

COMPUTER EVALUATION OF DISTILLATION PROCESSES WITH PARALLEL STREAMS

P. MIZSEY*, I. MÉSZÁROS[†] and Z. FONYÓ

(Technisch-Chemisch Laboratorium, Swiss Federal Institute of Technology, ETH-Zentrum, 8092 Zürich,
Switzerland

* Technical University of Budapest, Department of Chemical Engineering, 1521, Budapest, Hungary

[†] SULZER Brothers Ltd., 8401, Winterthur, Switzerland)

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Mathematical models and iterative methods are developed for simulating alternative multicomponent distillation processes with parallel flow streams (vapour and liquid streams) in order to study the variation of separating effects. In the parastillation process, the uprising vapour stream is divided into two equal parts at the bottom of the distillation column and the whole amount of the falling liquid is stage-by-stage alternatively contacted with both parts of the vapour. In the metastillation process, the falling liquid is separated into two equal parts at the top of the column, while the whole amount of the uprising vapour is stage-by-stage alternatively contacted with both liquids flows (*Fig. 1*). According to our previous study [6], the parastillation process results in smaller column with less investment or operating cost than distillation. In this study the metastillation process is investigated and it is found that the required theoretical number of stages increases roughly by 50 %. However, the following liquid and vapour patterns on the trays, as specified by Lewis [5], can change significantly the stage efficiency as well as the economics of the alternative processes.

Introduction

It can be proved that under certain circumstances the separation efficiency by counter current processes can be increased by dividing a flowing phase into several parallel streams. HEUCKE [2] determined for two-component mixtures the extent of efficiency increase by simple graphically representation. A mass transfer apparatus was developed by JENKINS [3,4] and later referred to as parastillation by CANFIELD [1]. With experimental analyses and non-rigorous computer simulation CANFIELD pointed out that parastillation process under total reflux condition provides roughly 33 % greater efficiency than distillation. MÉSZÁROS and

FONYÓ [6] developed a mathematical model and an iterative procedure for simulating any kind of multi-stage, multicomponent parastillation with arbitrary structures in order to judge the effectiveness of these novel devices at conditions other than total reflux. Compared to conventional distillation the results show significant energy or column height reduction assuming identical tray efficiency. However, the adverse impact on the tray efficiency is also indicated owing to the larger liquid/vapour ratio, which results in significantly smaller tray efficiency and thus parastillation process loses a lot from its attractiveness.

The objective of this study is to extend the investigation to the so called metastillation process, where instead of the uprising vapour stream the downwards

