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# The Effects of Interstage Backmixing on the Design of a Multicomponent Distillation Column

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Interstage backmixing is encountered as entrainment in many distillation columns. Bidirectional backmixing is common in liquid-liquid extraction. These effects, which reduce the effectiveness of a separation process, may interfere with its operation even to the extent of shutdown. The design engineer and process operator need to recognize the effects of backmixing and must quantify them to take effective countermeasures. A procedure is developed which describes the effects of interstage bidirectional backmixing in multistage separations. It is implemented on an existing simulation for multicomponent distillation and is used to show the effect of backmixing on product purity as well as on the temperature and bulk flow profiles within the column. These profiles are compared with profiles generated by the specification of nonequilibrium stages to obtain the same product purity. The designer may then identify backmixing and nonequilibrium effects independently and allow for them quantitatively in his design.

## Introduction

Entrainment and deviation from equilibrium are the major factors which prevent distillation and extraction units from operating as counter-current equilibrium processes. The increasing requirement for more precision in column design forces the engineer to include both effects quantitatively in his work. Entrainment arises in a column as a result of interstage hydraulics but incomplete mass transfer upon a stage leads to stage product streams which have not reached equilibrium. The disparate origins of these factors require their independent evaluation and consideration in process design work.

The standard measure of nonequilibrium is an efficiency factor such as that developed by Murphree (1925). The efficiency factor may be used to draw a pseudo-equilibrium line on a McCabe-Thiele diagram or to locate an actual overflow composition on a phase envelope. When greater precision is required, an efficiency factor may be included in the material balance algorithm of a multistage multicomponent separator program. It may be stated directly (Holland, 1963) or indirectly (Holland, 1963; Waggoner and Loud, 1977). Nonequilibrium may thus be included in the column design for either an approximate or a very precise representation.

Entrainment has been studied for many years and procedures for including its effects in the operating line of a McCabe-Thiele diagram have been presented as early as 1934 (Rhodes) and as recently as 1977 (Standart *et al.*). The causes of entrainment have been identified (Kageyama, 1969) and the relation of entrainment to tray hydraulics has been described (Fair and Matthews, 1958). A procedure is presented to enable the design engineer to use the estimate of the entrainment present in a column to determine its effect on column operations and separations when he is working with a conventional multicomponent distillation program.

When a computer program is used to aid distillation design the approach is altered from the one used for a graphical design. Graphical methods (McCabe-Thiele, Ponchon-Savarit, etc.) are design procedures. The product qualities are specified, the operating rates chosen, and the diagrams are drawn to determine the number of stages needed for the separation. In contrast, the computer programs are rating methods. The tower design is first completely described and the program is used to determine its internal operating rates and its product separation. The design parameters are then adjusted and the program re-run until the desired product separation is

achieved. To effectively use the rating program and, also, include entrainment effects in a design, the engineer must develop an understanding of the ways in which entrainment affects the operating rates and product qualities and how its effects are evident in the data he obtains from the program.

## Entrainment in Distillation Columns

Entrainment has long been recognized as a problem in distillation. In column operation increased entrainment may lead to flooding evidenced by excessive holdup in the downcomer (Hausch, 1964) and may reach the point that the column becomes inoperable (Teller and Rood, 1962). The work of Fair and Matthews (1958) relates entrainment to an approach to flooding in which the liquid in the column continues to recirculate between adjacent trays and little material continues down from stage-to-stage. Even though tray hardware has been designed to minimize the effect of entrainment (Nutter, 1971) it still constitutes an important operating problem and a source of concern in column design.

The effect of occlusion has seldom been included in distillation studies. When it has been observed, the column has been operating close to a flooding point (Martin, 1975) and the actions taken by the operator to avoid flooding would eliminate the occlusion.

**Entrainment Results from Hydraulic Effects.** The rate of entrainment,  $E_j$ , is a function of a number of operational parameters, particularly the gas to liquid ratio on each tray (Kageyama, 1969). Sherwood and Jenny (1935) determined that the rate of entrainment is an increasing function of the boil-up rate. The work of Fair and Matthews (1958) confirms this effect and points out that the rate of entrainment can be expected to vary with the rate of the carrying vapor stream. An entrainment factor,  $e_j$ , may be defined (Colburn, 1936) so that the entrainment rate above each tray may be included in the material balances as the product term,  $e_j V_j$  (Figure 1).

Fair and Matthews (1958) define a similar entrainment factor,  $\Psi$ , as the ratio of the recirculating material to the total flow in the downcomer (Figure 2). The factor is a measure of the entrainment occurring and is related to the approach to flooding through tray hydraulics. They state that use of this factor is not meant to imply that the entrainment rate is a function of the overflow rate.

**Design Methods May Include Entrainment.** Over four decades ago, the effect of entrainment was introduced into

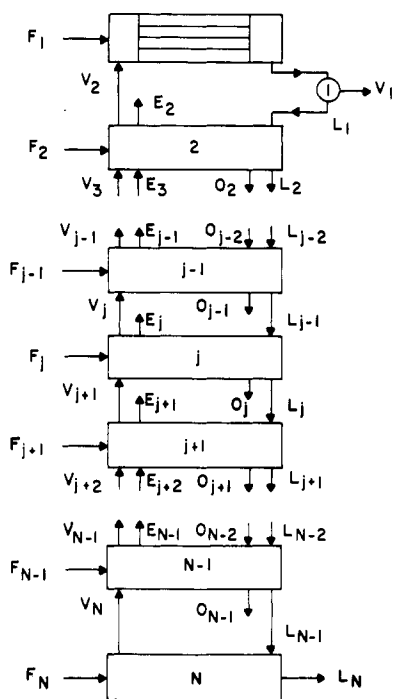


Figure 1. Interstage flow diagram for bidirectional backmixing.

