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A SIMPLE SYNTHESIS METHOD
BASED ON UTILITY BOUNDING FOR
HEAT INTEGRATED DISTILLATION SEQUENCES
by

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ABSTRACT

In this paper a new method is presented which will enable engineers to select better heat integrated distillation systems quickly and easily. The key to this method is making the assumption that OAT, the product of the condenser or reboiler duty and the temperature difference between the reboiler and condenser, is constant for a single distillation task over a wide range of pressures. Using this assumption and the principles of multieffect distillation, a lower bound on the utility use for single distillation tasks and for distillation sequences is readily calculated for designs involving simple two product columns that may or may not be multieffected. This paper also describes methods which can be used to synthesize distillation systems which approach these bounds. Finally, an algorithm is presented which develops the least cost distillation system for separating a multicomponent feed. The methods in this paper are illustrated with a five component example problem.

SCOPE

For many years design engineers have had to face the problem of selecting the least expensive distillation sequence for separating multicomponent mixtures. Many methods have been developed, but most, of these only consider the use of simple, sharp separators. (A simple separator is one which separates a feed stream into two product streams. A sharp separator is one in which each component entering in the feed stream leaves in only one of the product streams.) Harbert(1957) investigated the separation of ternary mixtures using simple, sharp distillation columns and proposed two heuristics which are still used: 1) do the easiest separation first and 2) favor separations in which the distillate and bottoms flows are nearly equal. Other investigators (Heaven, 1969; King, 1971, 1980; Seader and Westerberg, 1977; Nath and Motard, 1981; Henley and Seader, 1981) have suggested additional heuristics. Later investigators (Thompson and King, 1972; Hendry and Hughes, 1972; Westerberg and Stephanopoulos, 1975; Rodrigo and Seader, 1975; Gomez and Seader, 1976) developed algorithms based on tree searches to find the best sequence for a given separation problem. A rigorous search algorithm has the advantage that it will always find the optimal solution *to the problem posed*, although the computational expense may be high. Heuristics and search techniques have been combined in several very effective methods (Seader and Westerberg, 1977; Nath and Motard, 1981). In these methods heuristic rules are initially used to find good sequences; these sequences are then modified by making small evolutionary changes in the structure where the heuristics are in conflict.

All of the methods mentioned above assume that the heating and cooling requirements of the separation processes are supplied by utilities. In a distillation sequence it is possible for the condenser of one column to provide some or all of the heating required in the reboiler of another column which is operating at a lower temperature. If this type of heat integration between

columns is allowed, the separation sequence synthesis problem becomes much more difficult because not only must the best distillation sequence be chosen, but the column pressures and a heat exchange network must be specified.

The first studies of heat integrated distillation sequences were by Rathore, Van Wormer, and Powers(1974a,b) who presented an algorithm based on dynamic programming. Freshwater and Ziogou(1976) and Siirola(1978) have used case studies to demonstrate the economic advantages of using heat integrated distillation sequences. Umeda et al (1979) used heat availability diagrams to improve the heat integration for a specified distillation sequence, but did not extend the work to propose a general separation synthesis procedure. Sophos, Stephanopoulos, and Morari(1978) and Morari and Faith(1980) used lagrangian methods to develop a branch and bound algorithm. All of these methods involve considerable computational effort. Sophos, Stephanopoulos, and Linnhoff(1981) have recently demonstrated that the heuristics used to choose the best separation sequences without considering heat integration are also good heuristics for choosing which sequences are the best candidates for heat integration. Other investigators (Petlyuk, et al, 1965; Stupin and Lockhart, 1972; Tedder and Rudd, 1978a,b) have studied how thermally coupled distillation columns impact energy use. Naka, et al(1982) have recently published a paper in which they show how to develop a heat integrated distillation sequence which minimizes the loss of available energy. Their method considers structures based on simple, sharp separators and permits multiple heat sources and sinks which may be either utility or process streams. In their method they use a bound which is different from the bounds which we will propose later, but they use a diagram which is very similar to one which we shall present. The purpose of this paper is to develop a design methodology for heat integrated distillation processes, particularly those which allow the use of multieffect structures.

CONCLUSION AND SIGNIFICANCE

In this paper we have shown how to use multieffect distillation to calculate a simple lower bound on the minimum utility use for a given distillation sequence which is comprised of simple columns that may or may not be multieffected. We have presented a method for developing distillation systems whose utility use approaches this bound. Finally we have shown how to combine these insights in a method to discover the distillation structure based on simple or multieffected columns which has the lowest annualized cost for a multicomponent separation.

The method can be used for columns effecting nonsharp splits if the user will himself enumerate any of these tasks which might be useful for the problem he is solving.

INTRODUCTION

In the first part of this paper we shall define an example problem which is used to illustrate the methods we present. Next we shall briefly describe two important concepts. The first is multieffect distillation; the second is the importance of the product QAT for a distillation problem. These concepts will then be used to calculate a lower bound on the utility use for a given distillation *task*. We shall also show how to develop distillation systems which approach this lower bound. Next we shall extend our insights from single distillation tasks to distillation *sequences*. We shall then discuss the implication of these insights on restricted distillation problems, on selecting a *priori* which combination of hot and cold utilities will result in the lowest utility costs, and on integrating distillation systems with process streams. Finally we shall present and illustrate an algorithm which determines the least expensive distillation system for a multicomponent separation where utilities provide the residual heating and cooling.

PROBLEM DESCRIPTION

The problem we are addressing in this paper is how to find the least expensive configuration of distillation columns which separates a given multicomponent feed into a set of desired products. In addition to specifying the feed conditions (temperature, pressure, composition) and the product compositions, it is also necessary that the temperatures at which utilities are available and the costs of the utilities be specified.

The data for the example problem used in this paper are presented below. This problem is taken from King(1971).

Component	x_F	V^K
A. Ethanol	0.25	351.5
B. Isopropanol	0.15	355.4
C. N-Propanol	0.35	370.4
D. Isobutanol	0.10	381.0
E. N-Butanol	0.15	390.9

Feed flow * 0.139 kgmol/s

Feed is saturated liquid at 100 kPa.

Recovery of key components in each column is 0.98.

$AT_{m_i} \ll 10 \text{ K}$

K-values and physical properties are calculated assuming ideal behavior.

The available utilities are:

Utility	$T_{u, K}$	Cost, $10^3 \$/10^{12} \text{ J}$
Cooling Water	305	0.16
Exhaust Steam	373	1.08
Steam(448 kPa)	421	2.63
Steam(1069 kPa)	462	3.51
Steam(4241 kPa)	527	4.01

MINIMUM UTILITY USE FOR A SINGLE DISTILLATION TASK

The first step in finding the best configuration of simple two product distillation columns which may or may not be multieffected in a given separation synthesis problem is to calculate a lower bound on the minimum utility use for each possible sequence. Before doing this it is necessary to understand multieffect distillation and the significance of QAT, the product of

Q, the reboiler or condenser duty in a given column, and AT, the difference between the reboiler and condenser temperatures in the same column.

Multieffect distillation is a well-known (King, 1971), but not widely used, method for reducing the utility use of a distillation column. Instead of sending the entire feed through a single column with one condenser and one reboiler, the feed is split into two parts and sent to two columns. The pressure in one of the columns is chosen to be high enough so that its condenser temperature is hotter than the reboiler temperature of the low pressure column. The heat rejected in the condenser of the high pressure column can then be used to replace steam or other hot utility in the reboiler of the low pressure column. If the condenser and reboiler duties are about equal and are not strongly affected by moderate pressure increases, it is possible to cut the utility use in half by using two columns instead of one.

The disadvantage of multieffect distillation is that the heat used is degraded across a larger temperature range than for a single column. In a two column multieffect distillation the heat which is provided by the hot utility is degraded across twice the temperature range of a single column. This means that for the same minimum condenser temperature, the temperature of hot utility in a multieffect distillation must be higher than the temperature of hot utility which would be required in a single column. As more effects are added, the utility savings decrease and the reboiler temperature increases. The utility use and cost of a multieffect distillation sequence decrease approximately proportional to $1/N$, and the maximum reboiler temperature in a distillation sequence increases approximately proportional to N , where N is the number of effects. A multieffect distillation sequence is shown in Figure 1.

Multieffect distillation is important in this work because, for given utilities, it can be used to predict a lower bound on the minimum utility use for a single distillation task. The utility use for a single column can be cut in half by the addition of one column and the use of multieffect distillation.

Additional effects reduce the utility use further. The minimum utility use for any given distillation task is obtained by determining the maximum number of effects which can be placed between the coldest cold utility and the hottest hot utility and by evaluating the utility use for a multieffect distillation system with that number of effects.

The number of effects for a given distillation task is limited several ways. The first limits are the available utility temperatures. No reboiler may operate at a temperature higher than that of the hottest hot utility; no condenser may operate at a temperature lower than that of the coldest cold utility. This limits the number of effects because as the number of effects is increased either the reboiler temperature of the hottest column increases or the condenser temperature of the coldest column decreases or both. The temperature range for multieffect distillation is also limited by the critical temperatures of the products. No reboiler may operate above the bottoms critical temperature, and no condenser may operate above the distillate critical temperature. This constraint may be more stringent than the utility bound. The final constraints on the temperature interval which is available for multieffect distillation are the maximum and minimum design pressures or temperatures specified by the engineer. These could be to avoid thermal decomposition or running at vacuum pressures. Pressure constraints can be converted to temperature constraints by calculating the bubble temperature of the bottoms product at the maximum design pressure and the bubble temperature of the distillate product at the minimum design pressure. The temperature range for multieffect distillation, $AT^{^^}$, can be defined as the difference between the lowest limit on the hot utility temperature and the highest limit on the cold utility temperature.

A lower bound on the minimum utility use for a given distillation task can be easily estimated from the quantity QAT which characterizes that task. The quantity Q can be either the reboiler or condenser duty for a given

separation task. For a distillation column with a saturated liquid feed and with distillate and bottoms products removed as saturated liquids, the effect of these streams on the overall column energy balance is small, and any heat added in the reboiler is essentially removed in the condenser. This assumption is particularly true for difficult separations with high reflux ratios where condenser and reboiler duties are even more dominant. The quantity AT is a measure of the temperature range over which heat is degraded to effect a given separation. The temperature drop across a column is the difference, between the reboiler and condenser temperatures. Although multicomponent products may reboil or condense over a temperature range, in this paper we assume that the reboiler and condenser temperatures are the bubble point temperatures of the distillate and bottoms. The reason for this is that in a total condenser all of the heat is rejected at temperatures at or above the bubble point, and in a partial reboiler heat is required at or slightly above the bubble temperature of the bottoms. A minimum driving force for heat transfer, AT_{mm} , must be added in both condenser and reboiler. In a thermally integrated system, however, each column involved in an energy match need only supply a driving force of $AT_{min}/2$ so that the minimum thermal driving force of two columns joined in a heat exchanger will be AT_{mm} .

