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### MATHEMATICAL MODELS FOR RECTIFICATION PROCESSES

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A large number of mathematical models for the dimensioning of rectifying column and the description of the process of rectification can be found in literature. However, all these models use the concept of plate or column efficiency. In the present paper, a mathematical model is proposed for the case of continuous and non-continuous rectification which, by application of the diffusion model, dispenses with the necessity of the knowledge of the efficiency. Numerical examples were elaborated for the illustration of the models. The calculations were carried out by an electronic computer.

#### INTRODUCTION

Rectification is an operation which enables a vapour to be obtained that is substantially richer than the liquid left in the still. This operation is very frequently applied in the chemical industry. In the fractionating columns used to carry out the operation, heat and material transfer processes occur simultaneously. In order to determine the main dimensions of such columns, the McCabe-Thiele method is most frequently applied, and the Ponchon-Savarit method [1] in the case of non-constant overflow is used. A number of papers were published in recent years [2] dealing with

this subject and proposing models which enable more accurate theoretical description of the processes. Efforts were made to try to describe the simultaneous heat and material transfer by analytical methods. The most important drawback of the above-mentioned graphical methods is the fact that the determination of the plate or column efficiency is difficult [3].

In the present paper a mathematical model is proposed for the numerical dimensioning of two-component fractionating columns. The treatment is basically valid for plate-type columns, but - with slight modifications - it can also be used for packed columns.

A diffusion model is applied in connection with the plate. The relations are presented for continuous and batch operation, the application is illustrated by a numerical example.

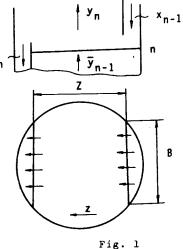
#### CONTINUOUS OPERATION

As mentioned in the foregoing, graphical methods, and - in the case of certain operational conditions - analytical procedures [e.g. Fenske-Underwood equation (1)] can be used for the determination of the theoretically necessary number of plates in continu-

ous rectifying columns. The real number of plates can be determined if the column or plate efficiency is known.

# Mathematical Model

Let be considered the  $n^{th}$  plate of the column (Fig. 1). The concentration of the liquid entering the plate (z=0) is  $x_{n-1}$ . The liquid,



during its progress along the plate, meets the vapour arising from

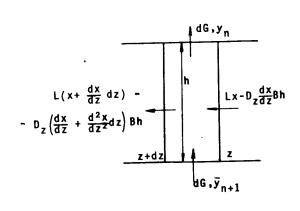


Fig. 2

plate n+1. This vapour is well mixed and consequently its concentration along the co-ordinate z is constant and it leaves the plate enriched in the more volatile component. This concentration is, naturally, a function of the co-ordinate z. The liquid, having passed a plate of the length Z, leaves it at a concentration x<sub>n</sub>.

As a first step, the material balance of the more volatile component is written for an elementary liquid layer of the height h (Fig. 2):

$$L (x + \frac{dx}{dz} dz) - D_z (\frac{dx}{dz} + \frac{d^2x}{dz^2} dz) Bh + dGy_n =$$

$$= Lx - D_z \frac{dx}{dz} Bh + dG\overline{y}_{n+1}$$

and

$$L \frac{dx}{dz} dz - D_z \frac{d^2x}{dx^2} dzBh = dG(\bar{y}_{n+1} - y_n)$$
 (1)

The material transport between the liquid and the vapour phases can be described by the material transfer coefficient on the side of the vapour:

$$dG(\bar{y}_{n+1} - y_n) = \beta_g(y_n - y^*)dfe$$
 (2)

(It is to be mentioned that the vapour concentration varies between the values  $\bar{y}_{n+1}$  and  $y_n$  and consequently Equation (2) is, at the same time, the equation defining the vapour side transfer coefficient.)