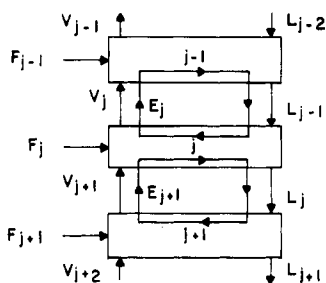


Figure 2. Recirculating entrainment flow described by Fair and Matthews (1958).

distillation design procedures. Rhodes (1934, 1935) and Sherwood and Jenny (1935) include entrainment factors in the McCabe–Thiele plot and develop a modified operating line. Colburn (1936) defined an apparent plate efficiency,  $E_a$ .

$$E_a = \frac{E_j^M}{1 + E_j^M \left( \frac{e_j V_j}{L_j} \right)} \quad (1)$$

This expression combined the effects of entrainment and deviation from equilibrium into a single factor which could be used to draw a conventional pseudoequilibrium line. It was never intended to imply that entrainment per se had an effect on the approach to equilibrium within the confines of the material held on the tray. It is necessary to combine the effects in order to obtain a single factor which could be included in the construction of the McCabe–Thiele diagram. The Colburn procedure was widely accepted and was recommended by AIChE (1958) in the “Bubble Tray Design Manual”. The approach of including entrainment in a single tray efficiency factor was studied in detail by Kageyama (1969), who determined a single plate efficiency factor as a function of several parameters in addition to point efficiency. These factors include the Peclet number and the weeping fraction, as well as entrainment.

Mecklenburgh and Hartland (1969) continued the development of graphical techniques to describe the separation of

binary mixtures. Their design method is a manual calculation which accounts for finite mass transfer, entrainment, occlusion, and variable molar enthalpy. Procedures have been presented for determining stage-to-stage compositions in the separation of a binary mixture (Standart and Kastanek, 1966; Rhodes, 1934). In the most recent work on entrainment, Standart et al. (1977) reexamine the apparent efficiency of Colburn (1936) and develop an expression designated as the reduced efficiency. They relate the overall plate efficiency to entrainment, point efficiency, and operating parameters without reference to Colburn’s hypothetical plate without entrainment. The method is implemented by using a modified operating line on a McCabe–Thiele construction. Graphical methods are limited to binary separations. The effect of entrainment on internal flows could be implied from the completed diagram, but with one exception (Mecklenburgh and Hartland, 1969) the effect of enthalpy on the bulk-flow rates is not considered in the computations.

**Entrainment Affects Multicomponent Distillation Operations.** In order for entrainment to be considered in multicomponent distillation design, it must be made a part of the computer program used to rate trial designs. When it is made an integral part of the material balance and energy balance algorithms, the designer may proceed with his parameter search without increasing his computer cost or time.

Since he works with a rating program in multicomponent distillation, the designer must consider the characteristics of entrainment in the column description as he adjusts his design parameters. An entrainment factor may be estimated from the operating parameters and fluid properties (Fair and Matthews, 1958; Kageyama, 1969). The rating program may be used to describe the column operation for the estimated entrainment and by manipulating the entrainment factor, the designer may determine whether the cost of reducing entrainment is justified in improved product separation.

Computer simulations described in this work have shown the effects of entrainment to be most evident in the overflow and boil-up rates and thereby to be significant in the reboiler and condenser duties. In the product streams, the middle components are distributed in a characteristic manner that permits entrainment to be identified separately from non-equilibrium. To illustrate the effects of entrainment on multicomponent distillation, a three-component hydrocarbon separation has been specified (Table I). The column description is obtained from a conventional digital computer program modified to include bidirectional backmixing in the material balance and energy balance algorithms. The following observations are obtained from a series of runs for this example.

#### The Effect of Entrainment on the Overhead Product.

Since entrainment characteristically carries the heavy components up the column, ideal separation cannot be achieved

Table I. Column Specifications<sup>a</sup>

Feed condition: boiling point liquid	
Feed composition (mole fraction):	0.30 <i>n</i> -pentane
	0.35 <i>n</i> -hexane
	0.35 <i>n</i> -heptane
Feed rate: 500 lb-mol/h	
Distillate rate: 250 lb-mol/h	
Reflux rate: 400 lb-mol/h	
Number of stages: 10	
Feed stage location: 5	
Type of condenser: total	
Column pressure: 300 psia	

<sup>a</sup> Thermodynamic data is taken from Appendix A of Holland (1963).

(Table IV). As the entrainment of a system is increased, the overhead product shows increasing quantities of the heaviest component and decreasing quantities of both the lighter components. The ratio of the light to the middle component remains nearly constant as entrainment increases.

**The Effect of Entrainment in the Column Profiles.** The first deviation noted from the desired operation is that a quantity of liquid is carried overhead from the top tray to the condenser. A similar quantity of liquid is carried into the froth on the top tray by vapor rising from the tray below it. The internal reflux from the top tray would, thus, not be appreciably changed by an increase in entrainment. So long as the rate of entrainment remains approximately the same from tray-to-tray the effect on the overflow rate down the column should not be appreciable. This effect does not extend to the bottom tray above the reboiler. This tray does not receive entrained liquid from the reboiler, but a portion of its material is entrained to the stage above, and as shown in Figure 5 the overflow to the reboiler is reduced. The next consequence is that, since the bottoms rate is determined by the material balance and the specified distillate rate, the boil-up rate must be reduced and consequently the reboiler duty is reduced as well (Table IV). There is no internal effect to make up the reduced boil-up rate so that vapor continues at a reduced rate up to the condenser (Figure 7).

