Part II. Heuristic Optimization

State optimization should not be ignored in the evaluation of distillation alternatives. However, heuristic rank order algorithms can greatly simplify the analysis. Optimal operating pressures correlate well with feed bubble points, and intertower economic interactions are often small.

SCOPE

A detailed economic evaluation of a distillation train requires optimization on the operating state of each tower. In such calculations, models are formulated which include estimates of the tower dimensions, internal requirements, heat exchanger areas and duties, and pumping requirements. Often, pretreatment of the feed is possible which may include heating or cooling this stream as well as the pumping requirements to attain the tower operating pressure.

In scoping studies, however, it is often desirable to find attractive distillation configurations without performing a detailed economic analysis. One approach to simplifying the problem is to assume an operating state and carry out an economic evaluation of the system on that basis. In distillation evaluation, for example, it is common to fix the vapor rate at some constant ratio greater than the minimum (see Lockhart, 1947; Rod and Marek, 1959; Thompson and King, 1972; Freshwater and Henry, 1974). In addition, the overhead pressure of a tower and the feed fractional vaporization are frequently ignored as optimization variables because of the computational complexities which ensue.

In this study, the venture cost of operating a single distillation tower is examined as a function of the overhead operating pressure, the feed fractional vaporization, and the vapor to minimum vapor rate ratio. One variable is changed parametrically, while the two remaining are fixed at their optimal values. The percentage increase in cost above the minimum is shown. The relative significance of each variable is discussed. A method is presented for estimating the optimal overhead operating pressure of a distillation tower.

Simplified methods for calculating relative tower costs are evaluated. These methods utilize estimates of the Underwood minimum vapor rate, the Fenske minimum theoretical stages, and the temperature drop up the tower, or combinations thereof. Simplified rank order methods suggested by Rudd et al. (1973) are also considered and discussed. These alternative ranking methods are evaluated by comparing their predicted ranking with the ranking obtained from a detailed economic evaluation of the distillation towers, including a gradient search over the operating state to minimize the venture cost of each tower considered. The Spearman rank correlation coefficient is used to compare the effectiveness of the various methods.

Consideration of the economic interactions between two towers in a train is also important in the evaluation of alternatives. It is often necessary to neglect any interactions which may occur in order to synthesize highly integrated systems (see Rathore et al., 1974). A study of these interactions between towers in the direct and inverted configurations (see Part I) is presented. Observed interactions between towers in complex design configurations are also discussed.

CONCLUSIONS AND SIGNIFICANCE

The overhead operating pressure can be more economically significant than the ratio of vapor to minimum vapor in the tower, which in turn is more significant than the feed fractional vaporization. Increasing utility rates increases the importance of optimizing over all three variables, although the effect is most pronounced on the operating pressure, especially if refrigerants are utilized in overhead condensation.

The rank order algorithm provides a useful screening device for eliminating many design configurations, although it is limited in applicability to the simple direct and inverted sequences. The recommended correlation provides a significant improvement in accuracy over the common assumption that costs are proportional to the Underwood minimum vapor requirements, but the computational difficulties are only slightly greater than those associated with the latter estimation technique.

The economic interactions between towers in the simple direct and inverted configurations were found to be negligible. Distillation trains comprised of towers in these simple configurations may be optimized sequentially, starting with the upstream tower and proceeding in the same direction as material flow. When all possible towers have been state optimized once, then the optimal train may be synthesized, starting with the downstream towers. The process synthesis occurs in a direction opposite to that of the material flows (see Hendry and Hughes, 1972). The absence of significant interactions between the towers facilitates the separation of the state and structural optimization into two sequential and distinct steps and minimizes the state optimization requirements.

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Process synthesis is closely related to system analysis. In order to compare two processing structural alternatives, it is necessary to first optimize the processing state for each and compare some suitable economic indicator like venture cost. However, many processing alternatives of industrial interest have excessive degrees of freedom. So, to simplify the problem, the designer frequently resorts to comparisons in which certain of the optimization variables have been arbitrarily fixed. In distillation evaluation, for example, it is common to fix the vapor rate at some constant ratio greater than the minimum. In addition, overhead pressure, feed fractional vaporization, or subcooling or superheating product streams are frequently ignored as optimization options, at least in preliminary analysis, if their economic effects are considered small. To the extent that these assumptions are valid, they constitute viable heuristics. However, relatively few evaluations have actually been carried out to ascertain specifically the correctness of such assumptions.

As a further simplification of the network analysis, some workers have chosen to optimize heuristic objective functions. Rudd et al. (1973) and Harbart (1957), for example, suggest comparisons utilizing simple functions based on feed mass rates, and the normal bubble points of pure components to be separated. When distillation alternatives are compared on this basis, cost variables such as capital investment and utilities are considered only by inference. These heuristics are appealing because of their simplicity, but their ability to rank a collection of towers according to relative costs has not been previously measured.

