A MODEL FOR A NARROW-CUT FRACTIONATING COLUMN

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ABSTRACT

A mathematical model was developed to simulate the operation of a narrow-cut fractionating column. The model can calculate boiling point and dew point on the feed plate, the number of liquid and vapour moles , the enthalpy of feed and the final product distribution at the top and bottom of the column. The θ-method of convergence for predicting the product composition in bottom product and distillate corresponding to different operating conditions was used. The model was tested using different top pressures (5-30 psig), different feed temperatures (77-107°F) and different reflux ratios (1:1 to 1:3). The most effective variable was found to be top pressure. Decreasing the number of plates improved the convergence. Also increasing the number of iterations gave better convergence.

Keywords: Distillation, Model, Narrow-cut

NOMENCLATURE

A_{ji}	:	absorption factors
b_i	:	flow rate of component i in the bottoms 1b. mole/hr
B	:	total flow rate of bottoms, 1b-mole/hr
C	:	total number of components
d_i	:	flow rate of component i in the distillate, 1b.mole/hr
D	:	total flow rate of the distillate, 1b-mole/hr
f^L_i , f^V_i	:	fugacities of component i in the liquid and vapor phases, (composed òf any number of components) respectively, evaluated at the total pressure and temperature of the two-phase system
f (T)	:	bubble point function
F (T)	:	dew point function
F	:	total flow rate of the feed, 1b-mole/hr

$g(\theta)$: a function of θ; defined by equation (6)

h_{Fi}, H_{Fi} : enthalpies of pure component i, evaluated at the temperature T_f and pressure P of the flash, Btu/1b-mole

h_F : $\sum\limits_{i=1}^{c} hjiXji$, for an ideal solution, evaluated at the temperature T_F, and pressure P of the flash , Btu/1b-mole

h_j : $\sum\limits_{i=1}^{c} hjiXji$ $h_{ji} X_{ji}$,for an ideal solution ;evaluated at the temperature T_j , pressure and composition of the liquid leaving the j th plate, Btu/1b-mole

H : enthalpy per mole of feed, regardless of state, Btu/1b-mole

H_j : $\sum\limits_{i=1}^{c} H_{ji} Y_{ji}$, for an ideal solution

$H(x_j)K$: $\sum\limits_{i=1}^{c} H_{ki} X_{ji}$, for an ideal solution ; evaluated at the temperature and pressure of the vapor leaving the K th stage and at the composition of the liquid leaving the j th stage

$h(y_i)K$: $\sum\limits_{i=1}^{c} j_{ki} y_{ji}$ for an ideal solution evaluated at the temperature and pressure of the liquid leaving the K th stage and at the composition of the vapor leaving the j th stage

K_{ji} : equilibrium vaporization constant; evaluated at the temperature and pressure of the liquid leaving the j th stage

l_{ji} : flow rate at which component i in the liquid phase leaves the j th mass transfer section, 1b mole/hr

l_{oi} : flow rate of component i in the liquid reflux, 1b-mole/hr

$l_{Fi} V_{fi}$: flow rates of component i in the liquid and vapor parts respectively, of a partially vaporized feed, 1b.mole/hr. For bubble point liquid and subcooled feeds, $l_{Fi} = Fx_i$ and $V_{fi} = 0$. For dew point vapor and superheated feeds; $V_{fi} = F_{xi}$ and $l_{Fi} = 0$

L_j : total flow rate at which liquid leaves the j th stage, 1b-mole/hr

N : total number of plates

P_i : vapor pressure of component i, atm

P : total pressure, atm

$P(\psi)*$: flash function

q : a factor related to the thermal condition of the feed

Q_c : condenser duty, Btu/hr

Q_R : reboiler duty, Btu/hr

S_{ji} : K_{ji} V_j $/L_j$, stripping factor for component i, evaluated at the conditions of the liquid leaving the j th stage

T : temperature $T_{B.P.}$ = bubble point temperature and $T_{D.P.}$ = dew point temperature, ºF

T_F : flash temperature, ºF

V_{ji} : flow rate at which component i in the vapor is leaving the j th stage, 1b-mole/hr

X_{fi} : mole fraction of component i in the liquid leaving a flash process

X_{ji} : mole fraction of component i in the liquid leaving the j th stage

X_{bi} : mole fraction of component i in the bottom

X_i : abscissa of the point of intersection of the operating lines for a binary mixture

X_i : total mole fraction of component i in the feed (regardless of state)

X_{di} : total mole fraction of component i in the distillate (regardless of state)

