

OPTIMAL REFLUX RATE POLICY DETERMINATION FOR MULTICOMPONENT BATCH DISTILLATION COLUMNS

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Abstract—This paper describes a procedure to obtain optimal reflux or optimal distillate rate policy for multicomponent batch distillation columns using the Pontryagin's continuous maximum principle. For application to multicomponent systems, a reduced order model is used using short-cut procedure developed specifically for analysis and design of batch columns.

Scope—The two well-known methods of operating batch columns are the constant reflux operation and the variable reflux operation. The optimal reflux rate policy, which is essentially a trade-off between the two methods, is based on the ability to yield the most profitable operation. Existing literature has dealt with the problem of determining the optimal reflux rate policy for batch distillation columns handling binary systems using dynamic programming, variational calculus, or Pontryagin's maximum principle. Similar studies on multicomponent systems, however, are sporadic in the current literature and have been limited to three components. Systematic design-optimization procedures which are computationally efficient are not yet available for multicomponent batch distillation problems. This is perhaps due to the inherent complexity of the problem, a rigorous treatment of which calls for solution of a set of differential equations which can be stiff in nature. Our earlier studies on several ideal multicomponent systems and selected non-ideal binary systems have shown that the use of a short-cut method, in place of rigorous techniques, for preliminary design, gives results which are not appreciably different from that given by the rigorous method especially for columns with negligible plate holdup. This approach has been extended for determination of optimal reflux rate policy.

Conclusions and Significance—The use of short-cut method to simplify the model equations is shown to be a potentially alternative and feasible approach towards finding optimal reflux rate policy for multicomponent batch distillation columns. The approach offers considerable reduction in computation time without compromising much on the accuracy of the solution.

INTRODUCTION

The optimal reflux rate policy for the operation of batch distillation columns falls between the two conventional policies and in this neither the reflux ratio nor the instantaneous distillate composition remains constant. The optimal reflux policy can usually be determined by solution of one of the following optimization problems.

1. Maximum distillate problem [1, 2]—collection of maximum amount of distillate of a specified concentration in a prescribed length of time.

2. Minimum time problem [3-11]—minimization of distillation time needed to produce a prescribed amount of distillate of a specified concentration.

The work on the maximum distillate problem was first reported by Converse and Gross [1]. They solved the problem using Pontryagin's continuous maximum principle, dynamic programming and calculus of variation. Murty *et al.* [2] used the same model and compared the solution obtained by using different optimization techniques. Their work is restricted to binary systems and with very small number of plates.

Coward [3, 4], Robinson [5-7], Mayur and Jackson [8], have all applied the minimum time problem to the same model and Price [9] to a slightly complex model. Egly *et al.* [10] solved the problem for a tray column with hold up and with possibility of reaction. Recently, Hansen and Jorgensen [11] reported optimal solution for both tray and packed columns, using collocation techniques to solve the two-point boundary value problem.

Kerkhof and Vissers [12] solved the optimization problem using profit as the objective function.

Most of the work reported above is restricted to binaries. Egly *et al.* [10] have considered a multicomponent system but no details are given. A ten-component system has been used by Robinson [5] but it is treated as an effective binary system. Robinson [6] and Mayur and Jackson [8] considered a ternary system. However, they have also discussed the difficulties of extending the method to systems involving more than three components, since it calls for solution of an increased number of equations because of an increase in the number of components. Another difficulty with their problem formulation is that the number of equations also increases with an increase in the number of plates and hence results in addi-

tional memory and computational time requirement. Gallier and Ryan [13] have considered the problem of maximization of profit for a batch distillation operation using rigorous dynamic models. However, the optimal policy proposed by them has been in a heuristic manner and is not based on a rigorous optimization procedure.

In the present work, the problem of an increase in computational time due to the reasons stated above is circumvented by using a short-cut method which is based on an extension of the short-cut method commonly used for continuous columns. The method has been widely tested for variable reflux and for constant reflux problems [14, 15]. The maximum distillate problem has been solved and the results are compared with the earlier reported results for binary systems. Results of a quaternary system are also shown.

PROBLEM FORMULATION

For the system shown in Fig. 1, if we assume that the distillation is carried out under constant boil-up rate V , an overall differential material balance over a differential time dt gives:

$$\frac{dX_1}{dt} = \frac{dB}{dt} = -\frac{V}{R_t + 1}, \quad X_1(0) = B(0) = F, \quad (1)$$

where, F is the feed, which is initial condition to $X_1(t)$. A material balance for the key component, over the differential time, dt , gives:

$$x_D^{(1)} \cdot \frac{V}{R_t + 1} dt = -d(X_1 X_2) \\ = -X_1 dX_2 - X_2 dX_1. \quad (2)$$

Substitution of equation (1) in equation (2) results in:

$$\frac{dX_2}{dt} = \frac{V}{(R_t + 1)X_1} (X_2 - x_D^{(1)}), \quad X_2(0) = x_F^{(1)}. \quad (3)$$

For equations (1) and (3):

X_1 = quantity of charge remaining in the still, B , (mol),

X_2 = composition of the key component in the still, $x_D^{(1)}$, (mol fraction),

R_t = reflux ratio (function of time),

V = vapour boil up rate (mol h^{-1}),

$x_D^{(1)}$ = overhead composition of key component (mol-fraction),

t = time of operation (h).

