Simple, Analytical Criteria for the Sequencing of Distillation Columns

A quantitative criterion for the selection of simple distillation sequences is derived for ideal mixtures. A simple cost model, along with a short-cut solution of Underwood's equations, gives an analytical form for the total vapor rate, which is the key design variable. The results for column sequencing that are based on the analytical criterion agree well with more exact solutions, but they indicate that in numerous situations the commonly accepted heuristics are incorrect.

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SCOPE

The synthesis of a distillation separation sequence is often a key step in the invention of a process flowsheet. Heuristics are normally used for this step in the process synthesis. However, some heuristics, such as "remove the lightest component first," depend only on volatility, whereas other heuristics, such as "remove the most plentiful component first," depend only on feed composition. Thus, it should not be surprising that the previously published heuristics can be contradictory.

Since we expect that the selection of the best separation sequence must depend both on relative volatility and feed composition, we need to have a criterion available that includes both quantities. A few functions of this type have been proposed (Lu and Motard, 1982; Tedder and Rudd, 1978), but the functional forms chosen are based on intuition. As an alternate approach, we show how an appropriate functional form can be derived that is based on approximate solutions of the design equations and an order of magnitude analysis of the cost equations. The results indicate that the new analytical approach gives better predictions than the qualitative heuristics.

CONCLUSIONS AND SIGNIFICANCE

Conflicts and inaccuracies in heuristic or rank-order approaches to the selection of a distillation sequence can be eliminated using the analytical criterion developed here. The approximate, but accurate, solution of the design equations, along with a simple cost model, are sufficient for process synthesis. For ternary mixtures separated in a simple column sequence, the optimal sequence and, more importantly, the sensitivity of this decision to the composition and thermodynamic information are shown by Eq. 23. Mixtures containing more components can be easily investigated with similar expressions.

Many of the most widely used heuristics are contradictory, and the associated rank-order functions based on these heuristics are often in error. For example, in contradiction to many of the previous studies, we find that the most difficult separation should often be done first rather than last. The quantitative treatment presented here delineates the region where the heuristic is applicable, as well as the magnitude of potential errors that are possible using previously published heuristics in regions where they are not valid. Several examples are presented, and the results are compared with those of other investigations based on more rigorous simulations.

INTRODUCTION

In the development of a process it is usually necessary to specify a sequence of distillation columns for the fractionation of multicomponent mixtures. At the preliminary design stage in industrial practice the selection of the sequence is normally based on heuristics. Similarly, most of the recent process synthesis algorithms rely on heuristics both to reduce the size of the search space and to provide good initial solutions for the evolutionary procedures. Some of the most common heuristics are

1. Remove the lightest component first
2. Remove the most plentiful component first
3. Save difficult separations until last
4. Favor 50–50 splits

A much more extensive listing, as well as a quite complete evaluation of the literature, is presented in the review paper by Nishida et al. (1981) or the more recent paper by Nadgir and Liu (1983).

CONTRADICTORY HEURISTICS

The separation sequencing heuristics, such as those listed above, were developed either as generalizations of experience or as generalizations obtained from large sets of computer-aided design case

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TABLE 1. PERFORMANCE OF SEVERAL RANK-ORDER FUNCTIONS

j	Model	SS_j/SS_1
1	$V_{\min}^{0.648}N_m^{0.184}\Delta T^{0.144}$	1.00
2	$90.22V_{\min} + 153.9N_m + 344.2\Delta T$	1.05
3	$107.7V_{\min} + 203.3\Delta T$	1.20
4	$V_{\min}$	1.36
5	$88.34V_{\min} + 912.1N_m$	1.46
6	$0.2996CAP + 0.520P$	1.52
7	$V_{\min}N_m\Delta T$	1.83
8	$V_{\min}N_m$	2.48
9	Feed rate/boiling point diff. of keys	2.98
10	$V_{\min}\Delta T$	6.49

studies. However, in contrast to the rules of thumb for many other problems, sometimes the heuristics for separation systems give contradictory results. For example, rules 1 and 2 above will be in conflict if the heaviest component is the most plentiful. In order to resolve these conflicts, Powers (1972), Hartmann (1979), and Hartmann and Hacker (1979) assigned subjective weights to a list of heuristics, although they do not present guidelines for selecting these weights. Similarly, Seader and Westerberg (1977) and Nadgir and Liu (1983) present ordered sets of heuristics, where the order itself represents a heuristic.