Y_{ji} : mole fraction of component i in the vapor leaving plate j

Subscripts:

ca : calculated value

co : corrected value

f : feed plate

F : variables associated with a partially vaporized feed

i : component number, i = 1, 2,......c or ($1 \le i \le c$)

j : plate number, j = 0 for the accumulator. For the top plate = 1, for the feed plate j = f, for the bottom plate j = N, and for the reboiler j = N+ 1, that is , j = 0,1,2,...,f,...N₁, N+1 , or ($0 \le j \le N+1$)

n : trial number

N : total number of plates

r : rectifying section

s : stripping section

Superscripts:

L : liquid phase

V : vapor phase

Mathematical Symbols:

$\sum\limits_{i=1}^{c} X_i$: sum of overall values X_i,, $i = 1,2,...c$, or $(1 \le i \le c)$

(X_j) : set of all values X_j belonging to the particular set under consideration

$\prod\limits_{i=1}^{c} Xj$: $X_1, X_2, ... X_{c-1}, X_c$,product of the X_i's from $j = 1$ through $j = c$.

INTRODUCTION

Conventional distillation columns mathematical problems are solved most rapidly by the Lewis and Matheson procedure and using the θ-method . For more complex column problems the Thiele and Geddes procedure using a modification of the θ-method is more suited (1).

The θ-method of convergence is used for (2):

1- Predicting the product composition corresponding to new operating conditions.
2- Determining the operating conditions necessary to meet product purity.
3- Determining the ratio of the flow rates of a component in distillate and bottoms when the reflux ratio is changed.

Other techniques have been recently used to develop empirical models for distillation columns as spread sheets (11) and neural networks (12, 13).
The aim of this work is to develop a model for a distillation column operating at steady state to separate multi component mixtures .

PLANT DESCRIPTION AND ANALYSIS

Field tests were performed on the depentanizer column for mixed hexanes production plant located in Alexandria Petroleum Company in Mex, Alexandria, Egypt.

The feed to the plant is light straight run naphtha treated by the Merox process to remove mercaptanes. The plant was designed to produce 10,000 MT/Year hexane solvent (64 - 68 °C). The flow diagram of the hexane plant is shown in Fig. 1.
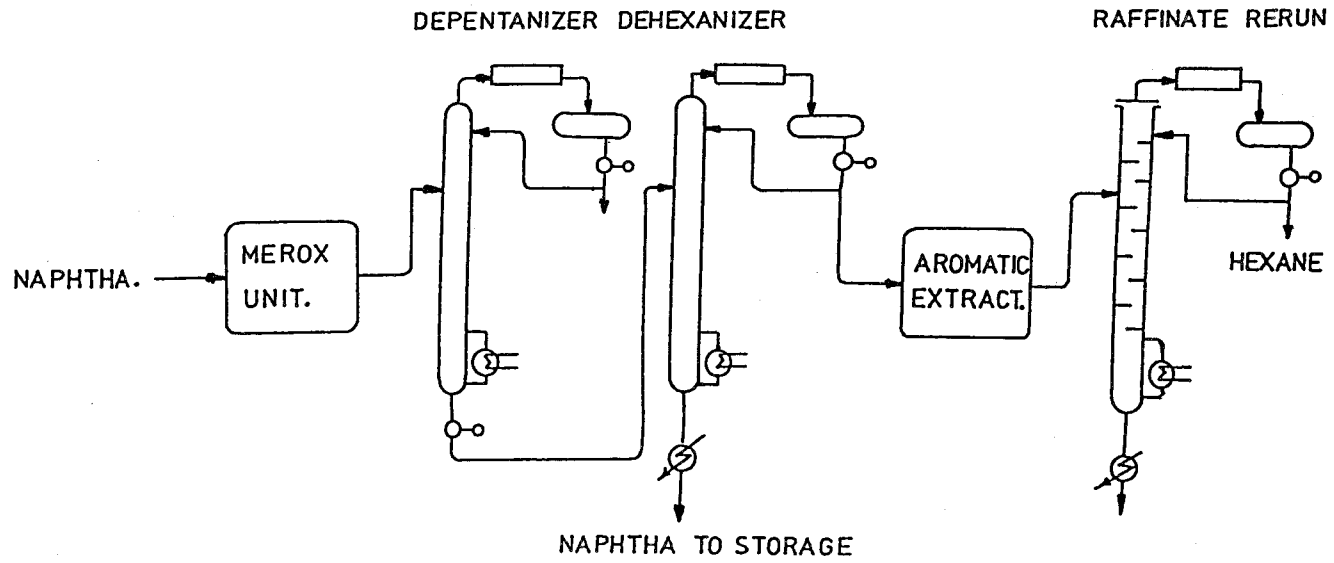
Fig. 1. Flow diagram of the hexane plant

The naphtha from Merox process is then fed to the depentanizer column. The overhead product consists mainly of C_5 and lighter components which are cooled by an air cooler and accumulated. The temperature at the top of the column is 63 °C and the reflux flow rate is 5.75 MT/hr. The bottom product is composed of mixed hexanes and heptanes and heavier components. The dehexanizer top and bottom temperatures are 99 °C and 126 °C . The treated product is introduced to a rerun column for further adjustment of the final boiling point.