Heuristics play an important role in simplifying the system analysis and optimization, so that the higher goals of process synthesis can be achieved. For example, a general heuristic and evolutionary synthesis approach was taken by Rudd (1968), Masso and Rudd (1969), Siirola et al. (1971), and Siirola and Rudd (1971). In this work, the objective was to discover good, and hopefully optimal, design structures via completely heuristic means and to carry out a direct search over the structural alternatives. Deductive reasoning was employed. The heuristic scheme was considered valid if it found economically attractive designs. Powers (1971) further suggested that weighting factors be applied to a list of heuristics for choosing alternative design sequences. Using these rules, the AIDES program worked interactively with the design engineer by suggesting structures which appeared to have a high probability of optimality. The search through alternative tasks was evolutionary. The AIDES program learned to recognize attractive design patterns. It also assumed the ability to decompose a process into nearly independent subproblems, although the validity of this assumption was not determined. Moreover, the significance of the heuristic rules was not evaluated in any systematic way.

Thompson and King (1972) also developed a heuristic method for synthesizing separation networks. They compared different separators by using heuristic weighting factors which reflect the estimated cost of the separators. Initially, the weighting factors were given arbitrarily low values in order to encourage their investigation by the computer synthesis program. The system converged by eliminating structural alternatives. The weighting factors were periodically updated during the deductive synthesis by detailed analysis of the unit costs. This cost analysis, however, did not include state optimization.

These heuristic and evolutionary methods of synthesizing separation networks have the common feature of beginning a synthesis starting with the original feed to be separated. The heuristics are invoked at each step along the way until all the products have been generated, and no extra streams are unaccounted for. This approach to design is a logical one, since it is desirable to move from the upstream towers downstream when performing the calculations. The same computational approach is utilized when more detailed simulation with equilibrium stage models are performed, since it is convenient to pass information in that direction.

The algorithmic approach to synthesizing separation networks begins with the downstream towers. Hendry and Hughes (1972) showed how a list splitting operation could be used together with dynamic programming (Bellman, 1957) to synthesize separation networks. In this method, the components in the original feed mixture are first ranked according to some physical property. In the case of straight distillation, decreasing volatility is a convenient ranking, but the method is applicable for any ranking of separation factors in general. Hendry and Hughes also showed that the method can easily be applied to extractive distillation. If the ranking changes, say with pressure, then both rank lists can be formed and the pressure optimization appropriately constrained. So the method is quite general.

For any one ranked list L_N so formed for an N component mixture, two contiguous rankings can be formed from it, by deleting either the first or the last component from L_N. This process can be continued until $N - 1$ lists, each containing only two contiguous components, are formed. In this manner, all the subproblems derived from performing sharp cuts, without any distributed components, are represented by the subgroup lists.

Once the subproblems for all lists have been identified, then each subproblem is state optimized. The structural optimization is performed by working backwards using the subproblems as building blocks to synthesize the structure having the minimum venture cost. In this fashion one can generate the optimal structure for separating N components using knowledge of the optimal structures for separating $N - 1$, $N - 2$, . . 3 and 2 components. The extension to consider all of designs I through VIII (see Part I) by this method is straightforward, although a decomposition into a set of nearly independent subproblems requires that some subproblems consist of more than one tower.

The usefulness of this algorithmic approach for designing integrated networks with energy recycle has been demonstrated by Rathore et al. (1974). They have shown that the serial designs without energy recycle must form an upper bound for the cost of any integrated process. They also indicate systematic methods for proceeding with the energy integration. Using the serial solution as a base, they integrate the process by first optimizing two subproblems simultaneously, then three, etc. They show how the pressure range for optimization can be effectively reduced and a large number of alternatives eliminated without detailed consideration.

STATE OPTIMIZATION AND UTILITY RATE EFFECTS

In this work, design alternatives (see Part I) were compared after they had been optimized with respect to their operating state. The venture cost of each design was minimized by conducting a gradient search over the response surface and optimizing with respect to operating pressure, feed fractional vaporization, and the vapor to minimum vapor ratio. There is some question, however, as to whether or not this optimization is actually necessary. In order to obtain an answer, a single tower, like those comprising designs I and II in Part I, was chosen arbitrarily and optimized. This tower separates a feed containing equal amounts of iso and normal butanes. Each of the three optimization variables was then varied parametrically, while the others were set at their optimal values. In this manner Figures 1, 2, and 3 were obtained. These results are presented as percentage venture cost increase which is relative to the minimum venture cost and arbitrarily scaled as a percentage of \$250 000. Thus, for the low utility costs

$$\% = \frac{VC - \$140\,377}{\$250\,000} \times 100 \qquad (1)$$

and for the high utility costs:

$$\% = \frac{VC - \$430\,780}{\$250\,000} \times 100 \qquad (2)$$

so that the slopes of the curves in Figures 1, 2, and 3 are in comparable percentage units, although they have different reference points. (The utility rates are defined in Table 5, Part I.)

Figure 1 shows the effect of the vapor to minimum vapor ratio on the venture cost of a single tower. This effect was measured both for the low and high utility rates. It is clear that increasing the utility rates has a definite effect on the location of the minimum. As the cost is increased, the optimum vapor to minimum vapor ratio shifts from 1.113 3 to 1.026 7. Although this is a small difference numerically, if the tower is designed at the higher reflux ratio when the higher utility costs occur, it causes a 10% increase in the annual venture cost.

The venture cost of the tower appears to have the same asymptotic solution for both utility cost levels as the ratio approaches unity. This occurs because at the low reflux levels the costs are dominated by the capital investment term which remains the same.

