	0.0380	0.0409	0.0444	0.0484	0.0504	0.0610	0.0951	0.2195	0.0471	0.0367	0.0231	0.0144	0.0054
17	0.0641	0.0447	0.0269	0.0420	0.0380	0.0402	0.0344	0.0365	0.0389	0.0416	0.0445	0.0453	0.0528	0.0761	0.1763	0.0832	0.0650	0.0411	0.0259	0.0098
18	0.0089	0.0065	0.0040	0.0106	0.0120	0.0150	0.0148	0.0180	0.0215	0.0257	0.0306	0.0340	0.0439	0.0727	0.2047	0.1909	0.1512	0.0977	0.0638	0.0260

A8-c Temperature and Vapor Flow Rate Profiles (18 stages, 14 combined pseudocomponents)

Stage	T (deg. F)	V (lbmole/hr)
1	365.65	0.00
2	480.66	58.64
3	525.01	54.79
4	542.19	53.76
5	551.32	53.30
6	557.36	53.00
7	561.80	52.77
8	565.26	52.59
9	568.07	52.43
10	570.42	52.28
11	572.55	52.15
12	574.68	52.02
13	577.13	51.90
14	580.39	51.78
15	585.41	51.66
16	594.28	51.53
17	612.90	51.37
18	711.12	46.79

APPENDIX B

SOURCE CODE OF PROGRAM

```
#include <iostream.h>
#include <stdio.h>
#include <math.h>
#include <conio.h>
#include <time.h>
#define R 10.73

// Parameters //
int     i,j,k,m,n;
double  Psys,Bottom,Reflux,Distil,Totalz,Tfeed,runtime,error;
double  API[40],MW[40][40],SG[40][40],w[40][40],Tb[40][40],Tc[40][40],lnPc[40],Pc[40][40],
        z[40][40],iTbr[40],iKp[40],feed[40],U[40],L[40],V[40],W[40];           // For Input Prop //
double  mi[40][40],Pr[40][40],Tr[40][40],Lij[40][40],ai[40][40],bi[40][40];    // For Thermo Prop //
double  asuml1[40],bsuml1[40],asuml2[40],Ail[40],Bil[40],Aipl[40][40],Bipl[40][40],
        ZL[40],lnfuL[40][40];                                                  // For Liquid //
double  asumv1[40],bsumv1[40],asumv2[40],Aiv[40],Biv[40],Aipv[40][40],Bipv[40][40],
        ZV[40],lnfuV[40][40];                                                  // For Vapor //
double  TrF[40],LijF[40],aiF[40],biF[40],asumf1,bsumf1,Aif,Bif,ZLF;           // For Feed //
int     comp,stage,vs,fs,checksum,Iter,Method;                                 // For System Prop //
double  X[40][40],T[40],Kij[40][40];                                           // For Process //
double  Afeed,A[40][40],B[40][40],C[40][40],D[40][40],P[40][40],Q[40][40],SumX[40];
                                                                               // For Calc Xij //
double  fT[40],fTp[40],Tn[40],part1V[40],part1L[40],part2V[40],part2L[40];
                                                                               // For Calc Tj //
double  Kp[40][40],CF[40][40],Ah[40][40],Bh[40][40],Ch[40][40],Acp[40][40],
        Bcp[40][40],Ccp[40][40];                                               //  For Coef H Ideal //
double  Hi[40][40],HidealL[40],HidealV[40],HidealF,Tdal[40],Tdav[40],Tdaf,H[40],h[40],HF;
                                                                               // For Calc hj & Hj //
```

```
// Parameters for Advance Calculate //
int     Oldcomp,count,xcount,Gcomp[20],Gsize,no_G,gr,bgin,bgroup,Iter2;
double  iMW[40],iTb[40],iTc[40],iPc[40],iw[40],iSG[40],iz[40];
double  iTbm[20][40],iTcm[20][40],iPcm[20][40],iwm[20][40],iSGm[20][40],izm[20][40],
        iXm[20][40],RatioX[40][40],F_Kij[40][40],F_X[40][40];



// Function Calculate Thermodynamic Properties each stage //
void ThermoProp(double T,int jj)
{
        for (i=0;i<comp;i++)
        {
                mi[i][jj]=0.48+1.574*w[i][jj]-0.176*w[i][jj]*w[i][jj];
                Pr[i][jj]=Psys/Pc[i][jj];
                Tr[i][jj]=T/Tc[i][jj];
                Lij[i][jj]=pow(1+(mi[i][jj]*(1-pow(Tr[i][jj],0.5))),2);
                ai[i][jj]=0.42748*pow(R*Tc[i][j],2)*Lij[i][jj]/Pc[i][jj];
                bi[i][jj]=0.08664*R*Tc[i][jj]/Pc[i][jj];
        }
}
```

```
// Function Z //
double ZF(double z,double A,double B)
{
        recalc :
        double Fz=pow(z,3)-pow(z,2)+(A-B-(B*B))*z-(A*B);
        double Dz=(3*z*z)-(2*z)+A-B-(B*B);
        double Zn=z-(Fz/Dz);
        if(fabs(Zn-z)< 0.0001)
                return Zn;
        else
        {
                z=Zn;
                goto recalc;
        }
}
// Function LN Fugacity //
double lnfu(double Zn,double A,double B,double Ap,double Bp)
{
  return -log(Zn-B)+(Zn-1)*Bp-(A/B)*(Ap-Bp)*log(1+(B/Zn));
}
// Function Calculate Z for liquid each stage //
void Z_liq(double T,int jj)
{
        asuml1[jj]=0;
        asuml2[jj]=0;
        bsuml1[jj]=0;
        for (int m=0;m<comp;m++)
        {
                asuml2[jj]=asuml2[jj]+(X[m][jj]*pow(ai[m][jj],0.5));
                bsuml1[jj]=bsuml1[jj]+(X[m][jj]*bi[m][jj]);
                for (n=0;n<comp;n++)
                        asuml1[jj]=asuml1[jj]+(X[m][jj]*X[n][jj]*pow(ai[m][jj]*ai[n][jj],0.5));
```

```
          }
          for (int i=0;i<comp;i++)
          {
                    Ail[jj]=asuml1[jj]*Psys/pow(R*T,2);
                    Bil[jj]=bsuml1[jj]*Psys/(R*T);
                    Aipl[i][jj]=2*pow(ai[i][jj],0.5)*asuml2[jj]/asuml1[jj];
                    Bipl[i][jj]=bi[i][jj]/bsuml1[jj];
                    ZL[jj]=ZF(0,Ail[jj],Bil[jj]);
                    lnfuL[i][jj]=lnfu(ZL[jj],Ail[jj],Bil[jj],Aipl[i][jj],Bipl[i][jj]);
          }
}
```

