

Multicomponent batch distillation column design

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λ_{ij} = diagonal elements of RGA

τ_1 = controller integral time (min)

ω_u = ultimate frequency

Registry No. Propylene, 115-07-1; propane, 74-98-6.

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SEPARATIONS

Multicomponent Batch Distillation Column Design

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Batch distillation is characterized as a system that is difficult to design because compositions are changing continuously with time. The models reported in the literature and used in the simulators like PROCESS and BATCHFRAC, etc., are too complex to use for obtaining optimal design because of high computational time and large memory requirement. In this work we are presenting a short-cut method for design of multicomponent batch distillation columns, operating under variable reflux and constant reflux conditions. The method is essentially a modification of the short-cut method widely used in the design of continuous multicomponent columns. The technique has been tested for both binary and multicomponent systems, and the results compare favorably with the rigorous methods of design. The method is very efficient and can be used for preliminary design and analysis of batch columns. The model used in this method has a number of tuning parameters that can be used for model adaptation. The main features of the short-cut method include lower computational time (which is independent of the number of plates in the column), lower memory requirements, and its adaptability to design.

1. Introduction

The design of a batch distillation column is much more complex in comparison with that of a continuous distillation column as it requires consideration of unsteady-state behavior. The complexity of the problem increases with the number of components in multicomponent systems.

The batch distillation column can be designed by taking into account two possible modes of operation: (1) variable

reflux and constant product composition of (a) all components and (b) one component; (2) constant reflux and variable product composition.

The design methods developed to date have some disadvantages. Most of the approaches are derived from the classical McCabe Thiele's method, which, for the batch distillation case, calls for an iterative solution procedure. Chao (1954) proposed a short-cut method based on the absorption separation factor method. Rose et al. (1950) and Houtman and Hussain (1956) have used the pole-height concept for design, which depends on the width of the intermediate fraction and is applicable only to sharp separations.

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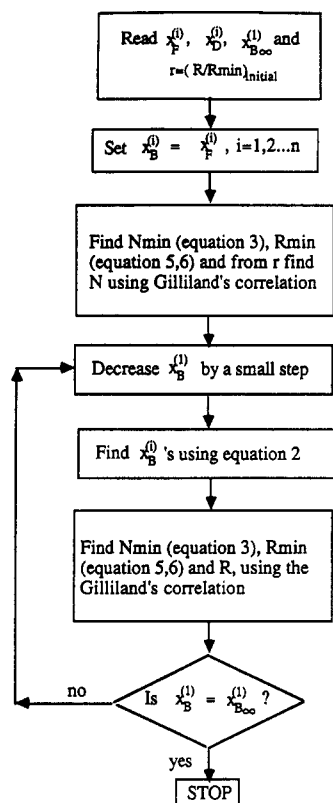


Figure 1. Design procedure for variable reflux condition (section 2.1.1).

The above methods are applicable only for binaries. The pole-height concept can be extended to a multicomponent system by assuming pseudobinaries.

All of the above work pertain to the constant reflux case. Rose (1979) has presented a model for the variable reflux case, considering a nonideal system, which takes large computational time and memory. However, this does not take into consideration the holdup effect.

A rigorous approach to simulation of a batch column that takes into account the plate holdup requires the use

Table I. Input Conditions and Maximum Percent Deviation in Key Component Still Composition (Variable Reflux Case)

no.	α_i	N	X_B^1	% dev
1	1.70	15	0.9	
	1.16			
	1.00			
2	2.0	20	0.9	
	1.5			
	1.0			
3	1.7	8	0.98	2.1
	1.16			
	1.0			
4	1.7	11	0.95	2.0
	1.16			
	1.0			
5	1.7	10	0.98	5.7
	1.16			
	1.0			
6	2.4	9	0.95	8.1
	1.0			
	1.0			
7	2.4	5	0.95	13.7
	1.0			
	1.0			

of dynamic models (Meadows, 1963; Distefano, 1968). Some of the commercial simulators (Boston et al., 1981) have this provision for simulation of batch columns. The use of a dynamic model requires a considerable amount of data and extensive computation time. Recently Galindez and Fredenslund (1988) proposed a method for rigorous simulation of batch columns, which assumes quasi-steady-state approximation at each time step Δt . The method is more efficient, but the accuracy of the results does depend upon the proper choice of Δt .

It is clear, therefore that there is a pressing need for the development of an efficient short-cut algorithm for multicomponent batch distillation that can be applied to both variable and constant reflux cases.

2. The Algorithm

This method is based on the reasonable approximation that the batch distillation column can be considered as a continuous distillation column with changing feed. In