DESCRIPTION OF THE DEPENTANIZER COLUMN

The fractionator consists of a total condenser, rectifying and stripping sections, a feed mixing section and a reboiler. The upper rectifying section of the columns is 90 cm in outside diameter and 16 meters in height with 25 (pass-one-pass) sieve trays. The lower stripping section is 90 cm in outside diameter and 14.4 meters in height.

The total number of actual trays is 50. The column has a total condenser and thermosyphonic kettle reboiler. The feed enters above tray number 26. The source of heat is steam at 4.5 kg/cm² gauge pressure and 155°C temperature. An air cooled total condenser is associated with an overhead accumulator. The column pressure is controlled by a split range pressure control using the nitrogen blanket system.

COLLECTION AND TREATMENT OF DATA

For each run samples were withdrawn from the feed, the distillate and bottom lines, and analyzed by gas chromatography (5840 A- HEWLETT PACKED Gas Chromatograph) which was equipped with (ov-1, capillary column, flame ionization detector, and a linear temperature programmer). The analysis of the liquid samples in the column was carried out under a pressure of 1.05 kg/cm²g. The percentage area was used for calculating the weight percent values using a AGC, Terminal Integrator.

THEORETICAL BACKGROUND

The Thiele and Geddes Method

In this method the plate temperatures, number of plates and vapor and liquid flow rates are used as independent variables. The material balance equations are

written in the rectifying section for a given plate and the condenser. In the stripping section each material balance equation is written for a given plate down to the reboiler. The calculations are commenced at one end of the column to the other end. The copmonent flow rates in each section of the column b_i and d_i obtained by calculation are compared with existing data(3).

The Lewis and Matheson Method

In this method the distribution of component between the top and bottom products are used as independent variables. The calculations are started from both the top and bottom of the column up to the feed plate and a comparison is made between the actual composition of the feed plate and that obtained by calculation.(3)

The θ-method of convergence is usually used; where the rate of convergence, to determine the operating conditions, can be improved by using the K_b method and taking advantage of the tridiagonal matrix form of steady state equation(4). Matrix calculation at the total and minimum reflux ratio conditions for different input parameters is presented for the special case for which iterative calculation is used with the total amounts of product components both in distillate and bottoms given (5). A hypothetical component method for estimating the bubble and dew points for each stage is presented. It increases the convergence rate in iterative calculations (6), and is used with tridiagonal matrix to calculate the liquid phase composition (7).

The overall problem of multi component distillation columns is solved by partitioning the whole system of equations describing the system into 3 subsets. Steady state and theoretical tray behavior are assumed. The component material balances and equilibrium equations are solved in terms of temperatures and new equilibrium compositions profile. Total flow material balances, enthalpy balances and data equations are solved in terms of total flows of the liquids and vapors and heat duties to non adiabatic trays. A temperature T-promoter is used, whose main task is to correct liquid and vapor components flow rates, is used to accelerate convergence of material balance and equilibrium equations (8). A procedure based on successive approximations with adjustment of the number of equilibrium stages in each column section between iterations to meet the given reflux flow and feed- stage composition was applied to a number of distillation design problems(9).

Separation of Multicomponent Mixtures

For a column at steady state operation consider the case in which the following specifications are made:

(1)   number of plates in each section of the column.
(2)   quantity, composition, and thermal condition of the feed.
(3)   column pressure.
(4)   type of overhead condenser (total or partial).
(5)   reflux ratio, L_o / D, or V_1 or L_o, and
(6)   one specification of the distillate such as the total flow rate D.

Steady-state operation means that no process variable changes with time. For this set of operating conditions, the problem is to find the compositions of the top and bottom product. Thus, by solving this kind of problem the characteristics of the top and bottom products can be determinated. The set equations required to represent such a system for all components ($i = 1, 2, 3, \ldots\ldots c$) are as follows:

Equilibrium relation ships

$$Y_{ji} = K_{ji} X_{ji} \qquad\qquad (j = 1, 2, \ldots, ..N)$$

$$\sum_{i=1}^{c} Yji = 1 \qquad\qquad (j = 1, 2, \ldots, ..N)$$

$$\sum_{i=1}^{c} Xji = 1 \qquad\qquad (j = 1, 2, \ldots, ..N)$$

Material balances

$$V_{ji} \times Y_{j+1.i} = L_j X_{ji} + DX_{Di} \qquad (j = 1, 2, \ldots, f-2)$$
$$V_{fi} \times Y_{fi} + V_F = L_{f-1} X_{f-1.1} + DX_{Di}$$
$$V_{j+i} \times Y_{j+1.i} = L_j X_{ji} - BX_{Bi} \qquad (j = f, f+1, ..N-1)$$
$$FX_i = DX_{Di} + BX_{Bi}$$

Enthalpy balances

$$V_{j+1} \times H_{j+1} = L_j h_j + DH_D + Q_c \qquad (j = 1, 2, \ldots, f-2)$$
$$V_f H_f + V_F H_F = L_{F-1} h_{f-1} + DH_D + Q_c$$
$$V_{j+1} \times H_{j+1} = L_j h_j - Bh_B + Q_R \qquad (j = f, f+1, \ldots N-1)$$
$$FH = Bh_B + DH_D + Q_c - Q_R$$

A schematic representation of the component - material balances is shown in Fig.2. The behavior assumed on the feed plate is demonstrated by Fig.3.
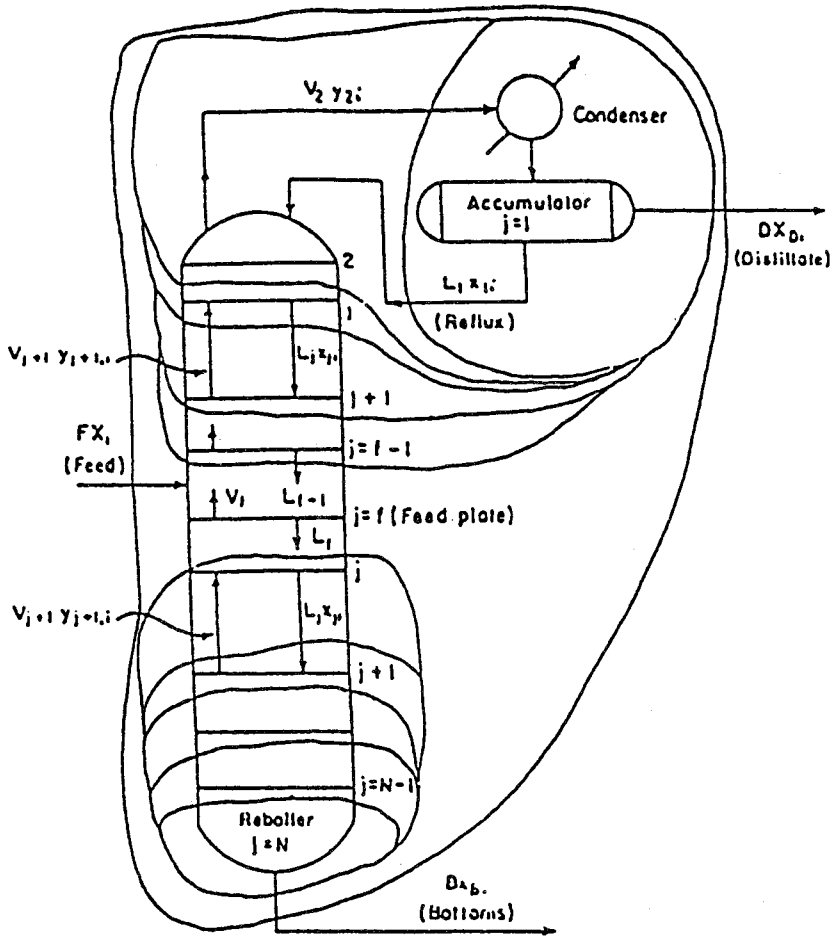
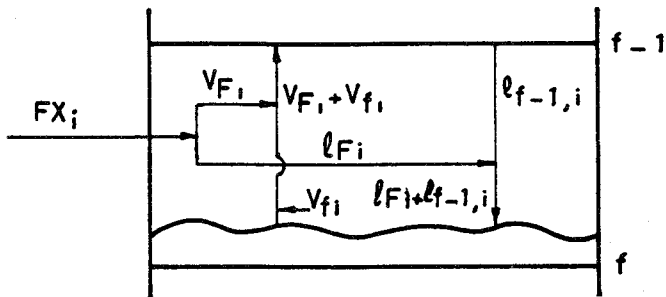**Fig. 2. Representation of the component-material balances (3)**

Fig. 3. Model 2 for the behavior of the feed plate (3)

ENTHALPY CONSTANTS DETERMINATION

During the mathematical modeling of a super fractionator to produce narrow cut components, an equation relating the enthalpy , specific heat and temperature was developed to calculate the enthalpies of these components (in the liquid and vapor phases) at specific working temperatures and that is shown below (equation 1). The enthalpy-temperature dependencies show a polynomial equation of the form:

$$H_T = AT + BT^2 + CT^3 + D \qquad (1)$$

at the working temperature range, 60-270 °F i.e 520-730 °R, where A,B,C and D are constants. The values of A, B, C and D for some light components of the feed are shown in Tables 1 and 2. The enthalpies of both liquid and vapor phases were obtained from Ref. 10.