Increasing the utility rates, however, has a pronounced effect on the venture cost at ratios greater than the optimum. Many investigators have suggested that a tower be designed on the basis of a fixed reflux at 1.25 times the minimum. It is interesting to note that increasing the vapor rate by this factor has a small effect on the processing costs at the lower utility levels. From Figure 1, the percentage cost increase is only about 1%. But when the utility costs are increased by a factor of 10, the cost increase for the same tower is 23% above the minimum. Such a large increase is not acceptable and shows that at the higher cost levels a failure to optimize over the reflux ratio can perhaps make the results meaningless.* This is not necessarily the case if all designs have similar curves as in Figure 1. But this study indicates that the minimum venture cost for different designs occurs at different values of the vapor to minimum vapor ratio. It is likely, therefore, that the curves are not identical.

The curves in Figure 1 look qualitatively very similar to those in McCabe and Smith (1967) and Robinson and Gilliland (1950) for cost vs. reflux ratio. Both curves appear very smooth, and there are no apparent discontinuities in the slope which can be detected at the minima or elsewhere.

Figure 2 shows the effect of the feed fractional vaporization on the venture cost of the same tower. This curve shows a strong linear behavior on either side of the minimum. Its most distinctive feature is the discontinuity in the slope at the minimum. The minimum for this downstream tower occurs when the feed is subcooled. Increasing the utility rates shifts this minimum from −0.2 to −0.287. At the high utility rates, the common assumption of sending a bubble point feed to the tower leads to a 5% cost increase over the minimum possible venture cost. Thus, the venture cost is less sensitive to the feed fractional vaporization than to the tower vapor rate.

The discontinuity in slope which occurs at the minima in Figure 2 is a consequence of the Underwood equations. A typical percentage vapor increase, shown as a function of the feed fractional vaporization, is linear on either side of the minimum. The change in slope occurs when the minimum vapor rate is controlled by the upper rather than the lower section of the tower. In that region of the figure where the slope is negative, the minimum vapor rate is determined by the lower section of the tower. As the feed fractional vaporization is increased, the vapor requirements in this section of the tower are reduced. The minimum occurs at a bubble-point feed. At positive feed fractional vaporization, the minimum vapor rate is greater in the upper section of the tower and it controls. This control is reflected in the section of Figure 2 with a positive slope.

Figure 3 shows the effect of the overhead pressure on the cost of a single tower. This surface also has discontinuities in slope. The discontinuities at the low pressures are caused by an inability to satisfy approach for the warmer refrigerants. As the overhead pressure is increased, the reflux condenser can be supplied with warmer ammonia refrigerant which leads to the apparent discontinuities as the condenser routine switches from the colder to the warmer and less expensive refrigerant.

The curve for the high utility rates is very flat between 0.1 and 0.5 MN/m^2. Ammonia refrigerant is required in this region. For some feed mixtures, the slope in areas like this becomes positive, so that a local minimum occurs in that region of the pressure curve. When this occurs, the optimization routine can get stuck on the local minimum if it was started from the low pressure side. This figure then illustrates the wisdom of the heuristic suggested by Rudd et al. (1973), "avoid excursions in temperature and pressure, but aim high rather than low."

It is also clear from Figure 3 that smaller errors result if the overhead pressure is greater than the optimum, than if it is less. An atmospheric tower operating at the high utility rates leads to over 900% greater annual costs. The use of refrigerants is the cause of this increase. Cooling water is always used at the global minimum in this study, and a local minimum is suspected if a tower is found using any refrigerant.

A blowup of conditions at the optimum points for both utility costs is presented in the upper right-hand corner of Figure 3. Increasing the low utility rates by a factor of 10 causes the optimum pressure for the same tower to shift from 0.796 to 0.910 MN/m^2. This effect has been observed with other towers, and the shift for the fractional feed vaporization shown in Figure 2 is always negatively correlated with it. Generally speaking, as the optimum overhead pressure is observed to increase, the optimum feed fractional vaporization decreases. A discontinuity at the minima can also be seen in the blowup in Figure 3. Like that discontinuity in Figure 1, this is a consequence of the Underwood equations.

It is clear from Figure 3 that the pressure is an important optimization variable. But the range of the variable is usually large, and it is not clear where the optimum lies. It can vary considerably from feed to feed. Optimal operating pressures have been found as low as 0.06 MN/m^2 (8 $lb/in.^2$abs) and as high as 1.59 MN/m^2 (230 $lb/in.^2$abs). It is observed, however, that the optimal overhead pressure exhibits a strong correlation with the nor-

* In practice, a tower would probably be operated with vapor rates greater than the optimum to provide controllability, especially when the optimum rate is very close to the minimum. Under such conditions, the primary significance of the optimum vapor rate is that it provides a uniform, economic basis for comparing alternatives.

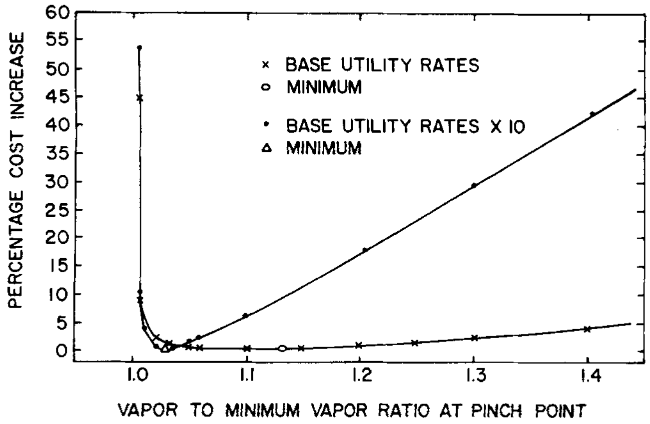

Fig. 1. Effect of the vapor to minimum vapor ratio on the venture cost of a tower.