The product QAT is a function of the temperature (or pressure) at which a distillation column is operated. We have found that both the heat duty, Q , and the difference between the reboiler and condenser temperatures, AT , increase with pressure, and that the increase in each quantity is approximately linear with the temperature level resulting for the column. The product QAT may double over a pressure range of 100 to 2500 kPa (1 to 25 atm). In the remainder of this work however, it will be assumed that both Q and AT are constant and independent of the column operating conditions. Use of this assumption allows the basic characteristics of this synthesis problem to be explored.

A T-Q diagram, Figure 2, gives insight into the use of $Q\Delta T$ for predicting a lower bound on the minimum utility use for a given distillation task. The quantity $Q\Delta T$ is an area on this diagram. If a second column is added, and multieffect distillation is used, the heat load, Q , is cut in half, but ΔT doubles. The area $Q\Delta T$ remains the same for this separation although two columns are used. If more multieffect columns are added, Q will decrease, ΔT will increase, but the area, $Q\Delta T$, remains constant. As explained earlier, the limits on the addition of new columns are the maximum and minimum temperatures which are allowed. A lower bound on the minimum utility use for a given separation is obtained by distributing the area $Q\Delta T$ across the temperature range between the coldest possible condenser temperature and the hottest possible reboiler temperature. This is also shown in Figure 2. A driving force for heat transfer is needed in any heat exchange with utilities so the effective temperature of any hot utility must be decreased by $\Delta T_{\min}/2$ and the effective temperature of any cold utility must be increased by $\Delta T_{\min}/2$. The lower bound on the minimum utility use is the width of the T-Q diagram whose height is ΔT_{avail} and whose area is $Q\Delta T$.

This bound is easily calculated. First determine the quantities $Q\Delta T$ and ΔT_{avail} . The ΔT_{avail} is easily calculated from the problem specifications. In this paper we evaluate $Q\Delta T$ at 100 kPa. The values of $Q\Delta T$ for the separations in the alcohol problem are shown in Table 1. If both Q and ΔT increase with temperature, we can guarantee a lower bound calculation by evaluating $Q\Delta T$ at the lowest temperature range allowed for the task. However to a good approximation we may simply evaluate $Q\Delta T$ at some nominal conditions for the task.

This method is used to calculate a bound on the minimum utility use for the separation of n-propanol and isobutanol. The hottest hot utility is available at 527 K and the coldest cold utility is available at 305 K. Using a ΔT_{\min} of 10 K, ΔT_{avail} can be calculated:

$$AT_{min} = (527 - 10/2) - (305 \cdot 10/2) = 212 \text{ K}$$

Since the normal boiling point of n-propanol is 370.4 K, any column operating with a condenser temperature between 305 K and 370.4 K will be operating under vacuum. If the constraint is added that columns must operate at or above atmospheric pressure, the temperature range for heat integration is reduced:

$$AT_{min} = (527 - 10/2) - 370.4 = 151.6 \text{ K}$$

Since the condenser temperature, 370.4 K, is more than AT_{min} above the cooling water temperature, no driving force for heat transfer should be added. From Table 1 QAT for this separation is 2640 kJ-K/gmol. The lower bound for the minimum utility use for this separation is:

$$Q_{min} = 2640 \text{ kJ-K/gmol} / 151.6 \text{ K} = 17.4 \text{ kJ/gmol}$$

The actual utility use for this separation which would be obtained by using six multieffect distillation columns is 19.9 kJ/gmol of high pressure steam and 23.2 kJ/gmol of cooling water. This system is shown in Figure 3.

This simple method predicts the steam use within 14%, the cooling water use within 27%, and the total utility use within 21%. This error is caused mainly by the discrete nature of multieffect distillation. In estimating the minimum utility use the entire temperature range, AT_{avail} is used; in the multieffect design the configuration AT is smaller than AT_{avail} so the utility use is higher. If the configuration AT were used rather than AT_{avail} , the predicted utility use would be 19.1 kJ/gmol which is within 4% of the actual minimum steam use and within 18% of the actual minimum cooling water use.

MINIMUM UTILITY USE FOR A DISTILLATION SEQUENCE

The quantity QAT is important in calculating a lower bound on the minimum utility use for a single distillation task, but it can also be used to evaluate which distillation sequences are best for separating a given multicomponent feed.

Using distillation to separate a feed stream containing three or more

components into pure component products requires a sequence of distillation columns, each performing a single separation task. The sequence which separates a multicomponent feed into pure products is not unique; as the number of components in the feed increases, the number of possible distillation sequences increases rapidly. If only simple, sharp separators are used, there are only two sequences which separate a three component feed into pure products; there are 42 possible sequences for a six component feed. For the five component alcohol problem the 14 possible sequences are shown in Figure 4. The engineer must choose the distillation sequence which produces the desired products at the lowest cost.

If the designer can propose tasks useful for the separation that do not produce sharp splits, then these too can be used to develop even more sequence alternatives. One would be assuming negligible pressure effect on the ratios of the flows for the distributed components experienced for such tasks, an assumption that would have to be checked for the tasks included.

A lower bound on the minimum utility use for a single distillation task is calculated by determining QAT for that separation and by dividing this quantity by the available temperature range. In a similar way a lower bound on the minimum utility use for a sequence of distillation tasks is obtained by determining QAT for the entire sequence. The sequence QAT is the sum of the QAT's for the individual separations in the distillation sequence. A lower bound on the minimum utility use for a distillation sequence, k, is calculated by

$$Q_{\min}(k) \geq \sum_{j \in S(k)} (QAT)_j / AT_{\text{avail}}$$

where $S(k)$ is the set of indices of all tasks needed in sequence k. AT_{avail} is

the maximum temperature found useful for any of the tasks less the minimum temperature found useful for any of the tasks. It is likely larger than AT_{avail}

for any individual task. While this larger range will not be useful in its

entirety for each task, each portion of the range will be useful to some task. Being the largest range possible, clearly the above equation gives a lower bound on the utility use for the sequence. This lower bound on the utility use is one criteria which can be used to choose the best distillation sequences in a given separation problem. Lower bounds on the utility use for each sequence in the alcohol problem are shown in Table 2.

A SYNTHESIS METHOD FOR MINIMUM UTILITY SEQUENCES

In addition to estimating a lower bound for $Q_{\text{min}}(k)$ for a given sequence, it is also possible to use this bound and the T-Q diagram to develop a multieffect design which will be very close to the predicted minimum utility use. On the T-Q diagram first divide the QAT for each separation task into widths equal to the lower bound on the utility use. Each subdivision represents one distillation column. Next "stack" these columns on a T-Q diagram between the maximum hot utility and minimum cold utility temperatures in such a way that the width of this stacking remains as narrow as possible. The width of this stacking will remain close to the lower bound on the utility use, but the discrete nature of the actual problem and the fact that a lower bound is being used make it impossible to obtain a system with a utility use equal to the bound. This stacking procedure is illustrated in Figure 5 and the minimum utility configuration this stacking represents is shown in Figure 6. Note that this procedure implicitly selects the pressure and feed flow rate for every column.

FURTHER IMPLICATIONS OF THESE CONCEPTS

Minimum Utility Bounds for Restricted Problems

Although we have previously used multieffect distillation to obtain minimum utility bounds, our method is not restricted to the use of multieffect distillation systems. If multieffect distillation is not used, a bound on the minimum utility use is:

$$Q_{\min}(k) \geq \max_{j \in S(k)} Q_j$$

where Q_j is the heat duty of column j . This is illustrated in Figure 7 by stacking the tasks in Figure 7a as shown in Figure 7b.

If the distillation system is restricted by a bound on the number of columns, a similar procedure can be followed. First solve the problem with the minimum number of columns (no multieffect distillation). Then add one column. In Figure 7b it is clear that the only way to reduce the utility use is to split distillation task 2. If the utility use of each of the columns created by splitting distillation task 2 is less than the utility use of distillation task 1, then distillation task 1 establishes the minimum utility bound for this new configuration. A second multieffect column should then be added to split task 1 unless the temperature interval for the problem will be exceeded. The extension of this method for larger problems is obvious.

It is interesting to note at this point how easy it is to bound the utility use for these restricted structures which have been much studied. These bounds, once calculated, can be used many ways. The first use is to evaluate quickly the minimum utility cost for a given distillation configuration. Calculation of the bound also shows which column limits a further decrease in the utility use. As seen in Figure 7b, cutting the utility use of distillation task 3 would not result in any decrease in the utility use of the sequence, but any decrease in the utility use of distillation task 2 directly reduces the utility use of the whole sequence. Another use of this bound is to identify columns whose replacement by other separation processes, such as absorption, would significantly reduce the utility use of a separation sequence. Again column 2 in Figure 7b is the one which must be considered first for replacement.

Selecting Least Cost Utilities

In the development of our algorithm it is assumed that the temperature levels of the hot and cold utilities are specified. In most problems a choice must be made among several hot and several cold utilities. Suppose several

different hot utilities are available at temperature levels T_{Hj} and unit costs G_j , and several different cold utilities are available at temperatures T_{Ck} and unit costs C_{Ck} . If we assume that we can find a distillation system whose utility use is close to the predicted lower bound, we can write:

$$C_{util} = C_{Kj} + C_{Ckf} Q_{min}$$

If we substitute for Q_{min} we can write:

$$C_{util} = C_{Hj} + C_{Ck} \left(\frac{Q_{AT}}{T_{Hj} - T_{Ck} - \Delta T_{min}} \right)$$

If ZQAT is fixed for a given sequence, the utility cost can be minimized by picking the utility pair (H_j, C_{Ck}) which minimizes the ratio:

$$(G_j \cdot C_{Ck}) / (T_{Hj} - T_{Ck} - \Delta T_{min})$$

This ratio does not depend on the separation problem. Values of this ratio for the alcohol problem are shown in Table 4.

Integrating with Existing Process Streams

Although in the paper thus far we have assumed that heating and cooling are supplied by outside utilities, many of the principles we have developed can also be used to integrate distillation systems with existing process streams. In this situation although it is no longer easy to calculate a bound on the minimum heating and cooling required for a given distillation sequence, it is still possible to use QAT's and a T-Q diagram to synthesize distillation systems. Rather than attempting to stack a sequence QAT between specified utilities, QAT must be stacked between the existing process streams. This is shown in Figure 8. The stackings may not be unique, and it may be possible **that** several different sequences could be operated between the given process streams. This problem was considered by Naka, et al (1982) to find the sequence of columns which minimizes the available energy loss. They do not consider multieffect columns however. In the limit, sequences which use only process streams for heating and cooling are without utility cost, and the engineer must then minimize the capital investment to obtain the least expensive sequence.

When an engineer is integrating distillation sequences with existing process streams, he must not heat integrate across a process pinch point. Dunford and Linnhoff(198D have shown that integrating across a pinch point will prevent us from achieving the minimum utility use for the entire process.