The specific contact area referred to unit volume is introduced:

$$\varepsilon = \frac{dfe}{dV} = \frac{1}{Bh} \frac{dfe}{dz}$$
 (3)

Considering Equations (2) and (3), Equation (1) becomes

$$L \frac{dx}{dz} - D_z \frac{d^2x}{dz^2} Bh + \beta_g(y^* - y_n) Bh\varepsilon = 0$$

With the introduction of the dimensionless variables

$$\xi = \frac{z}{Z}$$
, Pe =  $\frac{LZ}{BhD_z}$ , No =  $\frac{\beta g \epsilon Bh}{L} Z$ 

the Equation (4) attains the following final form:

$$\frac{dx}{d\xi} - \frac{1}{Pe} \frac{d^2x}{d\xi^2} + No (y^* - y_n) = 0$$
 (4)

where

$$0 \le \xi \le 1$$
 and  $x_{n-1} \le x \le x_n$ ;

The calculation of the concentration of the vapour rising from the plate should now be examined. Considering Equation (3), Equation (2) can be written in the form

$$\frac{dG}{dz} = \frac{\beta_g \varepsilon Bh(y_n - y^*)}{y_{n+1} - y_n}$$

but, the molar mass fluxes are constant and accordingly

$$\frac{dG}{-} = constant = -$$

$$dz$$

and consequently

$$\bar{y}_{n+1} - y_n = \frac{L}{c} No(y_n - y^*)$$
 (5)

For the case of the rectifying section, the ratio L/G can be expressed by the reflux ratio:

$$\frac{L}{G} = \frac{R}{R+1}$$

and accordingly

$$y_n = \frac{NoR}{R+1} (y^* - y_n) + \bar{y}_{n+1}$$

Rearranging:

$$y_{n} = \frac{\overline{y}_{n+1} + No \frac{R}{R+1} y^{*}}{1 + No \frac{R}{R+1}}$$
(6)

The average concentration of the vapour rising from the plate is

$$\bar{y}_{n} = \frac{1}{z} \int_{0}^{z} y_{n} dz = \int_{0}^{1} y_{n} d\xi$$
 (7)

The value of y\* can be determined on the basis of the equilibrium curve

$$y^* = \varphi(x) \tag{8}$$

An equation essentially similar to Equation (5) can be written for the stripping section, with the difference that is this case  $\bar{L}$  and  $\bar{G}$  values are used which correspond to the change in material flux caused by the feed:

$$\mathbf{y_n} = \frac{\mathbf{\bar{y}_{n+1}} + \mathbf{\bar{N}oL}/\mathbf{\bar{G}y^*}}{1 + \mathbf{\bar{N}oL}/\mathbf{\bar{G}}}$$

The  $f^{ ext{th}}$  plate, i.e. the plate where the feed enters will now

be examined in order to determine the relation between the concentrations in the rectifying and the stripping sections, resp. (cf. Fig. 3).

Supposing that a thorough mixing has occurred between the feed and the liquid leaving plate (f - 1) in the

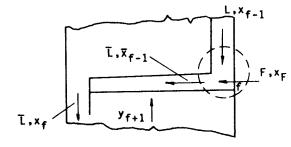


Fig. 3

downcomer tube prior to entering the plate, the material balance for the volatile component is:

$$L_{x_{f-1}} + F_{x_{f}} = \overline{L}_{x_{f-1}}$$

or

$$\mathbf{x}_{\mathbf{f}-\mathbf{l}} = \frac{\bar{\mathbf{L}}}{L} \quad \bar{\mathbf{x}}_{\mathbf{f}-\mathbf{l}} - \frac{\mathbf{F}}{L} \mathbf{x}_{\mathbf{F}} \tag{9}$$

It is apparent that only the relation between the material fluxes need to be given. This can be done on the basis of the overall material and heat balances of the feed plate (Fig. 4).