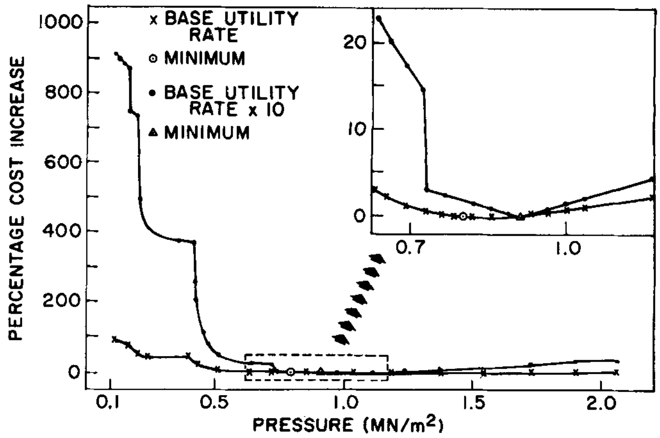

Fig. 3. Effect of the operating pressure on the venture cost of a tower.

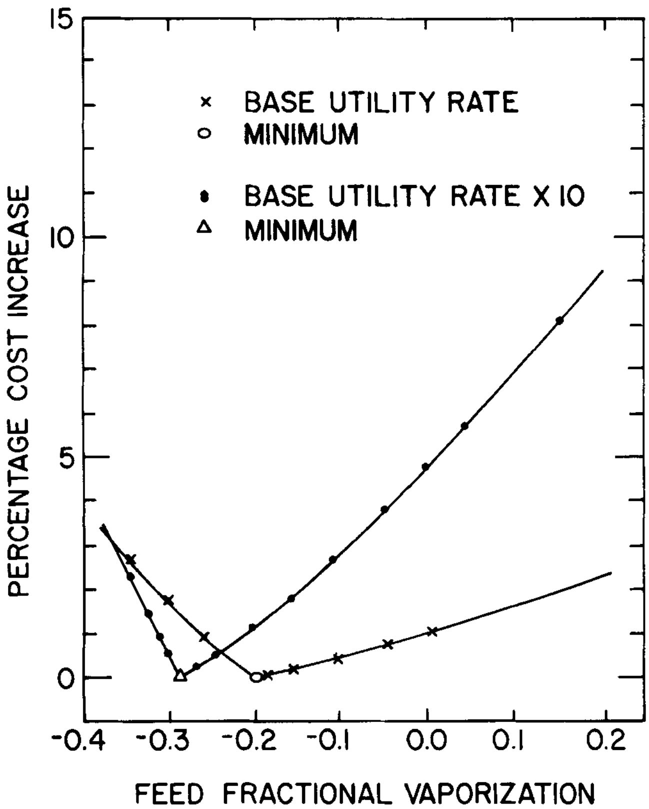

Fig. 2. Effect of the feed fractional vaporization on the venture cost of a tower.

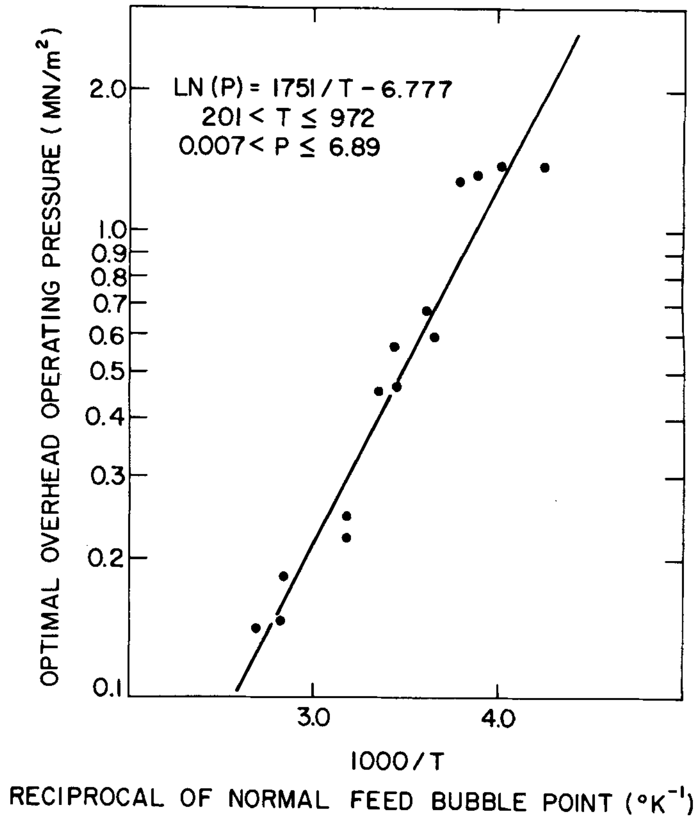

Fig. 4. Correlation of optimal overhead operating pressure with the normal feed bubble point.