TREE SEARCH SYNTHESIS ALGORITHM FOR LEAST COST CONFIGURATIONS

From Figure 6 it is clear that although this solution has a low utility cost, it has a high capital cost. Decreasing the number of columns decreases the capital cost, but increases the utility cost. The least expensive configuration is a compromise between the increased capital cost and the decreased utility cost associated with the addition of more columns.

The trade-offs between the number of columns and the utility use can easily be seen by looking at QAT for each column in a sequence. If the minimum number of columns is used (NC-1 columns to separate a feed containing NC components into pure products using sharp separators), the minimum utility use for that sequence will be the utility use of the column which uses the most utilities:

$$Q_{\min}(k) \geq \max_{j \in S(k)} Q_j$$

The capital cost for this configuration will be lowest (fewest columns), but the utility cost will be highest. If one more column is added to this sequence, it must reduce the utility use; otherwise it cannot be economical to add that column. Therefore the additional column must split the separation task for the column which has the highest utility use. The minimum utility use is then calculated as:

$$Q_{\min}(k) \geq \max_{j \in S(k)} (Q_j/N_j)$$

where N_j is the number of columns of type j which are being used in a given configuration. The annualized capital costs associated with adding an extra column can be compared with the utility savings to determine if it is economical to add that column. As we show below this process can be systematized to use bounds effectively to find the least expensive

configuration of columns for a given task sequence. The least expensive configuration for the whole separation problem is obtained by searching all of the task sequences, again using bounds to limit the search space. The procedure for finding the least expensive column configuration to effect a multicomponent separation is described in the following algorithm.

LEAST COST ALGORITHM

1- **Identify and** list all of the distillation task sequences which will produce the required products. The list splitting technique of Hendry and Hughes(1972) may be useful in this step if only simple, sharp separators are permitted. All such sequences for the alcohol separation problem are shown in Figure 4.

2- **List all** of the distillation tasks which occur in any of the task sequences generated in Step 1. Use (shortcut) techniques to size and cost each task when implemented in a single column at a nominal pressure. In this paper we have used 100 kPa as the nominal pressure. Calculate Q , the column duty, ΔT , the temperature drop across the column, and their product, $Q\Delta T$. As explained earlier, Q may be either the reboiler or condenser duty. To obtain ΔT across a column it is necessary to add ΔT_{mm} to the difference to provide a driving force for heat transfer. The results of these calculations for the alcohol example are shown in Table 3.

3- **For each** task sequence calculate the minimum utility cost, the minimum capital cost, and the minimum annualized cost. The minimum utility use for each sequence is given by:

$$Q_{min}(k) = \sum_{i \in S(k)} Q_i \Delta T_i / \Delta T_{avail}$$

The minimum utility cost for each sequence is obtained by multiplying the minimum utility use, $Q_{min}(k)$, by the cost of the hot

utility, C_{HU} , and by the cost of the cold utility, C_{CU} , and adding these two quantities:

$$C_{util,min}(k) = Q_{min}(k) [C_{CU} + C_{HU}]$$

The minimum capital cost for a configuration is the sum of the costs of the individual columns in the configuration:

$$C_{cap,min}(k) = \sum_{i \in S(k)} C_{cap,i}$$

The minimum annualized cost of each configuration is given by (Sophos, Stephanopoulos, and Linnhoff, 1981): -

$$C_{ann,min}(k) = (1/a) C_{cap,min}(k) + \beta C_{util,min}(k)$$

where a is the payout time for the capital investment and β is a factor reflecting the income tax rate. In this paper a is 2.5 years and β is 0.52. The cost of each configuration calculated here is a lower bound on the sequence cost since the minimum number of columns and the minimum utility use will not occur in the same configuration. The capital cost for any actual configuration will be at least the capital cost of the bound, and the utility use will be greater than that of the bound. Rank the task sequences by the lower bounds for their annualized costs, cheapest first. The results of these calculations are shown in Table 5.

4. Set Z^* , an upper bound on the optimal solution, equal to M , a large number. For this problem let M equal five times the lower bound cost of the most expensive sequence. Set Z^* to 8815.
5. From the list generated in Step 3, choose the sequence with the lowest lower bound for annualized cost. If the list is empty, stop; the best solution is the configuration corresponding to the current value of Z^* . Otherwise, knowing Z^* , $C_{cap,min}(k)$, and $C_{util,min}(k)$, it is possible to calculate upper bounds on the utility use and capital

cost of this sequence. The upper bound on the utility use is:

$$Q^+(k) = (Z^* - C_{cap,min}(k)/a) / \beta (C_{TU}^* \cdot C_{CU})$$

Any configuration of sequence k with a utility use greater than $Q^+(k)$ cannot be cheaper than Z^* . The upper bound on the capital investment is:

$$\leq \beta, \ll * a (Z^* - fi Q_{min}(k) t C^{\wedge} C_{cu}])$$

Any configuration of this sequence with a capital cost greater than $C_{cap}^*(k)$ cannot be cheaper than Z^* . For the alcohol example the cheapest sequence is Sequence 1. With the value of Z^* set to 8815, the value of $Q^+(D$ is 120 MW, and the value of $C^+(1)$ is

cap

21.000.

6. Determine an initial configuration for the sequence chosen. This configuration must have $Q_{min}(j,k) < Q^+(k)$ and $C_{cap}(j,k) < C^+(k)$.

mm

cap *

cap

- a. To find this configuration start with the minimum number of columns, one for each separation task. The minimum utility use for this configuration is:

$$Q_{TM}^{<j^k>} = \sum_i Q_i / N_i$$

where N_i is the number of columns of separator i in configuration j of sequence k . If

$$Q_{min}(j,k) \geq Q^+(k)$$

go to part (b). Otherwise add to configuration j one column of that separation task which will reduce the utility use. Repeat this process until $Q_{min}(j^k) < Q^+(k)$.

- b. Assume that $Q_{min}(j,k)$ can be obtained and calculate $C_{cap}^*(j,k)$. If $C_{cap}(j,k) > C_{cap}^*(k)$, eliminate sequence k from the list generated in Step 3 and return to Step 5. Otherwise, use

$Q_{min}(j,k)$ and $C_{cjp}(j,k)$ to calculate a lower bound for Z , the annualized cost of configuration j of sequence k . If $Z < Z^*$, go to Step 7. If $Z > Z^*$ configuration j of sequence k cannot be less expensive than the current best solution. Set $Q^*(k) = Q_{min}(j,k)$ and return to part (a) of this step.

7. Determine if the configuration chosen in Step 6 can be operated between the hottest hot utility temperature and the coldest cold utility temperature. Also determine the minimum utility use for this configuration. This can be done in several steps.

a. If $Z_{i,c} \leq \sum_{i=1}^N \frac{AT_i}{U_i} \leq AT_{avail}$, the configuration is feasible and $Q(j,k) = Q_{min}(j,k)$. Go to Step 8.

b. Divide the heat duty of each separation task into blocks of width $Q_{min}(j,k)$. For most separations there will be a remainder with a width less than Q_{min} . From the original $AT_{i,c}$ subtract the appropriate AT for each block of heat duty which has a width of $Q_{min}(j,k)$. If the remaining blocks can be **stacked** in the $AT_{i,c}$ which remains and if they can be **stacked** with no combined width greater than $Q_{min}(j,k)$, the configuration is feasible and $Q(j,k) = Q_{min}(j,k)$. Go to Step 8. This step is shown in Figure 7. This step may be **combinatorial** - the approach used by Naka, et al(1982) could be used.

c. If the configuration must operate with a duty greater than $Q_{min}(j,k)$ the following procedure may be followed. Starting with $Q_{min}(j,k)$, increase $Q(j,k)$ by small increments and reapply the procedure described in part (b). The lowest value of $Q(j,k)$

which gives a feasible stacking is an estimate of the minimum utility use for this configuration. If $Q(j,k) < Q^*(k)$, go to Step 8. If $Q(j,k) > Q^*(k)$, this configuration cannot decrease the cost. If $C_{cap}(j,k) < C_{cap}^*(k)$, go to Step 6. Otherwise eliminate Sequence k from the list and return to Step 5.

8. If $Q(j,k) > Q_{min}(j,k)$, recalculate Z, the cost off configuration j of sequence k. Otherwise, continue.
- If $Z < Z^+$. set $Z^+ = Z$ and recalculate $Q^*(k)$ and $C_{cap}^*(k)$ as in Step 5. Return to Step 6.
 - If $Z > Z^+$ and $C_{cap}(k) < C_{cap}^*(k)$, set $Q^*(k) = Q(j,k)$ and return to Step 6.
 - If $Z > Z^+$ and $C_{cap}(k) \geq C_{cap}^*(k)$. eliminate sequence k from the list generated in Step 3. Also eliminate from the list any other sequences with $C_{ann,min}(k) > Z^+$.
- Return to Step 5.

APPLICATION OF THE LEAST COST ALGORITHM

The results of Steps 1 to 3 of this algorithm as applied to the alcohol problem are shown in Figure 4 and in Tables 3 and 5. In Step 4 an initial upper bound for the optimal solution is calculated. We set Z^+ equal five times the lower bound of the most expensive sequence, sequence 14.

$$Z^+ \ll 5 \times 1763 = 8815$$

Next, we choose the least expensive sequence in Table 5; this is sequence 1. We then calculate upper bounds on the utility use and the capital cost for sequence 1. These bounds are:

$$Q^*(1) \ll 120 \text{ MW}$$

$$C^d) \ll 21,000 \cdot 10^3 \text{ \$/yr}$$

In Step 6 we choose a configuration of sequence 1 which has a utility use less than $Q^*(1)$ and a capital cost less than $C_{cap}^*(1)$. First choose a configuration in which one column performs each separation. This will be called the **1-1-1-1** configuration of sequence 1. Each number refers to the number of columns which are used to perform each split. The first number refers to the A/B split, the second to the B/C split, the third to the C/D split, and the fourth to the D/E split. This notation is used for other sequences, but it should be noted that the column type which performs each split may differ from sequence to sequence. In other words, the A/B split may refer to any of the following column types depending on the sequence: A/B, A/BC, A/BCD, A/BCDE. For configuration 1-1-1-1 of sequence 1 the minimum utility use is:

$$Q_{min} * \text{Max}(20.53, 6.42, 8.64, 4.91) = 20.53 \text{ MW}$$

Since this is less than Q^+ (120 MW), this configuration is acceptable based on the utility use. The capital cost must be compared with $C_{cap}^*(1)$ also. This calculation shows that:

$$C_{cap}^{(j,k)} \leq 2153 < C_{cap}^{*(1)} = 21,000$$

Sequence 1 is acceptable based on both the utility use and the capital cost upper bounds.