The overall material balance is:

$$L + F + \overline{G} = G + \overline{L}$$

The heat balance is:

$$\text{Li}_{L} + \text{Fi}_{F} + \overline{\text{Gi}}_{g} = \text{Gi}_{G} + \overline{\text{Li}}_{L}$$

Fig. 4

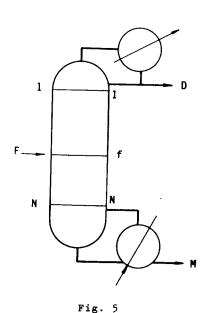
Assuming that

$$i_L \approx i_{\overline{L}}$$
 and  $i_G \approx i_{\overline{G}}$ 

the ratio of the change in molar flux of the liquid to the feed flux is q:

$$q = \frac{\bar{L} - L}{F} \tag{10}$$

It follows from this and the previous two balance equations that



$$\frac{\tilde{G} - G}{F} = q - 1 \tag{11}$$

and

$$q = \frac{i_{G} - i_{F}}{i_{G} - i_{L}}$$
 (12)

Summarizing the equations obtained, and taking Fig. 5 into consideration, we obtain

$$\frac{dx}{d\xi} - \frac{1}{Pe} \frac{d^2x}{d\xi^2} + No(y^* - y_n) = 0 \quad (4)$$

where

$$Pe = \begin{bmatrix} LZ/BhD_z & \text{if } 1 \leq n \leq f-1 \\ -LZ/BhD_z & \text{if } f \leq n \leq N \end{bmatrix}$$

$$y_{n} = \frac{\bar{y}_{n+1} + No (L/G)y^{*}}{1 + No (L/G)}$$
 (6)

where

No L/G = 
$$\frac{\frac{\beta_g \epsilon Bh \ Z}{G}}{\frac{\beta_g \epsilon Bh \ Z}{G}} \quad \text{if } 1 \le n \le f-1$$

e 41

$$\bar{\mathbf{y}}_{\mathbf{n}} = \int_{0}^{1} \mathbf{y}_{\mathbf{n}} \, \mathrm{d}\boldsymbol{\xi} \tag{7}$$

$$y^* = \varphi(x) \tag{8}$$

$$\mathbf{x}_{\mathbf{f}-\mathbf{l}} = \frac{\bar{L}}{L} \mathbf{x}_{\mathbf{f}-\mathbf{l}} - \frac{\mathbf{F}}{L} \mathbf{x}_{\mathbf{F}}$$
 (9)

$$\bar{L} - L = Fq \tag{10}$$

$$\overline{G} - G = F(q-1) \tag{11}$$

$$q = \frac{i_G - i_F}{i_G - i_L}$$
 (12)

In order to make the model complete, the boundary conditions are to be defined.

## Boundary Conditions

$$x(1) = x_n \qquad 1 \le n \le N$$
 (13)

and

$$\frac{dx}{dE} (1) < 0 \tag{14}$$

i.e. the derivative of the concentration function of the liquid leaving the plate is a constant, which is characteristic of the plate (and of the degree of the material transfer) whose value is different at every plate. As a first approximation, it was supposed that the value of this constant was zero. In order to establish the validity of the material balance, the value of the constant was varied by iteration until the material balance was true to the prescribed degree of accuracy. It should be noted here that

the value of Equation (14) cannot be zero, as it is generally assumed in literature [e.g. (5)]; this would be true only in the case of a plate of infinite width.

. The concentration of the distillate should be known, i.e.:

$$x_1 < x(\xi) = x_D \qquad 0 \le \xi \le 1$$
 (15)

Equation (15) should be formulated like this, since it cannot be prescribed that

$$x_1 < x (0) = x_D$$

if the value of Z is fixed.