mal feed bubble point. This correlation is shown as Figure 4, where the logarithm of the optimal pressure appears to give a straight line when plotted against the reciprocal of the normal feed bubble point in absolute temperature units. A good regression model for this correlation is given by

$$LN(P) = 1\,751/T - 6.777 \qquad (3)$$

The regression should not be extrapolated beyond the temperature and pressure ranges given by

$$201 < T \leq 972 \qquad (4)$$

$$0.007 < P \leq 6.89 \qquad (5)$$

The coefficient of determination for this correlation is 0.94 using fourteen observations. In the absence of any prior knowledge as to where the optimum operating pressure lies, Equation (3) is useful for obtaining an initial estimate. It should be a valid approximation so long as the relative utility costs are as shown in Table 5, Part I. In the event that steam costs are significantly greater than cooling costs, then the validity of Equation (3) is somewhat diminished, as is the heuristic ". . . aim high rather than low."

HEURISTIC PREDICTION OF RANK ORDER

Heuristic objective functions and rank order functions have been commonly used in process design and synthesis for some time. In distillation, the most common rank order function results from specifying that the reflux be fixed at some constant above the minimum.

Consider a set of M different alternative designs which can be arranged arbitrarily and numbered with subscripts j, where $j = 1, 2, \ldots M$. Associated with each of these designs is an economic observation X_j which will normally be the best possible estimate of the economic cost or profitability of the j^{th} design. These observations can be obtained either from a highly detailed and complex optimizing cost model (see Tedder, 1975) or, preferably, from actual construction and operating experience. If the observations are compared, then an integer can be assigned to each according to its relative magnitude. The integer rank 1 is assigned to the smallest observation and rank M to the largest. Thus, for the original list of observations

$$(X_1, X_2, \ldots X_j, \ldots X_M) \tag{6}$$

there is a corresponding integer list whose elements are assigned according to the rank order magnitude of the observations:

$$(I_{X_1}, I_{X_2}, \ldots I_{X_j}, \ldots I_{X_M}) \tag{7}$$

A rank order function is defined as any function which predicts the rank order given in (7) by generating a set of observation estimates Y_j whose subscripts correspond to the same designs as in (6). An integer can also be assigned to each of these estimates according to their relative magnitudes. Thus, for the rank order function yielding the set of estimates

$$(Y_1, Y_2, \ldots Y_j, \ldots Y_M) \tag{8}$$

there is the corresponding integer list

$$(I_{Y_1}, I_{Y_2}, \ldots I_{Y_j}, \ldots I_{Y_M}) \tag{9}$$

In the event that the rank order function is a perfect indicator of the true design cost ranking, then there is a one-to-one correspondence in magnitude between all the elements of the two integer lists; that is

$$I_{X_j} = I_{Y_j} \quad J = 1, 2, \ldots M \tag{10}$$

Often the rank order function will generate a set of estimates whose relative magnitudes do not match those of the true cost observations for some of the designs. The goodness of the match for any rank order function can be measured, however, by calculating the Spearman rank correlation coefficient (see Mendenhall and Schaeffer, 1973) defined by

$$R_S = 1.0 - 6 \left[\sum_{j=1}^{M} d_j^2 \right] \Big/ [M(M^2 - 1)] \tag{11}$$

where

$$d_j = I_{X_j} - I_{Y_j} \quad J = 1, 2, \ldots M \tag{12}$$

A number of investigators have compared designs in distillation by assigning costs which are proportional to the Underwood minimum total vapor rate V_j^U .By doing this, they are in essence assuming that the rank order list for the observations X_j is adequately represented by

$$Y_j = V_j^U \tag{13}$$

All design methods which specify the vapor as a constant ratio to the minimum vapor without considering the height of the distillation tower in essence assume Equation (13) as their rank order function.

Rudd et al. (1973) have suggested an interesting rank order function given by

$$Y_j = \text{feed rate/boiling-point difference} \tag{14}$$

The boiling-point difference is between those boiling points of the components being separated. While Equation (13) requires trial and error calculations, Equation (14) is especially simple to evaluate, since all the necessary data are readily available.

The ability of Equations (13) and (14) to predict the rank order in venture costs of a collection of similar distillation towers has been tested along with several other slightly more complicated rank order functions. In this test, the set of observations X_j is given by the observed minimum venture cost at the low utility rates associated with 136 simple towers. All the towers compared are like those used in designs I and II (see Part I). The upstream towers in design V were also included, since they are of the same structure, but not designs III, IV, VI, or VII. Because Equation (14) generates the same numerical estimates for many of these towers, only a subset of thirty-one observations was used to evaluate this function, for which it gave numerically different estimates.

Equation (14) is evaluated from the feed rate and the difference in pure component normal bubble points. The remaining rank order functions require some combination of the minimum vapor rate V_j^U, the minimum number of theoretical stages N_j (Fenske equation), and the observed temperature drop up the tower δT_j.

The results of evaluating several functions are presented in Table 1. In addition to R_s, the sum of the squared deviates Σd_j^2 is also presented. The third column in Table 1 shows the sum of the squares for the various models divided by that observed for model 1 which has the strongest correlation. The sum of squares shown for model 9 was calculated from its observed R_s and Equation (11) assuming 136 observations. The actual observed sum of squares was 805 for the thirty-one observations.