In an alternate approach Nath and Motard (1978) and Lu and Motard (1982) presented a quantitative evaluation function, which estimates the total sequence cost and takes into account most of the commonly used heuristics. The expression proposed is

$$H_L = \frac{\log\left\{\dfrac{SP_{LK}}{1 - SP_{LK}}\dfrac{SP_{HK}}{1 - SP_{HK}}\right\}}{\log\alpha_{LK\text{-}HK}}\left(1 + \frac{2D}{D + B}\right) \times\left(1 + \left|\frac{D - W}{D + W}\right|\right) \quad (1)$$

$$H_D = EML \cdot AVE \cdot W \quad (2)$$

The H_L function estimates the cost of a current separation per unit mass, and it is the product of three terms. The first term is the minimum number of trays, which Lu and Motard (1982) relate to their heuristics of favoring large α separations early in the sequence and saving difficult separations to last. The second term is included to account for their heuristic of favoring less distillate product, and the third term is included to account for the heuristic of favoring 50–50 splits. The choice of a triple product with unit weighting factors and the use of minimum trays instead of minimum reflux was arbitrary. The H_D function then accounts for downstream separations, and estimates of the terms EML, AVG, and W are detailed by Lu and Motard (1982).

Rod and Marek (1959) also proposed a quantitative criterion, which is based on the heuristic that the cheapest separation sequence is that with the smallest vapor rate. For ternary mixtures, their result for the difference in vapor rates between the indirect and direct sequence is

$$\frac{\Delta V}{F} = \frac{(\alpha_{AC} + 0.25)X_A - 1.25X_C}{\alpha_{AC} - 1} \quad (3)$$

Since this relationship does not include the volatility values for all the components, it cannot reproduce many of the current heuristics. Rudd et al. (1973) estimate the relative cost of a distillation separation, to a first approximation, as

$$\text{Distillation Cost} \sim \frac{\text{Feed Rate}}{\text{Boiling Point Difference}} \quad (4)$$

which also corresponds to some of the heuristics. Nadgir and Liu (1983) propose a coefficient of ease of separation, which is defined as

$$CES = \frac{D}{F - D}\Delta T, \quad \text{or} \quad 100\frac{D}{F - D}(\alpha - 1) \quad (5)$$

Tedder and Rudd (1978) considered numerous combinations of rank-order functions (see Table 1).

A NEW APPROACH

Instead of using intuition to propose functions that might indicate the best separation sequence and then using case studies to evaluate these functions, we use approximate solutions of design equations or commonly accepted approximations of functions, coupled with order of magnitude arguments, to derive the quantities of interest. The great advantage of this analytical approach is that the limitations of the results are clearly identified by the assumptions introduced in the analysis.

Relationships Between Previous Criteria

In addition, an elementary analysis can often be used to demonstrate under what conditions two apparently different criteria are essentially the same. For example, for small values of α (which corresponds to large and expensive columns), a Taylor series expansion gives that

$$\ln\alpha \simeq \alpha - 1 \quad (6)$$

Also approximately

$$\ln\alpha = \ln\frac{P_1^o}{P_2^o} = \ln\exp\left\{-\frac{\Delta H_v}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)\right\} = C_o(T_1 - T_2) \quad (7)$$

Thus, the use of ΔT or $(\alpha - 1)$ in Nadgir and Liu's (1983) expressions in Eq. 5 should be essentially the same for small values of α.

Similarly, Rudd et al.'s (1973) criteria can be written as

$$\text{Distillation cost} \sim \frac{F}{\Delta T} \sim \frac{F}{\ln\alpha} \simeq \frac{F}{\alpha - 1} \quad (8)$$

For a binary mixture with a saturated liquid feed, we can write, approximately, that

$$V = (R + 1)D = \left\{\frac{1.2X_D}{(\alpha - 1)X_F} + 1\right\}\frac{FX_F}{X_D} = \left(\frac{1.2}{\alpha - 1} + \frac{X_F}{X_D}\right)F \quad (9)$$

so that the distillation cost proposed by Rudd et al. (1973) is essentially proportional to the vapor rate.

Column Cost Model

In order to derive a criterion for column sequencing, we start by considering the separation costs. An approximate model for estimating the total annualized cost of a distillation column in terms of the number of trays, N, and the vapor rate, V, is (Marquez, 1982)

$$TAC = C_oN^{0.82}V^{0.53} + C_1V^{0.65} + C_2V \quad (10)$$

The first term represents the annualized capital cost from Guthrie's correlation and assumes that the column height is proportional to the number of trays and that column diameter depends on the square root of the vapor rate. The second term corresponds to the combined annualized costs for the reboiler and condenser from Guthrie's correlation and assumes that the heat exchanger areas are directly proportional to the column vapor rate. The third term is the combined cost of the steam and the cooling water, assuming that the utility flows are proportional to the vapor rate. The cost coefficients depend on cost factors, boiling points, heats of vaporization, etc., and they can be evaluated for any system of interest (see Marquez, 1982). Colburn's (1936) incremental cost model

$$TAC = TAC_o + (G_1N + G_2)V \quad (11)$$

essentially represents a linearization of Eq. 10. Estimates for the constants G_1 and G_2 can be found in Happel and Jordan (1975). For the purposes of our study, we use a linearization of Eq. 10 around a base case design

$$TAC = TAC_o + K_1N + K_2V \quad (12)$$

We can make the linearization agree as closely as we desire to Eq.