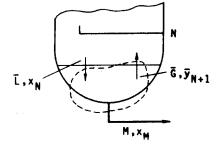
Generally the concentration of the bottom product is also prescribed; however, this is not adequate to be chosen as a boundary condition. Considering Fig. 6 the material balance for the more volatile can be constructed:

$$\bar{L}x_N = \bar{G}\bar{y}_{N+1} + Mx_M$$

and from this

$$x_{N} = \frac{\bar{G}}{\bar{L}} \bar{y}_{N+1} + \frac{M}{L} x_{M}$$

Assuming equilibrium in the boiler:



$$\bar{y}_{N+1} = \phi(x_M)$$

l '\"M' Fig. 6

and consequently

$$x_{N} = \frac{\bar{G}}{\bar{L}} \quad \varphi(x_{M}) + \frac{M}{\bar{L}} x_{M} \tag{16}$$

The material fluxes can be determined on the basis of the top and bottom product concentrations, as well as the condition - Eq.

(12) -, amount and concentration of the feed, for a given reflux ratio, since

$$R = \frac{L}{D}$$

and on the basis of Fig. 7

$$Fx_F = Dx_D + Mx_M$$

and

$$F = D + M$$

The value of D and M can be determined from this equation, and on the basis of

$$L = RD$$

and

$$G = L + D$$

the material fluxes in the rectifying section are L and G. By the application of the values of q and F and on the basis of Equations (10) and (11), the  $\bar{L}$  and  $\bar{G}$  values will be known.

Moreover, the location of the feed, i.e. the value of f should be known. Considerations concerning this problem will be described in the following.

# Numerical Solution

In the determination of the boundary conditions, cases were considered where the degree of separation was predetermined and the necessary number of plates was sought. The algorithm enabling the calculation of this problem will be described here.

The calculation will be started at the bottom of the column, at the  $\textbf{N}^{\text{th}}$  plate, considering the conditions

$$x(1) = x_N$$

and

$$\frac{dx}{-} (1) = constant (N)$$

The equilibrium curve can be written, with the application of the relative volatility, in the following form

$$y^* = \frac{\alpha x}{1 + (\alpha - 1) x} \tag{17}$$

where generally  $\alpha = \alpha(x)$ , i.e. the y\* pertaining to a given x value can be determined. The value of  $y_n$  for the lower section is obtained on the basis of Equation (6):

$$\mathbf{y}_{n} = \frac{\mathbf{\bar{y}}_{n+1} + \mathbf{y} \cdot \mathbf{\bar{N}} \circ \mathbf{\bar{L}} / \mathbf{\bar{G}}}{1 + \mathbf{\bar{N}} \circ \mathbf{\bar{L}} / \mathbf{\bar{G}}}$$

Accordingly,  $\mathbf{x}(\xi)$  can be calculated with the application of Equation (4). By proceeding along the plate to the value  $\xi=1$ , the function  $\mathbf{y}_n(\xi)$  is obtained, by whose integration the average concentration of the vapour arising from the plate is obtained [cf. Equation (7)]. If the place of feed has been reached, the change in concentration due to the feed can be calculated by Equation (9), where

$$\bar{x}_{f-1} = x(0)$$

for the f<sup>th</sup> plate.

Using Equations (10), (11), and (12), the material fluxes, as well as the No and Pe values of the rectifying section can be determined. The calculation is then carried on until the condition

$$x(\xi) \ge x_D$$

comes true. The plate on which this occurs will be the first plate.

Hereupon the calculation is repeated with various feed places taken until the particular feed place giving the minimum number of plates is found.

In order to illustrate the aforesaid, a numerical example will be presented. The calculations were carried out using digital computer type ODRA 1204.

# Numerical Example

Data used in the calculation of the example:

D	=	88.8 kilomoles/hour	F	=	216.8 kilomoles/hour
M	=	128 kilomoles/hour			0.916
x <sub>M</sub>	=	0.00565	х <sub>г</sub>	=	0.36
		303.4 kilomoles/hour	x <sub>D</sub>		0.87
G	=	174.45 kilomoles/hour	<u>p</u>	=	0.0782 hour/kilomole
α	=	5			303.4 hours/kilomole
			where Pe	=	$\overline{p}$ L and $\overline{e} = L$ No.

The material transfer surface area and the material transfer

coefficient were determined on the basis of HOBLER [4], whereas the diffusion coefficient can be calculated on the basis of GERSTER [3].

