

STEADY STATE SIMULATION OF ATMOSPHERIC CRUDE DISTILLATION TOWER

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ABSTRACT

Computer simulation of multicomponent separation processes like complex distillation is carried out at steady state condition using the very well known equilibrium stage model.

The equations that describing the model equilibrium stage are: the material balances equations, the energy balances equations and the equilibrium equations for each stage (the MESH equations), which are lead to a nonlinear system, the non-linearity in these equations necessitate the use of some iterative scheme to obtain the desired solution. The set of equations were collected and setup in a block-tridiagonal structure, namely, Jacobian matrix to minimize both storage and CPU times. The coefficients of Jacobian matrix represent the partial drivatives of all the MESH equations with respect to all the independent variables. This structure permits solution by means of Thomas algorithm. Thus, the model employs a multivariate Newton Raphson procedure for solving all equations simultaneously to determine the corrections of the independent variables at each iteration.

The thermodynamic quantities (K-values and enthalpies) within the MESH equations are calculated by means of Soave-Redlich-Kwong (SRK) equation of state (Soave,1972). The solution is reached quite rapidly within less than 10 trials.

INTRODUCTION

The final design of equipment for the separation of multicomponent mixtures is often based on the solution of the steady state or the unsteady state equation and requires rigorous determination of temperature, pressure, stream flowrates, stream composition and heat load at each stage, this is can be done by using the MESH equations for each stage. Most algorithm for solving the MESH equations fall into one of two categories

1. Tearing methods, in which the equations are divided into groups and solved separately.
2. Simultaneous correction methods, in which all of the equations are solved simultaneously.

A wide variety of iterative solution procedures for solving these equations have appeared in the literatures, such as that given by Fenske (1932), Lewis Matheson (1932), Amundson and Pontinen (1958), Holand (1963), Ferraries and Donati (1974), Holand (1976), Kinoshita and Hushimoto (1983).

In this work a modification of the Naphtali and Sandholm (1971) method for stage wise, countercurrent gas liquid contacting devices calculations at steady state has been proposed.

For the equilibrium stage model the MESH equations (Wang and Henke 1966). The thermodynamic quantities (K-values and enthalpies) Soave, 1972 within these equations led to make them highly nonlinear equations, they are grouped by stage and then linearised using Taylor series approach, therefore, the difficulties resulting from non linearity can be avoided. To obtain the desired solution, some iterative scheme must be used.

The linearised MESH equations are collected and put in a block-tridiagonal form, namely, Jacobian matrix, which having an elements represent the partial derivatives of all the equations with respect to all the independent variables. These structure which permits solution by means of Thomas algorithm. Thus, the model employs a multivariate Newton Raphson procedure for solving all equations simultaneously to determine the corrections of the independent variables.

Choice of Stage temperature, total liquid and vapor flowrates and liquid composition as independent variables, reduce the block size to $(m+3).(m+3)$ instead of $(2m+1).(2m+1)$ that for NS method

The Model Equations (The MESH Equations)

For a complex distillation column where the stages (tray or plate) are numbered down from the top, with the condenser as the first stage and the reboiler as the *n*th stage as shown in Figure 1.