Two phenomena take place to cause deviations in the temperature profile. The liquid feed to each stage is relatively unchanged in quantity but contains heavier material (from the stage below) than if there were no entrainment. The temperature on all stages would then be increased. The reduced boil-up reduces the mass transfer between phases on the tray. The individual trays and the entire column are used less effectively and the degree of separation throughout the tower is reduced. This effect would cause the stages in the rectifying section to operate with additional heavy material and thus show higher temperatures than for perfect interstage transfer. The stages in the stripping section, however, would operate with more lights and would exhibit reduced temperatures. The temperature profiles shown in Figure 3 indicate that the latter effect is predominant, illustrated by higher rectifying temperatures and lower stripping temperatures.

**The Effect of Occlusion on Column Operations.** If occlusion were to take place in the operation of a distillation

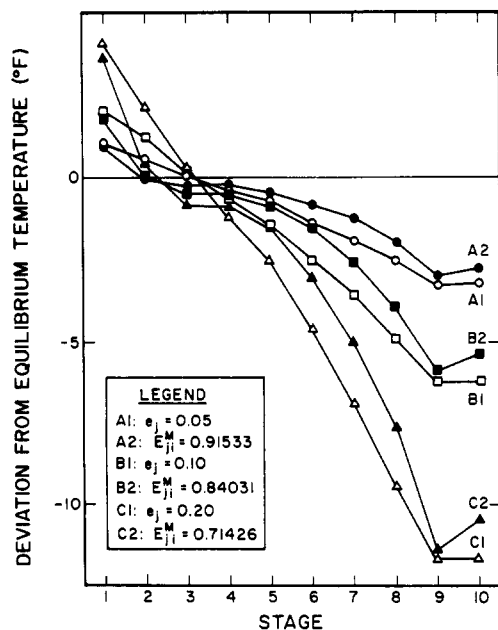


Figure 3. Effect of entrainment on the temperature profile of a distillation column.

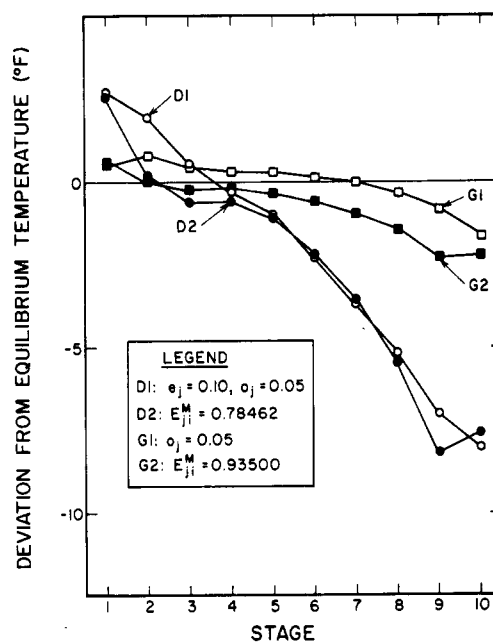


Figure 4. Effect of occlusion and bidirectional backmixing on the temperature profile of a distillation column.

column, the primary effect would be the deviation in the boil-up rates as shown in Figure 8. Even though internal recycle is increased, all of the increase in boil-up is diverted downward, entrapped in the liquid overflow, Figure 6. The ultimate effect is a less effective separation evident as increased tray temperatures in the rectifying section and lowered temperatures in the stripping section (Figure 4). This set of conditions, indicating occlusion, should warn the operator that the column may be approaching flooding conditions.

**A Material Balance Algorithm May Include Bidirectional Backmixing in Distillation Computations.** Entrainment and occlusion may be included in conventional multicomponent distillation computations if the algorithms used to solve the component-material balances for composition and the energy and bulk flow balances for bulk flow rates are modified to describe the flow pattern shown in Figure 1. The technique for modifying individual portions of larger multicomponent distillation programs has been described by Waggoner and Loud (1977). It is equally applicable to all general methods for multicomponent distillation programs and is independent of the convergence algorithm. A bidirectional backmixing algorithm is developed to include occlusion as well as entrainment even though occlusion seldom occurs in distillation. For this algorithm, an occlusion factor,  $o_j$ , is defined analogous to the entrainment factor,  $e_j$ , (Colburn, 1936). Bidirectional backmixing is often encountered in extraction and such an algorithm may be developed within the context of the distillation program and subsequently be adapted to extraction.

The initial step in solving the set of component material balances which describe a distillation column is to state the balances in terms of compositions in one phase only by use of equilibrium relationships. The coefficients from these equations make up a sparse matrix, tridiagonal in format. When entrainment is included in these equations, the tridiagonal format is retained.

$$(1 + o_{j-1,i}K_{j-1,i}) \frac{L_{j-1}}{K_{j-1,i}} y_{j-1,i} - \left[ \left( 1 + \frac{e_{ji}}{K_{ji}} V_j \right) + (1 + o_{ji}K_{ji}) \frac{L_j}{K_{ji}} \right] y_{ji} + \left( 1 + \frac{e_{j+1,i}}{K_{j+1,i}} V_{j+1} \right) V_{j+1} y_{j+1,i} = -F_j X_{ji} \quad (2)$$

An effective algorithm has been developed to take advantage of the sparse property of the matrix in the solution of equations which take this format (Grabbe, 1958). When this algorithm is followed, two vectors,  $\bar{f}$  and  $\bar{g}$ , are computed. The final element of the  $\bar{g}$  vector takes the value of the composition or component flow from the bottom stage. The remaining compositions may then be computed sequentially from the bottom of the column to the top.