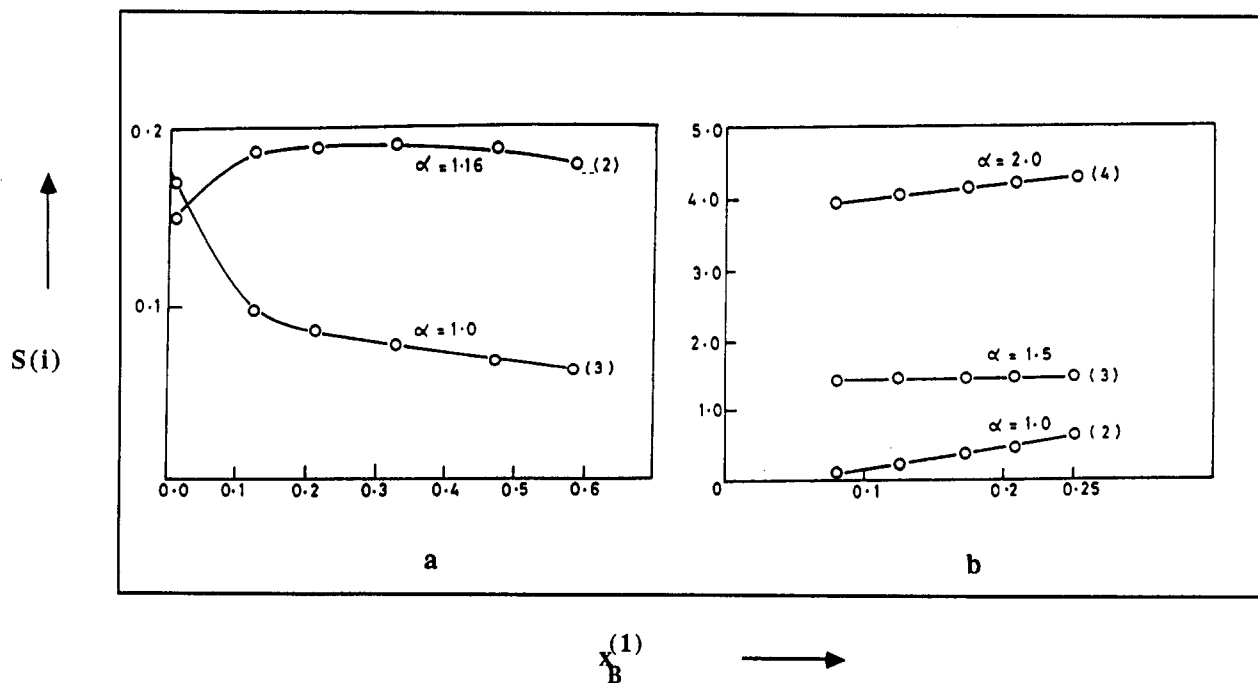


Figure 2. Sensitivity analysis (cases 1 (a) and 2 (b), Table I).

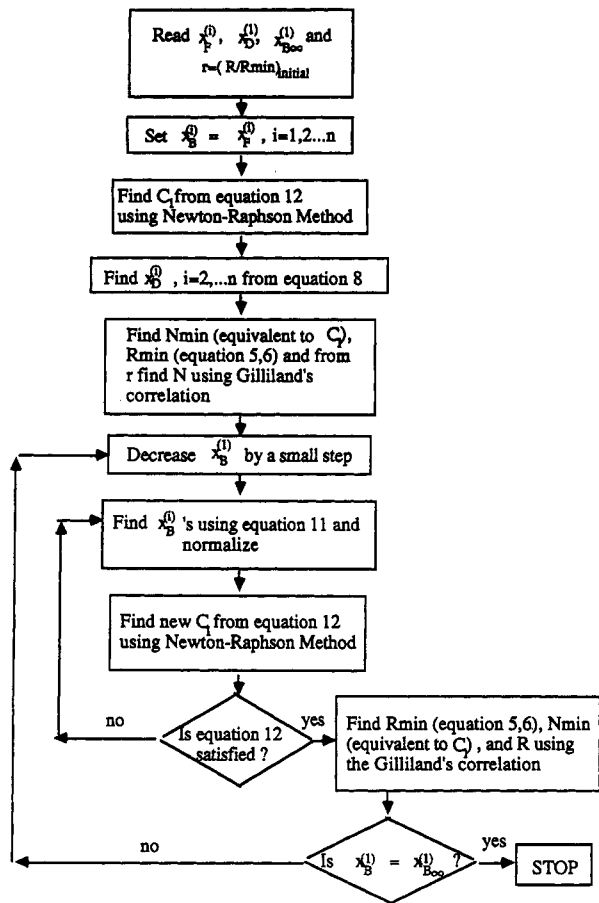


Figure 3. Design procedure for variable reflux condition (section 2.1.2).

other words, the bottom product of one time step forms the feed of the next time step. Note that the feed enters at the bottom plate and is at the boiling point. The Fenske–Underwood–Gilliland (FUG) method, which is widely used in continuous columns, has been modified to incorporate batch column design.

The batch time is implicit in the present analysis and can be calculated if the vaporization rate of the reboiler is known. For a small interval of time, the differential change of one component is considered. The relative changes of other component compositions are difficult to calculate for a multicomponent case, but this analysis makes it possible. In the following section, we will consider the development of the method for variable and constant reflux cases.

2.1. Variable Reflux Case. In this case, the short-cut method is developed initially for the assumption of constant product compositions of all the components. The validity of this assumption is checked by sensitivity analysis and a modified procedure is evolved to handle cases of changing compositions of the nonreference components.

2.1.1. Constant Product Compositions of All the Components. In this case, the product composition ($x_B^{(i)}$, $i = 1, 2, \dots, n$) is assumed to be constant throughout the operation. The differential material balance can be written as

$$d \ln (B/F) = dx_B^{(i)} / (x_B^{(i)} - x_B^i), \quad i = 1, 2, \dots, n \quad (1)$$

where x_B^i is the composition of the i th component in the still at any time t . If component 1 is taken as the reference, then the variation of composition of any other component