// Function Calculate Z for vapor each stage //

```
void Z_vap(double T,int jj)
{
          asumv1[jj]=0;
          asumv2[jj]=0;
          bsumv1[jj]=0;
          for (m=0;m<comp;m++)
          {
                    asumv2[jj]=asumv2[jj]+(Kij[m][jj]*X[m][jj]*pow(ai[m][jj],0.5));
                    bsumv1[jj]=bsumv1[jj]+(Kij[m][jj]*X[m][jj]*bi[m][jj]);
                    for (n=0;n<comp;n++)
                              asumv1[jj]=asumv1[jj]+(Kij[m][jj]*X[m][jj]*Kij[n][jj]*X[n][jj]
                                                  *pow(ai[m][jj]*ai[n][jj],0.5));
          }
          for (i=0;i<comp;i++)
          {
                    Aiv[jj]=asumv1[jj]*Psys/pow(R*T,2);
                    Biv[jj]=bsumv1[jj]*Psys/(R*T);
                    Aipv[i][jj]=2*pow(ai[i][jj],0.5)*asumv2[jj]/asumv1[jj];
                    Bipv[i][jj]=bi[i][jj]/bsumv1[jj];
                    ZV[jj]=ZF(1,Aiv[jj],Biv[jj]);
```

```
        lnfuV[i][jj]=lnfu(ZV[jj],Aiv[jj],Biv[jj],Aipv[i][jj],Bipv[i][jj]);
    }
}
// Function Calculate Z for Feed stage //
void Z_feed(double T)
{
    for (i=0;i<comp;i++)
    {
        TrF[i]=T/Tc[i][fs];
        LijF[i]=pow(1+(mi[i][fs]*(1-pow(TrF[i],0.5))),2);
        aiF[i]=0.42748*pow(R*Tc[i][fs],2)*LijF[i]/Pc[i][fs];
        biF[i]=0.08664*R*Tc[i][fs]/Pc[i][fs];
    }
    asumf1=0;
    bsumf1=0;
    for (m=0;m<comp;m++)
    {
        bsumf1=bsumf1+(z[m][fs]*biF[m]);
        for (n=0;n<comp;n++)
            asumf1=asumf1+(z[m][fs]*z[n][fs]*pow(aiF[m]*aiF[n],0.5));
    }
    Aif=asumf1*Psys/pow(R*T,2);
    Bif=bsumf1*Psys/(R*T);
    ZLF=ZF(0,Aif,Bif);
}
// Function Calculate Lj //
void Lj()
{
    for (j=1;j<stage-1;j++)
    {
        double Lsum=0;
        for (k=1;k<j;k++)
```

```
        {
            Lsum=Lsum+(feed[k]-W[k]-U[k]);
        }
        L[j]=V[j+1]+Lsum-(V[0]+U[0]);
    }
}
// Function Calculate A1,B1,C1,D1 & An,Bn,Cn,Dn //
void ABCD_1_n()
{
    for (i=0;i<comp;i++)
    {
        B[i][0]=-(V[0]*Kij[i][0]+L[0]+U[0]);
        C[i][0]=V[1]*Kij[i][1];
        D[i][0]=0;

        A[i][stage-1]=V[stage-1]+Bottom;
        B[i][stage-1]=-(V[stage-1]*Kij[i][stage-1]+Bottom);
        C[i][stage-1]=0;
        D[i][stage-1]=0;
    }
}
// Function Calculate Aj,Bj,Cj,Dj //
void ABCD_j()
{
    for (i=0;i<comp;i++)
    {
        for (j=1;j<stage-1;j++)
        {
        Afeed=0;
            for (k=1;k<j;k++)
                Afeed=Afeed+(feed[k]-W[k]-U[k]);
            A[i][j]=V[j]+Afeed-(V[0]+U[0]);
```

```
                }
                for (j=1;j<stage-1;j++)
                {
                        B[i][j]=-(((V[j]+W[j])*Kij[i][j])+A[i][j+1]+U[j]);
                        C[i][j]=V[j+1]*Kij[i][j+1];
                        D[i][j]=-feed[j]*z[i][j];
                }
        }
}
// Function Calculate Xij //
void Xij()
{
        for (i=0;i<comp;i++)
        {
                P[i][0]=C[i][0]/B[i][0];
                Q[i][0]=D[i][0]/B[i][0];
                for (j=1;j<stage-1;j++)
                P[i][j]=C[i][j]/(B[i][j]-A[i][j]*P[i][j-1]);
                for (j=1;j<stage;j++)
                        Q[i][j]=(D[i][j]-A[i][j]*Q[i][j-1])/(B[i][j]-A[i][j]*P[i][j-1]);
                X[i][stage-1]=Q[i][stage-1];
                for (j=stage-2;j>=0;j--)
                X[i][j]=Q[i][j]-P[i][j]*X[i][j+1];
        }
        for (j=0;j<stage;j++)
        {
                SumX[j]=0;
                for (i=0;i<comp;i++)
                        SumX[j]=SumX[j]+X[i][j];
                for (m=0;m<comp;m++)
                        X[m][j]=X[m][j]/SumX[j];
        }
```

```
}
// Function Calculate Tj //
void Tj(int j)
{
    fT[j]=-1;
    fTp[j]=0;
    for (i=0;i<comp;i++)
    {
        fT[j]=fT[j]+(Kij[i][j]*X[i][j]);
        part1V[j]=((Psys*bsumv1[j]/(R*T[j]*ZV[j]))/
                (1-(Psys*bsumv1[j]/(R*T[j]*ZV[j]))));
        part1L[j]=((Psys*bsuml1[j]/(R*T[j]*ZL[j]))/
                (1-(Psys*bsuml1[j]/(R*T[j]*ZL[j]))));
        part2V[j]=(Aiv[j]/Biv[j])*(Aipv[i][j]-Bipv[i][j])*( ((Psys*bsumv1[j]/
                (R*T[j]*ZV[j]))/(1+(Psys*bsumv1[j]/(R*T[j]*ZV[j]))))
                +log(1+(Psys*bsumv1[j]/(R*T[j]*ZV[j]))) );
        part2L[j]=(Ail[j]/Bil[j])*(Aipl[i][j]-Bipl[i][j])*( ((Psys*bsuml1[j]/
                (R*T[j]*ZL[j]))/(1+(Psys*bsuml1[j]/(R*T[j]*ZL[j]))))
                +log(1+(Psys*bsuml1[j]/(R*T[j]*ZL[j]))) );
        fTp[j]=fTp[j]+(Kij[i][j]*X[i][j]*((part1V[j]-part1L[j])/T[j]
            +(part2L[j]-part2V[j])/T[j]));
    }
}