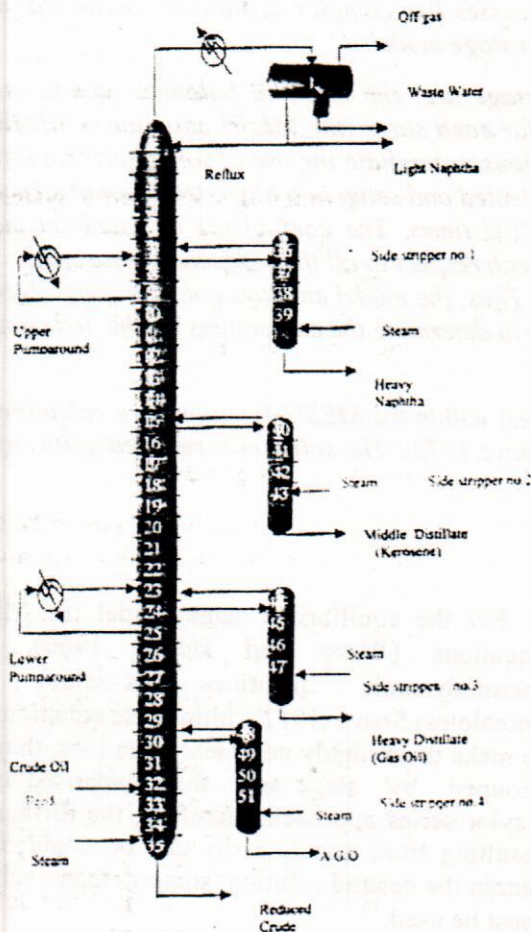


Fig. (1) Schematic diagram of atmospheric crude distillation tower

A general schematic representation of an equilibrium stage *j* is shown in Figure 2.

The steady state model for any stage *j* and any component *i* may be represented by four sets of equations are designated as MESH equations (Wang and Henke 1966). The MESH equations which must be satisfied in a rigorous equilibrium stage calculations, which are the material balance equation, the equilibrium equation, the summation equation of mole fraction and the heat balance equation. Depending on what variables are chosen and how the material and heat balances are

written, there are different ways to express the MESH equations. In this work the overall material and heat balances are written around each stage and the independent variables are the mole fractions of liquid, the temperature *T_j*, the liquid rate *L_j*, and the vapor rate *V_j*. The overall materials balance around stage *j* can be added to the MESH equations and then called MOSH equations by replacing the equilibrium equation by the overall material balance equation.

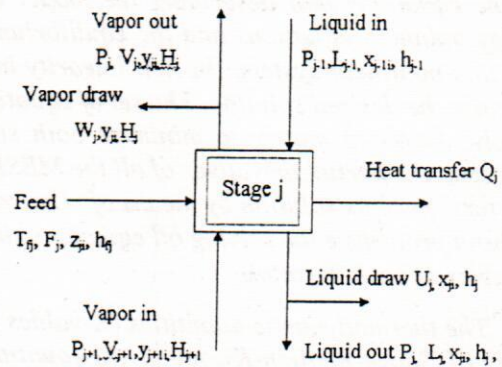


Fig. (2) Schematic diagram of general equilibrium stage

The MOSH equations are as follows:

Material balance of the *i*th component on the *j*th equilibrium stage:

$$M_{ji} = x_{ji}(L_j + U_j) + k_{ji}x_{ji}(V_j + W_j) - x_{j-1i}L_{j-1} - k_{j+1i}x_{j+1i}V_{j+1} - F_j z_{ji} \quad (1)$$

Overall material balance around stage *j*:

$$O_j = (L_j + U_j) + (V_j + W_j) - L_{j-1} - V_{j+1} - F_j \quad (2)$$

Summation of mole fractions on a stage:

$$S_j = \sum_{i=1}^m x_{ji} - 1 \quad (3)$$

Heat balance around stage *j*:

$$E_j = h_j(L_j + U_j) + H_j(V_j + W_j) - h_{j-1}L_{j-1} - H_{j+1}V_{j+1} - h_j F_j - Q_j \quad (4)$$

Furthermore we assume that the physicochemical properties in equations 1 to 4 are functions of temperature, pressure, and compositions of the liquid and the vapor phases

$$K_{ji} = K_{ji}(T_j, P_j, x_{ji}, y_{ji}) \quad i = 1, m, j = 1, n \quad (5)$$

$$h_j = h_j(T_j, P_j, x_{ji}) \quad i = 1, m, j = 1, n \quad (6)$$

$$H_j = H_j(T_j, P_j, y_{ji}) \quad i = 1, m, j = 1, n \quad (7)$$

The Tridiagonal Matrix Method

The usual approach for tray to tray calculation is to write the equation for the mass balance of each component entering and leaving each stage and then express the system of such equation for all stages in a matrix notation. At each stage

$$-l_{j-1,i} + l_{ji}(1 + U_j/L_j) + v_{ji}(1 + W_j/V_j) - v_{j+1,i} = f_{ji} \quad (8)$$