Since configuration 1-1-1-1 of sequence 1 is acceptable based on the upper bounds for both utility use and capital cost, it must now be checked to determine if this configuration is feasible based on the available temperature difference. The hottest hot stream is available at 527 K and the coldest condenser temperature can be 351.5 K, the normal boiling point of ethanol, if we specify that all columns must operate at or above atmospheric pressure. The available AT is

$$AT_{avail} * (527 - 10/2) * 351.5 * 170.4 \text{ K}$$

Applying part (a) of Step 8 gives

$$ZAT = 28.9 \cdot 30.6 \cdot 26.2 + 19.9 = 105.6 < 170.4 \text{ K}$$

which means that configuration 1-1-1-1 of sequence 1 is feasible.

Next calculate the annualized cost of this configuration. This cost is calculated based on the configuration capital cost of $2153 \cdot 10^3$ \$ and a utility use* of 20.53 MW. The cost is

$$Z \ll 2223 \cdot 10^3 \text{ \$/yr}$$

Since $Z < Z^*$, set $Z^* = 2223$ and recalculate Q^* and C_{cap}^* for sequence 1.

These values are:

$$\begin{aligned} Q^*(1) &= 20.53 \text{ MW} \\ C_{cap}^* &= 4472 \cdot 10^3 \text{ \$/yr} \end{aligned}$$

Now return to Step 6.

Returning to Step 6, we search for another configuration of sequence 1 with $Q < Q^*$ and $C_{cap} < C_{cap}^*$. The next configuration to be considered is 2-1-1*1 since only by cutting the utility use in column A/BCDE in sequence 1 can the cost be decreased. Calculation of $Q_{min}(j,k)$ for this configuration gives

$$Q_{min}(j,k) = \text{Max}\{(20.53/2), 6.42, 8.64, 4.91\} = 10.26 \text{ MW}$$

which is less than $Q^*(1)$.

The capital cost of this sequence is the sum of the individual costs of the columns. The costs in Table 3 were obtained at nominal flow rates. If the column feed flow rates are different from these nominal values, the six-tenths rule based on the ratio of feed flow rates has been used to scale the column costs. The ratio of column heat duties could be used instead since in this analysis the column cost is directly proportional to the feed flow rate. (This is done here only to keep the capital cost analysis simple.) The capital cost of configuration 2-1-1-1 of sequence 1 is

$$C_{cjp}(i,k) = 2420 \cdot 10^3 \text{ \$}$$

Since this is less than $C_{cap}^*(1)$, this configuration is acceptable based on the upper bounds. For this configuration the feasibility check in Step 7 gives

$$ZAT = 163.4 < 170.4 \text{ K}$$

so this configuration is feasible. The annualized cost of configuration 2-1-1-1

of sequence 1 which has a capital cost of $2420 \cdot 10^3$ \$ and a utility use of 20.52 MW is

$$2 * 1649 \cdot 10^3 \text{ \$/yr}$$

Reset $Z^* * 1649$, recalculate Q^+ and C^+ , and return to Step 5.

The remaining progress of this algorithm is shown in Table 6. The least cost configuration is the same configuration which was developed by the synthesis procedure for minimum utility use. This configuration is shown in Figure 6. Note how effectively the bounds limit the search space.

DISCUSSION

The development and use of the preceding algorithm are based on several assumptions concerning the structure and cost of distillation sequences. There are also extensions and modifications of this algorithm. These will be considered in this section.

The most important assumption in this work is that Q and AT for a distillation column are independent of the column operating conditions. As mentioned before both quantities increase as the column operating pressure increases. The assumption that QAT is constant does give a lower bound on the utility use for either a single distillation task or for a distillation sequence if QAT is evaluated at the lowest pressure allowed for each task. Then $ZQAT$ obtained by assuming that QAT is constant is less than $ZQAT$ which would be obtained if the actual column operating conditions were used. Work has just been completed to obtain more accurate lower bounds by including the variation of Q and AT with the column operating conditions. It will appear later. A conclusion from that work is that it was important to have done it, but it is not as important to understanding the design of systems of columns as the insights coming from this work.

In the development of the above algorithm, it is assumed that the distillation sequences for a given problem can be specified. It is easy to specify the sequences if the problem is separating a multicomponent feed into

pure products. The list splitting technique of Hendry and Hughes(1972) may be used. If the desired products are mixtures of components present in the feed, it may be possible or even desirable to use distillation columns with nonadjacent keys or to use distillation columns which do not sharply separate adjacent keys. The algorithm we have presented does not offer insight into how to choose which separation tasks to use, but it does allow the use of any distillation column, sharp or nonsharp, which separates its feed into two product streams.

Another assumption which has been made is that the sensible heat associated with preheating or precooling streams between columns is negligible compared to the latent heat required in condensers and reboilers. If it is assumed that the feed to a distillation system enters as a liquid at ambient temperature and that the products are removed as liquids at ambient temperature, it can be shown that the overall effect of the sensible heat on the distillation utility use is small. The sensible heat has been calculated for all streams in the least cost distillation system shown in Figure 6. All streams are assumed to enter and leave the distillation system as 364 K which is the temperature of the saturated liquid feed at 100 kPa. Most streams passing from one column to another must be heated to enter as saturated liquids. Most product streams must be cooled to reach 364 K. The net effect of this heating and cooling on the utility use of the problem is less than six percent after the sensible heat streams have been integrated with one another. The cooling curves for the merged hot and cold streams for this problem are shown in Figure 9.

Several assumptions have also been made in the calculation of column costs and sequence costs. The cost of each column type is determined at only one set of conditions: a pressure of 100 kPa, saturated liquid feed, a reflux ratio of 1.2 times the minimum, and the maximum flow rate which could occur in a particular problem. The methods of Cerda and Westerberg(1979,

1981) are used to calculate the minimum reflux ratio and the number of trays for each separation. If multiple columns are used for any separation, the six-tenths rule based on the feed flow rate is used to determine the cost of each column. Inherent in this method of determining the cost of columns is the assumption that the column cost is independent of the column pressure. Over small or even moderate pressure ranges this does not introduce much error, but at conditions far from those at which the size and cost were originally determined, the error may be substantial. A simple heuristic for handling this cost variation will be discussed later. Another assumption which has been made is that the cost of heat exchangers will not vary much from configuration to configuration or from sequence to sequence. If this is the case, exchanger costs need not be considered at all. Use of this assumption makes it easier to determine and compare configuration and sequence costs, but exchanger costs should be included in a final decision on the best configuration. The algorithm we have presented can be used to choose several configurations from the many possibilities. The heat exchanger costs for each of this smaller set of alternatives can be determined and then the best configuration can be chosen.

One deficiency of the algorithm we have presented is that the way in which columns are stacked between the allowable temperatures is not unique. The algorithm generates the appropriate heat duties for each column and suggests one possible stacking. This is shown in Figure 10. One way to handle this problem (suggested by George Stephanopoulos(1982)) is to rank the distillate compositions of the columns in a sequence in order of decreasing volatility. Stack the column with the most volatile distillate starting at the lowest temperature. Next stack the column with the second highest volatility, **and** so on. The advantage of this method of stacking is that it keeps the pressure in all of the columns low. Lower pressures are required to condense highly volatile compounds at lower temperatures than would be required at

higher temperatures; at high temperatures lower pressures are required to condense heavier distillates than would be required to condense lighter distillates. This ranking according to volatility could also be used in determining the nominal pressure at which to determine cost and QAT for each column. Rather than using a pressure of 100 kPa for all column types, the column types could be ranked by distillate volatility and the allowable temperature range could be evenly divided among the column types. The QAT and cost of each column type would then be determined at a pressure which would correspond to the temperature range assigned to that column type. Using this ranking procedure to determine column costs would also reduce errors introduced by assuming that column cost is independent of pressure since column conditions in an actual stacking will be closer to the nominal costs determined by ranking the distillate volatilities than to the nominal costs determined at conditions of 100 kPa.

NOTATION

$C_{\text{arm,mm}}(k)$	minimum annualized cost of distillation sequence k
$c_{\text{-p.i}}$	capital cost of column i
$C_{\text{cap}}(j,k)$	capital cost of distillation sequence k with configuration j
$C_{\text{cap}}^+(j,k)$	upper bound on the capital cost of sequence k with configuration j
$C_{\text{cap,min}}(k)$	minimum capital cost for sequence k
C_{CU}	unit cost of cold utility
$c_{\text{util,min}}(k)$	minimum utility use for sequence k
NC	number of components in the feed
N_i	number of columns of type j present in a distillation system
Q	reboiler or condenser duty of a column
q_j	reboiler or condenser duty of column j
$Q(j,k)$	utility use of sequence k with configuration j
$Q^+(k)$	upper bound on the utility use for sequence k
Q_{min}	minimum utility use for a given distillation task
$Q_{\text{min}}(j,k)$	minimum utility use for distillation sequence j with configuration k
$Q_{\text{min}}(k)$	minimum utility use for distillation sequence k
$S(k)$	index set of tasks in sequence k
T_b	normal boiling point
T_{cond}	bubble temperature of the distillate
T_{rcb}	bubble temperature of the bottoms
T_U	temperature at which a utility is available
Z	cost of a given distillation system
Z^+	upper bound on the cost of the distillation problem solution

*F v U . ' K ; X ; , in ;hc feed

Co: ct'r Letters

a ^r.yc«Jt time

; ^r.yc«Jt time ; Lcrr,€ taxes

_T ^ " < L .t t 1 ^ - ^ ^ ^ = d condenser
.L.) i . c ! ^ : t : i n c column

blem
v L .t t - J . i f L - i . i t t c t . v t e n h o t
C : L ^ c f v ; i l i ; i c i u s e d