10 by iterating, i.e., changing the base case design conditions to correspond to our new estimate of the optimum design. In fact, Nath and Motard (1978) have used this iterative procedure with Eq. 11.

In order to write this cost model in terms of compositions and α's, we first use Gilliland's approximation, $N/N_m = 2$, Fenske's equation for the minimum number of trays, and a 50% tray efficiency to eliminate N. Thus, we obtain

$$N = 4\,\frac{\ln\left\{\dfrac{SP_{LK}}{1 - SP_{LK}}\,\dfrac{SP_{HK}}{1 - SP_{HK}}\right\}}{\ln\alpha_{LK,HK}} = 4\,\frac{\ln S}{\ln\alpha} \tag{13}$$

which is almost the same as the first term in Motard's model, and is certainly within an order of magnitude of a more rigorous solution for N in constant α systems.

In order to estimate the vapor rate, we use the material balance expression and the commonly accepted rule of thumb $R = 1.2R_m$

$$V = (1.2R_m + 1)D \tag{14}$$

Then we use the approximate minimum reflux equations for saturated liquid feeds developed by Glinos and Malone (1983) for the ternary mixture

$$A/BC \qquad R_m = \frac{\alpha_B(X_A + X_B)}{fX_A(\alpha_A - \alpha_B)} + \frac{X_C}{fX_A(\alpha_A - 1)} \tag{15}$$

where f is a correction factor, given by $f = 1 + 1/(100X_B)$ (16)

$$AB/C \quad R_m = \frac{(X_B + X_C)/(\alpha_B - 1) + X_A/(\alpha_A - 1)}{(X_A + X_B)(1 + X_A X_C)} \tag{17}$$

and the approximations to Underwood's equations for the binaries

$$B/C \qquad R_m = \frac{1 - X_A}{(\alpha_B - 1)X_B} \tag{18}$$

$$A/B \qquad R_m = \frac{\alpha_B(1 - X_C)}{(\alpha_A - \alpha_B)X_A} \tag{19}$$

Thus, by combining Eqs. 12 through 19, we can develop a cost model for a separation system. Now we want to use these cost models to evaluate column sequences.

Sequencing Distillation Columns for Ternary Mixtures

We consider only the simplest, but the most common case, where $n - 1$ columns are used to separate n components in a train of distillation columns. Also, we restrict our analysis here to the case of ternary mixtures, where two alternative designs exist, the direct, I, and indirect, II, column sequences. The difference between the costs of these two configurations is denoted by Δ.

$$\Delta = TAC_I - TAC_{II} \tag{20}$$

The direct sequence is favored when Δ is negative and the indirect sequence is favored when Δ is positive. If we use Eq. 12 to describe the column costs and we assume that the cost coefficients of each column are roughly the same—i.e., roughly the same column pressures, same size columns, same vapor rates, etc.—then

$$\Delta = K_1\{N^I_{AB} - N^{II}_{AB} + N^I_{BC} - N^{II}_{BC}\} + K_2\{V^I_{AB} - V^{II}_{AB} + V^I_{BC} - V^{II}_{BC}\} \tag{21}$$

Effect of Number of Trays

Equation 13 gives $N^I_{AB} = N^{II}_{AB} = 4\ln S_{AB}/\ln\alpha_{AB}$, with a similar result for N_{BC}. Hence, the best separation sequence should be essentially independent of the split ratios. Small errors in this estimate are not amplified by the magnitudes of K_1 and K_2. In fact, typical values are $K_1/K_2 \simeq 0.1$ to 0.4. However, if component C, say, is highly corrosive, so that an expensive material must be used for both columns in the direct sequence but only for the first column in the indirect sequence, or if high pressures are required for two columns with the one sequence and only for one column with the other sequence, then the cost coefficients for the two column sequences will not be the same and the number of trays may have a significant effect on the most desirable sequence.