In a multicomponent case, for the columns in which the assumption of negligible hold up can be made, one can reduce the dimensionality of the state model to approximate further the terminal composition of the column. Instead of using time as an explicit variable (Mayur and Jackson [8]) the differential equations can be rewritten with component 1 as reference component. Then the variation of any other component i , can be expressed in terms of the reference component 1. This formulation has

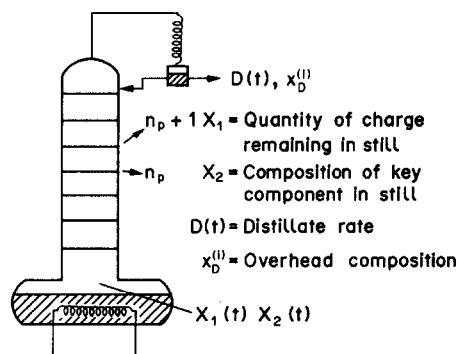


Fig. 1. Schematic diagram of a batch distillation system.

an advantage over the time explicit equations. The time implicit equations reduce the dimensionality of the problem, as the number of adjoint vectors and adjoint equations do not increase with the number of components. The differential material balance equations for component i with reference to component 1, can be written as:

$$\frac{d x_B^{(i)}}{(x_D^{(i)} - x_B^{(i)})} = \frac{d x_B^{(1)}}{(x_D^{(1)} - x_B^{(1)})}, \quad x_B^{(i)} \\ = x_F^{(i)}, \quad i = 2, \dots, n \quad (4)$$

From the simulation model developed using the proposed short-cut method, it can be shown that $x_B^{(i)}$ can be expressed as a function of $x_B^{(1)}$ and reflux ratio R .

Now the maximum distillate problem can be written as:

$$\max J = \int_0^T D(t) dt = \int_0^T \frac{V}{(R_t + 1)} dt, \quad (5)$$

subject to the constraint:

$$\bar{x}_D^{(1)} = \frac{\int_0^T \frac{x_D^{(1)} \cdot V}{(R_t + 1)} dt}{\int_0^T \frac{V}{(R_t + 1)} dt} = x_D^*, \quad (6)$$

by a proper choice of R_t , $0 \leq t \leq T$. Here, R_t has a constraint given by:

$$0 \leq R_t. \quad (7)$$

The constraint on the product purity is removed by employing the method of Lagrange multipliers.

Combining equations (5) and (6):

$$S = \int_0^T \frac{V}{(R_t + 1)} [1 - \lambda(x_D^* - x_D^{(1)})] dt, \quad (8)$$

where λ is the Lagrange multiplier. Now the objective is to maximize S , instead of J .

To solve the problem, an additional state variable X_3 is introduced which is given by:

$$X_3(t) = \int_0^t \frac{V}{(R_t + 1)} \\ \times [1 - \lambda(x_D^* - x_D^{(1)})] dt, \quad X_3(0) = 0 \quad (9)$$

The problem then can be written as:

$$\max_{\mathbf{R}_t} X_3(T)$$

subject to equations (1)–(4) and the constraint on \mathbf{R}_t , i.e. equation (7). The Hamiltonian function, which should be maximized, is:

$$H = \frac{-z_1 V}{(\mathbf{R}_t + 1)} + \frac{z_2 V}{(\mathbf{R}_t + 1)X_1} (X_2 - x_D^{(i)}) + \frac{V}{(\mathbf{R}_t + 1)} [1 - \lambda(x_D^* - x_D^{(i)})]. \quad (10)$$

Simplifying the adjoint vector functions and the Hamiltonian equations, the following differential equations are obtained:

$$\frac{dz_1}{dt} = \frac{z_2 V}{(\mathbf{R}_t + 1)} \frac{(X_2 - x_D^{(i)})}{X_1^2}, \quad z_1(T) = 0, \quad (11)$$

$$\frac{dz_2}{dt} = \frac{-z_2 V}{(\mathbf{R}_t + 1)X_1} \left[1 - \frac{\partial x_D^{(i)}}{\partial X_2} \right] - \frac{\lambda V}{(\mathbf{R}_t + 1)} \times \frac{\partial x_D^{(i)}}{\partial X_2}, \quad z_2(T) = 0 \quad (12)$$

and

$$H = \frac{-z_1 V}{(\mathbf{R}_t + 1)} + \frac{z_2 V}{(\mathbf{R}_t + 1)X_1} (X_2 - x_D^{(i)}) + \frac{V}{(\mathbf{R}_t + 1)} [1 - \lambda(x_D^* - x_D^{(i)})]. \quad (13)$$

By optimality conditions $\partial H / \partial \mathbf{R}_t = 0$, so

$$\frac{\partial H}{\partial \mathbf{R}_t} = \frac{z_1 V}{(\mathbf{R}_t + 1)^2} - \frac{z_2 V}{(\mathbf{R}_t + 1)^2 X_1} (X_2 - x_D^{(i)}) - \frac{z_2 V}{(\mathbf{R}_t + 1)X_1} \frac{\partial x_D^{(i)}}{\partial \mathbf{R}_t} - \frac{V}{(\mathbf{R}_t + 1)^2} [1 - \lambda(x_D^* - x_D^{(i)})] + \frac{V\lambda}{(\mathbf{R}_t + 1)} \times \frac{\partial x_D^{(i)}}{\partial \mathbf{R}_t} = 0, \quad (14)$$

where

$$\frac{\partial x_D^{(i)}}{\partial \mathbf{R}_t}$$

and

$$\frac{\partial x_D^{(i)}}{\partial X_2}$$

(calculated numerically) can be calculated using the simulation model presented in the next section. The equation for optimum \mathbf{R}_t can be written as:

$$\mathbf{R}_t = \frac{- \left[\frac{z_2}{X_1} (X_2 - x_D^{(i)}) - z_1 - \lambda(x_D^* - x_D^{(i)}) + 1 \right]}{\frac{\partial x_D^{(i)}}{\partial \mathbf{R}_t} \left(\frac{z_2}{X_1} - \lambda \right)} - 1. \quad (15)$$