Where l and f are the component molal liquid and feed flow rates respectively. Given the equilibrium relation $y_{ji} = K_{ji}x_{ji}$, and that the gross interstage flows, L and V are the sum of the component flows, the component vapor flow may be written in form of the liquid flow

$$v_{ji} = y_{ji}V_j = \frac{K_{ji}V_j l_{ji}}{L_j} \quad (9)$$

By substituting equation 9 into equation 8, the component mass balance becomes

$$-l_{j-1,i} + \left[(1 + U_j/L_j) + \frac{K_{ji}V_j}{L_j}(1 + W_j/V_j) \right] l_{ji} - \frac{K_{j+1,i}V_{j+1}}{L_{j+1}} l_{j+1,i} = f_{ji} \quad (10)$$

When the flow rates and composition of feed streams are given, and the amounts of all the product streams are specified, provided that the equilibrium ratios can be expressed as composition dependent which are assumed for a first trial, then the equation 10 is a linear system, which are put in a tridiagonal matrix form, over the whole tower.

$$\begin{bmatrix} B_1 & C_1 & 0 & 0 & 0 & \dots & 0 \\ -1 & B_2 & C_2 & & & & 0 \\ & -1 & B_3 & C_3 & & & 0 \\ & & & & \dots & & \\ 0 & & & & & & \\ 0 & & & -1 & B_{n-1} & C_{n-1} & \\ 0 & 0 & 0 & & -1 & B_n & \end{bmatrix} \begin{bmatrix} l_{1v} \\ l_{2v} \\ l_{3v} \\ \vdots \\ l_{n-v} \\ l_{ni} \end{bmatrix} = \begin{bmatrix} f_{1v} \\ f_{2v} \\ f_{3v} \\ \vdots \\ f_{n-v} \\ f_{ni} \end{bmatrix} \quad (11)$$

where

$$B_j = (1 + U_j/L_j) + K_{ji} \frac{V_j}{L_j} (1 + W_j/V_j)$$

$$\text{and } C_j = -\frac{K_{j+1,i}V_{j+1}}{L_{j+1}}$$

The solution of equation 11 for the l_{ji} is obtained by means of Thomas algorithm (Thomas 1966). The Thomas algorithm is a Gaussian elimination procedure, that involves forward elimination starting from top stage and working toward stage n to finally isolate the l_{ni} other values of l_{ji} are obtain starting with l_{ni} by backward substitution.

Equations 1 through 4, constitute a system of $n.(m+3)$ simultaneous nonlinear algebraic equations with $n.(m+3)$ unknowns (n temperatures, total liquid and vapor flows and $n.m$ liquid compositions) are setup and solved for a column.

Newton-Raphson Method

Newton-Raphson method has frequently been used to solve equilibrium stage model equations. The Newton-Raphson is an iterative method in which successive set of the output variables are produced until the values of the functions $F(\mathbf{X})$ are driven to within some tolerance zero during the iterations, the non zero values of the functions are called discrepancies or errors. The functions and output variables are grouped by stage to stage in order from the top to the bottom This can be done to obtain a block tridiagonal structure for the Jacobian matrix of the partial derivatives so that the Thomas algorithm can be applied.

Let

$$\mathbf{X} = [\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3, \dots, \mathbf{X}_j, \dots, \mathbf{X}_N]^T \quad (12)$$

and

$$\mathbf{F} = [\mathbf{F}_1, \mathbf{F}_2, \mathbf{F}_3, \dots, \mathbf{F}_j, \dots, \mathbf{F}_N]^T \quad (13)$$

Where \mathbf{X}_j is a vector of output variables for stage j arranged in the order

$$\mathbf{X}_j = [x_{1j}, x_{2j}, x_{3j}, \dots, x_{mj}, T_j, L_j, V_j]^T \quad (14)$$

and \mathbf{F}_j is a vector of functions for stage j arranged in the order

$$\mathbf{F}_j = [M_{1j}, M_{2j}, M_{3j}, \dots, M_{mj}, S_j, O_j, H_j]^T \quad (15)$$