The conclusion that the best sequence is insensitive to the number of trays also depends on the validity of Gilliland's correlation and the use of separation factors to specify the design. These approximations are quite good except for very difficult splits and highly imbalanced columns where the compositions of the outlet streams are specified rather than the fractional recoveries. A more detailed discussion is presented in the appendix.

Thus, the balance of the vapor rates in the columns is normally the dominant factor in the cost difference, and we can write

$$\frac{\Delta}{K_2F} = V^I_{AB} - V^{II}_{AB} + V^I_{BC} - V^{II}_{BC} \tag{22}$$

The coefficient K_2 reflects the magnitude of costs that are proportional, roughly, to the vapor rate in the system. This includes the annualized capital costs for the column and heat exchange equipment, as well as utilities costs. Expression (22) agrees with the empirical observation of Rod and Marek (1959), the results of Eliceche and Sargent (1981), and the common heuristic that vapor rate is the dominant factor in fixing the separation cost. However, this result is different from Motard's model.

Effect of Vapor Rate

When we substitute Eqs. 14 through 19 into Eq. 22, we obtain

$$\frac{\Delta V}{F} = 1.2\left\{\frac{X_B + X_C}{\alpha_B - 1}\,\frac{X_A X_C}{1 + X_A X_C} + \frac{1}{\alpha_A - 1}\,\frac{X_C - fX_A + X_A X_C^2}{f(1 + X_A X_C)} - \frac{\alpha_B(X_A + X_B)}{\alpha_A - \alpha_B}\,\frac{f - 1}{f}\right\} - X_A \tag{23}$$

as the criterion for sequence selection. It should be noted that the correction factor f, Eq. 16, is significant only when $X_B < 0.2$; otherwise it can be set equal to unity and the last term in Eq. 23 is eliminated. The factor f does not have a significant effect on the vapor rate given by Eq. 15 (the average error is 3.5% when $f = 1$), but it may have a significant effect on ΔV, since ΔV is often less than 10% of either vapor rate.

DISCUSSION OF THE SELECTION CRITERION MODEL

A comparison between Eq. 23 and the exact solution of Eq. 22 using Underwood's equations is shown in Figure 1 for some values of the design parameters. The accuracy is adequate for sequence selection, although not for a final design. Equation 23 is sufficiently simple that we can evaluate the effects of the various design variables.

First, note that terms involving X_A alone have a negative sign. This means that the direct sequence is favored for high X_A values.

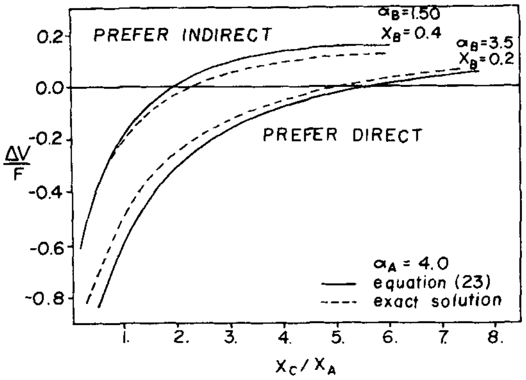

Figure 1. Comparison of the ΔV values obtained from Eq. 23 to the exact solutions of Underwood's equations.

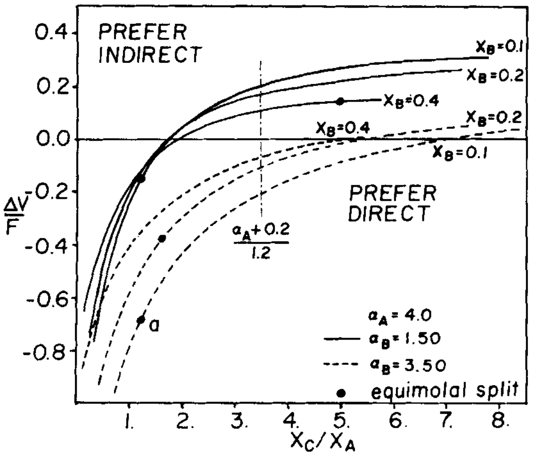

Figure 2. ΔV as a function of the ratio X_C/X_A, for $\alpha_A = 4$ and various values of X_B and α_B.

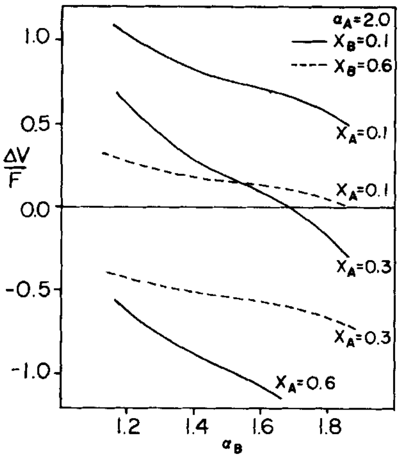

Figure 3. ΔV as a function of α_B for $\alpha_A = 2$ and various feed mole fractions.