SIMULATION MODEL

For expressing the relation between the still composition and the terminal product composition, the use of rigorous method will require extensive computation time which increases with the increase in number of plates and components.

In our earlier studies [14, 15], a short-cut procedure for batch columns has been developed and tested on several multicomponent systems and non-ideal binary systems. The equations used in the proposed short-cut method are: Hengstebeck–Geddes' equation,

$$x_D^{(i)} = \left(\frac{\alpha_i}{\alpha_1} \right)^{C_1} \frac{x_D^{(1)}}{x_B^{(1)}} x_B^{(i)}, \quad i = 2, \dots, n; \quad (16)$$

which can be related to the Fenske's equation,

$$N_{\min} = \frac{\ln \left[\frac{x_D(lk) x_B(hk)}{x_B(lk) x_D(hk)} \right]}{\ln \alpha_{lk}}, \quad (17)$$

Underwood's equations,

$$\sum_{i=1}^n \frac{\alpha_i x_B^{(i)}}{\alpha_i - \phi} = 0$$

$$\mathbf{R}_{\min} + 1 = \sum_{i=1}^n \frac{\alpha_i x_B^{(i)}}{\alpha_i - \phi}; \quad (18)$$

Gilliland's correlation,

$$y = 1 - \exp \left[\frac{(1 + 54.4X)(X - 1)}{(11 + 117.2X)\sqrt{X}} \right] \quad (19)$$

in which

$$X = \frac{\mathbf{R} - \mathbf{R}_{\min}}{\mathbf{R} + 1} \quad \text{and} \quad y = \frac{N - N_{\min}}{N + 1} \quad (20)$$

and

$$\sum_{i=1}^n x_D^{(i)} = 1. \quad (21)$$

In order to match the \mathbf{R}_{\min} predicted by the Underwood's equations (where the compositions $x_B^{(i)}$'s are used to calculate \mathbf{R}_{\min}) with the \mathbf{R}_{\min} obtained by the Gilliland's correlation (which uses N , \mathbf{R} and N_{\min} or equivalently C_1), the following additional condition is provided:

$$G(1) = \frac{\mathbf{R}_{\min u}}{\mathbf{R}} - \frac{\mathbf{R}_{\min g}}{\mathbf{R}}. \quad (22)$$

For a specific $x_B^{(1)}$ at each state, it is necessary to estimate $x_D^{(i)}$, $i = 1, \dots, n$ and $x_B^{(i)}$, $i = 2, \dots, n$. The differential material balance in equation (4) can be converted into a difference equation using old values (previous) of $x_B^{(i)}$'s and $x_D^{(i)}$'s and is given by:

$$x_{\text{new}}^{(i)} = x_{\text{old}}^{(i)} + \frac{\Delta x_B^{(1)} (x_D^{(i)} - x_B^{(i)})_{\text{old}}}{(x_D^{(1)} - x_B^{(1)})_{\text{old}}}, \quad i = 2, \dots, n. \quad (23)$$

To obtain initial values of $x_B^{(i)}$'s, the procedure given after equation (23) is used.

The Hengstebeck–Geddes equation along with equation (23) when substituted in equation (21) results in

$$\sum_{i=1}^n (\alpha_i/\alpha_1)^{C_1} \frac{x_B^{(i)}}{x_B^{(1)}} x_B^{(i)} = 1. \quad (24)$$

So,

$$x_B^{(i)} = \frac{1}{\sum_{i=1}^n (\alpha_i/\alpha_1)^{C_1} \frac{x_B^{(i)}}{x_B^{(1)}}}. \quad (25)$$

Substituting equation (25) in equation (16) and then using equation (22), one can obtain the value of C_1 and hence $x_B^{(i)}$'s. The Newton–Raphson procedure is used for the solution, the derivative required for which is given by:

$$\begin{aligned} \mathbf{R} \frac{\partial G(1)}{\partial C_1} = & - \sum_{i=1}^n \alpha_i (\alpha_i/\alpha_1)^{C_1} \frac{x_B^{(i)}}{x_B^{(1)}} \\ & \times \frac{\sum_{j=1}^n (\alpha_j/\alpha_1)^{C_1} \frac{x_B^{(j)}}{x_B^{(1)}} \ln(\alpha_j/\alpha_1)}{\sum_{j=1}^n \left[(\alpha_j/\alpha_1)^{C_1} \frac{x_B^{(j)}}{x_B^{(1)}} \right]^2 (\alpha_i - \phi)} \\ & + \sum_{i=1}^n \alpha_i \frac{x_B^{(i)} \ln(\alpha_i/\alpha_1)}{\alpha_i - \phi} - \frac{(\mathbf{R} + 1)}{(\mathbf{N} + 1)} \frac{dy}{dx}, \end{aligned} \quad (26)$$

where:

$$\begin{aligned} \frac{dy}{dx} = & (3187.84 X^3 + 4026.84 X^2 \\ & - 117.9 X + 5.5)/X/(11 \\ & + 117.2 X)^2/\sqrt{X} \cdot (y - 1). \end{aligned} \quad (27)$$