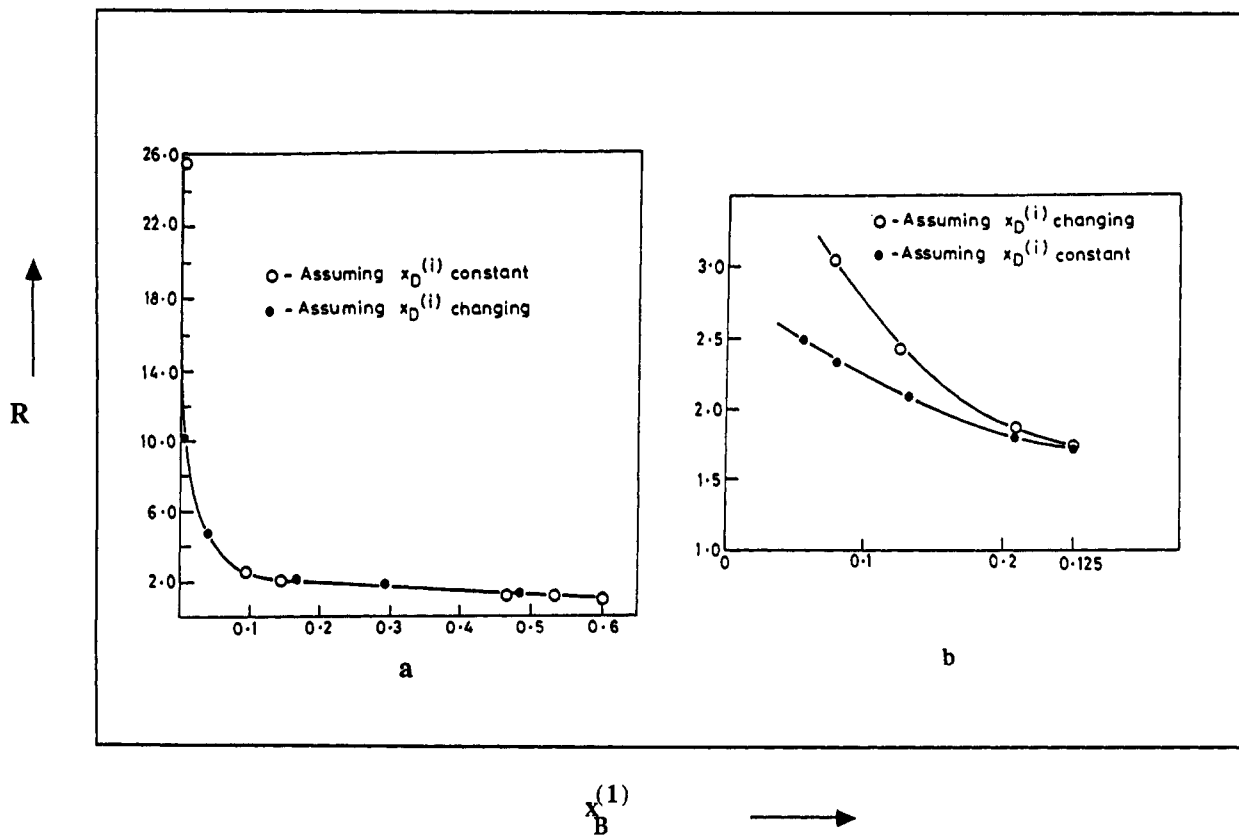


Figure 4. Comparison of R profiles (cases 1 (a) and 2 (b), Table I).

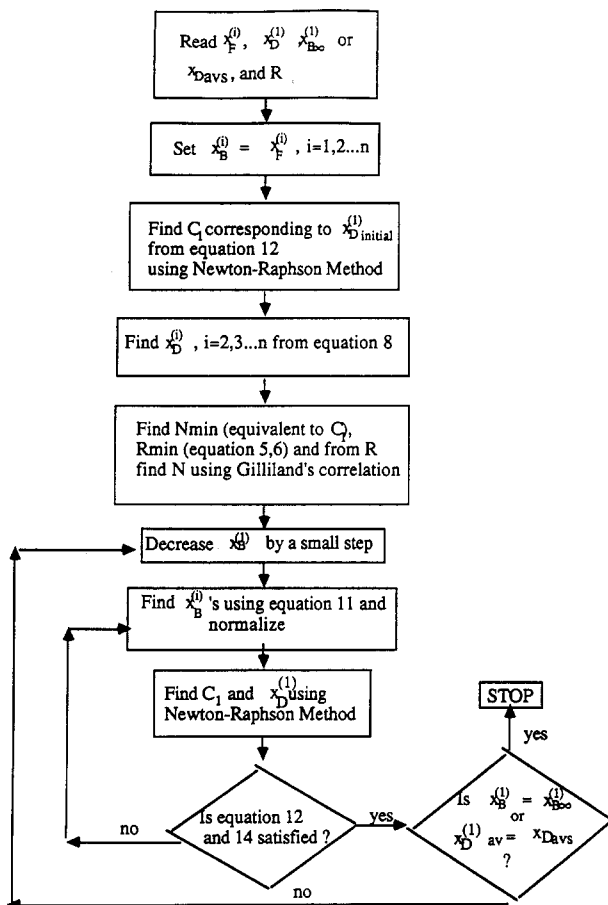


Figure 5. Design procedure for constant reflux condition (section 2.2).

i with respect to component 1, is given by the equation

$$x_B^i = x_B^i - \left[\frac{x_B^i - x_F^i}{x_B^i - x_F^i} (x_B^i - x_B^i) \right], \quad i = 2, 3, \dots, n \quad (2)$$

Once the still compositions are known at any time, the FUG method could be applied, resulting in the following equations:

Fenske equation

$$N_{\min} = \frac{\ln [x_B^k x_B^{hk} / x_F^k x_F^{hk}]}{\ln [\alpha_k / \alpha_{hk}]} \quad (3)$$

Underwood equations

$$1 - q = \sum_{i=1}^n \frac{\alpha_i x_F^i}{\alpha_i - \phi} \quad (4)$$

$$R_{\min} + 1 = \sum_{i=1}^n \frac{\alpha_i x_B^i}{\alpha_i - \phi} \quad (5)$$

with the feed at the boiling point ($q = 1$), eq 4 becomes

$$0 = \sum_{i=1}^n \frac{\alpha_i x_B^i}{\alpha_i - \phi} \quad (6)$$

Since, in this case, the x_B^i ($i = 1, 2, \dots, n$) are fixed, it follows that N_{\min} and R_{\min} are functions of x_B^i (x_B^i values in turn are dependent on x_B^i). Then the Gilliland correlation can be used to obtain the values of R .

The flow chart for the design procedure is shown in Figure 1.

The assumption that under variable reflux the product compositions of all the components can be held constant is not strictly valid. While the reflux can be varied to hold composition of the reference component 1 constant, the compositions of other components are expected to vary.

In order to estimate the variation of compositions of the nonreference components, a sensitivity function $S(i)$ has been defined as

$$S(i) = \frac{dx_B^i/x_B^i}{dx_B^1/x_B^1}, \quad i = 2, 3, \dots, n \quad (7)$$

From a study of the variation of $|S(i)|$ with x_B^1 , one can assess the extent of variation of compositions of nonreference components with x_B^1 (Appendix I).