None of the rank order functions are perfect. The parameters in the observed best function were obtained by nonlinear least squares. It is interesting to note that the simple least-squares linear model 2 gives results which are almost as good. (The least-squares constants are not shown for the linear models.) Excluding the constants, the least-squares coefficients are given for models 2, 3, 4, and 5. Model 6 is a function which uses the minimum vapor rate and the theoretical trays in the actual cost equations (Tedder, 1975). It is surprising that this model is less effective than model 4, which gives the results corresponding to Equation (13). Although the temperature drop up the tower and the minimum number of trays are statistically important in regression 2, it is clear that the most important variable of the three in that model is the minimum vapor rate. Thus, from a rank order standpoint, the common assumption that the costs are proportional to the minimum vapor rate is fairly good.

Equation (14) (model 9) does a surprisingly good job on those towers for which it is capable of predicting that some difference exists. Since it gives the same estimate for 105 of the towers, however, it cannot be as powerful as the other models whose correlations are based on all observations.

To further assess the significance of the best rank order function found, the observed rang order I_{X_j} was plotted against the predicted rank order I_{Y_j} for model 1. The re-

Table 1. Evaluation of Several Rank Order Functions

J	Model, Y_j	R_S	Σd_j^2	SS_J/SS_1
1	$(V_j^U)^{.648} N_j^{.184} \delta T_j^{.144}$	0.945	22 864	1.00
2	$90.22V_j^U + 153.9N_j + 344.2\delta T_j$	0.943	24 024	1.05
3	$107.7V_j^U + 203.3\delta T_j$	0.934	27 356	1.20
4	V_j^U	0.926	31 202	1.36
5	$88.34V_j^U + 912.1N_j$	0.920	33 338	1.46
6	$0.299\,6CAP_j + 0.520P_j$	0.917	34 640	1.52
7	$V_j^U N_j \delta T_j$	0.906	41 944	1.83
8	$V_j^U N_j$	0.864	56 810	2.48
9	Feed rate/boiling-point difference	0.837 7	68 039	2.98
10	$V_j^U \delta T_j$	0.646	148 452	6.49

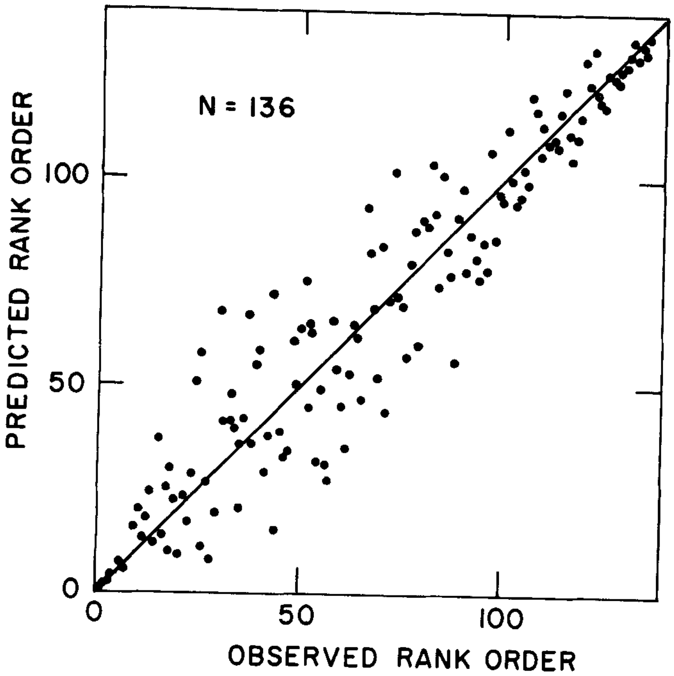

Fig. 5. Predicted rank order of towers using model 1 vs. the observed rank order from a detailed economic evaluation.

sults are shown in Figure 5. Deviations from the 45 deg line show up the model inadequacy. It is interesting to note that it correctly predicted the order of the best five designs. This result was also observed for model 4. However, there is still considerable scatter between the predicted and observed rank orders for model 1. Even so, there is sufficient correlation to use these functions as screening devices to eliminate many of design alternatives.

Although not shown, it has been observed that the rank order correlation for individual towers is about the same as the correlation observed for complete designs such as I and II consisting of two towers. When comparing designs, the rank order function becomes the sum of the estimates for the individual towers, just as the venture cost is a similar sum of individual tower costs. Given that the strength of the rank correlation is unchanged, then the observed rank discrepancies for the individual towers give a reasonable estimate of that expected for the rank order of the design alternatives.

The algorithm is suggested as a fairly simple method of identifying a few attractive designs from a large field of alternatives. These few attractive designs would then be examined in more detail. Model 1 in Table 1 gives the best estimate of the rank order, but that model also requires estimates of the minimum vapor rate, the minimum theoretical trays, and the temperature drop up the tower. In order to use this model, some method is needed to obtain these parameters. It is suggested that these calculations be performed by the algorithm presented below:

1. Obtain estimates of the overhead and bottom product compositions and rates for each tower (see Part III).
2. Estimate the optimal overhead operating pressure for each possible tower using the empirical correlation given by Equation (3).
3. Assume a nominal pressure drop for each section in the tower to estimate the pressure profile elsewhere.
4. Calculate the overhead bubble point and the bottoms dew point for the assumed compositions and pressures. Their difference is the desired temperature drop δT_j.
5. Calculate the minimum vapor rate using the Underwood equations. Assume bubble-point feeds. (Use the largest vapor rate calculated for all roots and sections.)
6. Calculate the minimum theoretical trays for each tower using the Fenske equation. (Calculate for all component pairs, use the largest value for each section, and sum for each tower.)
7. Calculate Y_j for each tower using model 1 or 2.
8. Form the rank order list of the estimates and examine the most attractive designs in more detail.