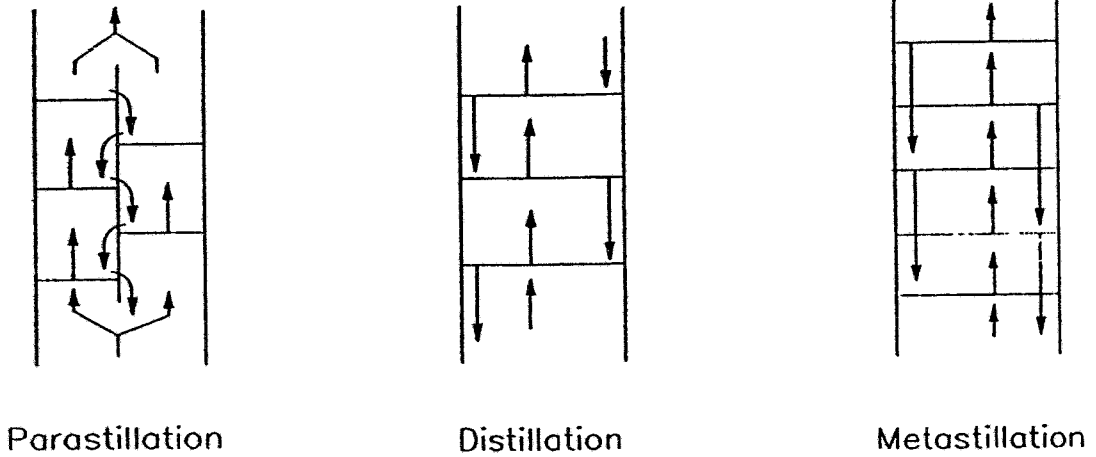


Fig. 1 Scheme of distillation with parallel streams

Mathematical Model

A new iterative method is developed for solving problems of multicomponent metastillation. This simulation method employs the tridiagonal matrix algorithm, which was introduced by WANG and HENKE [9] for the simulation of distillation columns. For the convenience of deriving the mathematical model of metastillation, a hypothetical column is shown in Fig. 2. This column has n equilibrium stages including a condenser (partial or total) and a reboiler as well. The stages are numbered from the top to bottom, i.e. the condenser is the first and the reboiler is the n th stage. Except for the the reboiler and the condenser at any stage side cooler/heater can be installed furthermore side streams (product/feed) are allowed.

In a rigorous equilibrium stage calculation four sets of equations must be satisfied. They are the material balance equations (M), the equilibrium equations (E), the summation equations of mole fractions (S) and the heat balance equations (H). These equations for metastillation column are summarized in Table 1. In the case of a metastillation column the situation is different to a common distillation column, because the internal liquid flow is divided into two practically equal parts. Each part flows into alternate stages.

The reflux flow rate is split and simultaneously fed into the first two stages. It is also advisable in the case of metastillation to divide the feed into two equal parts and introduce them into two consecutive stages to avoid the asymmetrical increase of the internal liquid flows.

Illustrative Examples

In order to demonstrate the effectiveness of the computer model and metastillation process three separation

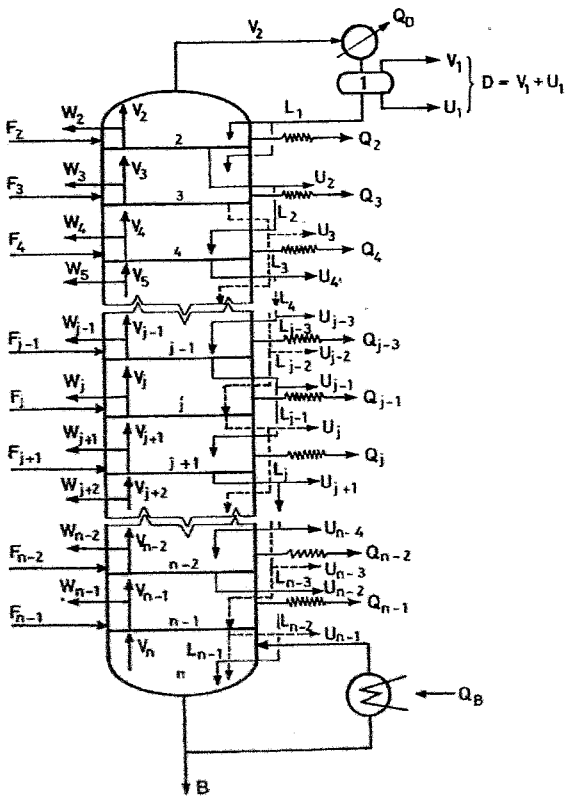


Fig. 2 Metastillation column model for simulation

flowing liquid is divided into two, practically equal parts and the whole amount of uprising vapour is stage-by-stage alternatively contacted with both liquid flows. First, the metastillation process is modelled and investigated by use of the equilibrium stage concept. After this, the alteration of the stage efficiencies of the alternative separation processes is elaborated and finally the necessary total-tray-areas are also compared.

Table 1 Model equations for metastillation column

M-Equations

$$M_{i,1}(x_{i,j}, v_j, T_j) = -[(U_1 + L_1) + V_1 * K_{i,1}] * x_{i,1} + V_2 * K_{i,2} * x_{i,2} = 0,$$

$$i=1, \dots, m$$

$$j=1, 2$$

$$M_{i,2}(x_{i,j}, v_j, T_j) = 0.5 * L_1 * x_{i,1} - [(U_2 + L_2) + (V_2 + W_2) * K_{i,2}] * x_{i,2} + V_3 * K_{i,3} * x_{i,3} + F_2 * x_{i,2} = 0,$$