The opposite happens with X_C, but the dependence of $\Delta V/F$ on X_C is usually much weaker. Another important thing to note is that the coefficient of $(\alpha_B - 1)^{-1}$ is always positive, which means that as α_B approaches unity, ΔV increases, that is, the indirect sequence is favored. Similarly, the coefficient of $(\alpha_A - \alpha_B)^{-1}$ is always negative, and as α_B approaches α_A, the direct sequence is favored, provided f is not very close to unity. Moreover, if α_B is close to α_A and both are large, we get $\Delta V \rightarrow X_A$ when $f \simeq 1$. This is in complete contradiction to what is commonly believed and to what the widely used heuristic "do the difficult separation last" suggests. The same contradiction arises when we examine the way in which the total number of trays is affected by the sequencing of the columns. As discussed in the appendix, "do the easy split last" always gives the fewest number of trays.

On the other hand, if $X_C > X_A$, the indirect sequence is favored for α_A and α_B near unity (and not for α_A near α_B). Also note that the dependence of ΔV on α_A is not clear, because the quantity $(X_C - fX_A + X_AX_C^2)$ can be either positive or negative.

If, in Eq. 23, we assume that $X_AX_C \simeq 0$, and set $f = 1$, we find that when

$$X_C/X_A > (\alpha_A + 0.2)/1.2 \tag{24}$$

then use the indirect sequence. This is exactly the criterion derived by Rod and Marek (1959) and by Marquez (1982). We expect this to be valid only when X_B is very large, because then it is true that $X_AX_C \simeq 0$ and $f \simeq 1$. In many other cases Eq. 24 can be misleading, particularly when α_B is close to unity.

The result obtained by Rudd et al. (1973), based on Eq. 4, could be

$$\text{Indirect if} \quad \frac{X_C}{X_A} \geq \frac{\ln\alpha_{AB}}{\ln\alpha_{BC}} \tag{25}$$

which we could also modify using Eq. 6 to give

$$\text{Indirect if} \quad \frac{X_C}{X_A} \geq \frac{\alpha_{AB} - 1}{\alpha_{BC} - 1} \tag{26}$$

The result based on Nadgir and Liu's (1983) model is obtained by comparing the quantities *CES*, given by Eq. 5, for the direct and indirect sequences. This result is

$$\text{Indirect if} \quad \frac{X_B}{X_AX_C} + 1 > \frac{\alpha_{AB} - 1}{\alpha_{BC} - 1} \tag{27}$$

Note that Eq. 27 indicates that whenever α_{AB} is approximately equal to α_{BC} or X_B is large, the indirect sequence should always be preferred. But this is not true in many cases. However, Nadgir and Liu base many of their design decisions of comparisons of the quantity *CES* for the various alternative splits.

The expressions based on Nath and Motard's model (1978) or Lu and Motard's model (1982) are much more complicated.

Validity of the Commonly Used Heuristics

In order to understand better the functional behavior of the quantity $\Delta V/F$, we plot it as a function of X_C/X_A and α_B in Figures 2 and 3. The values of the vapor rate used were the ones calculated with the approximate Eq. 23. We also use these graphs to understand the range of validity of the most widely used qualitative heuristics.

- "Remove the most plentiful component first." From Figure 2 it is clear that whenever $X_A > X_C$, the direct sequence is always better. However, the opposite is not always true. In fact, X_C may be as high as 5 times X_A and the direct sequence is still better (this happens for low X_B values and α_B close to α_A). Therefore, only "half" of this heuristic really holds, and it can often be misleading when $X_C > X_A$.
- "Make easier separation first" or "save difficult separations until last." We have already seen that Eq. 23 indicates an opposite trend, α_A being considered constant. This is illustrated in Figure 3, where $\Delta V/F$ is plotted against α_B. Note that all of the lines are approximately straight with a negative slope, which means that the direct sequence increases its chances of becoming better as α_B approaches α_A. The effect of α_B on $\Delta V/F$ is significant for low X_B values, while it is smaller (the slope is nearly equal to zero) for high X_B values. The latter is expected, since in this case Eq. 24 is approximately valid and ΔV is independent of α_B. The conclusion is that this heuristic is clearly misleading in many cases.
- "Favor equimolal splits." In Figure 2 we show some equimolal splits ($X_A + X_B = X_C$). Some of them correspond to negative $\Delta V/F$ values where the direct sequence is best, which contradicts this heuristic. In the case of large amounts of the heavy component, the heuristic is valid. In some cases, the economic penalty, associated with accepting the heuristic, is significant. For instance at point *a* we have that $X_C > X_A$, $\alpha_{AB} < \alpha_{BC}$ and that the *AB*/*C* split is equimolal. This heuristic, and in fact all three heuristics, suggest that the indirect sequence should be used. This is obviously not true, since the vapor rate required in the direct scheme is roughly 0.5 mol/mol of feed less than that for the indirect. Therefore, the heuristic of favoring equimolal splits is also not generally reliable, but can safely be used only when X_C/X_A is very large.