The Gaussian elimination and least square techniques were used to determine the constants of the modified equation which is the general relationship between enthalpy and absolute temperature. This work was done for all feed components. Any differences between the reported values for enthalpy (10) and those calculated using the obtained constants were very minor.

Table 1: Polynomial Constants for the Liquid Enthalpies Used for the Distillation Column for a Temperature Range of 60 °F to 270 °F at Atmospheric Pressure

Component	D	A	B	C
NBUT	0.377 E 04	0.184. E 02	0.292 E -01	0.160 E -04
IPEN	-0.253 E 04	0.124 E 02	0.197 E -01	0.109 E -04
NPEN	0.904 E 03	0.435 E 01	0.649 E -01	0.371 E -05
2MPE	0.441 E 04	-0.218 E 02	0.359 E -01	-0.190 E -04
3MPE	0.475 E 04	0.234 E 02	0.386 E -01	0.205 E -04
NHEX	-0.226 E 03	0.974 E 00	-0.971 E -03	0.706 E -06
MCPE	0.433 E 04	0.214 E 02	0.352 E -01	0.187 E -04
BENZ	-0.148 E 04	0.699 E 01	-0.106 E -01	0.566 E -05
CHEX	-0.107 E 04	0.495 E 01	-0.744 E -02	0.413 E -05

Table 2. Polynomial Constants for the Vapor Enthalpies Used for the Distillation Column for a Temperature Range of 60 °F to 270 °F at Atmospheric Pressure

Component	D	A	B	C
NBUT	0.839 E 04	0.403 E 02	0.659 E -01	0.353 E -04
IPEN	0.109 E 04	0.450 E 02	0.768 E -02	0.394 E -05
NPEN	0.316 E 03	0.147 E 01	0.242 E -01	0.129 E -04
2MPE	0.447 E 04	0.212 E 02	0.348 E -01	0.186 E -04
3MPE	0.618 E 04	0.295 E 02	0.484 E -01	0.259 E -04
NHEX	0.816 E 04	0.392 E 00	-0.641 E -01	0.344 E -04
MCPE	0.468 E 04	0.221 E 02	0.362 E -01	0.193 E -04
BENZ	0.659 E 04	0.313 E 02	0.512 E -01	0.274 E -04
CHEX	0.463 E 04	0.218 E 02	0.357 E -01	0.190 E -04

The feed consisted of n-Butane, iso-Pentane, 2-Methyl Pentane, 3-Methyl Pentane, n-Hexane, Methyl cyclo pentane, Benzene, Cyclo hexane, 2-Methyl hexane, n-Octane, n-Nonane.

The maximum percentage error for calculating liquid enthalpy was 6 % for 3-Methyl pentane, and for calculating vapor enthalpy it was not more than 1%.

EQUILIBRIUM CONSTANTS DETERMINATION

Equilibrium K values were determined at temperature intervals according to the data reported (10). The relation shows that a polynomial equation of the form:

$$3\sqrt{k / t} = a + bt + ct^2 + dt^3 \tag{2}$$

is a good empirical representation for the curve fit at the working temperature where a, b, c, and d are constants. The least square method and Gaussian elimination method were used to determine all these constants. The values of equilibrium K for feed components are shown in Table 3.