Similarly the values of

$$\frac{dx_B^{(i)}}{d\mathbf{R}}$$

required for solution of equations in the earlier section can be obtained as follows:

$$\frac{dx_B^{(i)}}{d\mathbf{R}} = \frac{dx_B^{(i)}}{dC_1} \frac{dC_1}{d\mathbf{R}}, \quad (28)$$

where

$$\frac{dC_1}{d\mathbf{R}} = - \frac{\partial G(1)}{\partial \mathbf{R}} \bigg/ \frac{\partial G(1)}{\partial C_1} \quad (29)$$

$$\begin{aligned} & = \left[\frac{(\mathbf{R}_{\min g} - \mathbf{R}_{\min u})}{\mathbf{R}^2} \right. \\ & \left. - \frac{(\mathbf{R}_{\min g} + 1)}{(\mathbf{R} + 1)\mathbf{R}} \right] \bigg/ \frac{\partial G(1)}{\partial C_1} \end{aligned} \quad (30)$$

and

$$\frac{dx_B^{(i)}}{dC_1} = \frac{- \sum_{i=1}^n (\alpha_i/\alpha_1)^{C_1} \frac{x_B^{(i)}}{x_B^{(1)}} \ln(\alpha_i/\alpha_1)}{\left[\sum_{i=1}^n (\alpha_i/\alpha_1)^{C_1} \frac{x_B^{(i)}}{x_B^{(1)}} \right]^2}. \quad (31)$$

SOLUTION STRATEGY

Basically now the problem is reduced to finding out the solution of equation (15) using equations (1), (3), (11) and (12) along with the short-cut method simulation model. The equations also involve the Lagrange multiplier, which is a constant for a specific value of time T . This means that the solution involves trial and error on the multiplier λ . So, equations (1), (3), (11) and (12) must be solved for different values of λ , until the constraint equation [equation (6)] is satisfied.

It can be seen that the solution of equations (1), (3), (11) and (12) also involves a two point boundary value problem. Converse and Gross [1] obtained the solution, by assuming $X_1(T)$ and $X_2(T)$ and then performing backward integration. This optimal solution, however, is valid only for the values of $X_1(0)$ and $X_2(0)$ obtained at the end of this integration step. The exact solution for the starting values can then be obtained by iterating on $X_1(T)$ and $X_2(T)$. This asks for additional computational time and hence has not been reported by Converse and Gross [1]. Here we are using the method of steepest ascent of Hamiltonian [16], since due to being a multi-component system a backward integration of equations (1) and (2) is not possible. This method is given below.

Here we are seeking to maximize H , by choosing the decision vector \mathbf{R}_i in such a way that the Hamiltonian is a maximum. The method of steepest ascent of Hamiltonian accomplishes this by using an iterative procedure to find \mathbf{R}_i , the optimal decision vector. An initial estimate of \mathbf{R}_i is obtained and \mathbf{R}_i is corrected during each iteration. For the i th component of the decision vector the following rule is used for proceeding from the j th to $(j + 1)$ th approximation:

$$\mathbf{R}'_i(i) = \mathbf{R}_i(i) + K \frac{\partial H}{\partial \mathbf{R}_i(i)}, \quad i = 1, 2, \dots, r \quad (32)$$

where the prime denotes the $(j + 1)$ th iteration and the unprimed quantities, the j th iteration and where K is a suitable constant. This iterative method is used until there is no further change in \mathbf{R}_i . The values of K should be small enough so that no instability will result, yet large enough so that convergence will not be too slow. It should be noted that the sign of K is also important, because $\partial H/\partial \mathbf{R} \rightarrow 0$ at and near total reflux conditions, which gives minimum value of H .

The flowchart to obtain optimal reflux rate policy is shown in Fig. 2.

RESULTS AND DISCUSSION

The short-cut method used in this study is based on three key assumptions, namely, zero hold up, constant molal overflow and constant relative volatility. The method, however, has been extensively tested for cases with small holdup for several systems, for both variable reflux and constant reflux operations and the