min ; ^ , . V . L o / t ^ r . c t b e t w e e n
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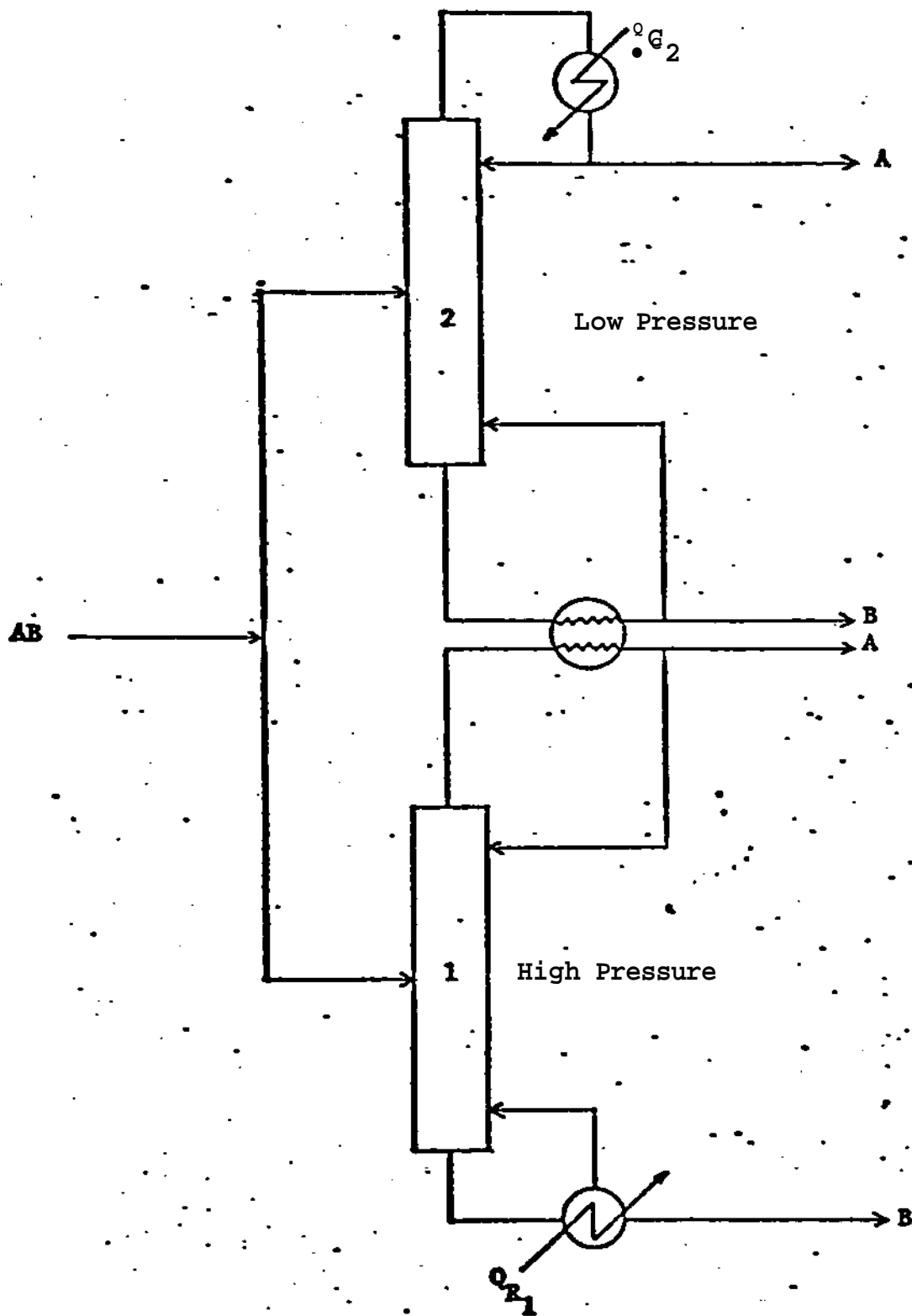