Table 3. Equilibrium k-values Data

Component Name / TEMP. R	NBUT	IPEN	NPEN	2MPE	3MPE	NHEX	MCPE	BENZ	CHEX	MHEX	MCHE	NHEP	TOLU	MHEP	NOCT	NNON
492	0.90	0.40	0.24	0.09	0.08	0.06	0.06	0.04	0.04	0.04	0.015	0.015	0.009	0.006	0.009	0.001
528	2.00	0.80	0.60	0.25	0.22	0.17	0.15	0.11	0.10	0.10	0.05	0.048	0.033	0.024	0.029	0.004
564	3.20	1.60	1.00	0.47	0.42	0.35	0.31	0.23	0.22	0.22	0.13	0.120	0.076	0.057	0.043	0.013
600	5.20	2.50	2.00	1.00	0.80	0.70	0.68	0.50	0.47	0.47	0.27	0.300	0.200	0.155	0.127	0.039
636	8.00	4.00	3.00	1.60	1.40	1.20	1.10	0.92	0.85	0.85	0.55	0.580	0.403	0.319	0.265	0.092
672	11.50	5.60	4.50	3.00	2.80	2.30	2.00	1.50	1.40	1.40	0.85	0.910	0.720	0.580	0.490	0.187
708	15.20	8.40	7.00	4.40	3.90	3.00	3.00	2.50	2.40	2.40	1.70	1.560	1.181	0.700	0.887	0.367
744	20.00	11.00	9.00	6.00	5.50	4.20	4.40	3.70	3.60	3.60	2.50	2.000	1.812	1.600	1.311	0.578
780	23.00	13.50	12.00	7.30	7.00	6.00	5.50	5.20	4.60	4.60	3.00	2.784	2.293	2.000	1.800	0.900
816	27.00	18.00	15.00	9.60	9.00	8.20	7.00	7.00	6.30	6.30	5.00	4.600	3.946	3.387	3.000	1.509
852	33.00	21.00	18.50	13.00	12.00	11.00	10.50	9.00	8.80	8.80	7.00	6.588	5.631	4.894	4.383	2.327

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MODEL DEVELOPMENT

The model uses basically, the Thiele and Geddes procedure modified to suit the digital computer. In this method the following data for the column under investigation are specified.
- Complete description of the feed, whether liquid, vapor, or partially vaporized, subcooled, saturated or super-heated.
- The heat content or temperature of the feed.
- The maximum and minimum vapor flow rates at the top and bottom of the column.
- Type of condenser, whether, total or partial condenser .
- A correlation for K_{ji} , H_{ji} and h_{ji} and temperature, for each component at pressure P.

The aim of the model was to estimate the product distribution d_i and b_i , the molar rate of component i in the top and bottom products of the column, for component $i = 1, 2, ..., C$. This is done as follows:

Step 1: Top and bottom temperatures are used to calculate the temperature profile. Then overall material balance is used to calculate V_j and L_j The bubble and dew points of the feed are determined.

Step 2: Using these values and Tridiagonal Matrix procedure, a material balance for each component i , is done for all plates. Each of the C component matrices are solved for (l_{ji}) and (v_{ji}).

Step 3: Using the fact that the column should be in overall balance for each component, i.e.

$$Fx_i = d_i + b_i \tag{3}$$

$$g(\theta) = \sum_{i=1}^{c} (d_i)_{co} - D \tag{4}$$

A multiplier θ, defined by equation 5 is calculated by trial and error up to the positive value of θ which will make g (θ), tent to zero:

$$(b_i / d_i)_{co} = \theta (b_i / d_i)_{ca} \tag{5}$$

$$g(\theta) = D - \sum_{i=1}^{c} Fx_i / (1 + \theta (b_i / d_i)_{ca}) \qquad (6)$$

Step 4: If the difference $(\theta - 1)$ is less than the convergence e, where e is a prescribed small value, the calculation is terminated, otherwise the calculation is continued.

Step 5: This multiplier θ is used to calculate a corrected set of X_{ji} and Y_{ji} using equations 7-10; where:

$$(d_i)_{co} = FX_i / (1 + \theta (b_i / d_i)_{ca}) \qquad (7)$$

$$(b_i)_{co} = FX_i - (d_i)_{co} \qquad (8)$$

$$X_{ji} = (L_{ji} / b_i)_{ca} (B_i)_{co} / \sum_{i=1}^{c} (L_{ji} / b_i)_{ca} (b_i)_{co} \qquad (9)$$

$$Y_{ji} = (V_{ji} / b_i)_{ca} (d_i)_{co} / \sum_{i=1}^{c} (V_{ji} / b_i)_{ca} (d_i)_{co} \qquad (10)$$

Step 6: A new temperature profile (T_j), is computed, on the basis of the latest set of X_{ji} and Y_{ji}, by performing a bubble point calculation on each plate, using equation (11).

$$f(T_j) = \sum_{i=1}^{c} k_{ji} X_{ji} - 1 \qquad (11)$$

Step 7: New set of L_j and V_j are calculated by heat balance, using equations 12 and 13:

$$H_j = \sum_{i=1}^{c} H_{ji} Y_{ji} \qquad (12)$$

$$h_j = \sum_{i=1}^{c} h_{ji} X_{ji} \qquad (13)$$

Eq. (14) is used to calculate L_j at each plate.

$$L_{j-1} = [D (H_D - X_D H_{ji}) + Q_c] / (X_{j-1,i} H_{ji} - h_{j-1}) \qquad (14)$$

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Step 8: Using the new sets of V_j, L_j and T_j steps 2 to 7 are repeated until a good convergence is attained.