The variation of $|S(i)|$ with x_B^1 is presented in Figure 2a,b, for cases 1 and 2 of Table I, respectively.

For the system shown in Figure 2a, C_1 , the Hengstebeck-Geddes constant (eq 8) is small, so $|S(i)|$ is decreasing for component 2 but is increasing for component 3 as x_B^1 is decreasing. If the maximum value of $|S(i)|$ ($S(2) = 0.18$) is small, one need not consider the composition changes of nonreference components. However, for the problem in Figure 2b, C_1 is large, hence $|S(i)|$ is decreasing with decreasing x_B^1 , for all the components. Since the maximum value of $|S(i)|$ ($S(4) = 4.27$) is large, it is necessary to consider a design procedure that can account for the composition changes of the nonreference components in the product.

2.1.2. Consideration of Composition Changes of the Nonreference Components. Here the application of the short-cut method becomes a little more complex as x_B^i ($i = 2, 3, \dots, n$) is not constant.

In order to relate the compositions in the still and overhead, the Hengstebeck-Geddes (Hengstebeck, 1946; Geddes, 1958) equation and the differential material balance equations are used.

Hengstebeck-Geddes equation

$$\frac{x_B^i}{x_B^1} = \left(\frac{\alpha_i}{\alpha_1} \right)^{C_1} \frac{x_B^i}{x_B^1}, \quad i = 2, 3, \dots, n \quad (8)$$

differential material balance equation

$$dx_B^i/(x_B^i - x_B^1) = dx_B^1/(x_B^1 - x_B^1), \quad i = 2, 3, \dots, n \quad (9)$$

$$\sum_{i=1}^n x_B^i = 1 \quad (10)$$

Integrating the material balance equation and substituting in eq 8 yields

$$x_{B_{\text{new}}}^i = x_{B_{\text{old}}}^i \exp \left[\frac{\Delta x_B^1}{(x_B^1 - x_B^1)} \left(\left(\frac{\alpha_i}{\alpha_1} \right)^{C_1} \frac{x_B^i}{x_B^1} - 1 \right) \right] \quad (11)$$

Combining eqs 9-11 gives

$$G(1) = \sum_{i=1}^n \left(\frac{\alpha_i}{\alpha_1} \right)^{C_1} \frac{x_{B_{\text{new}}}^i}{x_B^1} x_B^i - 1 = 0 \quad (12)$$

[The above equations are obtained by substituting new values of x_B^i and x_B^1 in the integration of eq 9. However, the derivation of the equation permits the use of old values, which reduces the computation time further, and is used by Diwekar et al. (1987).] The objective is to determine the value of C_1 , using the Newton-Raphson method for the solution of eq 12.

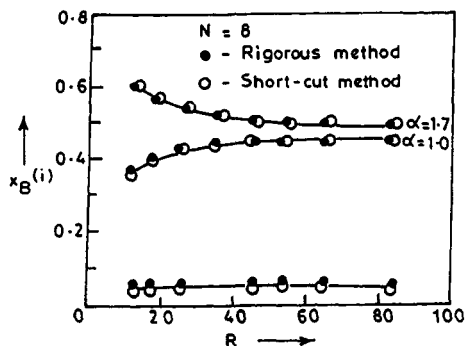


Figure 6. Composition profiles, variable reflux condition (case 3, Table I).

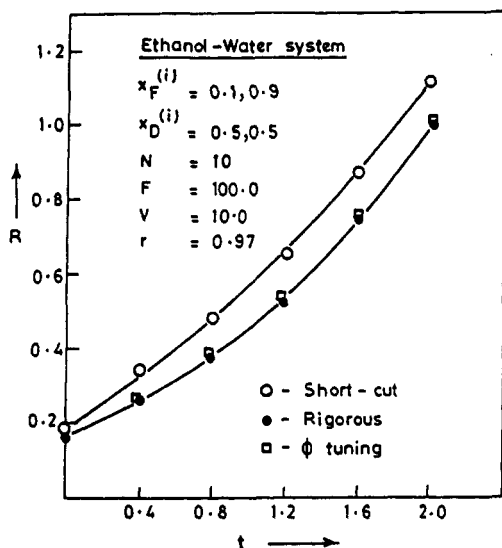


Figure 7. Reflux rate profile for a nonideal system (ethanol-water, variable reflux).

Since the intermediate values of x_B^i may not add up to unity, these values are transformed into normalized variables, x_{BN}^i :

$$x_{BN}^i = x_{B_{new}}^i; \quad x_{BN}^i = \frac{x_{B_{new}}^i}{\sum_{j=2}^n x_{B_{new}}^j} (1 - x_{B_{new}}^1), \quad i = 2, 3, \dots, n \quad (13)$$

These normalized variables are included in eq 12.

After obtaining the value of C_1 , x_D^i values can be calculated from eq 8 and the Underwood equation can be solved to obtain R_{min} . Assuming equivalence of C_1 to N_{min} , R can be obtained by using the Gilliland correlation.

The flow chart for the design procedure is shown in Figure 3.

A comparative study of the reflux ratio profile obtained by applying the methods developed in sections 2.1.1 and 2.1.2 to cases 1 and 2 (Table I) is presented in Figure 4a,b.

For case 1, the maximum value of $S(i)$ is small; hence the difference between the two profiles is marginal (Figure 4a), and the changes in product composition can be neglected, so the design procedure shown in Figure 1 can be used.

For case 2, the maximum value of $S(i)$ is large; the difference between the two profiles is large, as can be seen from Figure 4b. Hence, it is necessary to consider the composition changes, and the design procedure shown in Figure 3 can be used.