The results obtained are illustrated in Figs. 8, 9 and 10. Figs. 8 and 9 show the changes in liquid and vapour concentrations along the plate, resp. Fig. 10 shows the concentration of the liquid entering the plate and the average composition of the vapour leaving the plate along the height of the column.

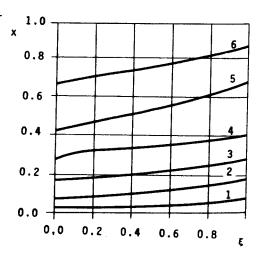
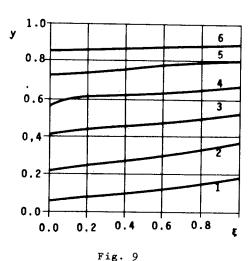


Fig. 8



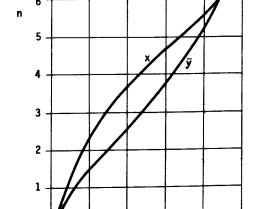


Fig. 10

0.8

0,2

0,0

### BATCH OPERATION

In the case of batch fractionating columns, two modes of operation can be distinguished, according to the aim of the process:

- operation with a distillate of constant composition,
- operation at a constant reflux ratio.

From the two modes of operation mentioned above, the first is applied more frequently. This necessitates a continuous variation of the reflux ratio.

A batch fractionating column will now be considered and its mathematical model constructed, together with necessary initial and boundary conditions. Heat and material balances will be employed.

### Mathematical Model

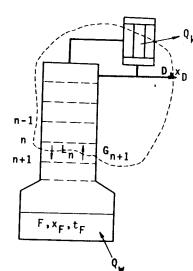
The fractionating column is shown in Fig. 11. The material balance of the column will now be constructed for time instants  $\tau$  and  $\tau$  +  $d\tau$ . The overall material balance is

$$F = (F + \frac{dF}{d\tau} d\tau) + D d\tau$$

from where

$$D = -\frac{dF}{d\tau} \tag{18}$$

The material balance for the more volatile component is



$$Fx_{F} = (F + \frac{dF}{d\tau} d\tau)(x_{F} + \frac{dx_{F}}{d\tau} d\tau) + Dx_{D} d\tau$$

and rearranging

$$\frac{\mathrm{d}\mathbf{x}_{\mathbf{F}}}{\mathrm{d}\mathbf{r}} = -\frac{\mathrm{D}}{\mathrm{E}} \left( \mathbf{x}_{\mathbf{D}} - \mathbf{x}_{\mathbf{F}} \right) \tag{19}$$

The following two equations are deduced from the material balances applied to the column.

The overall material balance, for the part enclosed by the control surface is

$$D + L_n = G_{n+1}$$
 (20)

The material balance for the more volatile component, for the part enclosed by the control surface is

$$Dx_{D} + L_{n}x_{n} = G_{n+1} y_{n+1}$$

from which

$$x_{n} = \frac{G_{n+1}}{L_{n}} y_{n+1} - \frac{D}{L_{n}} x_{D}$$
 (21)

Further relations can be derived by constructing the heat balance:

$$Fi_{F} + qAd\tau = (F + \frac{dF}{d\tau} d\tau)(i_{F} + \frac{di_{F}}{d\tau} d\tau) + Di_{D}d\tau + (D + L_{n}) M_{D}r_{D}d\tau$$