Figure 1. A Multieffect Distillation System

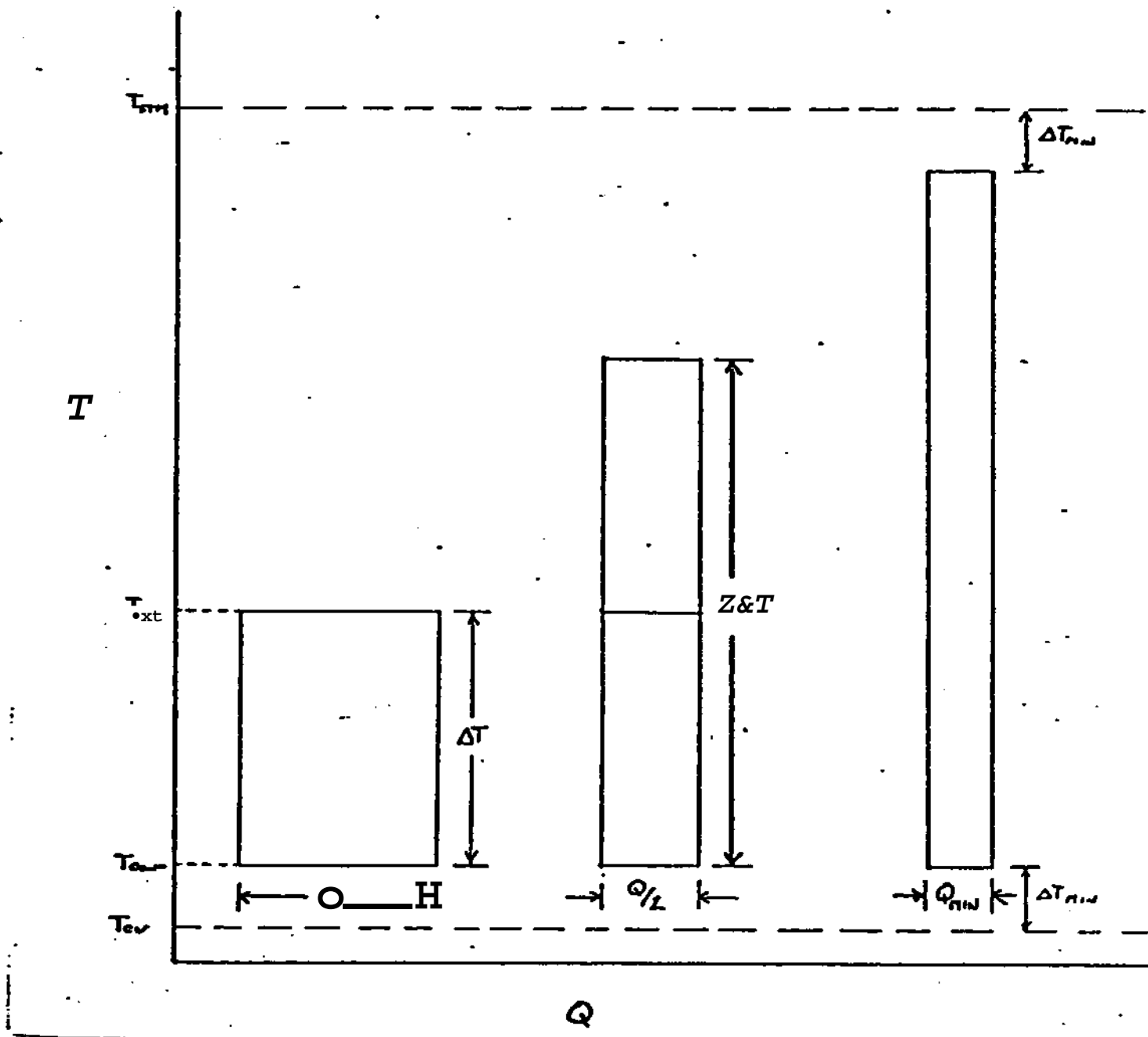


Figure 2: Multieffect Distillation on a T-Q Diagram

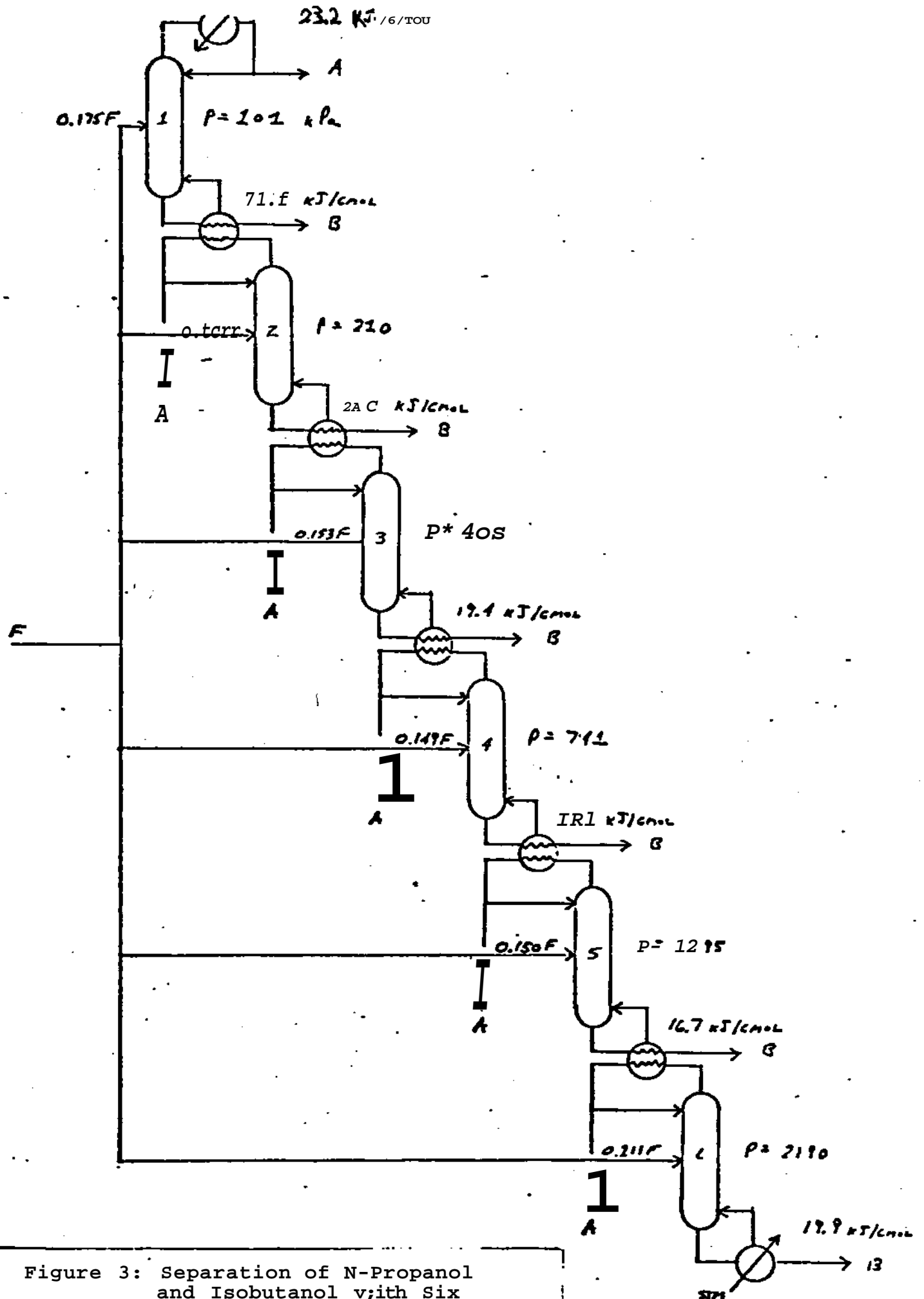


Figure 3: Separation of N-Propanol and Isobutanol with Six Multieffect Columns

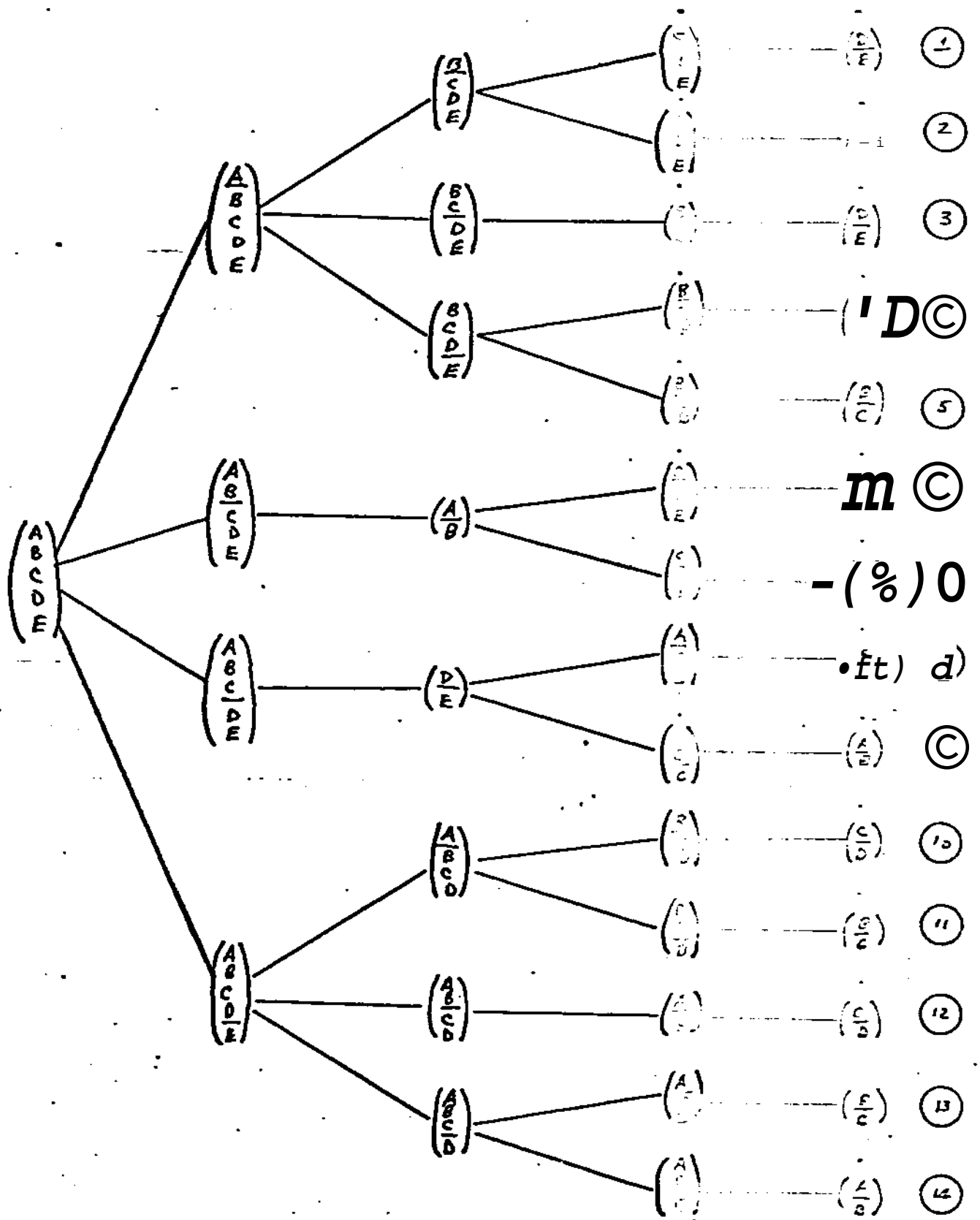


Figure 4: Distillation Sequences for the Alcohol example. PreTeX, s111

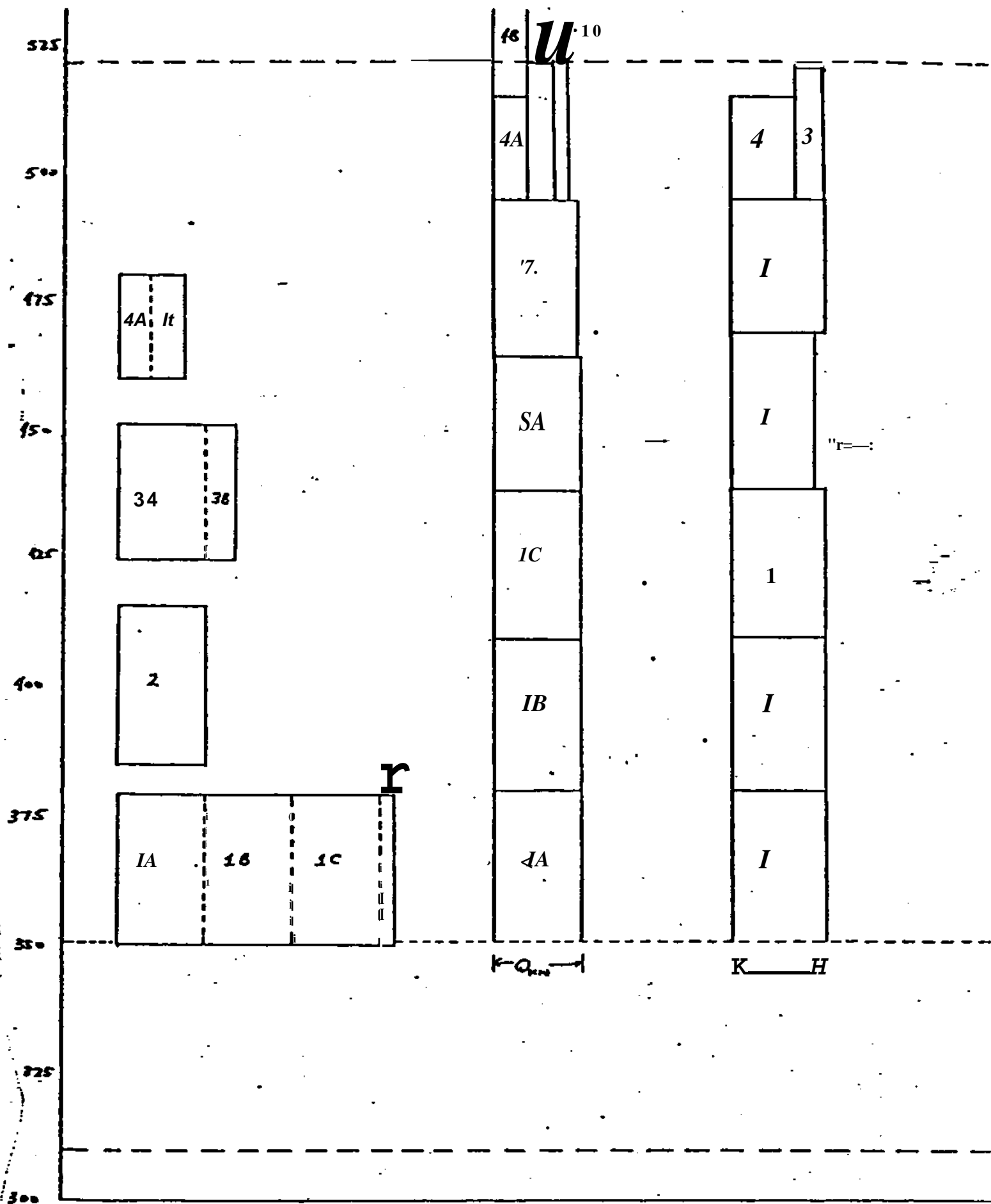


Figure 5: Column "Stacking" to Obtain a Minimum Utility Distillation System .

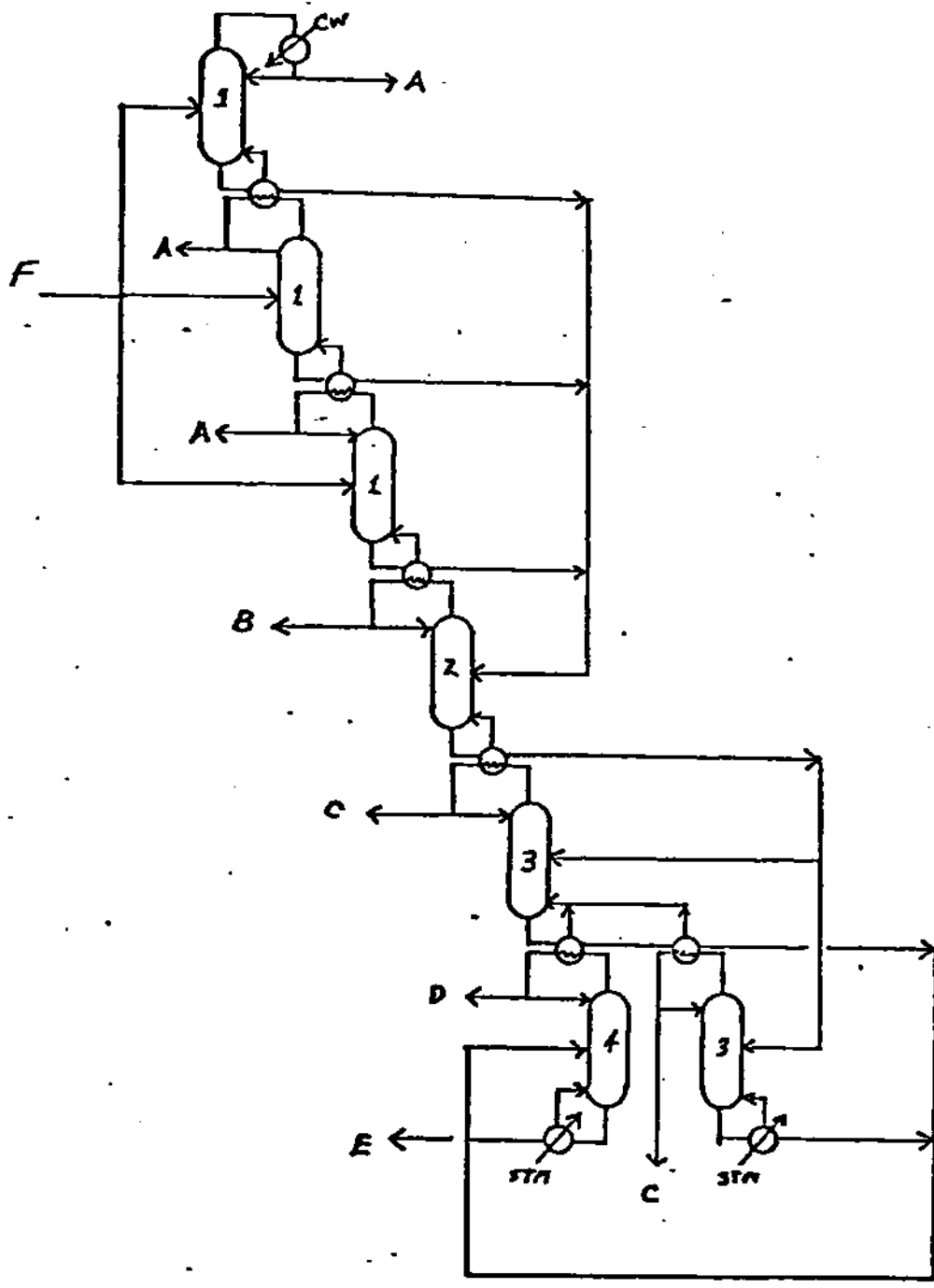


Figure 6: The Minimum Utility Configuration Developed by Column "Stacking"