SUBPROBLEM INTERACTIONS

Study in the area of process synthesis has revealed two basic approaches to the problem. There are integrated methods which reduce a network to its optimal configuration and decomposition methods which synthesize the optimal structure from design subunits.

The integrated methods have been discussed by Umeda et al. (1972) and Ichikawa and Fan (1973). A network is formulated which contains all feasible designs as subunits. An optimization is performed which minimizes the network objective function by varying the process state variables and the mass rates between the different processing units. The optimal design is obtained by splitting streams to alternative routes within the enlarged structure. When the optimized splitting ratios are close to 0 or 1, alternative streams can be eliminated, and the optimal processing structure has been found.

Brosilow and Lasdon (1965), Umeda et al. (1972), and Tazaki et al. (1972) have explained how a process can be divided into subproblems by forming Lagrangian objective functions. On the lower level of the optimization, the subproblems are optimized individually. On the upper level, the optimization between the subproblems is coordinated using Lagrange multipliers in order to effectively account for any interactions. Umeda et al. (1972) have used this method to solve a three subsystem problem. But it is too complicated to be useful in the general synthesis problem.

Process decomposition can be used in conjunction with dynamic programming to state optimize a set of subproblems, as has been done by Aris (1961) for sequential reactors. Beveridge and Schechter (1970) give a review of the large number of different applications for dynamic programming in state optimization. Consider, for example, a process which has been divided into R subproblems which are arranged sequentially so that each except the first or R^{th} stage receives a feed from its immediate precursor. In general, each dynamic programming stage or subproblem may yield any number of products, but they do not affect the optimization since they are not interconnections or links between the stages.

In distillation, the logical stages are based on the towers themselves. If the mass rates of the feeds interconnecting two towers which are not thermally coupled are specified, then the feed state for each of the downstream towers is fixed when the pressure and enthalpy are determined. If the convention is adopted that the feeds are at their bubble point when they enter the subproblem, then the feed pressure is the single state variable which must be considered in the dynamic programming optimization to account for subproblem or intertower interactions. A bubble-point product is always taken from the upstream tower and sent as feed to a downstream tower where it may be cooled or heated as desired within that subproblem. Under these conditions, a grid of feed pressures, say p pressures, must be chosen such that they include upper and lower bounds on the optimal pressure for operating the upstream tower. If the operating pressure in the upstream tower is to be treated as a continuous variable in the state optimization for that subproblem, then a regression expression for the venture cost of operating the downstream tower as a function of its feed pressure should be obtained from the

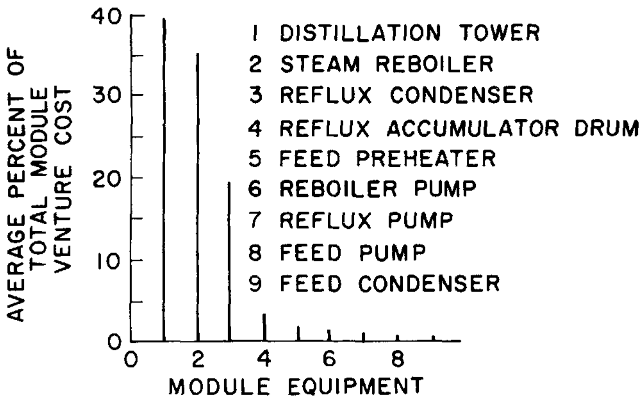

Fig. 6. Typical relative costs of equipment item in a simple distillation tower.

grid of p feed pressure points. Consequently, each downstream tower must be state optimized p times. If s subproblems are considered from the process decomposition, then $p(s - 1) + 1$ state optimizations must be performed.

A much simpler approximate method is given by starting with the R^{th} tower, optimizing it alone, then calculating from the optimal overhead pressure the required feed pressure and enthalpy to the downstream tower. The interactions between the towers are then ignored, but only s state optimizations must be performed, one for each tower.

The essential differences between the rigorous and approximate optimization methods are then as follows. The rigorous method starts with the downstream tower and works upstream, taking all the interactions between the towers into account. The approximate method starts with the upstream tower and works downstream, assuming that there are no significant interactions between the towers. The rigorous method can optimize designs I or II in $p + 1$, three-dimensional optimizations.

In order to assess the significance of any interactions between the subproblems in the direct and inverted sequences, these designs (I and II in Part I) were optimized using both the approximate and rigorous methods described above. This analysis gave estimates of the venture cost for each design obtained by the rigorous and approximate methods for a total of fifty-six observations. In all fifty-six cases, obtained using the low utility costs, the observed differences were less than 2%. The interactions are really insignificant, since cost differences between designs are often greater than 10% over a large portion of the composition surface. Most interactions observed were only slightly greater than zero. Moreover, the cumulative function for these small tower interactions shows that they are lognormally distributed. The expected deviation obtained is 0.13% of $250 000 in annual venture cost.