It is supposed that a perfect condensation occurs in the condenser, where the amount of heat to be removed is

$$Q_{k} = (D + L_{n}) M_{D}r_{D}$$

the same, expressed with the reflux ratio; is

$$Q_k = D(R + 1) M_D r_D$$

The relation can be simplified by supposing the additivity of the enthalpy:

$$i = [xc_1 + (1 - x)c_2]t$$
 (22)

and

$$\frac{di}{d\tau} = \frac{\partial i}{\partial \tau} \frac{dt}{d\tau} + \frac{\partial i}{\partial x} \frac{dx}{d\tau}$$

where

$$\frac{di}{dt} = xc_1 + (1 - x)c_2$$
 (23)

$$\frac{di}{dx} = (c_1 - c_2)t$$

The above equation can be simplified - the group of Equations (23) is, for the sake of conciseness, not give -

$$qA = F \frac{\partial i_F}{\partial t_F} \frac{dt_F}{d\tau} + F \frac{\partial i_F}{\partial x_F} \frac{dx_F}{d\tau} + D (i_D - i_F) + (D + L_n) M_D r_D$$
 (24)

The following should be added to the connections obtained in the above:  $\cdot$ 

$$t_{F} = \varphi(x_{F}) \tag{25}$$

and

$$\frac{dt_F}{d\tau} = \frac{dt_F}{dx_F} \frac{dx_F}{d\tau} = a(x_F) \frac{dx_F}{d\tau}$$
 (26)

from where Equation (24), considering also Equation (19), will become

$$qA = D[i_D - i_F - (x_D - x_F)(\frac{\partial i_F}{\partial t_F} a(x_F) + \frac{\partial i_F}{\partial x_F}) + (1 + R) M_D r_D]$$

or

$$qA = D[i_D - i_F - (x_D - x_F)[(x_F c_1 + (1 - x_F) c_2)a(x_F) + (c_1 - c_2)t_F] + (1 + R) M_D r_D]$$
(27)

where the enthalpies  $i_D$  and  $i_F$  can be calculated from Equation (22), taking the corresponding concentrations  $\mathbf{x}_D$  and  $\mathbf{x}_F$  as well as the temperatures  $\mathbf{t}_D$  and  $\mathbf{t}_F$  into consideration.

The relations defined in the foregoing have to be supplemented with the equation of the equilibrium curve, as well as with the elementary material balances as written for a plate (cf. section 1.) and the definition of the reflux ratio.

$$\frac{dF}{d\tau} = -D \tag{18}$$

$$\frac{\mathrm{d}\mathbf{x}_{\mathbf{F}}}{\mathrm{d}\mathbf{r}} = -\frac{\mathbf{D}}{\mathbf{F}} \left( \mathbf{x}_{\mathbf{D}} - \mathbf{x}_{\mathbf{F}} \right) \tag{19}$$

$$D + L_n = G_{n+1}$$
 (20)

$$x_n = \frac{G_{n+1}}{L_n} y_{n+1} - \frac{D}{L_n} x_D$$
 (21)

$$qA = D\{i_D - i_F - (x_D - x_F)[(x_F c_1 + (1 - x_F)c_2)a(x_F)t_F] + (1 + R) M_D r_D\}$$
(27)

$$\mathbf{y}^* = \mathbf{\phi}(\mathbf{x}) \tag{8}$$

$$\frac{dx}{d\xi} - \frac{1}{Pe} \frac{d^2x}{d\xi^2} + No(y^* - y_n) = 0$$
 (4)

$$y_{n} = \frac{\bar{y}_{n+1} + No L_{n}/G_{n+1} y^{*}}{1 + No L_{n}^{*}G_{n+1}}$$
(6)

$$R = R(\tau) = \frac{L_n(\tau)}{D(\tau)} = \frac{L_n(\tau)}{G(\tau) - L_n(\tau)}$$
(28)

$$q = k(t_f - t_F)$$
 (29)

where  $\mathbf{t}_{\mathbf{f}}$  is the constant temperature of the heating medium and  $\mathbf{k}$  is the heat transfer coefficient.

It is supposed in the course of the solution of the set of equations that the molar material fluxes are unchanged along the column in a given time instant (i.e. the dynamic hold-up is constant along the column, but it may be dependent on time).

### Conditions

In order to solve the set of equations, the initial and boundary conditions, which, for Equation (4), are the following

$$x(1) = x_n \qquad 1 \le n \le N$$
 (13)

and

$$\frac{dx}{d\xi} (1) = constant(n)$$
 (14)

The constant described here is characteristic of the plate mentioned in the foregoing.