$$i=1, \dots, m$$

$$j=1, \dots, 3$$

$$M_{i,3}(x_{i,j}, v_j, T_j) = 0.5 * L_1 * x_{i,1} - [(U_3 + L_3) + (V_3 + W_3) * K_{i,3}] * x_{i,3} + V_4 * K_{i,4} * x_{i,4} + F_3 * x_{i,3} = 0,$$

$$i=1, \dots, m$$

$$j=1, 3, 4$$

$$M_{i,j}(x_{i,j}, v_j, T_j) = L_{j-2} * x_{i,j-2} - [(U_j + L_j) + (V_j + W_j) * K_{i,j}] * x_{i,j} + V_{j+1} * K_{i,j+1} * x_{i,j+1} + F_j * x_{i,j} = 0,$$

$$i=1, \dots, m$$

$$j=4, \dots, n-1$$

$$M_{i,n}(x_{i,j}, v_j, T_j) = L_{n-1} * x_{i,n-1} + L_{n-2} * x_{i,n-2} - [B + V_n * K_{i,n}] * x_{i,n} = 0,$$

$$i=1, \dots, m$$

$$j=n-2, n$$

E-Equations

$$E_j(x_{i,j}, v_j, T_j) = y_{i,j} - K_{i,j} * x_{i,j} = 0$$

$$i=1, \dots, m$$

$$j=1, \dots, n$$

S-Equations

$$S_j(x_{i,j}, v_j, T_j) = \sum_{i=1}^m y_{i,j} - 1 = 0$$

$$i=1, \dots, m$$

$$j=1, \dots, n$$

$$\text{or } S_j(y_{i,j}, v_j, T_j) = \sum_{i=1}^m x_{i,j} - 1 = 0$$

$$i=1, \dots, m$$

$$j=1, \dots, n$$

H-Equations

$$H_1(x_{i,j}, v_j, T_j) = -V_1 * H_1 - (L_1 + U_1) * h_1 + V_2 * H_2 - Q_D = 0,$$

$$i=1, \dots, m$$

$$j=1, 2$$

$$H_2(x_{i,j}, v_j, T_j) = 0.5 * L_1 * h_1 - (V_2 + W_2) * H_2 - (L_2 + U_2) * h_2 + V_3 * H_3 + F_2 * H_{f,2} - Q_2 = 0,$$

$$i=1, \dots, m$$

$$j=1, \dots, 3$$

$$H_3(x_{i,j}, v_j, T_j) = 0.5 * L_1 * h_1 - (V_3 + W_3) * H_3 - (L_3 + U_3) * h_3 + V_4 * H_4 + F_3 * H_{f,3} - Q_3 = 0,$$

$$i=1, \dots, m$$

$$j=1, 3, 4$$

$$H_j(x_{i,j}, v_j, T_j) = L_{j-2} * h_{j-2} - (V_j + W_j) * H_j - (L_j + U_j) * h_j + V_{j+1} * H_{j+1} + F_j * H_{f,j} - Q_j = 0,$$

$$i=1, \dots, m$$

$$j=4, \dots, n-1$$

$$H_n(x_{i,j}, v_j, T_j) = L_{n-1} * h_{n-1} + L_{n-2} * h_{n-2} - V_n * H_n - B * h_n + Q_B = 0,$$

$$i=1, \dots, m$$

$$j=n-2, n$$

The M-equations in matrix form:

$$\begin{bmatrix} C_{i,1} & D_{i,1} & & & & & & & \\ B_2 & C_{i,2} & D_{i,2} & & & & & & \\ A_3 & 0 & C_{i,3} & D_{i,3} & & & & & \\ & A_4 & 0 & C_{i,4} & D_{i,4} & & & & \\ & & & & & \ddots & & & \\ & & & & & & A_j & 0 & C_{i,j} & D_{i,j} \\ & & & & & & & & & \ddots \\ & & & & & & & & & & A_n & B_n & C_{i,n} \end{bmatrix} \begin{bmatrix} x_{i,1} \\ x_{i,2} \\ x_{i,3} \\ x_{i,4} \\ \vdots \\ x_{i,j} \\ \vdots \\ x_{i,n} \end{bmatrix} = \begin{bmatrix} E_{i,1} \\ E_{i,2} \\ E_{i,3} \\ E_{i,4} \\ \vdots \\ E_{i,j} \\ \vdots \\ E_{i,n} \end{bmatrix}$$