Solving for the correction ΔX to the output variables, which can be written in matrix form as follows, performs the Newton-Raphson iteration method.

$$\Delta X = - \left[\frac{\partial F(X)}{\partial X} \right]^{-1} F(X) \quad (16)$$

These corrections are used to compute the next approximation to the set of the output variables in the form

$$X^{k+1} = X^k + t \Delta X^k \quad (17)$$

where t is a non-negative scalar step factor in a range of 0 to 1. Different values of t are used to reduced the number of iterations to reach the convergence of solution, which is checked depends on the output vector or on the discrepancy function (Henley and Seader,1981). In this work the following criteria is used.

$$\text{Max.} \left(\left| \frac{X^k - X^{k+1}}{X^k} \right| \right) \leq \varepsilon$$

where ε is the tolerance error in range of $(10^{-3} - 10^{-5})$.

Jacobian Matrix

The partial derivatives of all the functions with respect to the vector of the output variables can construct a structure of square matrix, which is known the Jacobian matrix with a dimension of $[(m+3).n].[(m+3).n]$.

The Jacobian matrix for N-plates is then as follows

$$\begin{bmatrix} \frac{\partial F_1}{\partial X_1} & \frac{\partial F_1}{\partial X_2} & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\partial F_2}{\partial X_1} & \frac{\partial F_2}{\partial X_2} & \frac{\partial F_2}{\partial X_3} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\partial F_3}{\partial X_2} & \frac{\partial F_3}{\partial X_3} & \frac{\partial F_3}{\partial X_4} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & 0 & \frac{\partial F_{N-1}}{\partial X_{N-2}} & \frac{\partial F_{N-1}}{\partial X_{N-1}} & \frac{\partial F_{N-1}}{\partial X_N} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\partial F_N}{\partial X_{N-1}} & \frac{\partial F_N}{\partial X_N} \end{bmatrix}$$

Figure 3 Structure of the Jacobian matrix for N plates distillation column.

The Jacobian matrix $J = (\partial F/\partial X)$ of order $(N.N)$ is here very large, but it is evaluation is greatly facilitated by the fact the conditions on stage j only are influenced directly by the conditions on stages $j+1$ and $j-1$. As a result, the Jacobian becomes block-tridiagonal in structure, which permits rapid solution by the block elimination.

The structure of the Jacobian for the system of equations is then:

$$\begin{bmatrix} B_1 & C_1 & 0 & 0 & 0 & 0 & 0 & 0 \\ A_2 & B_2 & C_2 & 0 & 0 & 0 & 0 & 0 \\ 0 & A_3 & B_3 & C_3 & 0 & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & A_{N-1} & B_{N-1} & C_{N-1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & A_N & B_N \end{bmatrix} \begin{bmatrix} \Delta X_1 \\ \Delta X_2 \\ \Delta X_3 \\ \dots \\ \Delta X_{N-1} \\ \Delta X_N \end{bmatrix} = \begin{bmatrix} F_1 \\ F_2 \\ F_3 \\ \dots \\ F_{N-1} \\ F_N \end{bmatrix} \quad (18)$$

Where A , B and C are submatrices in order of $(m+3)$ by $(m+3)$ representing the partial derivatives of output variables and functions that given by equations 14 and 15. The elements below the diagonal B , contain the derivatives for stage j with respect to the variables on stage $j-1$, The diagonal elements of the Jacobian, B , contain the derivative of stage j with respect to the variables on stage j , The elements above the diagonal B , contain the derivatives for stage j with respect to the variables on stage $j+1$. A recurrence formula sometimes called Thomas algorithm (Thomas 1966) is applied to solve the block tridiagonal form of equation 18 for the corrections.

Description of the Problem

The atmospheric distillation tower shown in Figure 1 is used for the purpose of separating the crude oil feed F_1 into seven fractions (distillates and bottom products).