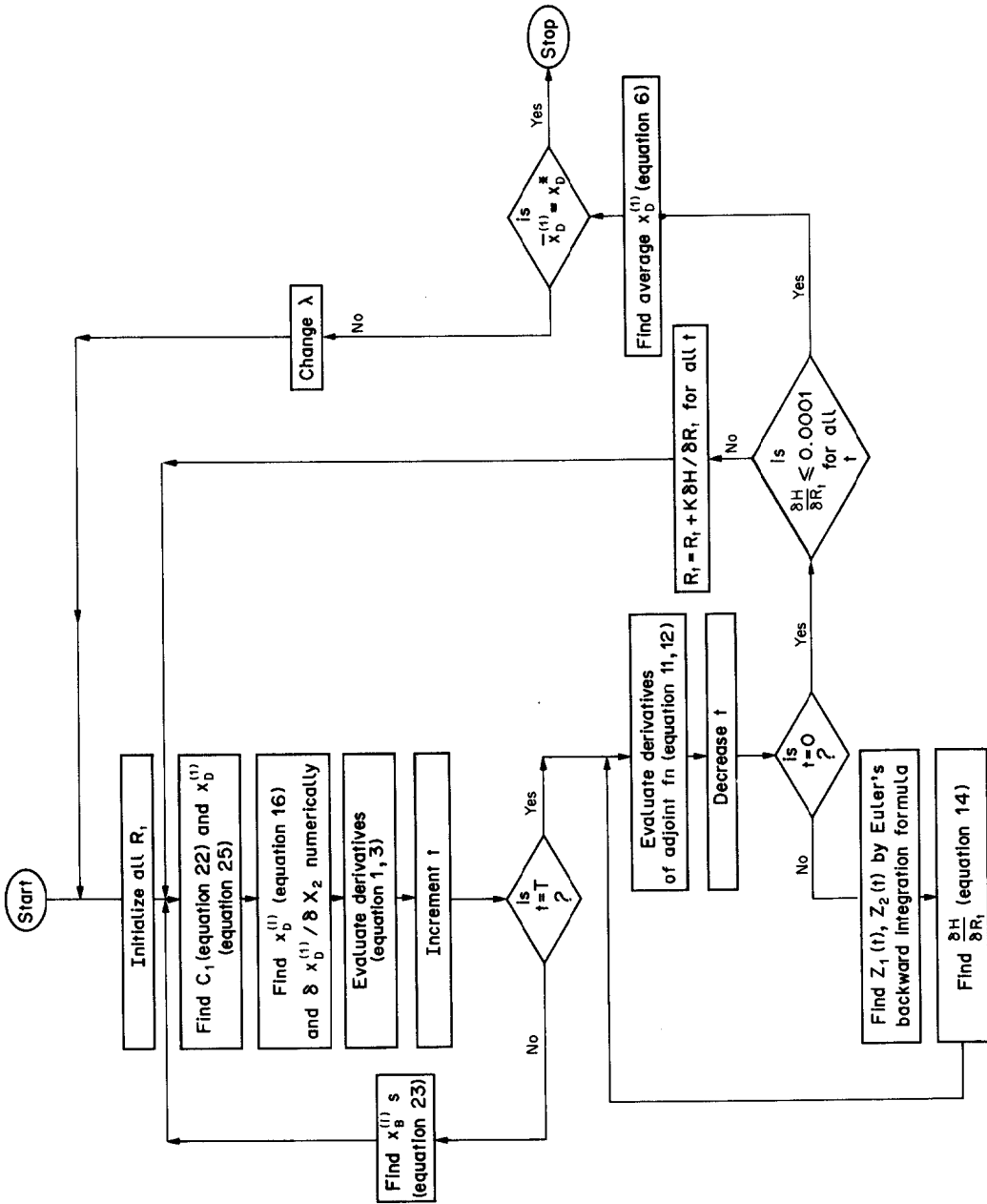


Fig. 2. Flowchart to obtain optimal reflux policy.

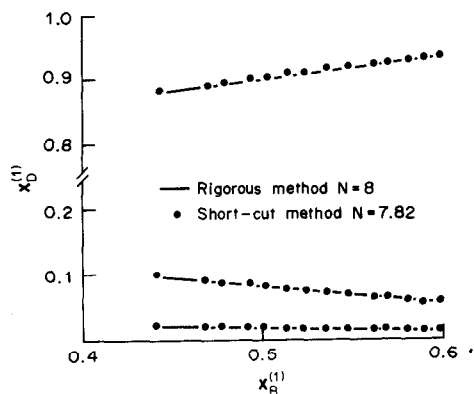


Fig. 3. Composition profiles for a ternary system (constant reflux).

results are reported in our previous work [14, 15]. These studies included multicomponent systems whose behaviour is close to ideal conditions. The results are satisfactory and the composition profiles for the top product obtained by the short-cut method show very close agreement to that obtained by the rigorous method. These profiles for a constant reflux case are shown in Fig. 3, which are reproduced here from our earlier work [15].

To test the performance of our short-cut method in determining the optimal-reflux rate policy using the Pontryagin's maximum principle, seven cases for the problem used in the study by Murty *et al.* [2] have been first tried. Table 1 includes the input conditions for all the seven cases for batch distillation model used by Murty *et al.* [2]. A comparison of results obtained using our short-cut method and results obtained by [2] is presented in Table 2 for the three operating policies, namely, the variable reflux, the constant reflux and the optimal reflux.

From the results in Table 2, it is seen that the values of J , the amount of distillate obtained by short-cut method seem to be consistently smaller than

Table 1. Input conditions for batch distillation model

| Case No. | $X_1(0)$ | $X_2(0)$ | x_B^* |
|----------|----------|----------|---------|
| 1 | 116.1 | 0.715 | 0.95 |
| 2 | 74.3 | 0.420 | 0.90 |
| 3 | 116.1 | 0.580 | 0.93 |
| 4 | 116.1 | 0.487 | 0.93 |
| 5 | 74.3 | 0.715 | 0.95 |
| 6 | 116.1 | 0.715 | 0.93 |
| 7 | 116.1 | 0.715 | 0.90 |

† $V = 110 \text{ mol h}^{-1}$; $N = 4$ (No. of plates = 3 + 1 for reboiler); $\alpha_i = 2.0, 1.0$; $T = 1 \text{ h}$.