The initial conditions are the following:

$$F(0) = F_{0}$$

$$x_{F}(0) = x_{F_{0}}$$

$$t_{F}(0) = t_{F_{0}}$$
(30)

The further conditions are dependent on the mode of operation and accordingly in the first mode

$$x_1 < x(\xi) = x_D = constant \quad 0 \le \xi \le 1$$
 (15a)

and

$$R(0) = R_0 \tag{31a}$$

whereas in the second mode of operation

$$\mathbf{x}_{\mathbf{D}}(0) = \mathbf{x}_{\mathbf{D}_{\mathbf{O}}} \tag{15b}$$

and

$$R(\tau) = R_0 = constant$$
 (31b)

### Numerical Solution

While defining the limiting conditions it was supposed that the number of the plates being present in the column is at first not defined, it will be decided on the basis of the initial condition with application of the model. The calculation is carried out according to the following:

the molar material flux of the destillate is determined from the given conditions by Equation (27) and hereafter the material fluxes are determined with the application of the initial value of the reflux ratio and with Equation (20). As the material fluxes are known, the composition of the liquid leaving the last plate ( $n \equiv N$ ) can be determined on the basis of Equation (21) and since the values

$$\overline{y}_{N+1} = \varphi(x_F)$$

$$y_N^* = \varphi(x_N)$$
(8)

can be calculated, the change in concentration along the plate can also be determined. The calculation is now carried out in accordance with the procedure described in Chapter 1, from plate to plate, as long as the condition given in Equation (15) is fulfilled. The number of plates determined in this manner will be constant in the following, and accordingly the calculation is carried on with a column of known number of plates.

The rates of changes can be determined on the basis of Equation (18) and (19) and the new values can be calculated if the time scale has been fixed. Accordingly:

$$F(\tau + \Delta \tau) = F(\tau) + \frac{dF}{d\tau} (\tau) \Delta \tau$$

$$\mathbf{x}_{\mathbf{F}}(\tau + \Delta \tau) = \mathbf{x}_{\mathbf{F}}(\tau) + \frac{d\mathbf{x}_{\mathbf{F}}}{d\tau} (\tau) \Delta \tau$$

$$\mathbf{t}_{\mathbf{F}}(\tau + \Delta \tau) = \mathbf{t}_{\mathbf{F}}(\tau) + \frac{d\mathbf{t}_{\mathbf{F}}}{d\tau} (\tau) \Delta \tau$$

The course of further calculations is the following:

1. In the first mode of operation

the above described calculation is first repeated with unchanged reflux ratio and should the condition

$$|x_D - x_{DU}| \le \varepsilon_k$$

be fulfilled, the reflux ratio need not be modified. In the opposite case, the reflux ratio is to be modified (increased) until the condition is fulfilled (the prescribed margin of error is  $\epsilon_{\rm b}$ ).

2. In the second mode of operation

the calculation can be carried on without alteration, with the only remark that

$$x_{DU} = \bar{y}_1$$

i.e. the composition of the vapour leaving the uppermost plate gives the new composition of the distillate.

The calculation is carried on until the prescribed final composition is reached.

In order to illustrate the model a numerical example has been elaborated for the case of a constant reflux ratio. The calculations were carried out with digital computer type ODRA 1204.