24000 barrels/day of 36 °API crude oil after passing through a crude preheat train) is fed into a furnace, the hot pre-flash liquid leaving the furnace at 630 °F, the partially vaporised stream is then fed to the atmospheric crude column. The column operate with a total condenser as a first stage in which three phases are simultaneously present: Two liquids and one vapor. The two liquids are constituted of an organic phase, which is refluxed to the top plate of the main column with reflux ratio equal to one, and aqueous

phase, which is withdrawn as extra distillate. The vapor phase is mainly constituted of methane through n-butane. The main column is represented by 34 ideal stages excluding condenser. The Four side strippers are coupled with the main column, each one has 4 ideal stages. A naphtha product is produced an overhead, a heavy naphtha is produced from the first steam-stripped side stripper, a middle distillate (kerosene) is produced from the second steam-stripped side stripper, a heavy distillate (light gas oil) is produced from the third steam-stripped side stripper, and a heavy atmospheric gas oil (AGO) is produced from the fourth steam-stripped side stripper. The steam enters the main tower and the strippers as superheated steam at 285 °C and 150 psia with the rates of 8 kg per cubic meter of the hydrocarbons. The overhead condenser operate at 25 psia while the bottom stage operate at 50 psia.

In the present analysis water was regarded as being distributed between the vapor and liquid phases on stage 2 through 51.

For the theoretical column, the following variables could be specified:

1. Number of theoretical plates in fractionation tower.
2. Number of theoretical plates in each side stripper.
3. Quantity, composition, and thermal condition of all feeds (crude oil and steam).
4. Distillate product (all vapor, all liquid or flashed).
5. Column pressure and the pressure drop per stage.
6. Distillates and side streams rates and their positions.
7. The use of either a reboiler below plate N in main column or the use of steam stripping.
8. The reflux ratio or alternately, the condenser duty.
9. The pump around rates and their withdrawal and return positions.
10. The intercoolers duties for the pump around streams.

RESULTS AND DISCUSSION

To examine the applicability of the developed computer program for this work. The relevant data available for crude atmospheric tower in Al-Doura refinery was tested in the HYSIS simulation program and tested in the developed program. Figure 4 shows the applicability of the simulation results compared with the HYSIS

example. The deviation between the presented work and the HYSIS simulator is within 10%, which could be due to the complexity of the physical property (K-value and enthalpy) correlation and the form of the model equations being solved in each system. But it is obvious that the accuracy of prediction can be enough to allow us to use of the developed model of atmospheric crude tower for process investigation and optimization. Figure 4 shows that the profile of vapor and liquid flowrates throughout the column. The pattern of vapor flowrate can be divided into three regions, the first region top two trays at which the vapor flowrate increased rapidly because the large different between the amount of vapor in the condenser-accumulator section and the first top plate. The second region starts from the third upper plate to the flash zone section (i.e. stages 32 and 33) when the crude oil is fed to the fractionation tower. In this region the vapor flowrate decreased linearly with little fluctuations between stages 17 and 25 which could be due to the defect of the light components concentration down to the flash zone. The last region begin from the feed plate to the last stage in the main tower when the stripping steam is enter, the vapor flowrate profile decreasing rapidly due to the flashing of the petroleum and all the vaporised materials will be concentrated at the rectifying section.

Figure 4 showing that the liquid flowrate decreasing linearly with the number of stages, except at stages 17 and 24. in some portion. The flowrates of liquid always is less than the vapor flowrates however, at a certain positions these values are equal (i.e. stages 3 and 32).

The distribution of liquid and vapor flowrate throughout the side strippers is represented after stage 35 till stage 51, when the heavy gas oil is drawn as a heaviest product.

Figure 5 shows that the temperature profile is almost increased linearly with the number of stages from top down. The top temperature (stage 1) decreases rapidly due to the cooling in the total condenser, the streams leaving the top tray of the fractionation tower at 100 °C while the stream leaving the total condenser at 40 °C. The maximum value of the temperature occurs at the flash zone, when the mixed flowrate of crude oil is feed to the main column at stage 33 with temperature of 320 °C and pressure of 50 psia.