those reported by [2]. It would therefore appear that optimization using the short-cut method is not particularly effective compared to the methods reported by earlier researchers. From an analysis of average distillate composition predicted by our short-cut method and that by a rigorous method for a constant reflux, it is seen (Table 3) that the average composition predicted by the rigorous method is higher than that given by the short-cut method. Thus to produce the same average composition, the short-cut method predicts higher reflux than the rigorous method. Though the difference in the average composition is only of the order of 1–2%, its effect on the distillate collected is quite significant. This can easily be seen from Fig. 4, where x_D profiles for case 4 (constant reflux case) are shown for short-cut method and rigorous method. The profiles show that the difference in x_D values is 0.2% whereas it shows a difference of 25% in the value of J , as can be seen from Table 2. This is due to the fact that for the results in Table 2, the number of plates are very small. With small number of plates where

$$y = \frac{N - N_{\min}}{N + 1} \rightarrow 0,$$

the Gilliland's correlation becomes very sensitive to

$$R \left(\frac{dy}{dx} \rightarrow \infty \right)$$

Table 2. Comparison of results with results obtained by [2]

| Case No. | Method | J (Optimal reflux) | J (Constant reflux) | J (Variable reflux) | λ |
|----------|--------------|----------------------|-----------------------|--------------------------|-----------|
| 1 | Rigorous [2] | 25.979 | 26 (approx from Fig.) | 26.01 (approx from Fig.) | 27.15 |
| | Short-cut | 20.290 | 20.081 | 20.247 | 29.36 |
| 2 | Rigorous [2] | 6.082 | NR | NR | 42.69 |
| | Short-cut | 4.731 | 4.545 | 4.482 | 50.11 |
| 3 | Rigorous [2] | 16.397 | NR | NR | 28.54 |
| | Short-cut | 12.300 | 12.234 | 12.276 | 31.25 |
| 4 | Rigorous [2] | 4.379 | NR | NR | 102.93 |
| | Short-cut | 3.170 | 2.935 | 2.956 | 131.36 |
| 5 | Rigorous [2] | 22.827 | NR | NR | 25.76 |
| | Short-cut | 18.238 | 18.162 | 18.230 | 29.24 |
| 6 | Rigorous [2] | 38.752 | NR | NR | 13.06 |
| | Short-cut | 30.240 | 29.966 | 30.211 | 15.30 |
| 7 | Rigorous [2] | 46.204 | NR | NR | 10.40 |
| | Short-cut | 37.261 | 36.283 | 36.762 | 8.74 |

†NR = Not Reported.

Table 3. Comparison of results with rigorous method) constant reflux)

| Case No. | <i>J</i> Short-cut | <i>J</i> Rigorous | <i>x</i> _D [*] Short-cut | <i>x</i> _D [*] Rigorous |
|----------|--------------------|-------------------|--|---|
| 1 | 20.08 | 20.08 | 0.950 | 0.958 |
| 2 | 4.55 | 4.55 | 0.900 | 0.906 |
| 3 | 12.23 | 12.23 | 0.930 | 0.938 |
| 4 | 2.94 | 2.94 | 0.930 | 0.932 |
| 5 | 18.16 | 18.16 | 0.950 | 0.957 |
| 6 | 29.96 | 29.96 | 0.930 | 0.942 |
| 7 | 36.28 | 36.28 | 0.900 | 0.919 |

†*J* for rigorous is kept same as that of short-cut.

and so the values of

$$\frac{\partial \mathbf{R}}{\partial x_D} \rightarrow \infty.$$

Hence a small change in *x*_D results in large change in *J*. This can also be seen from Table 4 where number of plates vs *J* values obtained by the two methods are presented, for constant reflux case. It can be observed that as the number of plates increases both the methods show good agreement.

Table 5 and Figs 5 and 6 show results for a quaternary system. It can be seen from the results that optimal reflux rate policy always gives more distillate than both variable reflux or constant reflux cases though the difference is marginal sometimes.

The successful results of this method for multi-component systems shows that it can also be used to obtain solutions to the minimum time problem or the maximum profit problem, when the number of plates are large enough to avoid any discrepancy. However, to minimize the dependence of the optimal reflux rate policy on the number of plates, the following strategy can be used.

The optimal reflux rate composition profiles predicted by the short-cut method could be used as the programmed set points for the distillate composition control system manipulating the reflux. It is conjectured that the resulting reflux rate produced by the composition control system will correspond closely to the calculated optimal reflux policy, using a rigorous method. The proposed strategy has been tested for the problem in Table 1 (case 1) and has been found to produce results which match closely with the results presented by [2]. The computational time required for the determination of the optimal reflux policy is much large compared to variable reflux or

Table 4. Effect of increase in number of plates on amount of distillate collected (constant reflux)

| <i>N</i> | <i>J</i> Short-cut | <i>J</i> Rigorous |
|----------|--------------------|-------------------|
| 4 | 20.262 | 26.00 |
| 6 | 36.50 | 40.59 |
| 10 | 46.70 | 46.90 |
| 20 | 49.10 | 49.20 |

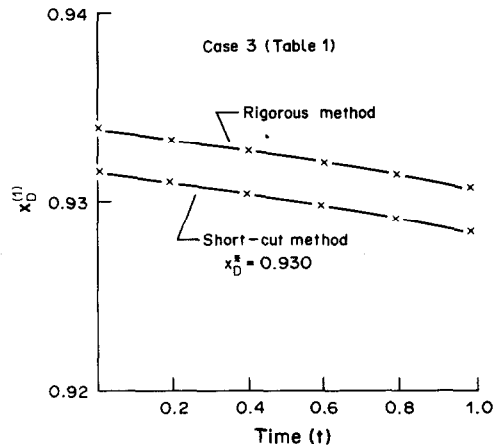


Fig. 4. Composition profiles (constant reflux).

constant reflux conditions. The convergence behaviour depends on initial profile of the *R*_{*i*} vector, initial value of *H*, initial value of *λ* and the value of *K*. The initial values of the *R*_{*i*} profile and the sign of *K* also affect the solution, as it may lead to a minimum value of *H* instead of a maximum.