2.2. Constant Reflux Case. In the constant reflux case, the product compositions x_D^i , ($i = 1, 2, \dots, n$) vary with

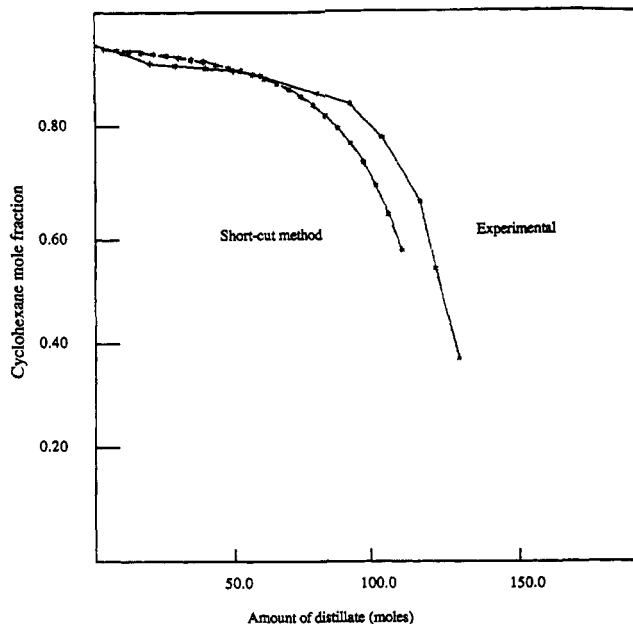


Figure 8. Experimental and theoretical distillation curves for a nonideal system (cyclohexane-toluene).

x_D^i . (To initiate the design procedure an initial value of x_D^i is to be specified for $x_B^i = x_D^i$.) Since x_D^i is changing in this case, an additional equation is needed to satisfy the extra degree of freedom. Assuming that C_1 is equivalent to N_{min} , $R_{min,g}$ calculated from the Gilliland correlation can be equated with the $R_{min,u}$ calculated from the Underwood equation (eq 5) to provide the following equation, which can relate R , N , C_1 , and compositions:

$$G(2) = \frac{R_{min,g}}{R} - \frac{R_{min,u}}{R} = 0 \quad (14)$$

Equations 12 and 14 can be solved to obtain the unknowns C_1 and x_D^i for a given change in x_B^i . For this, the Newton-Raphson method can be utilized. In order to handle the constraint on x_D^i (eq 15)

$$x_B^i < x_D^i < 1 \quad (15)$$

a variable transformation is done as follows:

$$x_D^i = x_B^i + \frac{1 - x_B^i}{1 + XM} XM \quad \text{for } XM > 1$$

$$= x_B^i + \frac{1 - x_B^i}{3 - XM} \quad \text{for } XM \leq 1$$

$$\text{as } XM \rightarrow +\infty, x_D^i \rightarrow x_B^i, \quad \text{and as } XM \rightarrow -\infty, x_D^i \rightarrow 1 \quad (16)$$

For $XM = 1$, both equations give the same solution.

The flow chart for the design procedure is given in Figure 5.

3. Algorithm Verification

The validity of the proposed procedure has been tested extensively for the problems in Table I for variable reflux and the problems in Table II for constant reflux conditions.

3.1. Variable Reflux Case. For each of the test cases, the R profile calculated by the short-cut method is used in the plate-to-plate method to estimate the still compositions. Table I gives the input conditions for the sample problems, and it also shows the comparison of the results using the proposed short-cut method and the plate-to-plate calculations in terms of the maximum percent deviation

Table II. Input Conditions and Maximum Percent Deviation in Composition of Key Components and Number of Plates (Constant Reflux Case)

no.	α_i	R	X_D^1	max % dev		% dev N
				X_D^1	X_B^1	
1	1.7, 1.16, 1.0	3	0.9412	<1	<1	2.25
2	2.0, 1.5, 1.0, 0.5	10	0.7400	<1	<1	3.2
3	2.0, 1.5, 1.0, 0.5	20	0.7400	2.9	3.8	1.45
4	1.7, 1.16, 1.0	3	0.8962	<1	<1	7.4
5	1.7, 1.16, 1.0	20	0.9482	<1	<1	<1
6	1.7, 1.16, 1.0	5	0.9183	<1	<1	<1
7	1.7, 1.16, 1.0	3	0.9349	<1	<1	1.8
8	1.7, 1.16, 1.0	10	0.9200	<1	<1	3.0

for the key component still composition.

It can be seen that the deviation is within the acceptable limits.

For a specific case of a ternary system (case 1, Table I) detailed results are shown in Figure 6. The profiles predicted by the short-cut method correspond closely to the profiles obtained from the plate-to-plate calculation.

3.2. Constant Reflux Case. For each of the test cases, the composition profiles and the number of plates N obtained by the plate-to-plate method (Robinson, 1975) are compared with the composition profiles and value of N obtained by the short-cut method, using the same value of reflux ratio R and the initial x_D^1 .

Table II gives the input conditions for the sample problems, and it also shows the comparison of the results in terms of the maximum percent deviation in the key component compositions and percent deviation in N . It can be seen that the deviations are small.

Table III shows the comparison of the results of the short-cut method, with BATCHFRAC (Boston et al., 1981) results, for the quaternary system consisting of propane, butane, pentane, and hexane. The CPU time required to solve this problem for the five fractions is 5 s on an ND560 (supermini, equivalent to VAX 11/785) system, compared to the time of 1.9 min on IBM 370 of BATCHFRAC.

In both cases the time constant τ of the stage ($\tau = \text{holdup}/(\text{reflux ratio } X \text{ distillate rate})$) is not large, so the results agree well.

4. Modification of the Short-Cut Method

The short-cut method has been tested extensively on a number of binary and multicomponent cases with the assumption of constant α and not for nonideal systems and columns with dominant holdup effects. It will be of interest to assess the capability of the method to handle nonideal systems and also situations where the holdup can be substantial.

4.1. Nonideal Systems. To analyze the capability of the short-cut method used in this study to simulate nonideal systems, problems on two systems have been studied, namely, ethanol-water and methanol-water with the assumption of the negligible holdup. Further experimental results reported by Domench and Enjalbert (1974) for the nonideal system consisting of cyclohexane and toluene with holdup are compared with the short-cut method.