where

$$B_2 = A_3 = 0.5 * L_1$$

$$A_j = L_{j-2} * v_{j-1} + \sum_{k=2}^{j-2} (F_k - W_k - U_k) - (D + L_{j-3}), \quad j=4, \dots, n$$

$$B_p = L_{p-1} * v_p + \sum_{k=2}^{n-1} (F_k - W_k - U_k) - (D + L_{p-2}),$$

$$C_{i,1} = -[(U_1 + L_1) + V_1 * K_{i,1}], \quad i=1, \dots, m$$

$$C_{i,j} = -[(U_j + L_j) + (V_j + W_j) * K_{i,j}], \quad j=2, \dots, n$$

Table 2 Separation problem specifications for simulation

Example No.	Separated mixture		Number of theor. stages	Distillate kmol/hr	Reflux ratio	Pressure, bar
	Component	kmol/hr				
1.	i-butane	75.0	20	198.6	1.3	7.0
	n-butane	150.5				
	i-pentane	25.4				
	n-pentane	8.8				
	n-hexane	1.8				
2.	benzene	100.0	10	100.0	2.0	1.0
	toluene	100.0				
3.	i-butane	2.0	10	2.1	1.5	3.0
	benzene	22.0				
	toluene	33.0				
	e-benzene	43.0				