The heuristics analyzed above are some of the most widely cited. The conclusion we make is that we should use quantitative methods and take both the compositions and the difficulty of separation into consideration. Judgment cannot be based on rules that decouple the feed compositions from the relative volatilities. We also note that the trend of the total number of trays with respect to the column sequencing changes similarly to the vapor rate, and in fact strengthens the results above.

Nath and Motard (1978), Lu and Motard (1982), and Nadgir and Liu (1983) developed methods to match the accepted heuristics. However, as shown above, these heuristics are often incorrect. Thus, caution must be exercised if the "best" column sequence is based on one of these models.

Examples

1. Consider an ideal ternary mixture with components A, B, and C having relative volatilities 2.0, 1.8, and 1.0 and feed mole fractions 0.40, 0.10, and 0.50, respectively. To separate this mixture in three nearly pure products, it is of interest to estimate the most efficient distillation sequence.

Setting the operating reflux equal to 1.2 times the minimum, and using Eq. 23, we find that $\Delta V = -0.60$ (evaluation of ΔV with the exact Underwood's equations yields $\Delta V = -0.63$). Since $\Delta V < 0$, we can say that the direct sequence is preferred. We can further convince ourselves by calculating the minimum number of total trays required for the two schemes. For 1% impurities in every outlet stream, we find that 170 theoretical trays are required for the direct and 200 trays are required for the indirect scheme. We can also use Eq. A2 of the appendix, which would predict a difference of 34 trays instead of 30.

We note that this design decision contradicts all of the traditional heuristics. In fact, all of them suggest exactly the opposite—i.e., the indirect sequence. The most difficult split is the A/B ($\alpha_{AB} = 1.1$), and heuristics dictate that we should perform it last. Second, the most plentiful component is C and the heuristics indicate that C should be removed first. Finally, the AB/C split is equimolal and is favored by heuristics. We see that the traditional heuristics are completely misleading in this case, although they do not contradict each other.

The criterion of Rod and Marek, Eq. 24, also favors the direct sequence, since $X_C/X_A = 1.25$ and $(\alpha_A + .2)/1.2 = 1.83$, but this happens accidentally. If α_B in our example was 1.1 instead of 1.8, this criterion would again suggest the direct sequence as being better, since it is independent of α_B. However, an evaluation of the vapor rates shows that the indirect sequence should now be preferred. Note that the most difficult split B/C is performed first in this case too.

2. Morari and Faith (1980) examined a five-component mixture and found the optimal separation sequence without heat integration through detailed costing and after having optimized the operating conditions for each of the 20 possible columns. The mixture was propane (A), i-butane (B), n-butane (C), i-pentane (D), and n-pentane (E) with feed mole fractions 0.05, 0.15, 0.25, 0.20, and 0.35, respectively. The best sequence they found was ABC/DE, A/BC, B/C, D/E with an annual cost of 351,510.

If we apply our simplified synthesis method by calculating the vapor rates required for all of the design alternatives using the approximate expressions of Glinos and Malone (1983), we find that the sequence ABC/DE, AB/C, A/B, D/E is preferred. This sequence has a total vapor rate of 28.2 moles per mole of feed while the sequence found by Morari and Faith has a consumption of 29.1. However, if we do the detailed costing of our sequence we get an annual cost of 351,630. Therefore, these two design alternatives are indistinguishable and both are essentially optimal.

3. Andrecovich and Westerberg (1983) developed a method for determining the preferred sequence with heat integration, and they applied their procedure to a five-component ideal mixture. The best sequence they found performs the most difficult split first. This split is of the type $A/BCDE$, where A represents ethanol and B represents isopropanol. The alpha for these two components is about 1.2. Note that this split is carried out in 4 columns integrated with each other.