Instead of constant α being used throughout the course of the distillation, the value of α is updated at each step by using appropriate correlations, to estimate the α values at the top and bottom of the columns. Here for the ethanol-water and the methanol-water systems, the values of α at the top and bottom are estimated at each step by the UNIQUAC equation and averaged by

$$\alpha = (\alpha_{\text{top}}\alpha_{\text{bottom}})^{1/2}$$

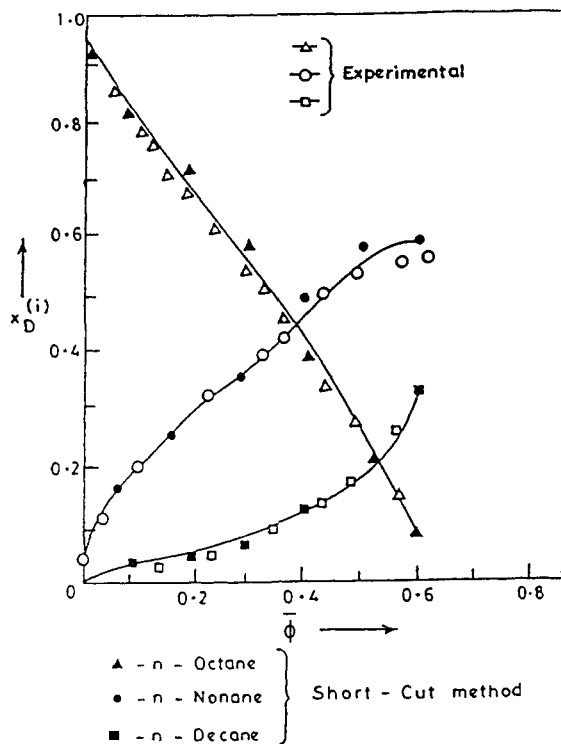


Figure 9. Experimental and theoretical distillation curves, ternary system (constant reflux).

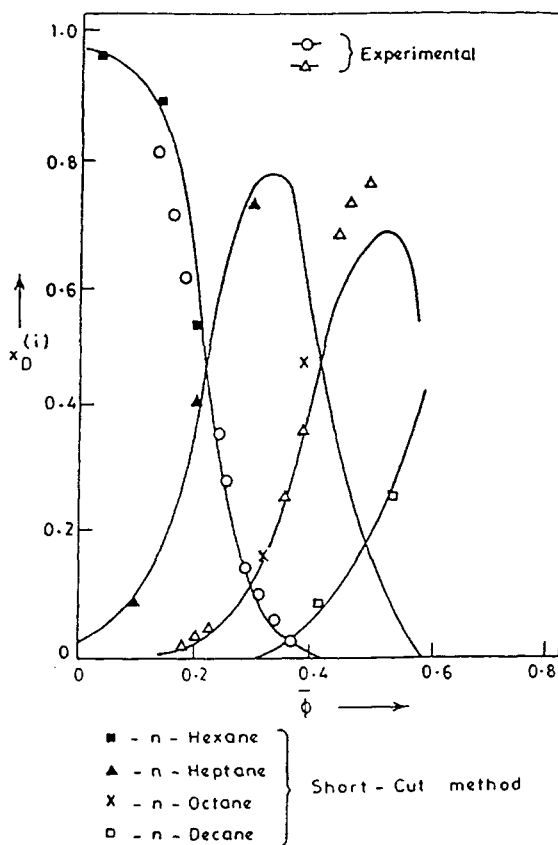


Figure 10. Experimental and theoretical distillation curves, five-component system (constant reflux).

A comparison of the results obtained by the short-cut method and the rigorous method are shown in Figure 7 for the specific case of the ethanol-water system.

In the case of cyclohexane and toluene, the UNIFAC method is used, and the results obtained are shown in Figure 8.

Table III. Comparison of Results of BATCHFRAC (Boston et al., 1981) with the Short-Cut Method

	propane removal				butane removal		pentane removal			
	fraction 1		fraction 2		fraction 3		fraction 4		fraction 5	
	BATCHFRAC	short-cut	BATCHFRAC	short-cut	BATCHFRAC	short-cut	BATCHFRAC	short-cut	BATCHFRAC	short-cut
reflux ratio	5	5	20	20	25	25	15	15	25	25
distillate rate	2	2	2	2	2	2	2	2	2	2
vapor rate	12	12	42	42	52	52	32	32	52	52
time	4.07	4.07	1.81	1.81	18.27	18.20	4.31	4.31	1.78	1.78
Distillate Composition (Mole Fraction)										
propane	0.8000	0.8173	0.0150	0.0190						
butane	0.2000	0.1817	0.9850	0.9742	0.1644	0.1593				
pentane				0.0063	0.8356	0.7521	0.8000	0.7638	0.0161	0.0168
hexane				0.0005		0.0886	0.2000	0.2362	0.9839	0.9832
Average Distillate Composition, at the End of Each Fraction (Mole Fraction)										
propane	0.9888	0.9853	0.5230	0.5220	0.0002					
butane	0.0112	0.0145	0.4770	0.4750	0.9900	0.9915	0.0058	0.0050		
pentane				0.0026	0.0098	0.0077	0.9845	0.9840	0.2994	0.3044
hexane				0.0004		0.0008	0.0097	0.0110	0.7006	0.6956
	8.1321	8.1220	3.6130	3.6000	36.543	36.388	8.6020	8.6015	3.6000	3.5390
Pot Composition (Mole Fraction)										
propane	0.0206	0.0217		0.0001						
butane	0.3254	0.3252	0.3191	0.3193	0.0006	0.0006				
pentane	0.1090	0.1088	0.1135	0.1134	0.1335	0.1335	0.0173	0.0174	0.0002	0.0002
hexane	0.5450	0.5442	0.5674	0.5672	0.8658	0.8658	0.9827	0.9826	0.9998	0.9998
	91.7350	91.8780	88.1240	88.1360	71.6000	71.7360	62.9980	62.9985	59.3890	59.4580

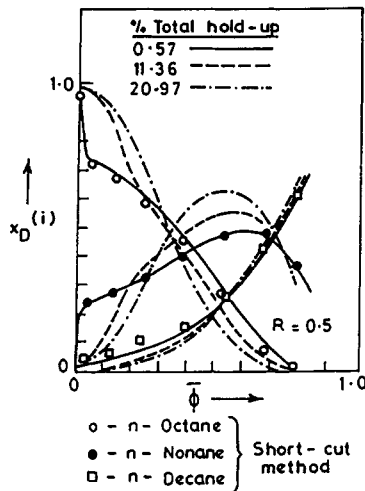


Figure 11. Theoretical distillation curves, ternary system (constant reflux).