A plot of the venture cost of the downstream tower vs. the feed pressure shows only a very weak dependence. As the pressure is increased, the observed venture costs decrease slightly since the tower is, in essence, receiving free energy from its feed. However, this free enthalpy, or the lack of it, is relatively unimportant compared to the total cost of the tower. Often the vapor and liquid traffic within a tower is much greater than the feed rate, so the internal molar rates tend to dominate the economic picture.

The bar chart, shown in Figure 6, illustrates another aspect of why the tower interactions are so small. This chart shows a breakdown of the percentage of the venture cost associated with the various processing items in simple towers like those in designs I and II. Nearly 95% of the total venture cost associated with the subproblem is due to the tower, the reboiler, and the overheads condenser, items 1, 2, and 3 in Figure 6. Processing items associated with the feed typically constitute less than 3% of the total venture cost associated with a subproblem. Since such a small percentage of the energy requirements are met by the feed enthalpy, the dependence of the module cost on it is very weak. This important observation was assumed by Rathore et al. (1974) and justifies their design method which only considered the first three items in Figure 6.

In designs I and II, the mass rate in the link connecting the two towers is always fixed by the overall material balances and does not change during the state optimization. This is not the case for design VIII (see Part I), where the fraction of the feed sent overhead is an optimization variable. In that design, the mass rates between towers 1 and 2 and between towers 1 and 3 do change during the state optimization. Surprisingly, however, significant interactions do not occur between sequential towers in this case, even when the material balances vary. For three cases, design VIII was optimized as a single problem with 10 deg of freedom. This optimization constitutes a rigorous solution, since the interactions are automatically taken into account if the design is not divided into subproblems. For these same cases, the upstream tower was then optimized separately with 4 deg of freedom. In all cases, the upstream tower had essentially the same final state and venture cost when optimized both ways. So, significant interactions do not occur between the towers of design VIII.

Comparison of the upstream tower final states obtained for design VIII, however, with those obtained for design V shows a significant difference in all cases. The final states were not the same. In particular, the amount of feed sent overhead in tower 1 of design V is usually significantly greater than tower 1 of design VIII. Consequently, that design cannot be decomposed into two independent subproblems.

The work of Hendry and Hughes (1972) showed how decomposition methods could be used in process synthesis as well as process optimization. In this approach, the optimal network is synthesized by aggregating the subproblems in a dynamic programming scheme. The resulting optimal design structure contains a subset of the subproblems generated by the analysis. Hendry and Hughes indicate that in the event significant interactions between the subproblems occur, then the decomposition method yields the optimal state for that design with the optimal structure and near optimal states for the remaining nonoptimal structures.

There are several implications from this study which make the decomposition and synthesis method of Hendry and Hughes even more attractive than before. First, when the interactions between the subproblems are small, then it is necessary to optimize each tower only once. This greatly reduces the number of state optimizations.

Secondly, when the interactions are negligible, it usually is more convenient to optimize the subproblems starting with that tower which is upstream. The state optimization of subsequent towers then proceeds in the same direction as the material flow. At the end of this process, when all towers have been state optimized, the optimal structure is then synthesized, starting with those towers which are downstream. The direction in which the process synthesis occurs is then opposite to that of the material flow. Thus, the absence of interactions between the subproblems facilitates the separation of the state and structural optimization into two sequential and distinct steps. The state optimization moves downstream, while the structural optimization moves upstream.

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NOTATION

CAP_j = capital investment required for j^{th} tower (see Tedder, 1975)
d_j = observed deviation in rank order between the predicted rank and the observed rank
I_{X_j} = observed rank order for j^{th} tower
I_{Y_j} = predicted rank order for j^{th} tower
N_j = minimum theoretical stages for j^{th} tower calculated from Fenske equation (see Part III)
OP_j = annual operating costs for j^{th} tower (see Tedder, 1975)
P = optimal overhead operating pressure, MN/m^2
R_s = spearman rank correlation coefficient
T = tower feed normal bubble point, °K
VC = annual venture cost (see Tedder, 1975)
V_j^U = minimum vapor requirements for j^{th} tower as calculated by the Underwood equation (see Part III)
X_j = observed minimum venture cost for j^{th} tower
Y_j = predicted minimum venture cost for j^{th} tower, minus the least-squares regression constant for models 2, 3, 4, 5, and 6 in Table 1, or divided by the multiplication constant for models 1, 7, 8, and 10.
δT_j = temperature drop up the j^{th} tower

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Part III. Design Methods and Their Evaluation

Distillation networks are described as sets of composition nodes which are used to estimate material and energy balances. Comparisons with equivalent, equilibrium stage models indicate that these simplified design methods consistently result in small, but acceptable, overdesign, even when applied to complex, thermally coupled tower configurations.

SCOPE

The incentives for state optimizing various processing trains increase with rising capital and operating costs. When a process design analysis is based on countercurrent equilibrium stage models, then each evaluation of the economic objective function requires a prior numerical convergence to the underlying energy and material balances. It is possible to use such a model to perform design optimization as has been done by Ricker and Grens (1974), but this method becomes exceedingly burdensome when

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