We anticipate that the difficult split should often be undertaken first if energy integration is considered. Even though the separation costs for a single column might be high, the small temperature drop, resulting from small α values, favors the breakdown of a single column into multiple, heat integrated units. Therefore, the traditionally most expensive separation may become the cheapest if heat integration is considered. The case of complex column configurations and heat integration will be addressed in another paper.

Sensitivity of the Design

It is important and very useful to know the sensitivity of a design alternative to changes in the operating conditions, the values of the physical properties, and/or the feed compositions. In other words, we would like to know the size of the neighborhood of the process variables in which the design alternative we chose is still nearly optimal. A design that is close to optimal but is flexible should be preferred over a slightly more optimal design that is very sensitive to small changes in the operating conditions. This is a problem that is not traditionally posed but that can often result in serious retrofit problems.

If analytical design criteria are available, such as those proposed here, the sensitivity of the optimality measure (vapor rate, cost, etc.) with respect to some variable can be easily evaluated by simply calculating its derivative. This will be always simple and straightforward to do. We give here some conclusions derived in this way for the ternary mixture case. The differentiation and the numerical calculations are simple and of no particular interest, so we don't present them here.

Systems with relatively small X_B or X_C feed compositions (corresponding to reactions such as $B \rightarrow A + C$ or $C \rightarrow A + B$, with high conversion) favor the direct sequence, and this design is nearly optimal even for strong disturbances, provided that α_B is not too small (say, $\alpha_B > 1.2$). Also, we find that the slope $d(\Delta V)/dx$, where x is the conversion per pass in the reactor, is always negative with a magnitude of about 1.0 or very often less than that. Therefore a conservative criterion for stability of the design can be stated as follows: "If ΔV is less than δx, where δx is an expected small conversion change, reconsider your choice of the design alternative or base it on operability considerations." For instance, if the conversion is expected to fluctuate between 50 and 60%, $\delta x = 0.1$.

Finally, we find that small α values generally result in optimal designs that are sensitive to perturbations, because their difference appears in the denominator of the derivative of ΔV. Also, the direct sequence is usually more stable than the indirect and should be favored when the decision is not clear.

Extensions to Other Systems

The problem of selecting a separation sequence for a process must be an iterative procedure. That is, the "best" separation sequence depends on the product distribution obtained in the reactor, but the "best" product distribution represents an economic trade-off between reactor size and selectivity losses balanced against recycle (which includes separation) costs (see Douglas, 1985). Since iteration is required, we prefer to use shortcut methods to develop good initial solutions and then to use more rigorous methods (see Hendry and Hughes, 1971, or Stephanopoulos and Westerberg, 1975) for final designs.

The shortcut method presented here is valid for a single feed stream, for constant values of the relative volatilities, and for sharp splits, which is the case previously considered in the literature. An extension of the analysis to more complicated multicomponent systems is simple since approximate expressions for minimum reflux ratios for these systems are available (see Glinos and Malone, 1983). Approximate expressions for the vapor rate required for sloppy splits are also available (Glinos and Malone, 1983), but the analysis needs to be extended to include the effect of recycling impure streams back to the reactor. Similarly, there are many processes that have multiple feed streams entering a distillation train; the synthesis procedure needs to be extended to include this case.

An extension of the analysis to nonideal systems (nonconstant α) will be much more difficult because neither Fenske's nor Underwood's equations will be valid. However, a promising approach is being developed by Doherty and co-workers (e.g., see Caldarola and Doherty, 1982; Levy et al., 1985; Van Dongen and Doherty, 1979).

APPENDIX

If we consider the simple case of a ternary mixture, we can easily evaluate the difference in the number of trays for the direct and indirect sequences. There are two cases of interest. Either the fractional recoveries are fixed or the impurities are specified. In the first case, the number of trays becomes independent of the way we sequence the columns when the recovery of each component is chosen to be the same in any column in which it is a key component (different recoveries between components are allowed). Also, the number of trays remains nearly independent of the sequencing if fractional recoveries and one product purity are specified. This is the approach followed in this paper, and we have already pointed out that the insensitivity of the number of trays to the sequencing of the columns becomes apparent from Eqs. 13 and 21. This is the most realistic case for the synthesis of a single product plant, where rules of thumb are used to choose the fractional recoveries of the splits in all the columns, except the product column.