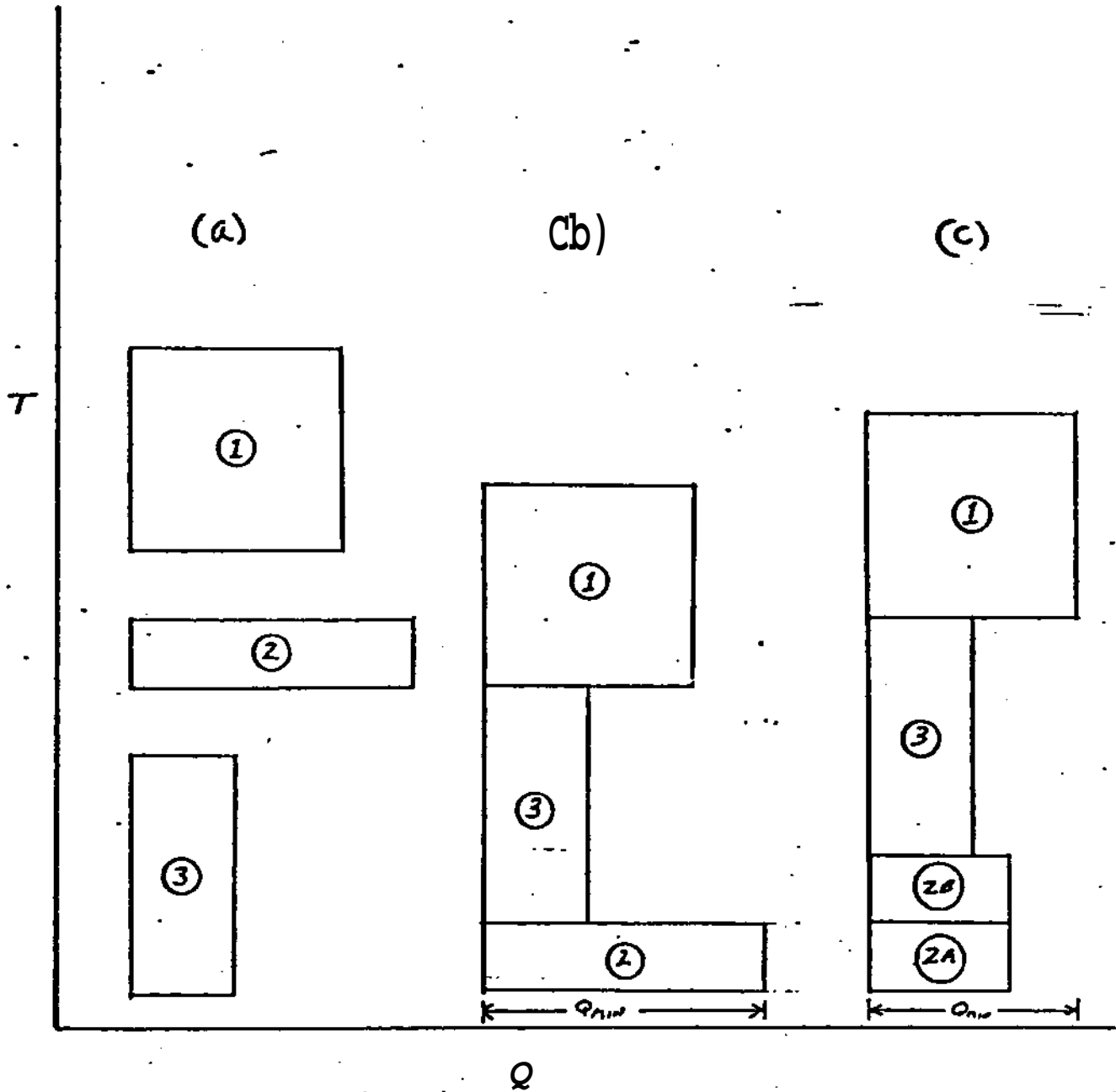


Figure 7: Minimum Utility Use for Restricted Problems

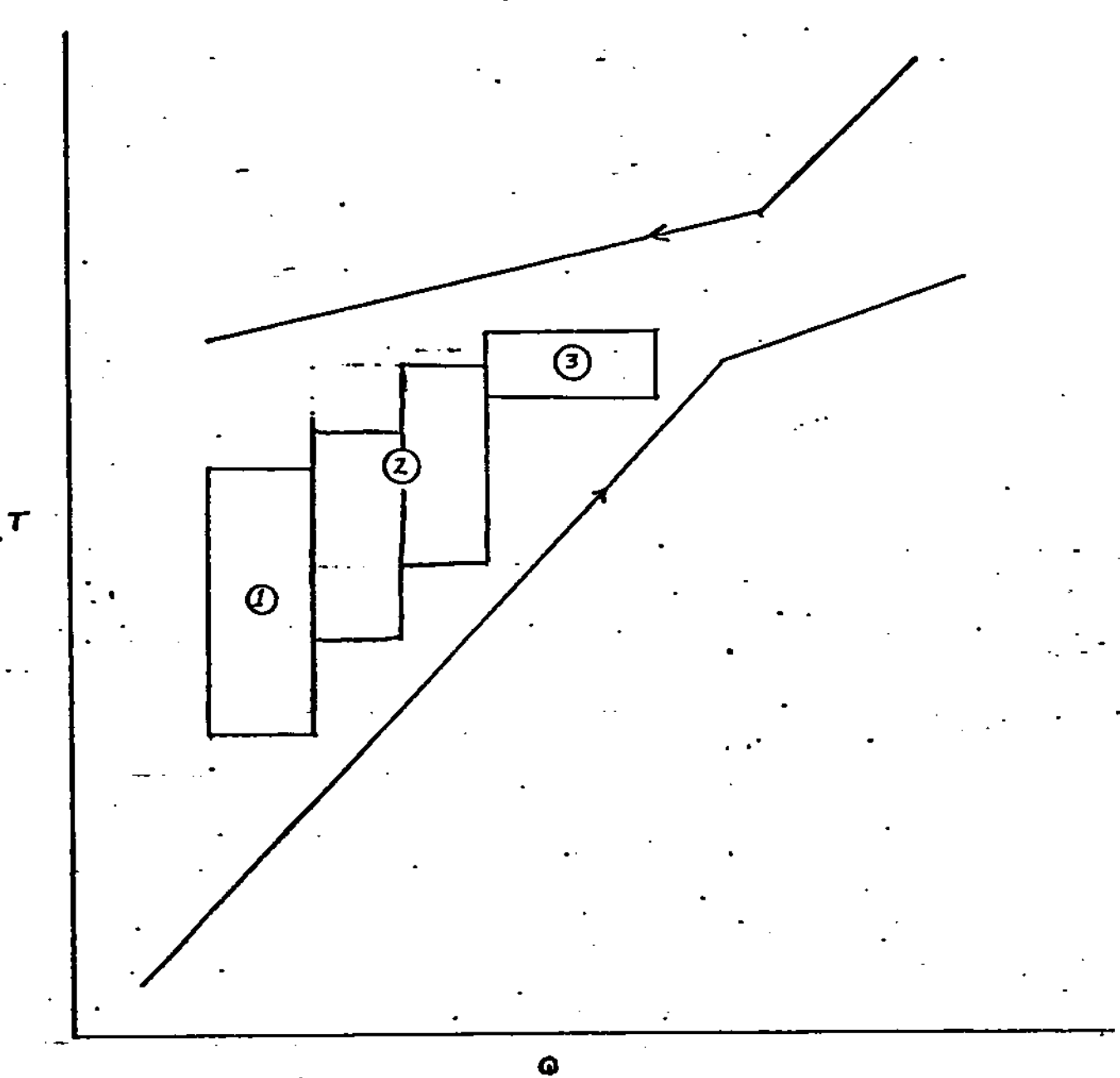


Figure 8: Integration of a Distillation Sequence with Process Streams

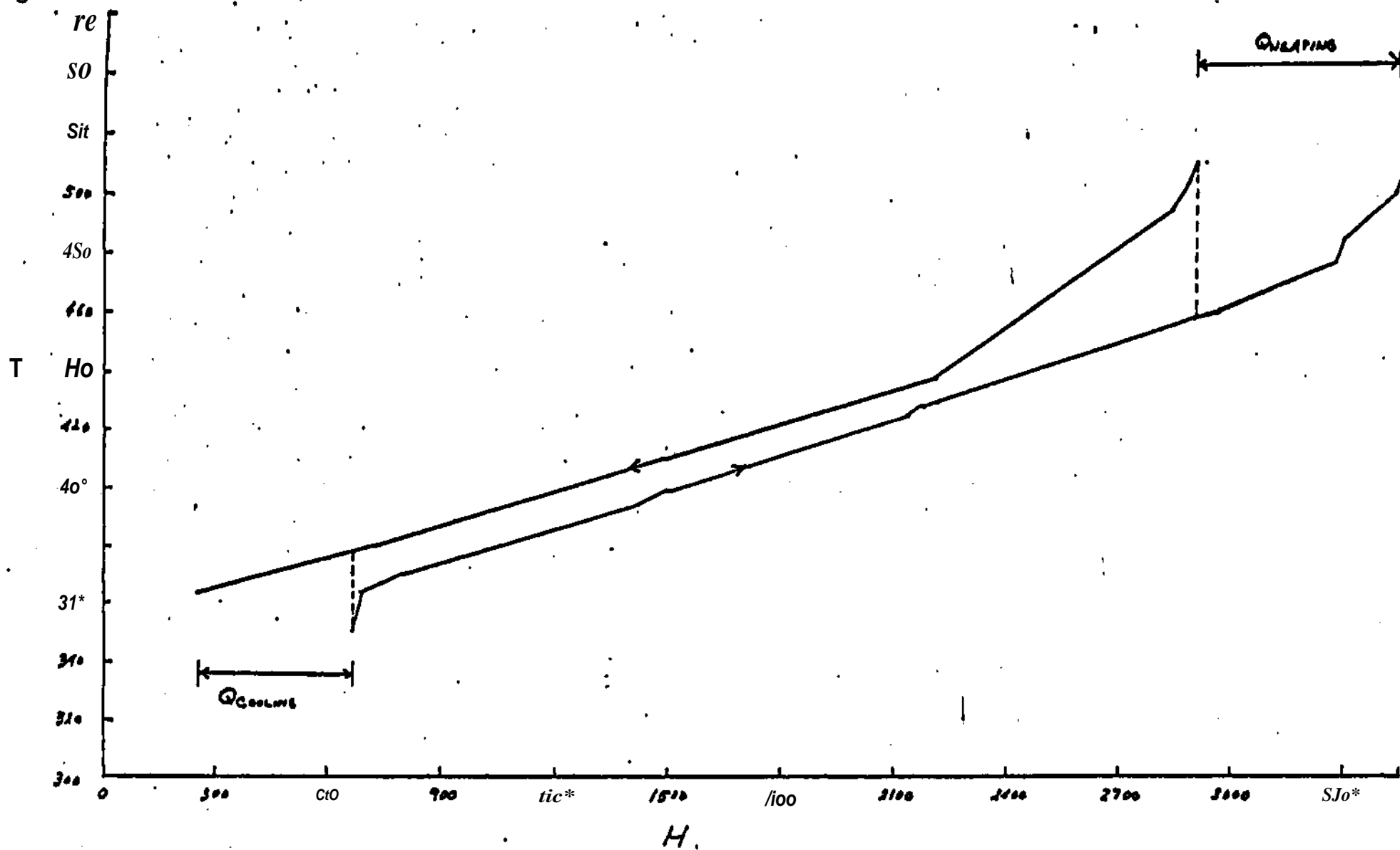


Figure 9: Composite Cooling Curves for Sensible Heat Effects In the Distillation Configuration of Figure 6