In the above-mentioned procedure to speed up convergence Newton's method and Interpolation methods of convergence were used. Also the Grabe recursion formula for solving tridiagonal matrices was used.

MODEL TESTING (RESULTS AND DISCUSSION)

The existing design data for the depentanizer column were used for testing the model. The agreement between the existing data and the model results was good. The basic model was used for studying the control of the distillation column. The model can be tuned automatically for any specific column and for the modeling of plate columns in separating multicomponent mixtures. The physical and chemical properties, material balance and vapor liquid equilibrium are considered. The model is thought to be very helpful in determining the yield of the vapor phase, distillates as well as for the design of new columns and their control. The model involves:

1. Determination of boiling point and dew point for the feed mixtures.
2. Calculating the enthalpy of the feed.
3. Determining the number of moles of vapor and liquid of the feed.
4. Calculating the number of moles of vapor and liquid on each tray.
5. Calculating tray temperature.
6. Determining product distribution.

The boundary conditions of the system (temperature and pressure) are known for the saturated vapor fed to the condenser and the boiling liquid in the reboiler. A correlation was developed for calculating the pressure drop in the column. The θ-method of convergence for predicting the product compositions in bottom and distillate corresponding to different operating conditions was used.

The data selected to demonstrate model applicability were top pressures (5-30 psig), feed temperatures (77° - 107°F) and reflux ratios (1:1 to 1:3). The criteria of selected data effect was the degree of separation of 2- Methyl pentane (the mid-distributed component) between the top and bottom products. The output data, presented in Figs. 4,5 and 6; and Tables (4) and (5) show that on increasing the feed temperature, the degree of separation very slightly increased, also on increasing the reflux ratio the degree of separation remained almost unchanged. The greatest effect was noticed on increasing the top pressure from 5
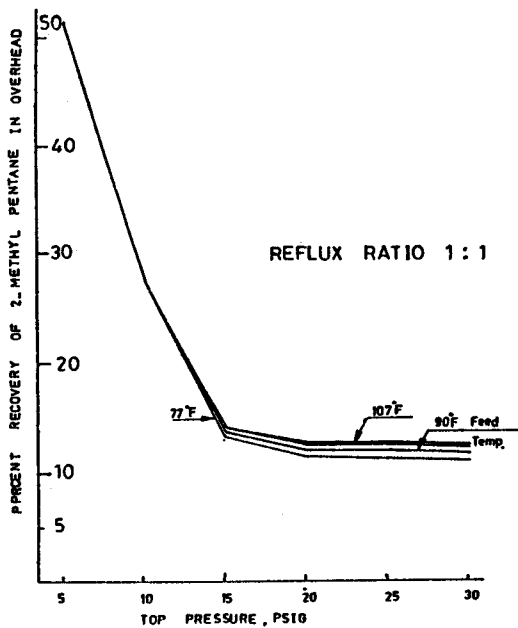
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Fig. 4. Effect of top pressure on percent recovery of 2-methyl pentane in overhead
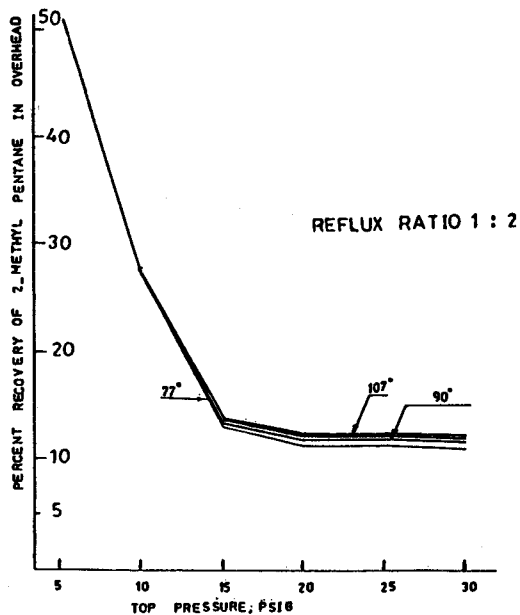

Fig. 5. Effect of top pressure on percent recovery of 2-methyl pentane in overhead