To analyze the capability of the short-cut method used in this study to simulate non-ideal systems, problems on two systems have been studied, namely an ethanol-water system and a methanol-water system with the assumption of zero hold up in both cases. In this the relative volatility value which is averaged using the values calculated by the UNIQUAC equation at the top and at the bottom, is updated for each increment in time space during the simulation. Comparisons of the results obtained by the short-cut method and rigorous method are shown in Figs 7 and 8 (variable reflux condition). Though the reflux ratio policies obtained by the two methods do not agree on an absolute scale, it can be seen that the trend of reflux profile obtained by the short-cut

Table 5. Input conditions and results for a quaternary system

| Component (<i>i</i>) | Feed comp. <i>x</i> _{<i>i</i>} ^(f) | Relative volatility <i>α</i> (<i>i</i>) |
|------------------------|--|---|
| 1 | 0.25 | 2.0 |
| 2 | 0.25 | 1.5 |
| 3 | 0.25 | 1.0 |
| 4 | 0.25 | 0.5 |

*x*_D^{*} = 0.90, *F* = 200 mol; *V* = 110 mol h⁻¹; *T* = 1 h.

| Case No. | <i>N</i> | <i>J</i> _{opt. ref.} | <i>J</i> _{const. ref.} | <i>J</i> _{var. ref.} | <i>λ</i> |
|----------|----------|-------------------------------|---------------------------------|-------------------------------|----------|
| 1 | 8.0 | 25.5420 | 24.7137 | 24.6960 | 265.12 |
| 2 | 10.0 | 20.4367 | 20.4296 | 19.9825 | 15.52 |

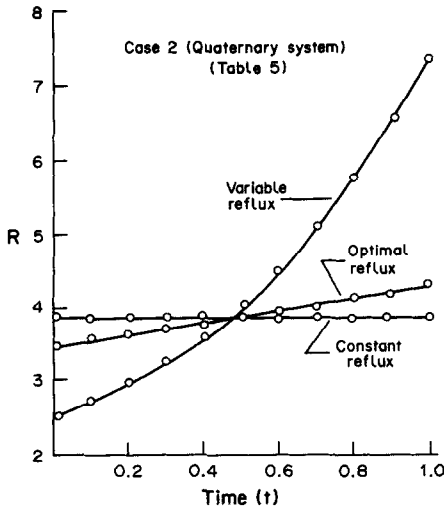


Fig. 5. Reflux rate policies for a quaternary system. (Constant reflux, variable reflux, optimal reflux).

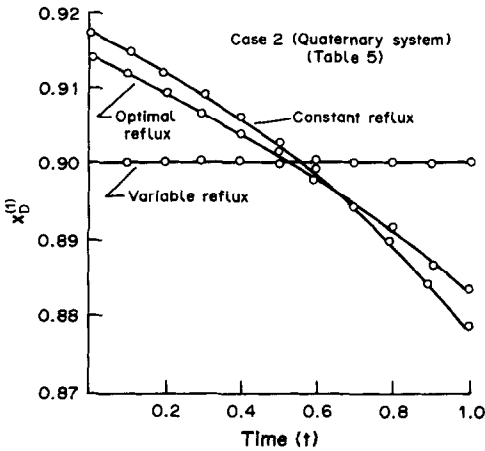


Fig. 6. Composition profiles for a quaternary system. (Constant reflux, variable reflux, optimal reflux).

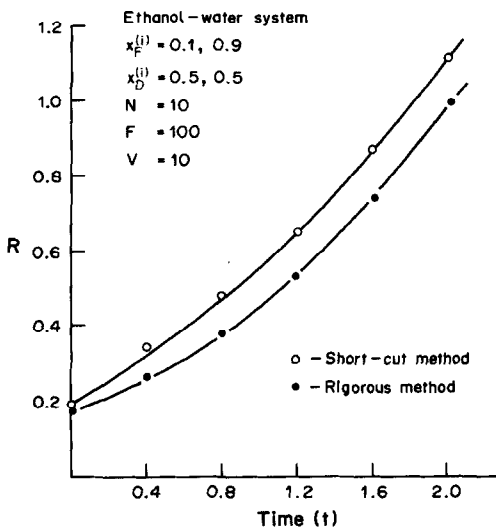


Fig. 7. Reflux rate policies for a non-ideal system (ethanol-water, variable reflux).