Though the profiles obtained by the two methods do not agree on an absolute scale, it can be seen that the trend of profiles obtained by the short-cut method is very close to that obtained by the rigorous method.

In order to force agreement between the short-cut and the rigorous cases, it may be necessary to look for tuning parameters in the short-cut model. Any discrepancies in ϕ to certain extent accommodated in updating the value of C_1 at each step (eq 12). Another parameter that could be explored as a tuning parameter is the value of ϕ , which occurs in the Underwood equation.

$$R_{\min} + 1 = \sum_{i=1}^n \frac{\alpha_i - x_b}{\alpha_i - \phi_{\text{tun}}} \quad (17)$$

where

$$\phi_{\text{tun}} = \gamma_1 \phi$$

ϕ is calculated from eq 6 using the estimated value of α_i .

With use of the simulation results obtained from the rigorous method, parameter γ_1 can be obtained by using either an initial estimate of α_i or an estimate of α_i over some part of the curve so that the deviation is minimum.

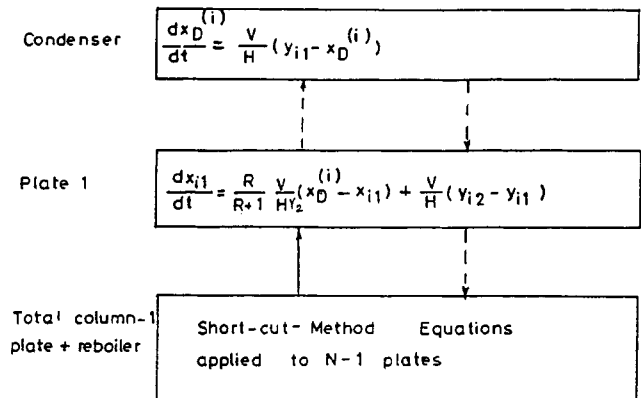


Figure 12. Batch distillation column, modified short-cut method model.

A comparison of the results of the tuned short-cut method with those of the rigorous case is shown in Figure 7 for the nonideal ethanol-water system. The proposed tuning procedure appears to be effective in handling the nonidealities.

4.2. Incorporation of the Holdup. To estimate the effect of holdup on the performance of the method, the results obtained by Stewart et al. (1973) are compared with the results obtained by our short-cut method (Figures 9-11). Here the initial total reflux condition is simulated by 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 the composition (Figure 11). This is due to the large time constant τ associated with large holdup and low reflux ratio ($\tau = \text{holdup}/(\text{reflux ratio} \times \text{distillate rate})$).

The short-cut method needs to be modified for such dynamic situations where the state variables associated with the plates have a dominant dynamic character.

In a batch distillation, the input variable that changes significantly is the reflux ratio. If one examines the transition from total reflux to a finite reflux condition, the

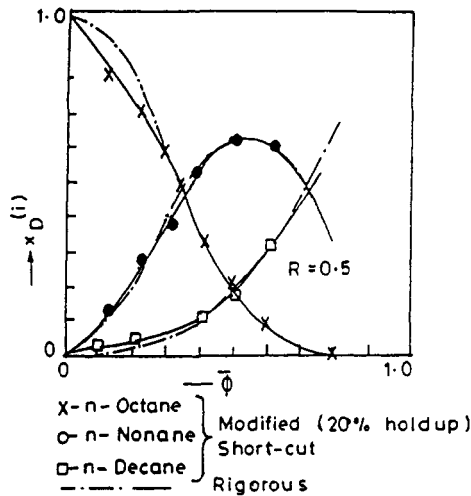


Figure 13. Theoretical distillation curves, ternary system.

short-cut method, which neglects holdup effect, predicts a sharp drop in the product composition (Figure 11), while in the actual case the top product composition varies in a gradual manner. To account for this dynamic effect, a lumped dynamic element is assumed to be located at the top of the column. A quasi-steady-state approximation is assumed for the remaining part of the column from the reboiler to the first plate, as the composition changes are slower in this part of the column. The short-cut method is used for that section of the column (Figure 12).

The modified form of the short-cut method involves the following: (1) dynamic model for the top plate 1 and the condenser; (2) short-cut method equations for $N - 1$ plates and reboiler.

The short-cut method equations use the compositions predicted by the dynamic model at the top, at each time step.

The results obtained by the modified short-cut method are compared with those obtained by using the rigorous dynamic model (Figure 13).

As can be seen in the figure, the inclusion of dynamic effect in the short-cut model permits closer correspondence with those predicted by the rigorous model. The holdup value of the lumped element at the top can be adjusted to forge a closer match with the results of the rigorous model. (Here, in this example the holdup is taken equal to the plate holdup only.)

For columns with a large number of plates, a single lumped element may not be adequate to represent the holdup effect; an appropriate model order may have to be chosen to represent the resulting dynamic effect.

5. Conclusions and Significance

The short-cut method proposed has been tested as a tool for both, preliminary design and optimization of batch distillation columns. An advantage of this method is that the increase in the number of plates does not affect the computation time and memory requirements. The presence of tuning parameters in the model permits the inclusion of nonideal behavior. The dynamic effect of holdup can be accommodated by inclusion of lower order models near the top of the column for the cases where the reflux rate is the major manipulated variable. The modified short-cut method, which incorporates the tuning parameters and the holdup effects, can be used for on-line application with adaptation features.