The temperature gradient through the tower is an important for separating the various fractions based on the vapor pressure and the average boiling point. The trend of the temperature profile after stage 35 are decreased rapidly due to the large difference of the temperature levels between the stages 35 and 36. At each side stripper, the temperature gradient increased slightly from the top down as shown in Figure 5, Figure 5 shows good agreement between the results from presented work and that of HYSIS simulator.

The internal reflux ratio (L/V) at each stage was explained in Figure 6, the ratio (L/V) almost less than one due to the amount of the generated vapor throughout the fractionation tower compared to the amount of descending liquid. But in some portions the ratio may be equal or greater than one, as at the bottom section of the column because that all the light materials are concentrated in the rectifying section, see Figure 4.

Figure 7 shows the concentration profiles of pseudocomponents among the various petroleum fraction distillates from the atmospheric crude oil unit. This Figure showing the successive peaks with different magnitude those represent the concentration profile of pseudocomponents among the overhead, the bottom, and the distillate products. The peaks of component mole fraction are light naphtha, heavy naphtha, light distillate, heavy distillate, heavy gas oil, and reduced crude product respectively. The position of peaks is due to the concentration of components in the product, for example, the component number of 2 to 7 are concentrated in the light naphtha, the component number of 8 to 12 are concentrated in the heavy naphtha (gasoline), the component number of 12 to 16 are concentrated in the middle distillate (kerosene), the component number of 13 to 23 are concentrated in the heavy distillate (gasoil), the component number of 22 to 26 are concentrated in the heavy gasoil naphtha, the component number 26 to 34 are concentrated in the bottom product. The light components especially light end, which are concentrated mainly in the liquid overhead product due to its low boiling point. Where the middle distillates are almost free from the light end, but enrich in the heavy materials which having high boiling point greater than 140 °C.

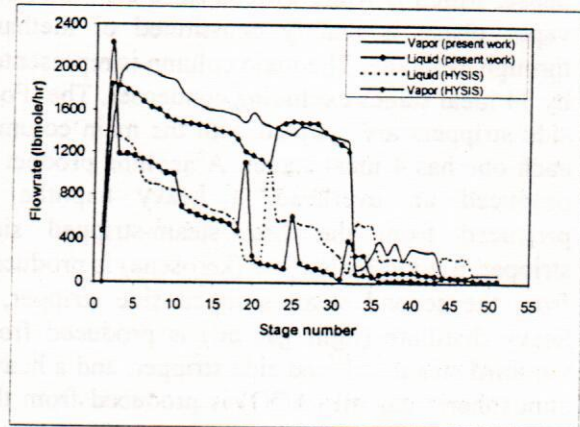


Fig. (4) comparison of flowrate profile along the main tower and the sidestrippers using the developed model with that of HYSIS

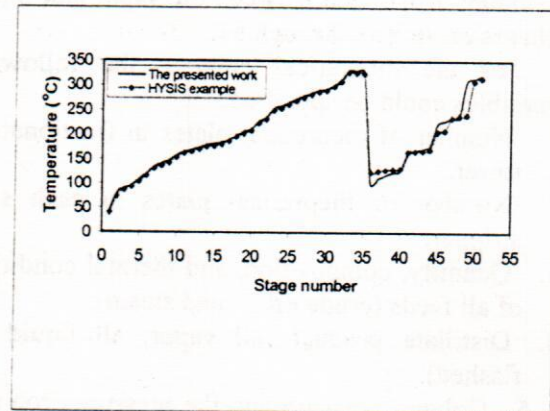


Fig. (5) Comparison of temperature profile along the main tower and the sidestrippers with that of HYSIS