// Function Calculate coeficient for H Ideal //
void CoefH(int j)
{
    for (i=0;i<comp;i++)
    {
        Kp[i][j]=pow(Tb[i][j],0.333333)/SG[i][j];
        CF[i][j]=pow((12.8/Kp[i][j]-1)*(10/Kp[i][j]-1)*100,2);
        Ah[i][j]=-0.0084773+0.080809*SG[i][j];
        Bh[i][j]=(2.1773-2.0826*SG[i][j])*pow(10,-4);
```

```
        Ch[i][j]=-(0.78649-0.70423*SG[i][j])*pow(10,-7);
        Acp[i][j]=-0.32646+0.02678*Kp[i][j];
        Bcp[i][j]=-(1.3892-1.2122*Kp[i][j]+0.03803*pow(Kp[i][j],2))*pow(10,-4);
        Ccp[i][j]=-1.5393e-7;
    }
}
// Function Calculate h Ideal //
double HiL(int j)
{
    double Hl=0;
    for (i=0;i<comp;i++)
    {
        Hi[i][j]=( (Acp[i][j]*(T[j]-492)) + (Bcp[i][j]*(pow(T[j],2)-pow(492,2))/2)
            +(Ccp[i][j]*(pow(T[j],3)-pow(492,3))/3))
            +CF[i][j]*((Ah[i][j]*(T[j]-492))+(Bh[i][j]*(pow(T[j],2)
            -pow(492,2))/2)+(Ch[i][j]*(pow(T[j],3)-pow(492,3))/3));
        Hl=Hl+X[i][j]*Hi[i][j];
    }
    return Hl;
}
// Function Calculate H Ideal //
double HiV(int j)
{
    double Hv=0;
    for (i=0;i<comp;i++)
    {
        Hi[i][j]=( (Acp[i][j]*(T[j]-492)) + (Bcp[i][j]*(pow(T[j],2)-pow(492,2))/2)
            +(Ccp[i][j]*(pow(T[j],3)-pow(492,3))/3))
            +CF[i][j]*((Ah[i][j]*(T[j]-492))+(Bh[i][j]*(pow(T[j],2)
            -pow(492,2))/2)+(Ch[i][j]*(pow(T[j],3)-pow(492,3))/3));
        Hv=Hv+Kij[i][j]*X[i][j]*Hi[i][j];
    }
```

```
        return Hv;
}
// Function Calculate h Ideal Feed //
double HiF(double T)
{
        double Hf=0;
        for (i=0;i<comp;i++)
        {
                Hi[i][fs]=( (Acp[i][fs]*(T-492)) + (Bcp[i][fs]*(pow(T,2)-pow(492,2))/2)
                        +(Ccp[i][fs]*(pow(T,3)-pow(492,3))/3))
                        +CF[i][fs]*((Ah[i][fs]*(T-492))+(Bh[i][fs]*(pow(T,2)-pow(492,2))/2)
                        +(Ch[i][fs]*(pow(T,3)-pow(492,3))/3));
                Hf=Hf+z[i][fs]*Hi[i][fs];
        }
        return Hf;
}
// Function Calculate Tda for Liquid //
double TdaL(int j)
{
     double Tda=0;
     for (m=0;m<comp;m++)
     {
          for (n=0;n<comp;n++)
          {
               Tda=Tda+(X[m][j]*X[n][j]*mi[n][j]*pow((ai[m][j]*ai[n][j]*T[j]/
                         (Tc[n][j]*Lij[n][j])),0.5));
          }
     }
     return Tda;
}
// Function Calculate Tda for Vapor //
double TdaV(int j)
```

```
{
    double Tda=0;
    for (m=0;m<comp;m++)
    {
        for (n=0;n<comp;n++)
        {
            Tda=Tda+(Kij[m][j]*X[m][j]*Kij[n][j]*X[n][j]*mi[n][j]*
                    pow((ai[m][j]*ai[n][j]*T[j]/(Tc[n][j]*Lij[n][j])),0.5));
        }
    }
    return Tda;
}
// Function Calculate Tda for Feed //
double TdaF()
{
    double Tda=0;
    for (m=0;m<comp;m++)
    {
        for (n=0;n<comp;n++)
        {
            Tda=Tda+(z[m][fs]*z[n][fs]*mi[n][fs]*pow((aiF[m]*aiF[n]
                    *Tfeed/(Tc[n][fs]*LijF[n])),0.5));
        }
    }
    return Tda;
}
// Function Initial Group Properties //
void InitGprop()
{
       for (j=0;j<stage;j++)
       {
             count=0;
```

```
                xcount=0;
                for (m=0;m<no_G;m++)
                {
                        iTbm[m][j]=0;
                        iTcm[m][j]=0;
                        iPcm[m][j]=0;
                        iwm[m][j]=0;
                        iSGm[m][j]=0;
                        izm[m][j]=0;
                        iXm[m][j]=0;
                        for (n=0;n<Gcomp[m];n++)
                        {
                                iXm[m][j]=iXm[m][j]+X[xcount][j];
                                izm[m][j]=izm[m][j]+z[xcount][j];
                                xcount=xcount+1;
                        }
                        for (n=0;n<Gcomp[m];n++)
                        {
                                if (iXm[m][j]!=0)
                                        RatioX[count][j]=X[count][j]/iXm[m][j];
                                else
                                        RatioX[count][j]=1.00/Gcomp[m];
                                iTbm[m][j]=iTbm[m][j]+RatioX[count][j]*iTb[count];
                                iTcm[m][j]=iTcm[m][j]+RatioX[count][j]*iTc[count];
                                iPcm[m][j]=iPcm[m][j]+RatioX[count][j]*iPc[count];
                                iwm[m][j]=iwm[m][j]+RatioX[count][j]*iw[count];
                                iSGm[m][j]=iSGm[m][j]+RatioX[count][j]*iSG[count];
                                count=count+1;
                        }
                }
        }
}
```