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Nomenclature

- B = amount of material remaining in the still
 C_1 = Hengstebeck-Geddes constant
 F = amount of feed
 H = plate holdup
 H_D = condenser holdup
 hk = heavy key component
 lk = light key component
 n = number of components
 N = number of plates
 N_{min} = minimum number of plates
 q = feed condition, the Underwood equation
 $r = (R/R_{min})_{initial}$
 R = reflux ratio
 R_{min} = minimum reflux ratio
 $R_{min,g}$ = minimum reflux ratio using the Gilliland correlation
 $R_{min,u}$ = minimum reflux ratio using the Underwood equation
 R_t = reflux ratio at time t
 t = time
 V = vapor boilup rate of reboiler
 x_{ij} = liquid composition of component i , leaving plate j
 x_B^i = still composition of component i
 $x_{B\infty}^i$ = final still composition of component i
 x_{Dav}^i = average distillate composition of component i
 $x_{Dav_s}^i$ = specified average composition of component i
 x_D^i = distillate composition of component i
 x_F^i = feed composition of component i
 y_{ij} = vapor composition of component i , leaving plate j
 y_B^i = vapor composition of component i , leaving the still
- Greek Symbols**
 α_i = relative volatility of component i
 ϕ = Underwood equation constant
 ϕ = fraction distilled

Appendix I. Sensitivity Analysis for Variable Reflux Case

The sensitivity function $S(i)$ defined by eq 7 can be obtained by the procedure given below:

from eq 8

$$\frac{dx_B^i}{dx_B^{(1)}} = \left(\frac{\alpha_i}{\alpha_1}\right)^{C_1} \frac{x_B^i}{x_B} \frac{dx_B}{dx_B} - \left(\frac{\alpha_i}{\alpha_1}\right)^{C_1} \frac{x_B^i}{(x_B^i)^2} x_B^i + \left(\frac{\alpha_i}{\alpha_1}\right)^{C_1} \left[\ln \left(\frac{\alpha_i}{\alpha_1}\right) \right] \frac{x_B^i}{x_B} \frac{dC_1}{dx_B}, \quad i = 2, 3, \dots, n \quad (A1.1)$$

from eq 10

$$\frac{dx_B^i}{dx_B} = \frac{x_B^i}{x_B} \left[\frac{(x_B - x_B^i)}{(x_B - x_B^i)} - \frac{x_B^i}{x_B} \right] + x_B^i \left[\ln \left(\frac{\alpha_i}{\alpha_1}\right) \right] \frac{dC_1}{dx_B} \quad (A1.2)$$

Since $\sum_{i=2}^n dx_B^i = 0$,

$$\frac{dC_1}{dx_B} = \frac{\left[\sum_{j=2}^n \frac{x_B^j}{x_B^1} \left[\frac{(x_B^j - x_B^1)}{(x_B^j - x_B^1)} - \frac{x_B^j}{x_B^1} \right] \right]}{\left[\sum_{k=2}^n x_B^k \ln \left(\frac{\alpha_k}{\alpha_1} \right) \right]} \quad (\text{A1.3})$$

and substituting in eq A1.2 gives

$$S(i) = \frac{dx_B^i/x_B^1}{dx_B^i/x_B^1} = \left[\left(\left(\frac{\alpha_i}{\alpha_1} \right)^{C_1} \frac{x_B^i}{x_B^1} - 1 \right) / \left(\frac{x_B^i}{x_B^1} - 1 \right) - 1 \right] - \left(\left(x_B^i \ln \left(\frac{\alpha_i}{\alpha_1} \right) \right) / \left(\sum_{k=2}^n x_B^k \ln \left(\frac{\alpha_k}{\alpha_1} \right) \right) \right) \times \left[\sum_{k=2}^n \left(\frac{\alpha_k}{\alpha_1} \right)^{C_1} \left(\left(\left(\frac{\alpha_k}{\alpha_1} \right)^{C_1} \frac{x_B^k}{x_B^1} - 1 \right) / \left(\frac{x_B^k}{x_B^1} - 1 \right) - 1 \right) \right] \quad (\text{A1.4})$$

For components having a closer relative volatility, $\alpha_i \rightarrow \alpha_1$: i.e., for the limit $\alpha_i \rightarrow \alpha_1$, $S(i) \rightarrow 0$.

It can be seen from eq A1.4 that for large values of C_1 (C_1 increases as x_B^1 decreases), $(\alpha_k/\alpha_1)^{C_1}$ is small, so

$$|S(i)| \propto \left[1 / \left(\frac{x_B^i}{x_B^1} - 1 \right) + 1 \right] \quad (\text{A1.5})$$

for as x_B^1 decreases $|S(i)|$ decreases (Figure 2a). The initial value of $|S(i)|$ is sufficient to get the idea of whether or not composition changes should be considered.

For small values of C_1 (Figure 2a), the trend cannot be predicted initially. However, the maximum value among all the initial $|S(i)|$ ($i = 2, 3, \dots, n$) can still give a good estimate. This is generally true because in eq A1.4, since both the terms in square brackets are always negative, the maximum value of $|S(i)|$ is likely to occur when the magnitude of one of the terms is significantly higher than other. As an approximation one can assume that one of the terms will always be predominant and

$$\text{first term or second term} \propto \sum_{k=l}^m \left(\frac{\alpha_k}{\alpha_i} \right)^{C_1} \left[\left(\left(\frac{\alpha_k}{\alpha_1} \right)^{C_1} \frac{x_B^k}{x_B^1} - 1 \right) / \left(\frac{x_B^k}{x_B^1} - 1 \right) - 1 \right] = W \quad (\text{A1.6})$$

where $l = i$ and $m = i$ for the first term and $l = 2$ and $m = n$ for the second term.

Since $(\alpha_k/\alpha_1) < 1$ (1 being the most volatile component) as x_B^1 decreases, W decreases.

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