When the elements of the  $\bar{f}$  and  $\bar{g}$  vectors are computed from process variables, a solution is obtained which requires only two passes through the column for each component. When entrainment and occlusion are both included in the material balances, these vectors may be filled by the expressions

$$f_{1i} = -V_2(1 + e'_{2i})/(V_1 + L_1/K_{1i}) \quad (3)$$

$$g_{1i} = F_1 X_{1i}/(V_1 + L_1/K_{1i}) \quad (4)$$

$$f_{ji} = \frac{-V_{j+1}(1 + e'_{j+1,i})}{(1 + e'_{ji})V_j + (1 + o'_{ji})\frac{L_j}{K_{ji}} + (1 + o'_{j-1,i})\frac{L_{j-1}}{K_{j-1,i}}} f_{j-1,i} \quad (5)$$

$$g_{ji} = \frac{F_j X_{ji} + \frac{L_{j-1}}{K_{j-1,i}}(1 + o'_{j-1,i})g_{j-1,i}}{(1 + e'_{ji})V_j + (1 + o'_{ji})\frac{L_j}{K_{ji}} + (1 + o'_{j-1,i})\frac{L_{j-1}}{K_{j-1,i}}} \quad (\text{for } 2 \leq j \leq N) \quad (6)$$

Modified backmixing coefficients are defined to facilitate computations in eq 3-6

$$e'_{ji} = e_{ji}/K_{ji}$$

$$o'_{ji} = o_{ji}/K_{ji}$$

The backmixing streams must also be considered in the energy balance for those methods which combine the energy balance equations with the bulk flow balances to obtain corrected bulk flow profiles. The constant composition method (Holland, 1963) has proved to be stable and to minimize wide fluctuations between iterations when used for this computation. When bidirectional backmixing is included in these balances and the constant composition method is used, the following expression is used to determine the liquid flow rate for each stage

$$L_j = \frac{V_j H \left[ \frac{(1 + e'_{ji} y_{ji})}{(1 + e'_{j+1,i})} \right]_{j+1} + h \left[ \frac{(1 + e'_{ji})}{(1 + e'_{j+1,i})} e'_{j+1,i} y_{ji} \right]_{j+1} - H_j - e_j h_j}{h_j + o_j H_j - H \left[ \frac{(1 + o'_{ji})}{(1 + e'_{j+1,i})} x_{ji} \right]_{j+1} - h \left[ \frac{(1 + o'_{ji})}{(1 + e'_{j+1,i})} e'_{j+1,i} x_{ji} \right]_{j+1}} + \frac{L_{j-1} H \left[ \frac{(1 + o'_{j-1,i})}{(1 + e'_{j+1,i})} x_{j-1,i} \right]_{j+1} + h \left[ \frac{(1 + o'_{j-1,i})}{(1 + e'_{j+1,i})} e'_{j+1,i} x_{ji} \right]_{j+1} - h_{j-1} - o_{j-1} H_{j-1}}{h_j + o_j H_j - H \left[ \frac{(1 + o'_{ji})}{(1 + e'_{j+1,i})} x_{ji} \right]_{j+1} - h \left[ \frac{(1 + o'_{ji})}{(1 + e'_{j+1,i})} e'_{j+1,i} x_{ji} \right]_{j+1}} + \frac{F_j - H_F - H \left[ \frac{X_{ji}}{(1 + e'_{j+1,i})} \right]_{j+1} - h \left[ \frac{e'_{j+1,i} X_{ji}}{(1 + e'_{j+1,i})} \right]_{j+1}}{h_j + o_j H_j - H \left[ \frac{(1 + o'_{ji})}{(1 + e'_{j+1,i})} x_{ji} \right]_{j+1} - h \left[ \frac{(1 + o'_{ji})}{(1 + e'_{j+1,i})} e'_{j+1,i} x_{ji} \right]_{j+1}} \quad (7)$$

After the overflow rate is determined for stage  $j$ , the boil-up from the stage below may be computed.

$$V_{j+1} = V_j \frac{(1 + e_j)}{(1 + e_{j+1})} + L_j \frac{(1 + o_j)}{(1 + e_{j+1})} - L_{j-1} \frac{(1 + o_{j-1})}{(1 + e_{j+1})} - \frac{F_j}{(1 + e_{j+1})} \quad (8)$$

These material balance, component-material balance, and energy balance expressions have been used within the context of a multicomponent distillation program previously stored for general use. Their use in that program has been illustrated (above) in an analysis of the effect of entrainment on the operation or design of a distillation column. The development of these computational algorithms from the basic statement of the energy and material balances is given in Appendix A.

### Entrainment and Deviation from Equilibrium

Entrainment and deviation from equilibrium occur as distinct and separate phenomena in distillation. Entrainment is generated by hydraulic factors associated with the characteristics of the flow of inter-tray streams. Deviation from equilibrium is an intra-tray phenomenon and results when the interphase mass transfer is too slow for the mixture of vapor and liquid on the tray to reach equilibrium. The effects of entrainment and nonequilibrium on column operation are examined independently and subsequently compared.

**Deviation from Equilibrium is Described by the Murphree Efficiency.** The Murphree efficiency has been looked upon as the standard measurement for deviation from equilibrium since it was proposed (Murphree, 1925). Its format has been used continually but its definitions have been revised to facilitate computations. In the modified Murphree efficiency definition presented by Holland (1963) it is stated

$$E_{ji}^M = \frac{y_{ji} - y_{j+1,i}}{K_j x_{ji} - y_{j+1,i}} \quad (9)$$

The efficiency factor,  $E_{ji}^M$ , may be considered to represent the ratio of the change of the composition of component  $i$  in the vapor stream as it crosses tray  $j$  to the change which would have occurred if the vapor above the stage were in effective equilibrium with the liquid overflow from stage  $j$ . In certain cases the equilibrium coefficient for the overflow may be computed at temperatures other than the bubble point. This value for the Murphree efficiency is a function of plate parameters alone and is not affected by flow patterns external to the stage. Entrainment leaving stage  $j$  would be considered to have the same composition as the liquid overflow. The vapor occluded from the stage above would be added to the boil-up from the stage below to form a gross vapor inlet stream. The inlet vapor composition,  $y_{j+1,i}$ , would be that of the combined entering vapor streams.