// Function Advance Calculate //

```
void AdvCalc(int gr)
{
        comp=Gcomp[gr]+no_G-1;
        for (j=0;j<stage;j++)
        {
                bgin=0;
                for (i=0;i<gr;i++)
                {
                        bgin=bgin+Gcomp[i];             // Indicate first component of Group
                }
                for (m=0;m<Gcomp[gr];m++)
                {
                        Tb[m][j]=iTb[bgin];
                        Tc[m][j]=iTc[bgin];
                        Pc[m][j]=iPc[bgin];
                        w[m][j]=iw[bgin];
                        SG[m][j]=iSG[bgin];
                        z[m][j]=iz[bgin];
                        X[m][j]=X[bgin][j];
                        bgin=bgin+1;
                }
                k=0;
                for (n=Gcomp[gr];n<comp;n++)
                {
                        if (k!=gr)
                        {
                                Tb[n][j]=iTbm[k][j];
                                Tc[n][j]=iTcm[k][j];
                                Pc[n][j]=iPcm[k][j];
                                w[n][j]=iwm[k][j];
                                SG[n][j]=iSGm[k][j];
```

```
                z[n][j]=izm[k][j];
                X[n][j]=iXm[k][j];
            }
            else
            n=n-1;
            k=k+1;
        }
    }
}
// Function Recalculate Group Properties //
void Regroup(int gr)
{
    for (j=0;j<stage;j++)
    {
        iXm[gr][j]=0;
        bgin=0;
        for (i=0;i<gr;i++)
        {
            bgin=bgin+Gcomp[i];                // Indicate first component of Group
        }
        bgroup=Gcomp[gr];
        for (n=0;n<Gcomp[gr];n++)
            iXm[gr][j]=iXm[gr][j]+X[n][j];
        for (n=0;n<Gcomp[gr];n++)
        {
            if (iXm[gr]!=0)
                RatioX[bgin][j]=X[n][j]/iXm[gr][j];
            else
                RatioX[bgin][j]=1.00/Gcomp[gr];
            F_X[bgin][j]=X[n][j];
            F_Kij[bgin][j]=Kij[n][j];
            bgin=bgin+1;
```

```
				}
				for (n=0;n<no_G;n++)
				{
					if (n!=gr)
					{
						iXm[n][j]=X[bgroup][j];
						bgroup=bgroup+1;
					}
				}
		}
}
```