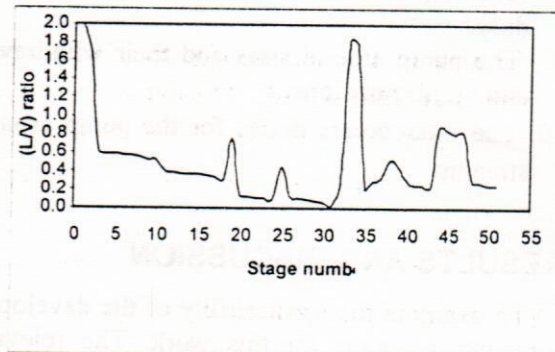


Fig. (6) Internal reflux ratio along the main tower and the sidestripper

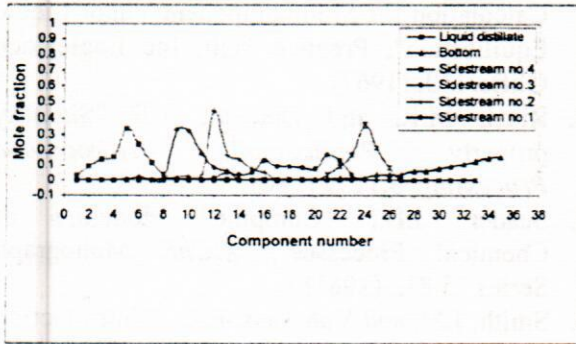


Fig. (6) Concentration of pseudocomponents in the petroleum fractions products

CONCLUSIONS

1. The linearisation procedure applied to simulate a complex distillation process can be applicable for different kinds of separating equipment, stripper, reboiled absorber and conventional distillation.
2. For the developed model the allowable of feeds and sidestreams is unlimited.
3. The multivariate Newton-Raphson method is a realistic method for solving industrial problems involving highly non-ideal solutions.
4. By assuming a linear temperature profile and a vapor rate profile corresponding to a constant molar overflow, a converged solution was obtained in less than ten iterations. So the number of iterations is usually lower than other method, such as NS method, θ -method and 2N Newton-Raphson method.
5. The size of the Jacobian matrix in the NS method is $[(2m+1) \cdot n]$. $[(2m+1) \cdot n]$ where in the present work is $[(m+3) \cdot n]$. $[(m+3) \cdot n]$. Thus, the computing time was less than that required for the NS method.
6. The method is robust and can be used to solve a wide range of highly nonlinear problems.
7. The advantage of the developed model is fast convergence, good stability and reliable requirements on computer memory.

NOMENCLATURE

A_j	Partial derivative of residual functions on plate j with respect to variables on plate $j-1$.
B_j	Submatrix partial derivative of residual functions on plate j with respect to variables on plate j .
C_j	Submatrix partial derivative of residual functions on plate j with respect to variables on plate $j+1$.
E_j	Enthalpy balance equation defined by equation (4).
F_j	Feed rate at stage j (lbmole/hr).
f_{ji}	Flow rate of component i in feed to stage j (lbmole/hr).
H_j	Enthalpy of vapor stream (Btu/lbmole).
h_j	Enthalpy of liquid stream (Btu/lbmole).
K_{ji}	Equilibrium ratio of component i at stage $j = y_{ji}/x_{ji}$.
L_j	Liquid stream flowing from j th stage down to the $(j+1)$ th stage (lbmole/hr).
l_{ji}	Molal liquid flow of component i on plate j (lbmole/hr)
M_{ji}	Material balance function as defined by equation (1)
m	Number of pseudocomponents.
n	Total number of stages in the complex column.
O_j	Overall material balance equation as defined by equation (3).
Q_j	Heat added or removed at stage j (Btu/hr).
S_j	Summation function as defined by equation (2).
T_j	Temperature at the j th stage ($^{\circ}$ F).
U_j	Liquid side stream from the j th stage (lbmole/hr).
v_{ji}	Molal vapor flow of component i on plate j (lbmole/hr).
V_j	Vapor stream leaving the j th stage to $(j-1)$ th stage above (lbmole/hr).
W_j	Vapor side stream from the j th stage (lbmole/hr).
X	vector of output variables.
x_{ji}	Mole fraction of the pseudo component i in the liquid phase leaving j th stage.
y_{ji}	Mole fraction of the pseudo component i in the vapor phase leaving j th stage.
z_{ji}	Composition of the feed stream entering the j th stage (mole fraction).

Subscripts

f	feed
i	component
j	stage
L	liquid phase
n	bottom tray
V	vapor phase

Superscripts

k	iteration index
T	transport

Greek letters

Δ	difference operator.
ϵ	tolerance error.
∂	partial derivative.

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