When a mass balance is written for the vapor phase on stage  $j$ , the Murphree efficiency may be expressed in terms of plate parameters (Waggoner and Loud, 1977).

$$(K_{GasZ})_{ji} = V_j \frac{E_{ji}^M}{1 - E_{ji}^M} \quad (10)$$

**Table II. The Effects of Entrainment and Nonequilibrium on Column Temperature Profile**

Stage	Temperature profile, °F						
	Base case	Entrainment factor			Modified Murphree efficiency		
		0.05	0.10	0.20	0.91533	0.84031	0.81426
1	380.51	381.55	382.58	384.60	381.40	382.31	384.16
2	402.05	402.60	403.14	404.20	402.07	402.15	402.44
3	418.07	418.14	418.21	418.39	417.82	417.59	417.24
4	429.20	428.85	428.52	427.97	428.97	428.76	428.33
5	436.84	436.12	435.46	434.33	436.44	436.05	435.32
6	446.32	445.00	443.80	441.68	445.53	444.76	443.28
7	457.71	455.81	454.04	450.88	456.43	455.17	452.71
8	471.44	468.94	466.58	462.32	469.49	467.55	463.79
9	488.21	485.03	482.03	476.56	485.23	482.34	476.83
10	509.30	506.12	503.11	497.61	506.56	503.92	498.84

**Table III. The Effects of Entrainment and Nonequilibrium on Column Overflow Profile**

Stage	Overflow rate, lb-mol/h						
	Base case	Entrainment factor			Modified Murphree efficiency		
		0.05	0.10	0.20	0.91533	0.84031	0.71426
1	400.00	400.00	400.00	400.00	400.00	400.00	400.00
2	390.95	390.79	390.73	390.80	390.00	389.21	388.08
3	389.92	389.80	389.77	389.92	388.13	386.55	384.05
4	390.31	390.37	390.48	390.82	389.39	388.57	387.16
5	912.26	910.37	908.72	906.14	909.99	908.01	904.74
6	940.40	936.16	932.38	926.14	936.38	932.85	926.97
7	975.36	968.55	962.36	951.83	969.46	964.13	954.93
8	1018.15	1008.64	999.84	984.47	1010.53	1003.17	989.70
9	1070.01	1022.00	978.72	904.25	1050.28	1031.91	999.45
10	250.00	250.00	250.00	250.00	250.00	250.00	250.00

A similar expression has been developed for the point efficiency (Holland, 1963).

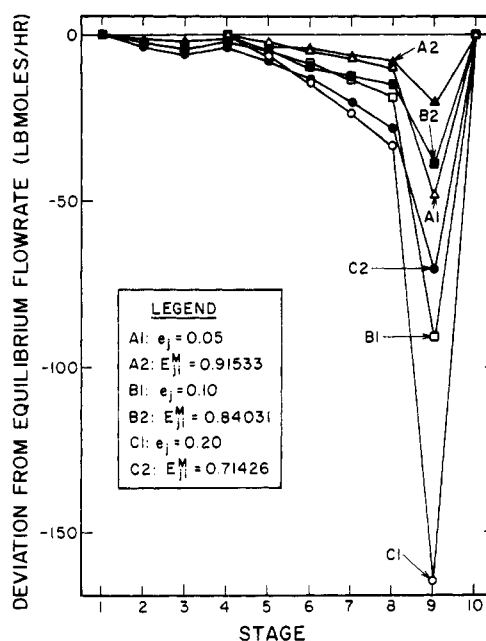
$$E_{ji}^M = 1 - \exp\left[-\frac{(K_{Gas}Z)_{ji}}{V_j}\right] \quad (11)$$

These differ conceptually in the location taken to measure the exiting vapor composition. In both cases the Murphree efficiency may be expressed as a power series in the set of plate parameters which make up the exponential term in eq 11. When they are compared, the difference in computed values would lie in the  $n$  division which appears in the second order and higher terms of the exponential expression but not in the other. Thus the two determinations would not differ greatly and both imply that Murphree efficiency values may be determined from mass transfer parameters alone.

**The Effects of Entrainment May Be Distinguished from the Effects of Nonequilibrium.** Both entrainment and deviation from equilibrium operate to reduce the effectiveness of a distillation column. Backmixing causes disruptions in the desired flow patterns between stages while nonequilibrium is encountered within the material held on the individual trays. Since entrainment is primarily hydraulic in origin and nonequilibrium is mass transfer related, they may exist independently and affect column operations or descriptions in ways which exhibit discernable differences.

A comparison of the effects of entrainment and deviation from equilibrium is illustrated for the three-component hydrocarbon system described in Table I. Entrainment factors are specified and the product split,  $x_D/x_B$ , for the light component is determined. Modified Murphree efficiency values are then determined such that the light component product split is identical with that obtained from the backmixing examples (Table IV). Column temperature and flow profiles for entrainment and nonequilibrium cases may be compared in Table II and III and Figures 5–8.

Differences in the effects of backmixing and deviation from equilibrium are found primarily in the product stream compositions. Entrainment causes the composition of the heavy



**Figure 5.** Effect of entrainment on the liquid overflow profile of a distillation column.

component in the distillate to exceed that caused by deviation from equilibrium. The middle component is more depleted from entrainment than from nonequilibrium effects. In the example comparison this depletion is increased by nearly three times.