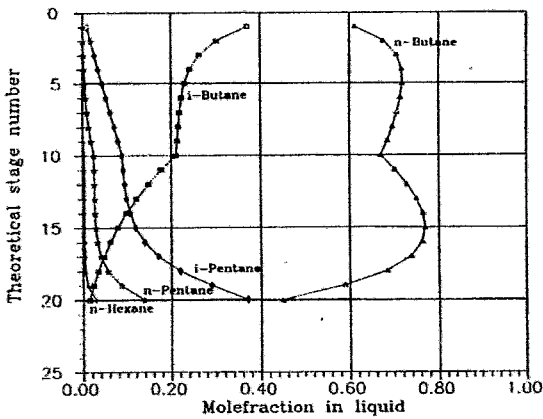


Fig.3 Composition profiles in distillation column for Example 1

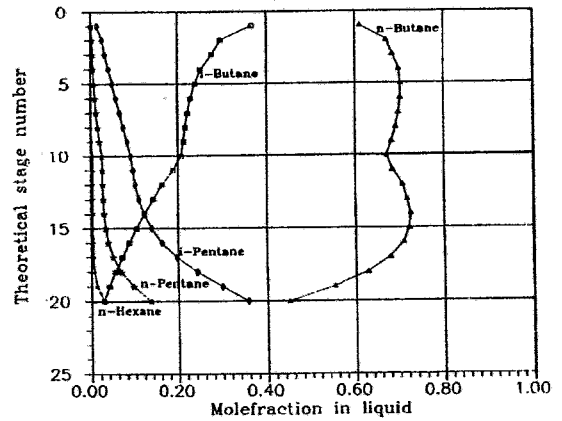


Fig.4 Composition profiles in metastillation column for Example 1

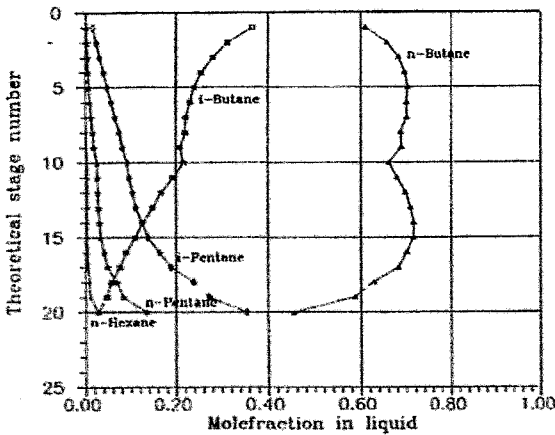


Fig.5 Composition profiles in parastillation column for Example 1

examples are selected (Table 2). For the sake of comparison all the three processes are modelled in example 1 with identical, 20 theoretical stages. The composition profiles and the temperature profiles along the column height are plotted in Figs.3-6 and the results are summarized in Table 3 as well. From Figs.3-5 and Table 3 it is obvious that with the same operating parameters (reflux ration, number of theoretical stages, pressure) identical separation effect cannot be reached with the three different separation processes. In order to obtain the same purity according to our experience at parastillation the number of theoretical stages has to be increased by roughly 40 % [6] and in the case of metastillation by 50 % which is in agreement with HEUCKE [2]. In Fig.6 the different temperature profiles are plotted. Due to the different pressure drops and degrees of separation the profiles are also different.

In examples 2 and 3 at metastillation the number of theoretical stages are increased by 50 % and it can be seen from Table 4 that the distillate purity is slightly better in the case of metastillation.

Table 3 Simulation data for Example 1 with identical numbers of theoretical stages

	Distillation	Parastillation	Metastillation
Number of theoretical stages	20	20	20
Reflux ratio	1.3	1.3	1.3
Top pressure, bar	7.0	7.0	7.0
Condenser heat load, kW	2802	2809	2808
Reboiler heat load, kW	2740	2251	2676
Distillate, kmol/hr			
i-butane	74.9	74.5	73.2
n-butane	122.7	122.5	122.3
i-pentane	1.0	1.6	2.9
n-pentane	0.0	0.0	0.2
Top temperature, °C	38.0	38.0	38.0
Bottom temperature, °C	85.4	79.3	76.0
Liquid flowrate, kg/hr	17850	17850	9000
Vapour flowrate, kg/hr	30970	16480	29880
Column diameter, mm	1210	950	980

Table 4 Simulation data for Examples 2 and 3

	Distillation		Metastillation	
	Example 2	Example 3	Example 2	Example 3
Number of theoretical stages	10	10	15	15
Condenser heat load, kW	3108	31	3124	31
Reboiler heat load, kW	3324	340	3293	302
Distillate, kmol/hr				
i-butane	—	1.997	—	1.983
benzene	94.2	0.084	94.8	0.099
toluene	5.8	0.017	5.2	0.015
e-benzene	—	0.004	—	0.002
Top temperature, °C	38.0	35.0	38.0	35.0
Bottom temperature, °C	112.5	155.4	112.8	155.4
Liquid flowrate, kg/hr	19490	12400	9530	6000
Vapour flowrate, kg/hr	27110	2810	25020	1770
Column diameter, m	1620	540	1540	400

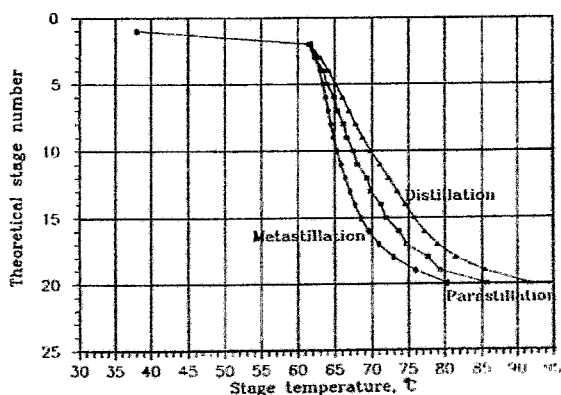


Fig. 6 Temperature profiles for Example 1

Results and Analysis

The effectiveness of the conventional and alternative separation processes is compared in the three separation examples. HEUCKE already studied these processes for binary mixture by using the McCabe-Thiele representation [2]. Since in the case of metastillation the required number of theoretical stages is roughly 50 % greater than at distillation:

1. In such operating range where the liquid flowrate determines the column diameter metastillation could provide smaller diameter because the liquid/vapour ratio is about 50 % of that of the distillation.