// Function Recalculate Xij //

```
void RecalcX()
{
		for (j=0;j<stage;j++)
		{
				bgin=0;
				for (n=0;n<no_G;n++)
				{
					for (i=0;i<Gcomp[n];i++)
					{
						X[bgin][j]=RatioX[bgin][j]*iXm[n][j];
						bgin=bgin+1;
					}
				}
		}
}
```

```
// Main Program ///////////////////////////////////////////////////////////////////////////

void main()

{

        comp=20;

        stage=18;

        Psys=14.696;

        for (j=0;j<stage;j++)                       //

        {                                           //

                U[j]=0;                             //          for set initial

                W[j]=0;                             //

                feed[j]=0;                          //

        }                                           //

        U[0]=20.75;

        vs=2;

        vs=vs-1;

        W[vs]=0;

        Bottom=5.58;

        Reflux=1.826;

        Distil=20.75;

        iTb[19]=1000.0;

// Input Tb ///////////////////////////////////////////////////////////////////////////////

//      20 component

        iTb[0]=140.0;

        iTb[1]=225.0;

        iTb[2]=294.0;

        iTb[3]=350.0;

        iTb[4]=395.0;

        iTb[5]=430.0;

        iTb[6]=458.0;

        iTb[7]=485.0;

        iTb[8]=507.0;

        iTb[9]=528.0;
```

```
        iTb[10]=548.0;
        iTb[11]=565.0;
        iTb[12]=585.0;
        iTb[13]=612.0;
        iTb[14]=650.0;
        iTb[15]=690.0;
        iTb[16]=735.0;
        iTb[17]=790.0;
        iTb[18]=875.0;
// Input API ////////////////////////////////////////////////////////////////////////////////
//      20 component
        API[0]=69.8;
        API[1]=58.5;
        API[2]=47.8;
        API[3]=42.0;
        API[4]=38.8;
        API[5]=36.5;
        API[6]=34.8;
        API[7]=33.0;
        API[8]=31.8;
        API[9]=31.0;
        API[10]=30.2;
        API[11]=29.3;
        API[12]=27.8;
        API[13]=25.5;
        API[14]=23.5;
        API[15]=22.5;
        API[16]=21.0;
        API[17]=17.5;
        API[18]=12.2;
        API[19]=6.0;
```

```
// Calculate Component Properties ////////////////////////////////////////////////////////

        for (i=0;i<comp;i++)

        {

                iSG[i]=(141.5/(API[i]+131.5));

                iTc[i]=768.071+(1.7134*iTb[i])-(1.0834e-3*pow(iTb[i],2))+(3.889e-7*pow(iTb[i],3))

                        -(8.9213e-3*iTb[i]*API[i])+(5.3095e-7*pow(iTb[i],2)*API[i])

                        +(3.2712e-8*pow(iTb[i],2)*pow(API[i],2));

                lnPc[i]=2.829+(9.421e-4*iTb[i])-(3.0475e-6*pow(iTb[i],2))+(1.5141e-9*pow(iTb[i],3))

                        -(2.0876e-5*iTb[i]*API[i])+(1.1048e-8*pow(iTb[i],2)*API[i])

                        +(1.395e-10*pow(iTb[i],2)*pow(API[i],2))-(4.827e-8*pow(API[i],2)*iTb[i]);

                iPc[i]=pow(10,lnPc[i]);

                iTb[i]=iTb[i]+460;

                iTc[i]=iTc[i]+460;

                iMW[i]=-122726.0+9486.4*iSG[i]+(4.6523-3.3287*iSG[i])*iTb[i]+(1-0.77084*iSG[i]

                        -0.02058*pow(iSG[i],2))*(1.3437-(720.79/iTb[i]))*(pow(10,7)/iTb[i])

                        +(1-0.80882*iSG[i]+0.02226*pow(iSG[i],2))*(1.8828-(181.98/iTb[i]))

                        *(pow(10,12)/pow(iTb[i],3));

                iTbr[i]=iTb[i]/iTc[i];

                iKp[i]=pow(iTb[i],0.333333)/iSG[i];

                if (iTbr[i]<0.8)

                        iw[i]=(log(Psys/iPc[i])-5.92714+(6.09648/iTbr[i])+1.28862

                                *log(iTbr[i])-(0.169347*pow(iTbr[i],6)))

                                /(15.2518-(15.6875/iTbr[i])-(13.4721*log(iTbr[i]))

                                +(0.43577*pow(iTbr[i],6)));

                else

                        iw[i]=-7.904+0.1352*iKp[i]-0.007465*pow(iKp[i],2)+8.359*iTbr[i]

                                +((1.408-0.01063*iKp[i])/iTbr[i]);

        }

// Feed Prop ////////////////////////////////////////////////////////////////////

        fs=17;

        fs=fs-1;

        feed[fs]=26.32;
```

```
        Tfeed=560.0;
// Input Mole Fraction of Feed ////////////////////////////////////////////////
//      20 component
        iz[0]=0.08739;
        iz[1]=0.08549;
        iz[2]=0.06725;
        iz[3]=0.06991;
        iz[4]=0.06041;
        iz[5]=0.06079;
        iz[6]=0.04939;
        iz[7]=0.04939;
        iz[8]=0.04939;
        iz[9]=0.04901;
        iz[10]=0.04787;
        iz[11]=0.04407;
        iz[12]=0.04331;
        iz[13]=0.04103;
        iz[14]=0.04217;
        iz[15]=0.03533;
        iz[16]=0.03495;
        iz[17]=0.02964;
        iz[18]=0.02964;
        iz[19]=0.02356;
// Generate for all stage /////////////////////////////////////////////////////////////
        for (j=0;j<stage;j++)
        {
                for (i=0;i<comp;i++)
                {
                        SG[i][j]=iSG[i];
                        w[i][j]=iw[i];
                        Tb[i][j]=iTb[i];
                        Tc[i][j]=iTc[i];
```

```
                        Pc[i][j]=iPc[i];
                        z[i][j]=iz[i];
                }
        }
// Initial Xij ///////////////////////////////////////////////////////////////////////////
//      20 component
        X[0][   0]=0.4196,X[1][   0]=0.2026,X[2][   0]=0.1151,X[3][   0]=0.0725,X[4][   0]=0.0479,X[5][
0]=0.0335,X[6][ 0]=0.0238,X[7][ 0]=0.0191,X[8][ 0]=0.0158,X[9][ 0]=0.0136,X[10][ 0]=0.0114,X[11][
0]=0.0092,X[12][ 0]=0.0102,X[13][ 0]=0.0052,X[14][ 0]=0.0004,X[15][ 0]=0.0000,X[16][ 0]=0.0000,X
[17][ 0]=0.0000,X[18][ 0]=0.0000,X[19][ 0]=0.0000;
        X[0][ 1]=0.1098,X[1][ 1]=0.1035,X[2][ 1]=0.0865,X[3][ 1]=0.0840,X[4][ 1]=0.0742,X
[5][ 1]=0.0692,X[6][ 1]=0.0617,X[7][ 1]=0.0591,X[8][ 1]=0.0573,X[9][ 1]=0.0573,X[10][
1]=0.0558,X[11][ 1]=0.0506,X[12][ 1]=0.0724,X[13][ 1]=0.0525,X[14][ 1]=0.0060,X[15][
1]=0.0001,X[16][ 1]=0.0000,X[17][ 1]=0.0000,X[18][ 1]=0.0000,X[19][ 1]=0.0000;
        X[0][ 2]=0.0513,X[1][ 2]=0.0549,X[2][ 2]=0.0508,X[3][ 2]=0.0564,X[4][ 2]=0.0558,X
[5][ 2]=0.0590,X[6][ 2]=0.0589,X[7][ 2]=0.0618,X[8][ 2]=0.0656,X[9][ 2]=0.0718,X[10][
2]=0.0766,X[11][ 2]=0.0749,X[12][ 2]=0.1268,X[13][ 2]=0.1181,X[14][ 2]=0.0170,X[15][
2]=0.0004,X[16][ 2]=0.0000,X[17][ 2]=0.0000,X[18][ 2]=0.0000,X[19][ 2]=0.0000;
        X[0][ 3]=0.0462,X[1][ 3]=0.0466,X[2][ 3]=0.0417,X[3][ 3]=0.0450,X[4][ 3]=0.0442,X
[5][ 3]=0.0472,X[6][ 3]=0.0485,X[7][ 3]=0.0524,X[8][ 3]=0.0580,X[9][ 3]=0.0666,X[10][
3]=0.0751,X[11][ 3]=0.0773,X[12][ 3]=0.1484,X[13][ 3]=0.1710,X[14][ 3]=0.0390,X[15][
3]=0.0009,X[16][ 3]=0.0000,X[17][ 3]=0.0000,X[18][ 3]=0.0000,X[19][ 3]=0.0000;
        X[0][ 4]=0.0460,X[1][ 4]=0.0456,X[2][ 4]=0.0399,X[3][ 4]=0.0417,X[4][ 4]=0.0400,X
[5][ 4]=0.0416,X[6][ 4]=0.0420,X[7][ 4]=0.0452,X[8][ 4]=0.0503,X[9][ 4]=0.0586,X[10][
4]=0.0678,X[11][ 4]=0.0718,X[12][ 4]=0.1510,X[13][ 4]=0.2095,X[14][ 4]=0.0471,X[15][
4]=0.0018,X[16][ 4]=0.0000,X[17][ 4]=0.0000,X[18][ 4]=0.0000,X[19][ 4]=0.0000;
        X[0][ 5]=0.0462,X[1][ 5]=0.0455,X[2][ 5]=0.0396,X[3][ 5]=0.0408,X[4][ 5]=0.0385,X
[5][ 5]=0.0392,X[6][ 5]=0.0388,X[7][ 5]=0.0410,X[8][ 5]=0.0451,X[9][ 5]=0.0522,X[10][
5]=0.0606,X[11][ 5]=0.0649,X[12][ 5]=0.1442,X[13][ 5]=0.2349,X[14][ 5]=0.0655,X[15][
5]=0.0032,X[16][ 5]=0.0001,X[17][ 5]=0.0000,X[18][ 5]=0.0000,X[19][ 5]=0.0000;
        X[0][ 6]=0.0463,X[1][ 6]=0.0455,X[2][ 6]=0.0395,X[3][ 6]=0.0405,X[4][ 6]=0.0379,X
[5][ 6]=0.0381,X[6][ 6]=0.0371,X[7][ 6]=0.0338,X[8][ 6]=0.0419,X[9][ 6]=0.0477,X[10][
```