A further significant difference between the two effects is seen in the bulk flow profiles. When backmixing is present, the deviation (from the base case) of these variables increases markedly at the trays next to the reboiler and condenser. These deviations are greatly reduced for liquid overflow and not evident for vapor boil-up when nonequilibrium is present alone. The temperature profiles for both phenomena show the

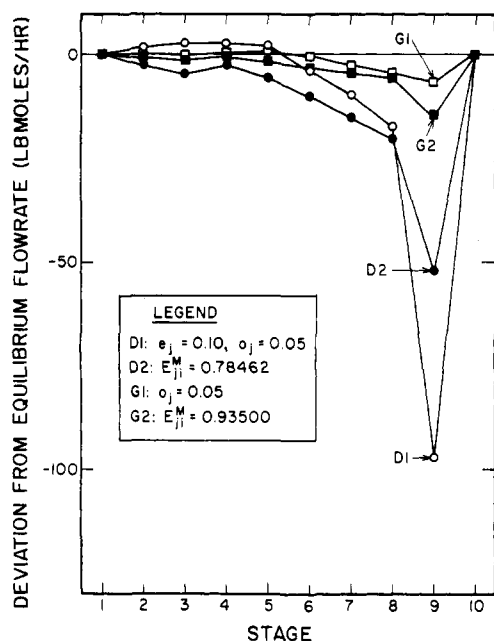


Figure 6. Effect of occlusion and bidirectional backmixing on the liquid overflow profile of a distillation column.

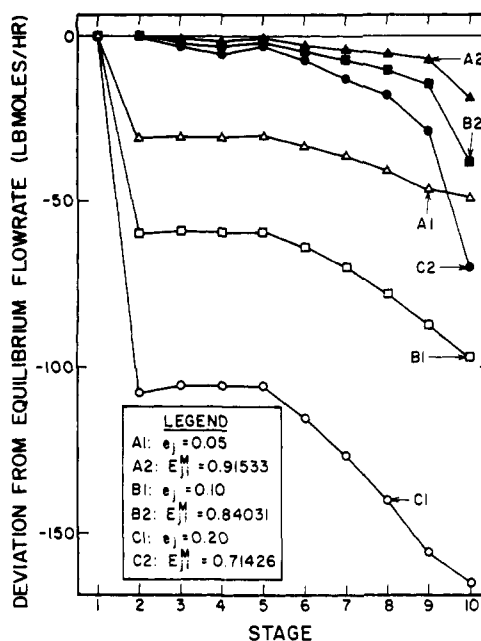


Figure 7. Effect of entrainment on the vapor profile of a distillation column.

same pattern of deviation from the equilibrium case. The magnitude of temperature deviation appears to be greater for backmixing than for deviation from equilibrium.

**Conclusion**

A simulation of entrainment in distillation shows that the presence of entrainment may be observed by examination of the column profiles. A distinctive characteristic of entrainment is a decreased overflow rate in the stripping section, particularly at the tray above the reboiler (Figure 5). Further, if the reflux rate is held constant, the reboiler duty and boil-up rate decrease as entrainment increases (Figure 7, Table IV). Component separation is reduced and consequently the temperature profile is raised in the rectifying section and lowered in the stripping section (Figure 3).

Entrainment and deviation from tray equilibrium are caused by different sets of factors; the first by hydraulics, the latter by mass transfer characteristics. Their effects on column operations, while similar, are sufficiently different to be identified in process simulations. In both cases, as conditions are changed further from the base case, the fraction of the light component in the distillate is reduced, but increasing entrainment causes a significant reduction in the middle component. Middle component reduction is not as noticeable when tray efficiency falls off (Table IV). Another difference is evident in the sharp decrease in the overflow to the reboiler observed when entrainment is increased. This deviation is not as noticeable when the trays are specified to operate further from equilibrium (Figures 5 and 6).

Interstage-backmixing may be described in a multistage

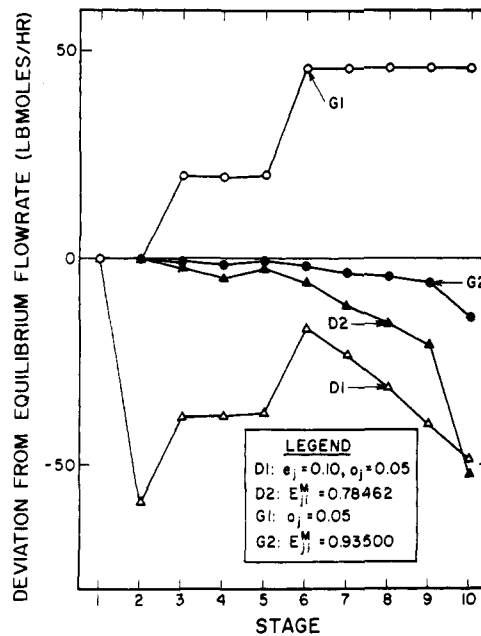


Figure 8. Effect of occlusion and bidirectional backmixing on the vapor profile of a distillation column.

distillation column program when the backmixing streams are included in the material balance equations and in the energy balance equations. Since the form of the component-material balance equations is not changed, the conventional tri-diag-

**Table IV. The Effects of Entrainment and Nonequilibrium on Product Separation**

Modified Murphree efficiency	Entrainment coefficient	Component distillate/bottoms composition, mole fraction			Reboiler duty 10 <sup>6</sup> Btu/h
		Pentane	Hexane	Heptane	
1.00000	0.00	0.55679/0.04321	0.35969/0.34031	0.08352/0.61647	5.41803
1.00000	0.05	0.55142/0.04858	0.35605/0.34394	0.09253/0.60748	5.16910
1.00000	0.10	0.54597/0.05402	0.35294/0.34705	0.10108/0.59892	4.94014
1.00000	0.20	0.53506/0.06494	0.34806/0.35194	0.11698/0.58312	4.53515
0.91533	0.00	0.55142/0.04857	0.35867/0.34133	0.08991/0.61010	5.35949
0.84031	0.00	0.54598/0.05401	0.35765/0.34234	0.09636/0.60365	5.30413
0.71426	0.00	0.53506/0.06493	0.35570/0.34429	0.10924/0.59077	5.20048

onal algorithm may be used to obtain a solution to the modified material balance expressions. The algorithm is not iterative and all of its initial, intermediate, and final elements may be contained in vectors. The procedure presented may be used by the design engineer to examine the effects of entrainment on his distillation design. It permits him to quantify the increased internal recycle required to obtain the designed separation for his column. He may then increase the column size, downcomer area, and reboiler only by that amount required to compensate for the degree of backmixing which he anticipates.