# Numerical example

Data used (ethyl alcohol-water system):

F = 200 kilomoles

 $x_{FO} = 0.3$ 

 $x_{Do} = 0.7$ 

R = 0.52

P = 1 atmosphere

A = 10 sq.metres

k = 200 kilocalories/sq.metres.hour.OC

t<sub>f</sub> = 150 °C

p = 0.125 hour/kilomole

### and

e = 86 hours/kilomole

 $\alpha$  = 46  $x^2$  - 38.2 x + 10.36, if 0 \le x \le 0.4

 $\alpha = 4.16 \times^2 - 8.2 \times + 5.02$ , if  $0.4 \le x \le 0.7$ 

### furthermore

$$t_{bp} = 144 x^2 - 100 x + 100,$$
 if  $0 \le x \le 0.4$   
 $t_{bp} = -8.5 x + 86.5$  if  $0.4 \le x \le 1$ 

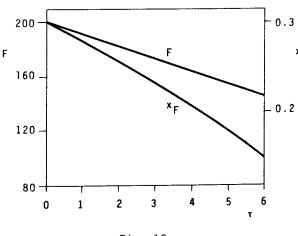


Fig. 12

The constants in the relations referring to the relative volatility or bubble point were determined by parabolic or linear approximation. If a higher degree of accuracy is required, the constants can be determined by regression analysis.

Fig. 12 shows the changes of the quantities F and  $\mathbf{x}_F$  plotted against time.

The numerical example can be calculated for changing the reflux ratio in the same manner.

### CONCLUSIONS

Table 1 clearly illustrates that the value of the initial derivate  $dx/d\xi(1)$  considerably differs from zero in the case of a number of plates and this accounts for the consideration of the final plate dimension.

It should be mentioned that the model enables the determination of the composition of the top and bottom products in continuous operation at a given plate

Table 1

Number of	dx .		
plate	<u>dξ</u> ξ=1		
1.	-0.025		
2.	-0.032		
3.	-0.084		
4.	-1,300		
5.	-0.350		
6.	-0.180		

number, i.e. in the case of a given column, if the feed plate and the conditions of feed are known. This could make possible the determination of the optimum feed place and calculation of the corresponding top and bottom products in the case of switching over to another product.

Further development of the models may also enable the consideration of a variable takeoff; however, in this case they become very complicated and the calculations are very difficult to carry out.

#### SYMBOLS USED

- a functional relation
- c specific heat (kilocalories/kilomole. OC)
- fe material transfer surface area (sq.metres)
- h height of liquid on the reay (metre)
- i molar enthalpy (kilocalories/kilomole)
- n number of trays
- heat flux density (kilocalories/sq.metre, hour), dimensionless variable (-)

```
latent heat (kilocalories/kilogram)
r
     temperature (°C)
t
     concentration of liquid
х
     concentration of vapour
У
     average concentration of vapour leaving the tray
ÿ
   · vapour concentration in equilibrium with x
у*
     heat transfer surface area (sq.metre)
Α
     width of plate (metre)
В
     material flux of destillate (kilomoles/hour),
D
        diffusivity (kilomoles/metre hour)
     material flux of feed (kilomole/hour),
F
        bottom product (kilomole)
     material flux of gas phase (kilomoles/hour)
G
     material flux of residue (kilomoles/hour),
М
        molecular weight (kilograms/kilomole)
     total number of plates
N
     heat removed by the condenser (kilocalories/hour)
     reflux ratio
R
     Peclet-number
Рe
```

### Greek letters

No

- relative volatility
- b heat transfer coefficient (kilomoles/sq.metre·hour)
- ε heat transfer surface area (sq.metres/cu.metre)
- sign of functional relation

dimensionless quantity

E dimensionless variable

#### Indexes

- f refers to the feed plate
- k refers to the condenser
- n serial number of plate
- y refers to the vapour side

- z direction of the co-ordinate z
- D refers to the destillate
- F refers to the feed or bottom product
- G,G refers to the vapour phase
- L,L refers to the liquid phase
- M refers to the residue
- N refers to the last plate

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#### PEGIUME

В литературе известен ряд математичесних моделей для рассчитивания рентифинационных оборудований и для описания процесса рентифинации. А все эти модели употребляют коэффициент полезного действия тарелон или нолонны. В настоящей работе описан математичесний модель, упразняющий с пользованием диффузионной модели необходимость знания коэффициента полезного действия. Для иллюстрации моделей выработань числовые примеры. Расчеты произведены на элентронновычислительных машин.