6]=0.0549,X[11][6]=0.0586,X[12][6]=0.1336,X[13][6]=0.2485,X[14][6]=0.0856,X[15][6]=0.0053,X[16][6]=0.0002,X[17][6]=0.0000,X[18][6]=0.0000,X[19][6]=0.0000;

X[0][7]=0.0464,X[1][7]=0.0455,X[2][7]=0.0394,X[3][7]=0.0403,X[4][7]=0.0376,X[5][7]=0.0376,X[6][7]=0.0363,X[7][7]=0.0375,X[8][7]=0.0400,X[9][7]=0.0449,X[10][7]=0.0508,X[11][7]=0.0537,X[12][7]=0.1221,X[13][7]=0.2522,X[14][7]=0.1069,X[15][7]=0.0086,X[16][7]=0.0004,X[17][7]=0.0000,X[18][7]=0.0000,X[19][7]=0.0000;

X[0][8]=0.0464,X[1][8]=0.0455,X[2][8]=0.0394,X[3][8]=0.0402,X[4][8]=0.0374,X[5][8]=0.0372,X[6][8]=0.0357,X[7][8]=0.0367,X[8][8]=0.0387,X[9][8]=0.0429,X[10][8]=0.0478,X[11][8]=0.0499,X[12][8]=0.1115,X[13][8]=0.2478,X[14][8]=0.1286,X[15][8]=0.0133,X[16][8]=0.0009,X[17][8]=0.0000,X[18][8]=0.0000,X[19][8]=0.0000;

X[0][9]=0.0465,X[1][9]=0.0455,X[2][9]=0.0394,X[3][9]=0.0401,X[4][9]=0.0373,X[5][9]=0.0370,X[6][9]=0.0353,X[7][9]=0.0361,X[8][9]=0.0379,X[9][9]=0.0416,X[10][9]=0.0457,X[11][9]=0.0471,X[12][9]=0.1021,X[13][9]=0.2371,X[14][9]=0.1496,X[15][9]=0.0200,X[16][9]=0.0018,X[17][9]=0.0000,X[18][9]=0.0000,X[19][9]=0.0000;

X[0][10]=0.0466,X[1][10]=0.0456,X[2][10]=0.0394,X[3][10]=0.0401,X[4][10]=0.0371,X[5][10]=0.0367,X[6][10]=0.0350,X[7][10]=0.0356,X[8][10]=0.0372,X[9][10]=0.0406,X[10][10]=0.0441,X[11][10]=0.0449,X[12][10]=0.0941,X[13][10]=0.2218,X[14][10]=0.1686,X[15][10]=0.0292,X[16][10]=0.0034,X[17][10]=0.0000,X[18][10]=0.0000,X[19][10]=0.0000;

X[0][11]=0.0467,X[1][11]=0.0456,X[2][11]=0.0394,X[3][11]=0.0400,X[4][11]=0.0370,X[5][11]=0.0365,X[6][11]=0.0347,X[7][11]=0.0352,X[8][11]=0.0366,X[9][11]=0.0397,X[10][11]=0.0429,X[11][11]=0.0431,X[12][11]=0.0873,X[13][11]=0.2033,X[14][11]=0.1843,X[15][11]=0.0413,X[16][11]=0.0062,X[17][11]=0.0000,X[18][11]=0.0000,X[19][11]=0.0000;

X[0][12]=0.0468,X[1][12]=0.0457,X[2][12]=0.0394,X[3][12]=0.0399,X[4][12]=0.0369,X[5][12]=0.0363,X[6][12]=0.0343,X[7][12]=0.0348,X[8][12]=0.0361,X[9][12]=0.0390,X[10][12]=0.0417,X[11][12]=0.0417,X[12][12]=0.0815,X[13][12]=0.1829,X[14][12]=0.1950,X[15][12]=0.0566,X[16][12]=0.0112,X[17][12]=0.0002,X[18][12]=0.0000,X[19][12]=0.0000;