However, the case commonly treated in the literature corresponds to the second approach. Here, we assume that all of the impurities are fixed from some design specifications. In fact, the unknown fractional recoveries correspond to optimization problems, rather than arbitrary design specifications. However, in order to understand the trends discussed by previous authors, we can examine the second case. If we write the expression for the number of trays, Eq. 13, in terms of mole fractions instead of fractional recoveries, we find

$$N_m \simeq 4\frac{\ln S}{\ln\alpha} = 4\frac{\ln\left\{\dfrac{X_{D,LK}}{X_{W,LK}}\dfrac{X_{W,HK}}{X_{D,HK}}\right\}}{\ln\alpha_{LK,HK}} \tag{A1}$$

In order to evaluate the difference in the number of trays in terms of stream compositions, we use Eq. A1 and assume the same level of impurities, p, in all streams and that the splits are relatively sharp. We then find

$$\Delta N = N^{\mathrm{dir}} - N^{\mathrm{ind}} = 4\left\{\frac{\ln(1 + X_A/X_B)}{\ln(\alpha_{BC})} - \frac{\ln(1 + X_C/X_B)}{\ln(\alpha_{AB})}\right\} \tag{A2}$$

This equation is useful to indicate the cases where the number of trays can be an important factor that has to be taken into account in the synthesis procedure. We see that if both relative volatilities are high (easy splits), the difference in the number of trays will be small and need not to be considered. Small errors in this approximation are not amplified by the magnitudes of coefficients K_1 and K_2 of Eq. 12. Using Eq. A2, we can examine the various limiting cases, where ΔN can be significant.

An interesting limiting case is when the A/B split is much more difficult than the B/C split, so that α_{AB} is close to unity and $\alpha_{BC} \gg \alpha_{AB}$. Then the first term on the right of Eq. A2 can be omitted, and we can write

$$\Delta N = -4\frac{\ln(1 + X_C/X_B)}{\ln(\alpha_{AB})} \tag{A3}$$

In this case, ΔN can be significant whenever $X_C \gg X_B$ and can be as large as 100 trays. Note here that ΔN is always negative, and therefore the direct sequence has a certain advantage, since it requires a smaller number of trays whenever $\alpha_{BC} > \alpha_{AB}$. This contradicts the heuristic "do the easy split first" and implies that the difficult separation should be carried out in the first column of the sequence. Also, it contradicts the heuristic "remove the most plentiful component first," since the magnitude of ΔN increases as X_C becomes bigger than X_B.

What is also of interest is the fraction of the total trays that ΔN represents. Dividing Eq. A3 by the number of trays in the direct sequence, we find that approximately

$$\frac{\Delta N}{N^{\mathrm{dir}}} = \frac{\ln(1 + X_C/X_B)}{2\ln p + \ln(1 + X_C/X_B)} \tag{A4}$$

The above equation gives that usually ΔN is less than 10 to 20% of the number of trays for the direct sequence. Essentially the same result is found when we evaluate ΔN as a percentage of N^{ind}. It is interesting to note that ΔN decreases as the sharpness of the split increases, that is, as p approaches zero. This is the opposite to what one might expect. Completely analogous equations and conclusions are derived when we assume $\alpha_{BC} \ll \alpha_{AB}$. Again, the difference in the number of trays favors the difficult split as the first to perform.

As a general conclusion, the total number of trays is insensitive to the way we sequence the columns if the fractional recoveries in all the columns are specified, or if purities are specified but the relative volatilities are not in the neighborhood of unity. For small volatilities, and especially when the feed compositions are not balanced, we should evaluate ΔN with an equation like A2 and probably take the number of trays into account, for example, by using the shortcut design equations with a cost model.

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NOTATION

CAP = capital investment required for a tower
CES = coefficient of ease of separation, defined by Eq. 5
C_o,C_1,C_2 = cost coefficients for the model of Eq. 10
D = distillate flow rate
F = feed flow rate
f = correction factor defined by Eq. 16
G_1,G_2 = coefficients for Colburn's cost model, Eq. 11
H_L,H_D = functions in Lu and Motard's model, Eqs. 1 and 2
K_1,K_2 = coefficients for the linear cost model, Eq. 12
N = actual number of trays
P = optimal overhead operating pressure
p = mole fraction of the heavy key (light key) in the distillate (bottoms)
S = separation factor, defined by Eq. 13
SP_i = fractional recovery of the light key (heavy key) at the top (at the bottom)
TAC = total annualized cost of a tower
V = vapor flow rate
W = bottoms flow rate
X_i = mole fraction of component i in the feed
x = conversion per pass in the reactor

Greek Letters

α_{ij} = relative volatility of component i with respect to component j. If j does not appear, the heaviest component is assumed
Δ = difference between the annualized costs of the direct and indirect sequences, defined by Eq. 20
ΔN = difference of the total number of trays required for the direct and indirect sequence
ΔT = temperature difference between the top and the bottom of a column
ΔV = difference of the vapor rates required for the direct and indirect sequence, per mole of feed

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