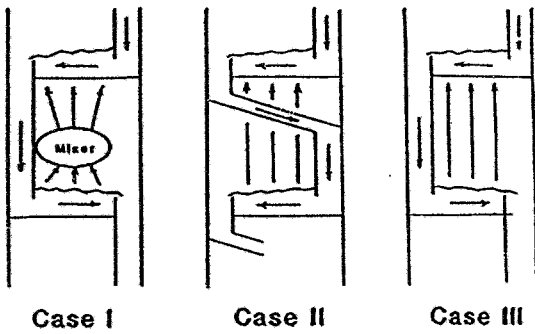


Fig. 7 Lewis cases for liquid flow pattern

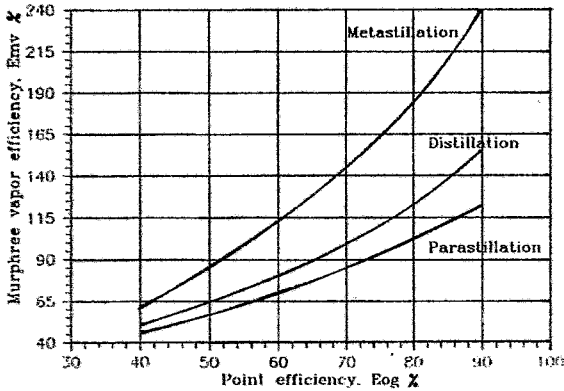


Fig. 9 Murphree vapour efficiency as function of point efficiency

2. According to LEWIS the tray efficiency greatly depends on the tray's flow pattern. In respect of flowing direction the parastillation serves the most advantageous flow pattern since the liquid on the trays in a given vapour side of the column always flows in the same direction (see Case II in Fig. 7)

In the following first the theoretical stage requirements and the effect of liquid and vapour flowrates on column diameter are discussed. Afterwards the tray efficiency is studied.

Theoretical Stage Requirement

HEUCKE showed in the case of binary mixtures that for the same separation different number of theoretical stages are needed at distillation and the alternative separation processes [2]. Our rigorous calculations justify these phenomena for multicomponent mixtures. As it is proved, the theoretical parastillation stage requirement 1.4 (with 1/2 tray spacing) and the theoretical

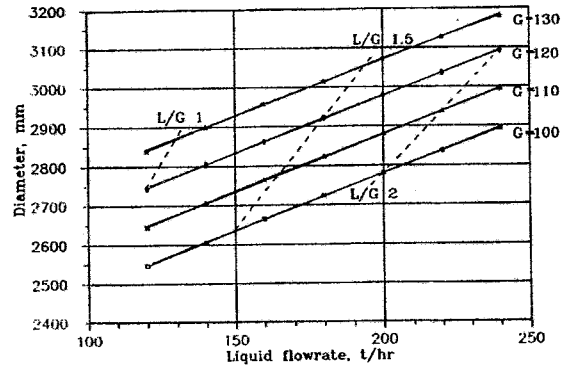


Fig. 8 Column diameter as function of liquid and vapour flowrate

metastillation stage requirement is 1.5 of that of the distillation.

Column Diameter

In Fig. 8 the column diameters are plotted against the liquid flowrate in the column for different vapour load. For calculation SULZER's METAWA type valve tray is considered [8]. The effect of varying liquid flowrate on the diameter is linear in a fairly wide range. It can be seen in Fig. 8 that decreasing the L/G ratio from 2 to 1, the column cross-section area decreases not greater than 30 % and this effect alone cannot compensate the increase of column height.

Tray Efficiency

Taking into account the efficiency differences caused by liquid flow direction on the trays for distillation and the alternative separation processes the Murphree vapour efficiency is determined in the function of point efficiency [7] (Fig. 9). It can be seen that although the flow pattern at parastillation is the most promising the E_{mv} proved to be the greatest in the case of metastillation due to the smallest L/G ratio. Selecting the 50 % point efficiency the numbers of theoretical and practical stages are plotted in the function of the theoretical stage requirement at distillation in Fig. 10. The distillation process shows smaller number of stages especially against the parastillation. This can also be observed in Fig. 11. However, it is to be noted that at parastillation one stage needs only half tray spacing compared to distillation. Furthermore, since the L/G ratios at parastillation and metastillation compared to distillation are doubled and halved, respectively, the column cross-section areas are only roughly 30 % greater and smaller, respectively. In