X[0][13]=0.0469,X[1][13]=0.0457,X[2][13]=0.0394,X[3][13]=0.0399,X[4][13]=0.0368,X[5][13]=0.0361,X[6][13]=0.0342,X[7][13]=0.0345,X[8][13]=0.0356,X[9][13]=0.0382,X[10][13]=0.0407,X[11][13]=0.0403,X[12][13]=0.0765,X[13][13]=0.1617,X[14]

```
[13]=0.1990,X[15][13]=0.0748,X[16][13]=0.0193,X[17][13]=0.0005,X[18][13]=0.0000,X[19]
[13]=0.0000;
        X[0][14]=0.0470,X[1][14]=0.0458,X[2][14]=0.0394,X[3][14]=0.0398,X[4]
[14]=0.0366,X[5][14]=0.0359,X[6][14]=0.0339,X[7][14]=0.0341,X[8][14]=0.0351,X[9]
[14]=0.0375,X[10][14]=0.0397,X[11][14]=0.0390,X[12][14]=0.0720,X[13][14]=0.1405,X[14]
[14]=0.1952,X[15][14]=0.0949,X[16][14]=0.0320,X[17][14]=0.0016,X[18][14]=0.0001,X[19]
[14]=0.0001;
        X[0][15]=0.0472,X[1][15]=0.0459,X[2][15]=0.0394,X[3][15]=0.0398,X[4]
[15]=0.0365,X[5][15]=0.0357,X[6][15]=0.0336,X[7][15]=0.0336,X[8][15]=0.0345,X[9]
[15]=0.0367,X[10][15]=0.0386,X[11][15]=0.0377,X[12][15]=0.0677,X[13][15]=0.1201,X[14]
[15]=0.1824,X[15][15]=0.1145,X[16][15]=0.0505,X[17][15]=0.0045,X[18][15]=0.0005,X[19]
[15]=0.0005;
        X[0][16]=0.0474,X[1][16]=0.0460,X[2][16]=0.0395,X[3][16]=0.0397,X[4]
[16]=0.0364,X[5][16]=0.0355,X[6][16]=0.0332,X[7][16]=0.0332,X[8][16]=0.0339,X[9]
[16]=0.0359,X[10][16]=0.0375,X[11][16]=0.0364,X[12][16]=0.0635,X[13][16]=0.1007,X[14]
[16]=0.1602,X[15][16]=0.1295,X[16][16]=0.0745,X[17][16]=0.0123,X[18][16]=0.0024,X[19]
[16]=0.0023;
        X[0][17]=0.0044,X[1][17]=0.0066,X[2][17]=0.0072,X[3][17]=0.0094,X[4]
[17]=0.0104,X[5][17]=0.0122,X[6][17]=0.0134,X[7][17]=0.0151,X[8][17]=0.0173,X[9]
[17]=0.0204,X[10][17]=0.0237,X[11][17]=0.0250,X[12][17]=0.0523,X[13][17]=0.1069,X[14]
[17]=0.2183,X[15][17]=0.2244,X[16][17]=0.1629,X[17][17]=0.0443,X[18][17]=0.0136,X[19]
[17]=0.0120;
// Initial L and V //////////////////////////////////////////////////////////////////
        L[0]=Reflux*Distil;             //Initial L1
        V[0]=Distil-U[0];               //Initial V1
        V[1]=L[0]+Distil+W[0];
        for (j=2;j<stage;j++)           //Initial V2 to last stage
        {
                V[j]=V[j-1]+W[j-1];
        }
```

```
// Initial Tj //////////////////////////////////////////////////////////////////////////////////
//          20 comp
            T[0]=257.12;
            T[1]=368.23;
            T[2]=433.97;
            T[3]=451.34;
            T[4]=457.05;
            T[5]=459.42;
            T[6]=461.53;
            T[7]=462.04;
            T[8]=463.02;
            T[9]=463.74;
            T[10]=464.40;
            T[11]=465.12;
            T[12]=465.80;
            T[13]=466.54;
            T[14]=467.38;
            T[15]=468.23;
            T[16]=469.26;
            T[17]=620.96;
// Convert Temperature Fahrenheit to Rankine ////////////////////////////////////////////////
            for (j=0;j<stage;j++)
                        T[j]=T[j]+460;
            Tfeed=Tfeed+460;
// Select Method ///////////////////////////////////////////////////////////////////////////////

//          Method=1;        // For Normal Technic
            Method=2;        // For Combined Technic
```

```
// Advance Input ////////////////////////////////////////////////////////////////////////
if (Method==2)
{
        Oldcomp=comp;
// Number of group ////////////////////////////////////////////////////////////////////////
        no_G=14;
// Number of group component ///////////////////////////////////////////////////////////////
        Gcomp[0]=3;
        Gcomp[1]=1;
        Gcomp[2]=1;
        Gcomp[3]=1;
        Gcomp[4]=1;
        Gcomp[5]=1;
        Gcomp[6]=1;
        Gcomp[7]=1;
        Gcomp[8]=1;
        Gcomp[9]=1;
        Gcomp[10]=1;
        Gcomp[11]=1;
        Gcomp[12]=1;
        Gcomp[13]=5;
// Calculate group properties //////////////////////////////////////////////////////////////
        InitGprop();
        gr=0;
// Advance Calculate ///////////////////////////////////////////////////////////////////////
        comp=no_G;
        for (j=0;j<stage;j++)
        {
                for (i=0;i<comp;i++)
                {
                        Tb[i][j]=iTbm[i][j];
                        Tc[i][j]=iTcm[i][j];
```

```
                Pc[i][j]=iPcm[i][j];
                w[i][j]=iwm[i][j];
                SG[i][j]=iSGm[i][j];
                z[i][j]=izm[i][j];
                X[i][j]=iXm[i][j];
            }
        }
    }
// Initial Kij /////////////////////////////////////////////////////////////////////////////////////////
    for (j=0;j<stage;j++)
    {
        for (i=0;i<comp;i++)
        {
            Kij[i][j]=1;
        }
        ThermoProp(T[j],j);
        Z_liq(T[j],j);
        Z_vap(T[j],j);
        for (i=0;i<comp;i++)
        {
            Kij[i][j]=exp(lnfuL[i][j])/exp(lnfuV[i][j]);
        }
    }
    Z_feed(Tfeed);
// Setup Iteration /////////////////////////////////////////////////////////////////////////////////////
    Iter=0;
// Looping ///////////////////////////////////////////////////////////////////////////////////////////////
Loop:
    Lj();                       // Calculate Lj
// Calculate Aj,Bj,Cj,Dj /////////////////////////////////////////////////////////////////////////////
    ABCD_1_n();                 // Calculate A1,B1,C1,D1 & An,Bn,Cn,Dn
    ABCD_j();                   // Calculate Aj,Bj,Cj,Dj
```

```
// Calculate Xij ///////////////////////////////////////////////////////////////////////////////
        Xij();                          // Calculate Xij
// Calculate Tj ////////////////////////////////////////////////////////////////////////////////
        error=0;
        for (j=0;j<stage;j++)
        {
                Tj(j);
                Tn[j]=T[j]-(fT[j]/fTp[j]);
                error=error+pow(Tn[j]-T[j],2);
                T[j]=Tn[j];
        }
// Calculate Kij ///////////////////////////////////////////////////////////////////////////////