## Appendix

### Development of an Algorithm for Bidirectional Backmixing

If a multistage system simulation is written to describe operations which include bi-directional interstage backmixing, the component-material balances, the bulk flow balances, and the energy balances differ from those used for the conventional column description. Since their composition and energy content differ appreciably from those of the carrier stream, the streams of entrained and occluded material cannot be included in the bulk flow stream descriptions but must be expressed independently.

**Component-Material Balances.** A component-material balance may be written for equilibrium stages and bidirectional interstage backmixing. If no interphase mass transfer takes place between stages, the entrained and occluded streams have the same composition upon entering a stage which they had when they left the adjacent stage. When a set of balances is used to describe distillation, backmixing effects may be limited to the streams which leave the column trays. Backmixing is not included in condenser and reboiler product streams.

The bulk flow pattern for a distillation column operating with bidirectional backmixing is illustrated in Figure 1. A total material balance around stage  $j$  may be written.

$$V_{j+1} + E_{j+1} + L_{j-1} + O_{j-1} + F_j = V_j + E_j + L_j + O_j \quad (\text{A-1})$$

The entrained stream,  $E_j$ , is defined.

$$E_j = \sum_{i=1}^c e_j x_{ji} V_j \quad (\text{A-2})$$

The occluded stream,  $O_j$ , is defined.

$$O_j = \sum_{i=1}^c o_j y_{ji} L_j \quad (\text{A-3})$$

The backmixing factors,  $e_j$  and  $o_j$ , imply that the rate of backmixing is a specified fraction of the flow rate of the carrier bulk stream (Fair and Matthews, 1958). Equations A-2 and A-3 may be rearranged and reexpressed to include the equilibrium relation and the modified backmixing factors eq 6.

$$E_j = \sum_{i=1}^c e'_{ji} v_{ji} \quad (\text{A-4})$$

$$O_j = \sum_{i=1}^c o'_{ji} l_{ji} \quad (\text{A-5})$$

A component material balance around stage  $j$  includes the backflowing streams.

$$(1 + e'_{j+1,i})v_{j+1,i} + (1 + o'_{j-1,i})l_{j-1,i} + f_{ji} = (1 + e'_{ji})v_{ji} + (1 + o'_{ji})l_{ji} \quad (\text{A-6})$$

This equation may then be rearranged and expressed in terms of vapor compositions for each component in the stream leaving each stage.

$$(1 + o'_{j-1,i}) \frac{L_{j-1}}{K_{j-1,i}} y_{j-1,i} - \left[ (1 + e'_{ji})V_j + (1 + o'_{ji}) \frac{L_j}{K_{ji}} \right] y_{ji} + (1 + e'_{j+1,i})V_{j+1} y_{j+1,i} = -F_j X_{ji} \quad (\text{A-7})$$

The reboiler and the overhead condenser are usually designed so that backmixing does not occur in their product streams. Equation A-7 may be modified to describe these stages and the tray adjacent to them. For stage 1, the condenser

$$(V_1 + L_1/K_{1i})y_{1i} - (1 + e'_{2i})V_2 y_{2i} = -F_1 X_{1i} \quad (\text{A-8})$$

stage 2, the top tray

$$\frac{L_1}{K_{1i}} y_{1i} - \left[ (1 + e'_{2i})V_2 + (1 + o'_{2i}) \frac{L_2}{K_{2i}} \right] y_{2i} + (1 + e'_{3i})V_3 y_{3i} = -F_2 X_{2i} \quad (\text{A-9})$$

stage  $N-1$ , the bottom tray

$$(1 + o'_{N-2,i}) \frac{L_{N-2}}{K_{N-2,i}} y_{N-2,i} - \left[ (1 + e'_{N-1,i})V_{N-1} + (1 + o'_{N-1,i}) \frac{L_{N-1}}{K_{N-1,i}} \right] y_{N-1,i} + V_N y_{Ni} = -F_{N-1} X_{N-1,i} \quad (\text{A-10})$$

stage  $N$ , the reboiler

$$(1 + o'_{N-1,i}) \frac{L_{N-1}}{K_{N-1,i}} y_{N-1,i} - \left( (V_N + \frac{L_N}{K_{Ni}}) y_{Ni} \right) = -F_N X_{Ni} \quad (\text{A-11})$$

The coefficients of this set of component-material balances take a tridiagonal form, and the equations may be solved to determine the vapor obtained from energy balances and bulk flow balances written for each stage. The backmixing streams are included in these balances and their rates are determined by the multipliers,  $e_j$  and  $o_j$ , defined for the component material balances. If no energy transfer occurs between the backmixing stream and its carrier stream, the backmixing stream has the same energy content when it enters a stage that it had when it left the adjacent stage.

The energy balance for a column with a conventional flow pattern may be written

$$V_{j+1}H_{j+1} + L_{j-1}h_{j-1} + F_j H_{Fj} = V_j H_j + L_j h_j \quad (\text{A-12})$$

Solutions for the conventional balances may become unstable and oversensitive to small changes in stage temperature if the vapor enthalpy,  $H_{j+1}$ , approaches the value of the liquid enthalpy,  $h_j$ . The constant-composition method presented by Holland (1963) may be used to minimize this instability. This method has been selected as the basis for a set of stage-to-stage energy balances written to describe a multistage operation which includes bidirectional backmixing.