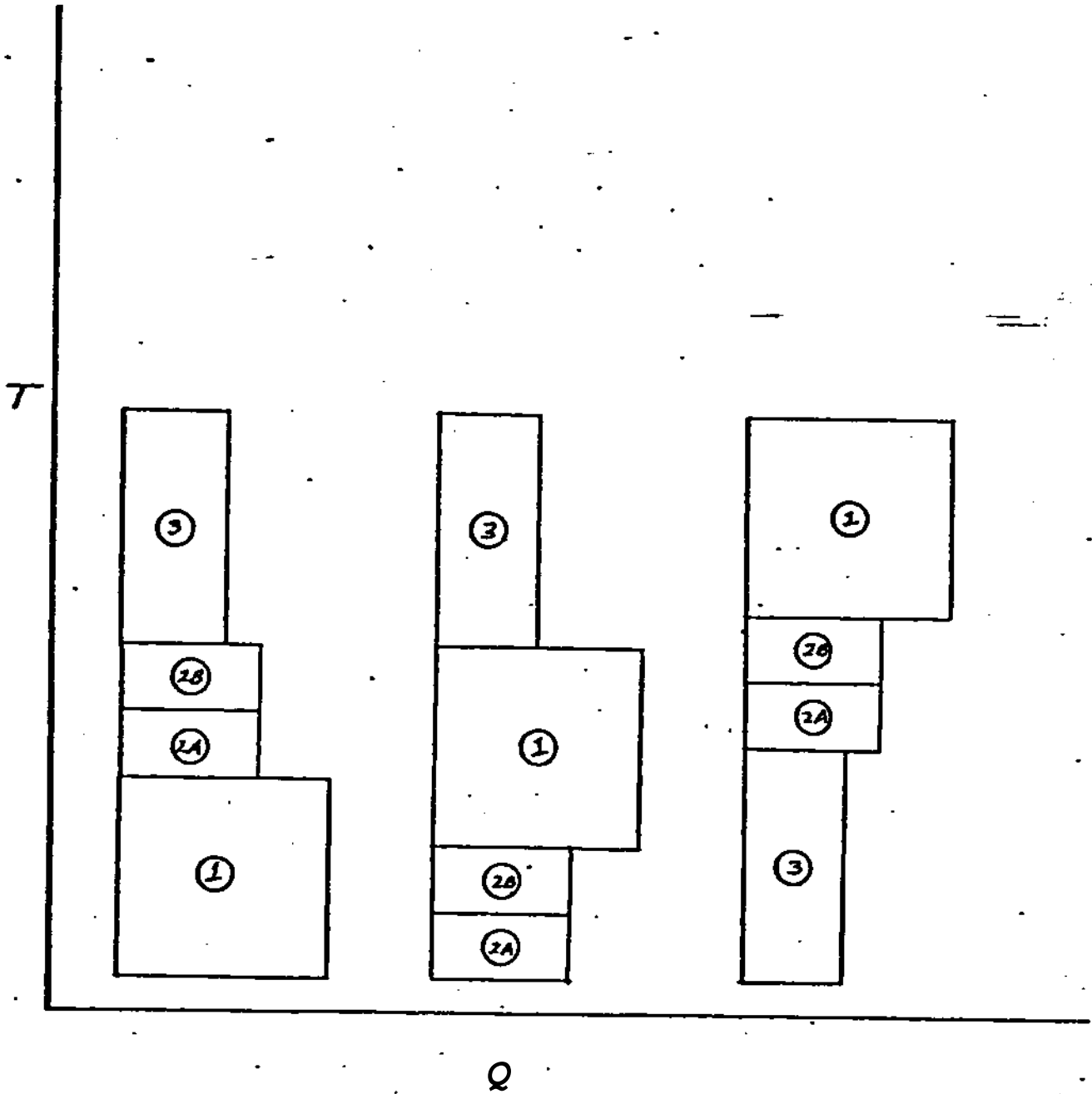


Figure 10: Alternate Stackings for a Given Sequence

Column	QAT
A/B	4190
B/C	2060
C/D	2640
D/E	2790
A/BC	4310
AB/C	1920
B/CD	1960
BC/D	2880
C/DE	2720
CD/E	2600
A/BCD	4270
AB/CD	1920
ABC/D	2910
B/CDE	1890
BC/DE	3000
BCD/E	2790
A/BCDE	4280
AB/CDE	1910
ABC/DE	3090
ABCD/E	2900

Table 1: QAT (kJ-K/gmol) for all Separators
in the Alcohol Example Problem.

Sequence fc	ZQAT MW-K	Klnimum UtJLlity Use KV
1	1114	6.54
2	1171	6.68
3	1146	6.73
4	1211	7.11
5	1266	7.43
6	841	4.94
7	898	5.27
8	1122	6.59
9	964	5.66
10	1234	7.25
11	1289	7.57
12	1024	6.01
13	1341	7.87
14	1182	6.94

Table 2: Lower Bounds on Utility Use for All Sequences
in the Alcohol Example Problem

Column	Cond Duty KW	Ret> Duty KW	Temp Diff K	QAT Ktf-K	Column Cost 10* \$
A/B	16.44	16.55	13.9	230.0	1832
B/C	5.28	5.73	25.0	143.2	319
C/D	8.42	7.96	20.6	164.0	624
D/E	4.70	4.91	19.9	97.7	474
A/BC	18.30	19.26	23.4	450.7	972
AB/C	6.85	7.48	27.5	205.7	373
B/CD	5.55	6.03	27.0	162.8	319
BC/D	9.49	9.16	26.1	239.1	588
C/DE	8.74	8.64	26.2	226.4	525
CD/E	7.31	7.61	28.5	216.9	484
A/BCD	18.70	19.74	25.5	503.4	910
Afi/CO	7.05	7.68	29.5	226.6	373
ABC/D	11.06	10.94	31.4	343.5	576
B/CDE	5.88	6.42	30.6	196.4	313
BC/DE	9.82	9.84	31.7	311.9	512
BCD/E	8.16	8.57	33.9	290.5	471
A/BCDE	19.27	20.53	28.9	593.3	841
AB/CDE	7.29	7.97	33.1	286.9	367
ABC/DE	11.30	11.63	37.0	430.3	511
ABCD/E	9.53	10.21	39.5	403.3	475

Table 3: Column Parameters and Costs for All Columns in the Alcohol Example Problem.

i	j	$C_i + C_j$	$\Delta T_{i,j}$	Ratio
CW	Ex Stm	1.24	68	0.0182
Ctf	448 kPa Stm	2.79	116	0.0241
CV	1069 fcPa Stm	3.67	157	0.0234
CW	4241 JcPa Stm	4.17	222	0.0188

Table 4: Ratio of Utility Costs to Available Temperature Difference for the Alcohol Example Problem

Sequence	Minimum Utility Use MW	Minimum Utility Cost 10*\$/yr	Minimum Capital Cost 10*\$	Minimum Annual Cost 10*\$/yr
1	6.54	834	2153	1295
3	6.73	859	2146	1305
8	6.59	841	2276	1348
2	6.88	878	2262	1361
4	7.11	907	2255	1374
5	7.43	948	2219	1381
10	7.25	925	2328	1412
11	7.57	966	2292	1419
13	7.87	1004	2342	1459
6	4.94	630	3198	1607
9	5.66	722	3190	1651
7	5.27	672	3307	1672
12	6.01	767	3304	1720
14	6.94	886	3256	1763

Table 5: Ranking of Distillation Sequences by Minimum Annual Cost

Table 6: Progress of Least Cost Algorithm

Sequence	Conflg	z^+ $10^3 \$/yr$	c^+ cap	Q^+ MW	\bar{c}^+ cap $10^3 \$$	Q MW	\bar{u}^+ ann $10^3 \$/yr$	Comment
1	1-1-1-1	8815	21000	120.00	2152	20.53	2223	
	2-1-1-1	2223	4473	20.52	2420	10.26	1649	
	3-1-1-1	1649	3038	10.26	2590	8.64	1609	
	3-1-2-1	1609	2937	8.64	2752	¹ 6.84	1555	
	4-1-2-1	1555*	2802	6.84	2854	6.54	1575	$c_{cap} > c_{cap}^+$
3	2-1-1-1	1555	2771	10.49	2415	10.26	1647	
	3-1-1-1	1555	2771	10.26	2510	9.84	1657	
	3-2-1-1	1555	2771	9.84	2761	6.84	1558	
	4-2-1-1	1555	2771	6.84	2822	6.73	1575	$c_{cap} > c_{cap}^+$
8	2-1-2-1	1555	2794	9.71	2710	9.63	1723	
	2-1-3-1	1555	2794	9.63	2975	6.60	1628	$c_{cap} > c_{cap}^+$
2	3-1-1-1	1555	2746	9.80	2717	7.96	1615	
	3-1-1-2	1555	2746	7.96	2801	7.61	1625	$c_{cap} > c_{cap}^+$
4	3-1-1-1	1555	2708	9.84	2692	8.57	1645	
	3-2-1-1	1555	2708	8.57	2785	7.96	1642	$c_{cap} > c_{cap}^+$
5	3-1-1-1	1555	2655	10.06	2632	9.16	1660	
10	2-3-1-1	1555	2685	9.40	2940	7.96	1704	$c_{cap} > c_{cap}^+$
11	2-3-1-1	1555	2632	9.62	2807	9.16	1731	$c_{cap} > c_{cap}^+$
13	2-2-3-1	1555	2582	9.32	3150	7.87	1782	$c_{cap} > c_{cap}^+$