        for (j=0;j<stage;j++)
        {
                ThermoProp(T[j],j);
                Z_liq(T[j],j);
                Z_vap(T[j],j);
                for (i=0;i<comp;i++)
                        Kij[i][j]=exp(lnfuL[i][j])/exp(lnfuV[i][j]);
        }
// Calculate H Ideal ///////////////////////////////////////////////////////////////////////////
        for (j=0;j<stage;j++)
        {
                CoefH(j);
                HidealL[j]=HiL(j);
                HidealV[j]=HiV(j);
        }
        HidealF=HiF(Tfeed);                     // Calculate H Ideal feed
// Calculate hj & Hj ///////////////////////////////////////////////////////////////////////////
        for (j=0;j<stage;j++)
        {
                Tdal[j]=-TdaL(j);
```

```
                Tdav[j]=-TdaV(j);
                h[j]=HidealL[j]+R*T[j]*(ZL[j]-1-Ail[j]*(1-Tdal[j]/asuml1[j])
                        *log(1+Bil[j]/ZL[j])/Bil[j]);
                H[j]=HidealV[j]+R*T[j]*(ZV[j]-1-Aiv[j]*(1-Tdav[j]/asumv1[j])
                        *log(1+Biv[j]/ZV[j])/Biv[j]);
        }
        Tdaf=-TdaF();
        HF=HidealF+R*Tfeed*(ZLF-1-Aif*(1-Tdaf/asumf1)*log(1+Bif/ZLF)/Bif);
// Calculate Vj ////////////////////////////////////////////////////////////////////////////
        for (j=2;j<stage;j++)
        {
                V[j]=((H[j-1]-h[j-1])*(V[j-1]+W[j-1])+L[j-2]*(h[j-1]-h[j-2])
                        -feed[j-1]*(HF-h[j-1]))/(H[j]-h[j-1]);
        }
// Check Iteration ////////////////////////////////////////////////////////////////////////
        if (error > 0.001)
        {
                 Iter=Iter+1;
                goto Loop;
        }
// Recalculate Xij ///////////////////////////////////////////////////////////////////////
if (Method==2)
{
        for (j=0;j<stage;j++)
        {
                for (i=0;i<comp;i++)
                        iXm[i][j]=X[i][j];
        }
        RecalcX();
        comp=Oldcomp;
```

```
// Regroup Prop ////////////////////////////////////////////////////////////////////////////////
        for (j=0;j<stage;j++)
        {
                for (i=0;i<comp;i++)
                {
                        Tb[i][j]=iTb[i];
                        Tc[i][j]=iTc[i];
                        Pc[i][j]=iPc[i];
                        w[i][j]=iw[i];
                        SG[i][j]=iSG[i];
                        z[i][j]=iz[i];
                }
        }
// Recal Kij ///////////////////////////////////////////////////////////////////////////////////
        for (j=0;j<stage;j++)
        {
                for (i=0;i<comp;i++)
                {
                        Kij[i][j]=1;
                }
                ThermoProp(T[j],j);
                Z_liq(T[j],j);
                Z_vap(T[j],j);
                for (i=0;i<comp;i++)
                {
                        Kij[i][j]=exp(lnfuL[i][j])/exp(lnfuV[i][j]);
                }
        }
// Calculate Aj,Bj,Cj,Dj //////////////////////////////////////////////////////////////////////
        ABCD_1_n();             // Calculate A1,B1,C1,D1 & An,Bn,Cn,Dn
        ABCD_j();               // Calculate Aj,Bj,Cj,Dj
```

```
// Calculate Xij and Tj ////////////////////////////////////////////////////////////////////////
        Xij();                          // Calculate Xij
        for (j=0;j<stage;j++)
        {
                Tj(j);
                Tn[j]=T[j]-(fT[j]/fTp[j]);
                T[j]=Tn[j];
        }
// Recalculate Kij ////////////////////////////////////////////////////////////////////////////
        for (j=0;j<stage;j++)
        {
                ThermoProp(T[j],j);
                Z_liq(T[j],j);
                Z_vap(T[j],j);
                for (i=0;i<comp;i++)
                        Kij[i][j]=exp(lnfuL[i][j])/exp(lnfuV[i][j]);
        }
// Calculate H Ideal ////////////////////////////////////////////////////////////////////////
        for (j=0;j<stage;j++)
        {
                CoefH(j);
                HidealL[j]=HiL(j);
                HidealV[j]=HiV(j);
        }
        HidealF=HiF(Tfeed);             // Calculate H Ideal feed
// Calculate hj & Hj ///////////////////////////////////////////////////////////////////////
        for (j=0;j<stage;j++)
        {
                Tdal[j]=-TdaL(j);
                Tdav[j]=-TdaV(j);
                h[j]=HidealL[j]+R*T[j]*(ZL[j]-1-Ail[j]*(1-Tdal[j]/asuml1[j])
                        *log(1+Bil[j]/ZL[j])/Bil[j]);
```

```
        H[j]=HidealV[j]+R*T[j]*(ZV[j]-1-Aiv[j]*(1-Tdav[j]/asumv1[j])
            *log(1+Biv[j]/ZV[j])/Biv[j]);
    }
    Tdaf=-TdaF();
    HF=HidealF+R*Tfeed*(ZLF-1-Aif*(1-Tdaf/asumf1)*log(1+Bif/ZLF)/Bif);
// Calculate Vj ////////////////////////////////////////////////////////////////////////////////////////
    for (j=2;j<stage;j++)
        V[j]=((H[j-1]-h[j-1])*(V[j-1]+W[j-1])+L[j-2]*(h[j-1]-h[j-2])-feed[j-1]
            *(HF-h[j-1]))/(H[j]-h[j-1]);
}
    Lj();                       // Calculate Lj
// Output Result ////////////////////////////////////////////////////////////////////////////////////////
    for (j=0;j<stage;j++)
    {
        //cout<<"T["<<j+1<<"],"<<T[j]-460<<"\n";
        //cout<<"V["<<j+1<<"],"<<V[j]<<"\n";
        //cout<<"L["<<j+1<<"],"<<L[j]<<"\n";
        for (i=0;i<comp;i++)
        {
            //cout<<X[i][j]<<",";
            //cout<<Kij[i][j]<<",";
        }
        //cout<<"\n";
    }
// Calc Run Time ////////////////////////////////////////////////////////////////////////////////////////
    runtime=clock();
    cout<<"Run Time = "<<runtime<<"\n";
}
```

VITA

Miss Patcharee Wongjirasawad graduated with high school diploma from Satri Si Suriyothai School in 1994 and received a Bachelor in Degree Chemical Technology from Chulalongkorn University in 1998.