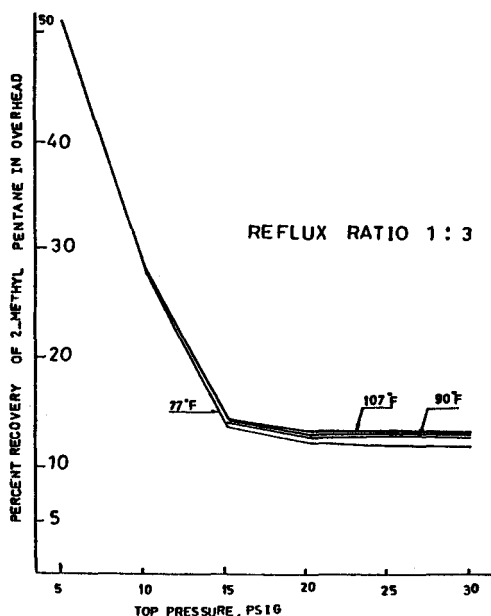Table 4. Percent Recovery of 2-Methyl Pentane in Overhead

*L/D • Temp °F ** Press	1:1				1:2				1:3			
	77	90	100.4	107	77	90	100.4	107	77	90	100.4	107
5	51.51	51.51	51.52	51.52	51.51	51.52	51.53	51.52	51.51	51.52	51.52	51.53
10	27.58	27.88	28.02	28.08	27.80	28.01	28.11	28.16	27.85	28.04	28.13	28.18
15	13.24	13.77	14.06	14.21	13.58	14.02	14.26	14.37	13.68	14.09	14.30	14.40
20	11.44	12.24	12.70	12.92	11.89	12.60	12.99	13.16	12.03	12.70	13.05	13.22
25	11.38	12.17	12.66	12.90	11.79	12.53	12.95	13.15	11.91	12.62	13.02	13.20
30	11.16	11.85	12.43	12.72	11.49	12.25	12.75	12.98	11.59	12.34	12.82	13.05

*   The ratio of reflux to product
**   Top pressure in Psig
•   The temperatures are the feed temperature

Table 5. Percent Recovery of n-Hexane in Bottom Product

*L/D • Temp °F ** Press	1:1				1:2				1:3			
	77	90	100.4	107	77	90	100.4	107	77	90	100.4	107
5	0.942	0.842	0.842	0.842	0.842	0.842	0.892	0.892	0.892	0.892	0.892	0.892
10	.957	0.958	0.958	0.958	0.959	0.958	0.958	0.958	0.958	0.958	0.958	0.958
15	0.982	0.982	0.981	0.981	0.982	0.981	0.981	0.981	0.982	0.981	0.981	0.981
20	0.984	0.980	0.983	0.982	0.984	0.983	0.982	0.981	0.983	0.983	0.982	0.982
25	0.982	0.981	0.981	0.981	0.982	0.981	0.981	0.981	0.982	0.981	0.981	0.980
30	0.982	0.982	0.981	0.980	0.982	0.981	0.980	0.980	0.9820	0.981	0.980	0.980

*   The ratio of reflux to product
**   Top pressure in Psig
•   The temperatures are the feed temperature

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Fig. 6. Effect of top pressure on percent recovery of 2-methyl pentane in overhead

psig to 20 psig through 10 and 15 psig. This led to almost 50 % decrease in the value of degree of separation in each step. Further increase in top pressure led to much lower effect. This can be attributed to the decrease of the vaporization driving force since the bottom pressure was fixed at 30 psig. Vaporization driving force is proportional to the pressure difference across the column, from column bottom to its top.

The above- mentioned results agree with the known theoretical principles of superfractionation. The model does not allow the feed temperature to exceed the mixture boiling point since this would mean a totally vaporized feed, a case causing the model to fail.

The model was subjected to round -off error at very high plate numbers. This round - off error is also a well known phenomenon and is a disadvantage in using tridiagonal matrixes in modeling conventional columns.

Decreasing the number of plates from 51 to 10 stepwise led to a noticeable improvement in convergence of θ (θ was equal to $0.97303 * 10^{-3}$ for 51 trays and 1.0146 for 10 trays). Also for the same number of trays an increase in the number

of iterations also gave better convergence as shown by the value of θ (1.0146 for 100 iterations compared to 1.18015 for 50 iterations for a number of plates = 10).

A double precision arithmetic method for improving the accuracy of the computation was used to overcome the round - off errors accumulation to the point where they obscure the actual result.

CONCLUSIONS

1. A model for calculating boiling point and dew point on the feed plate , the number of liquid and vapor moles , the enthalpy of feed and the final product distribution at the top and bottom of the column, was developed.

2. The θ-method of convergence for predicting the product composition in bottom and distillate corresponding to different operating conditions was used.

3. The model was tested using different top pressures (5-30 psig), different feed temperatures (77-107°F) and different reflux ratios (1:1 to 1:3). The most effective variable was found to be top pressure.

4. The model was subjected to round - off error at high plate numbers.

5. Decreasing the number of plates improved the convergence.

6. Increasing the number of iterations gave better convergence.

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