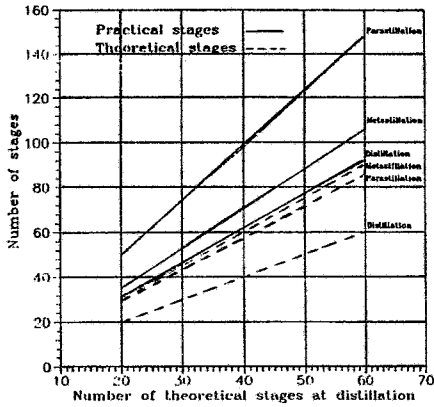


Fig. 10 Number of stages as function of number of theoretical stages at distillation ($E_{og} = 50\%$)

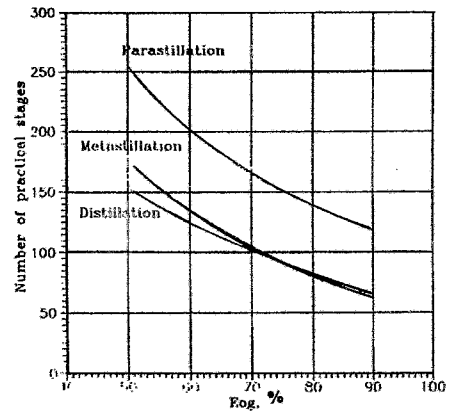


Fig. 11 Number of practical stages as function of theoretical stages ($N_{di} = 100, N_{pa} = 143, N_{me} = 150$)

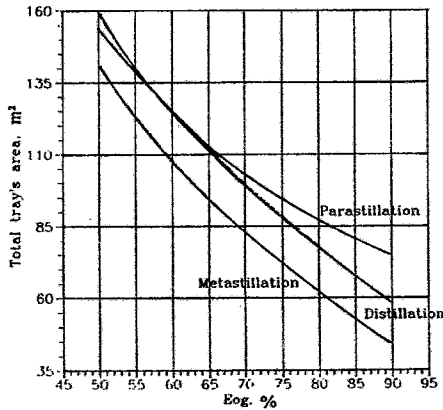


Fig. 12 Summarized tray's area in the column as function of point efficiency

Fig. 12 all these effects are summarized by expressing the total tray's area in the columns as a function of the point of efficiency. While this figure is proportional to the investment cost it is clear that at usual range of point efficiencies the parastillation cannot play any role and the metastillation seems to be the most promising.

Conclusions

The results of this study can be summarized as follows:

1. A new computer model using iterative approach is developed to simulate metastillation processes.
2. The effectiveness of separation is analyzed in several multicomponent examples and it is shown that in the case of metastillation the required number of theoretical stages increases by 50% compared to distillation.
3. In the case of metastillation the L/G ratio decreases by 50% compared to distillation, however the corresponding reduction of the column cross-section area (not greater than 30%) cannot compensate the growth of the column height.

4. Considering Murphree vapour tray efficiencies the metastillation shows the greatest values for given point efficiencies and thus this alternative separation process needs the smallest total separation area in the column.

SYMBOLS

A, B, C, D , see Table 1

E

B Bottom product, kmol/hr (Fig. 2)

D Distillate, kmol/hr (Fig. 2)

E_{mv} Murphree vapour efficiency, %

E_{og} Tray point efficiency, %

F Feed flowrate, kmol/hr

h Liquid enthalpy, kJ/kmol

H Vapour enthalpy, kJ/kmol

G Gas flowrate, kg/hr

K Equilibrium ratio

m Number of components

N_{di} Number of theoretical stages at distillation

N_{pa} Number of theoretical stages at parastillation

N_{me}, n Number of theoretical stages at metastillation

Q Heat duty, kJ/hr

Q_B Reboiler heat duty, kJ/hr

Q_C Condenser heat duty, kJ/hr

T Temperature, °C

U Liquid side product, kmol/hr

V Vapour flowrate, kmol/hr

W Vapour side product, kmol/hr

x Liquid molefraction

y Vapour molefraction

z Feed molefraction

Subscripts

i	component index
j	tray index
k	see <i>Table 1</i>
n	<i>n</i> th stage
p	see <i>Table 1</i>

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