The energy balance on stage  $j$  may be stated to include the effects of backmixing streams.

$$V_{j+1}H_{j+1} + E_{j+1}h_{j+1} + L_{j-1}h_{j-1} + O_{j-1}H_{j-1} + F_j H_{Fj} = V_j H_j + E_j h_j + L_j h_j + O_j H_j \quad (\text{A-13})$$

It may be reexpressed in terms of the backmixing coefficients.

$$(H_{j+1} + e_{j+1}h_{j+1})V_{j+1} = V_j(H_j + e_j h_j) + L_j(h_j + o_j h_j) - L_{j-1}(h_{j-1} + o_{j-1}H_{j-1}) - F_j H_{Fj} \quad (\text{A-14})$$

Energy in the boil-up stream for stage  $j+1$  may be described by the following expression.



$$V_{j+1}H_{j+1} = \sum_{i=1}^c H_{j+1,i}v_{j+1,i} \quad (\text{A-15})$$

An expression for  $v_{j+1,i}$  is obtained from the component-material balance.

$$v_{j+1,i} = \frac{(1 + e'_{ji})}{(1 + e'_{j+1,i})} v_{ji} + \frac{(1 + o'_{ji})}{(1 + e'_{j+1,i})} l_{ji} - \frac{(1 + o'_{j-1,i})}{(1 + e'_{j+1,i})} l_{j-1,i} - \frac{F_j X_{ji}}{(1 + e'_{j+1,i})} \quad (\text{A-16})$$

Equations A-15 and A-16 may be combined to obtain an expression for the enthalpy of the vapor stream,  $V_{j+1}$ .

$$V_{j+1}H_{j+1} = V_j \sum_{i=1}^c H_{j+1,i} \frac{(1 + e'_{ji})}{(1 + e'_{j+1,i})} y_{ji} + L_j \sum_{i=1}^c H_{j+1,i} \frac{(1 + o'_{ji})x_{ji}}{(1 + e'_{j+1,i})} - L_{j-1} \sum_{i=1}^c H_{j+1,i} \frac{(1 + o'_{j-1,i})}{(1 + e'_{j+1,i})} x_{j-1,i} - F_j \sum_{i=1}^c \frac{H_{j+1,i}}{(1 + e'_{j+1,i})} X_{ji} \quad (\text{A-17})$$

Equation A-17 may be expressed in the notation employed by Holland (1963) for the constant-composition method.

$$V_{j+1}H_{j+1} = V_j H \left[ \frac{(1 + e'_{ji})y_{ji}}{(1 + e'_{j+1,i})} \right]_{j+1} + L_j H \left[ \frac{(1 + o'_{ji})x_{ji}}{(1 + e'_{j+1,i})} \right]_{j+1} - L_{j-1} H \left[ \frac{(1 + o'_{j-1,i})x_{j-1,i}}{(1 + e'_{j+1,i})} \right]_{j+1} - F_j H \left[ \frac{X_{ji}}{(1 + e'_{j+1,i})} \right]_{j+1} \quad (\text{A-18})$$

The second coefficient of  $V_{j+1}$  in eq A-14 may also be expressed in notation for the constant composition method.

$$e_{j+1}V_{j+1}h_{j+1} = V_j H \left[ \frac{(1 + e'_{ji})e'_{j+1,i}y_{ji}}{(1 + e'_{j+1,i})} \right]_{j+1} + L_j h \left[ \frac{(1 + o'_{ji})e'_{j+1,i}x_{ji}}{(1 + e'_{j+1,i})} \right]_{j+1} - L_{j-1} h \left[ \frac{(1 + o'_{j-1,i})e'_{j+1,i}x_{j-1,i}}{(1 + e'_{j+1,i})} \right]_{j+1} - F_j h \left[ \frac{e'_{j+1,i}X_{ji}}{(1 + e'_{j+1,i})} \right]_{j+1} \quad (\text{A-19})$$

Equations A-13, A-18, and A-19 may be combined to obtain eq 7 which together with eq 8, the overall material balance, may be used to compute a bulk-flow profile for the column.

## Nomenclature

$a$  = effective interfacial area  
 $c$  = number of components  
 $e$  = moles of entrained liquid per mole of vapor  
 $e'$  = modified entrainment coefficient defined by eq 6  
 $E$  = flow rate of entrained material  
 $E_{ji}^M$  = modified Murphree efficiency

$F$  = feed rate  
 $f_j$  = component feed rate  
 $h_j$  = enthalpy of one mole of liquid leaving stage  $j$   
 $h(y_{ki})_j$  = molar enthalpy calculated on the basis of the component liquid enthalpies at the temperature of stage  $j$  and summed over the compositions,  $y_{ki}$  (Holland, 1963)  
 $H_j$  = enthalpy of one mole of vapor leaving stage  $j$   
 $H(x_{ki})_j$  = molar enthalpy calculated on the basis of the component vapor enthalpies at the temperature of stage  $j$  and summed over the compositions,  $x_{ki}$  (Holland, 1963)  
 $K$  = equilibrium coefficient  
 $K_G$  = mass transfer coefficient  
 $l$  = component liquid flow rate  
 $L$  = bulk liquid flow rate  
 $N$  = the number of stages in a column  
 $o$  = moles of occluded vapor per mole of dry liquid  
 $o'$  = modified occlusion coefficient defined by eq 6  
 $O$  = flow rate of occluded material  
 $s$  = effective area for mass transfer  
 $v$  = component vapor flow rate  
 $V$  = bulk vapor flow rate  
 $X$  = composition in a feed stream  
 $x$  = composition in liquid phase  
 $y$  = composition in vapor phase  
 $Z$  = height for mass transfer  
 $\Psi$  = entrainment factor defined by Fair and Matthews (1958)

## Subscripts

$F$  = feed  
 $i$  = component index  
 $j$  = stage index  
 $L$  = liquid phase  
 $N$  = final stage

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