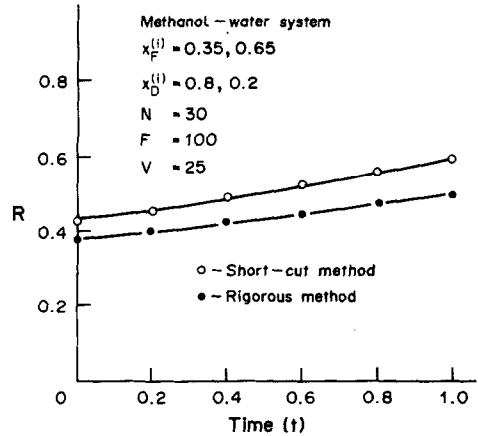


Fig. 8. Reflux rate policies for a non-ideal system (methanol-water, variable reflux).

method is very close to that obtained by the rigorous method. With a constant correction factor (here it is very close to 1), the reflux policy predicted by the short-cut method should provide a good initial policy for the actual conditions. Comparisons of the results obtained for the same systems for constant reflux policy and optimal reflux policy could not be presented here because of the convergence problems in the rigorous method for the cases of zero holdup.

To estimate the effect of holdup on the performance of the method, the results obtained by Stewart *et al.* [17] are compared with the results obtained by our short-cut method (Figs 9-11). Here the initial total reflux condition is simulated using $N = N_{min}$. It can be seen that the short-cut method results agree well with the results obtained for small holdup conditions. For large holdup values and low reflux ratio, the initial part of the composition profile for the more volatile component shows a gradual change for the rigorous models, while the short-cut method predicts a sharp drop in composition (Fig. 6). This is due to the large time constant (τ) associated with large holdup and low reflux ratio

$$\left(\tau = \frac{\text{Holdup}}{\text{Reflux ratio} \times \text{Distillate rate}} \right)$$

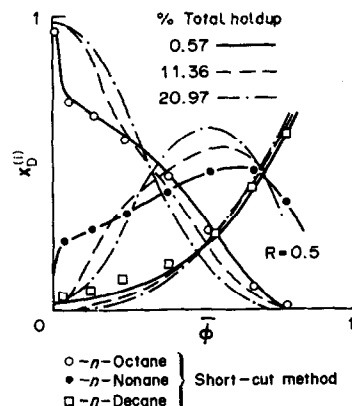


Fig. 9. Theoretical distillation curves, ternary system, $R = 0.5$ (constant reflux).

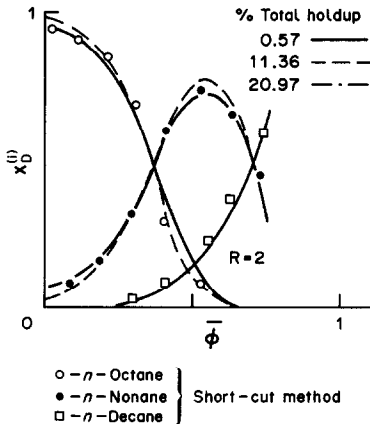


Fig. 10. Theoretical distillation curves, ternary system, $R = 2.0$ (constant reflux).

The short-cut method, which has only a few state variables associated with it, cannot be expected to approximate the dynamic situation where the state variables associated with each plate have a dominant dynamic character. There has been no reported literature on computation of optimal strategy for such situations, as a dynamic optimization procedure will call for extensive effort. The short-cut method can help to evolve an initial trial policy which could be systematically varied in a heuristic manner using a rigorous dynamic model to obtain the final optimal reflux policy.

CONCLUSIONS

A generalized model to obtain optimal reflux rate policy for a maximum distillate problem is presented here, which uses Pontryagin's continuous maximum principle and a short-cut method to simulate the column. The introduction of time implicit equations and use of the short-cut method reduce the number of equations and number of parameters, which in turn result in a reduction in the computational time and memory requirements. The method therefore can be applied to columns with large number of plates and a large number of components as well, where the system is near ideal and holdup is small. For highly

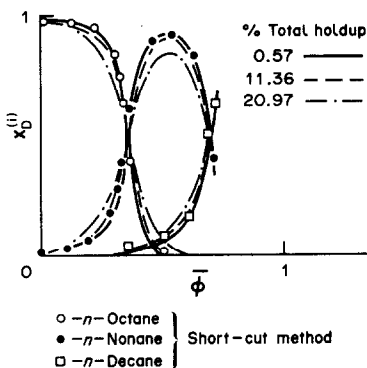


Fig. 11. Theoretical distillation curves, ternary system, $R = 8.0$ (constant reflux).

non-ideal systems, based on the limited systems studied, it can be said that the short-cut method can give a good initial estimate of the trend of reflux policy variation necessary to maintain the desired product compositions.

For a smaller number of plates, a strategy which accounts implicitly for the discrepancy of the short-cut model, is advocated to generate the optimal control policy.

Successful results from this method show that the method can also be extended to obtain solutions to the minimum time or maximum profit problems.

NOMENCLATURE

- B = Amount of material remaining in the still
- $D(t)$ = Distillate rate at time t
- F = Amount of feed
- hk = Heavy key component
- J = Amount of distillate collected
- lk = Light key component
- n = Number of components
- N_{\min} = Minimum number of plates
- R = Reflux ratio
- R_{\min} = Minimum reflux ratio
- R_t = Reflux ratio at time t
- T = Total time
- V = Vapour boil up rate
- $x_B^{(i)}$ = Still composition of component i
- x_F^* = Specified average composition of component i
- $x_D^{(i)}$ = Distillate composition of component i
- $x_F^{(i)}$ = Feed composition of component i

Greek symbols

- α_i = Relative volatility of component i
- λ = Lagrangian multiplier

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