# Parametric Studies in Industrial Distillation:

## Part I. Design Comparisons

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Minimum cost surfaces compare eight distillation systems separating ternary feeds. The region of optimality for a design varies with the species separated, but some tower configurations are always preferred at particular feed compositions.

### SCOPE

Industrial distillation networks frequently utilize complex, multiple-section fractionators. Towers often receive multiple feed streams and produce more than two products. Eight such configurations are compared economically with a computer design model. The venture cost, depending on the annual operating cost and the total capital investment, is first minimized for each design by changing its state vector. The dimensions of the state search range from two to ten. The minimum cost is then computed in sequences of parametric studies which compare the designs' characteristics.

Earlier study in process synthesis and design has been largely confined to the simpler, serial distillation configurations, where the N-1 rule is obeyed (see Hendry and Hughes, 1972; Hendry et al., 1973). Rathore et al. (1974) and Rathore and Powers (1975) develop algorithms for simultaneously synthesizing simple distillation networks and energy management systems; Rodrigo and Seader (1975), Gomez M and Seader (1976), and Stephanopoulos and Westerberg (1976) formulate systematic enumeration techniques. Here the objective is to discover rules of thumb by examining specific parametric case studies, involving mixtures of ideally behaved light hydrocarbons.

### CONCLUSIONS AND SIGNIFICANCE

Often the design engineer could synthesize complex separation flow sheets by hand, if he had simple, qualitative methods of defining likely, optimal candidates. For ternary mixtures, likely, optimal candidates, shown in Figures 1 through 4, are qualitatively defined by the feed composition and its Ease of Separation Index (ESI). Nonideal mixtures may also be so characterized, but with the feasible material balances and design options implicitly constrained by the designer. The expected feed composition regions of design optimality are shown as Figures 5 and 6. For ESI $<$ 1.6, the complex and simple designs are favored as shown in Figure 5, and by these rules

1. If 40 to 80% is middle product and nearly equal amounts of overhead and bottoms are present, then favor design V.
2. If more than 50% is middle product and less than 5% is bottoms, then favor design VI.
3. If more than 50% is middle product and less than 5% is overheads, then favor design VII.
4. If less than 15% is middle product and nearly equal amounts of overheads and bottoms are present, then favor design III.
5. Otherwise, favor design I or II, whichever removes the most plentiful component first.

For ESI $\geq$ 1.6, the complex and simple designs are favored as shown in Figure 6, and by these rules

1. If more than 50% is bottoms product, then favor design II.
2. If more than 50% is middle product and from 5 to 20% is bottoms, then favor design V.
3. If more than 50% is middle product and less than 5% is bottoms, then favor design VI.
4. If more than 50% is middle product and less than 5% is overheads, then favor design VII.
5. Otherwise, favor design III.

Thermally coupled designs III and IV should be considered as alternatives to designs I and II, respectively, if less than half the feed is middle product. In addition, designs III, IV, VI, and VII should be considered for separating all mixtures where a low middle product purity is acceptable.

Designs with good economic properties should be found by reducing the N component separation problem to sequences of pseudo ternary separations and performing the most difficult ternary separations last. This heuristic approach greatly increases the number of designs easily considered in the synthesis of a distillation train but does not guarantee structural optimality, nor explicitly consider all possible complex design alternatives.

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Distillation systems with far from simple topological structure play an important role in industrial operations, and it is well recognized that changes in the network configuration and operation can often result in more efficient operation. Consider the separation systems shown in Figures 2 through 4, for example. These more complex designs differ from the simpler, more conventional systems, I and II, with respect to the characteristics outlined in Table 1.

All designs except VI and VII could be operated with recycle between units, and the significance of this factor has not been completely examined here. If recycle is established between units 1 and 2 in design V, for example, the result is a thermally coupled system analogous to

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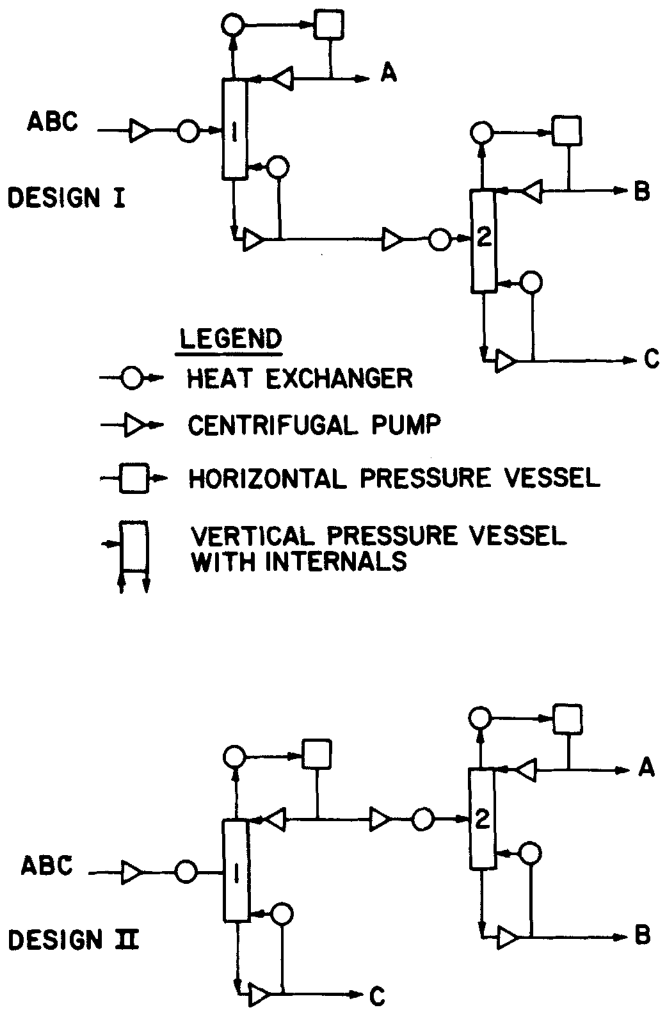


**Fig. 1. The simple direct (I) and inverted (II) sequences.**

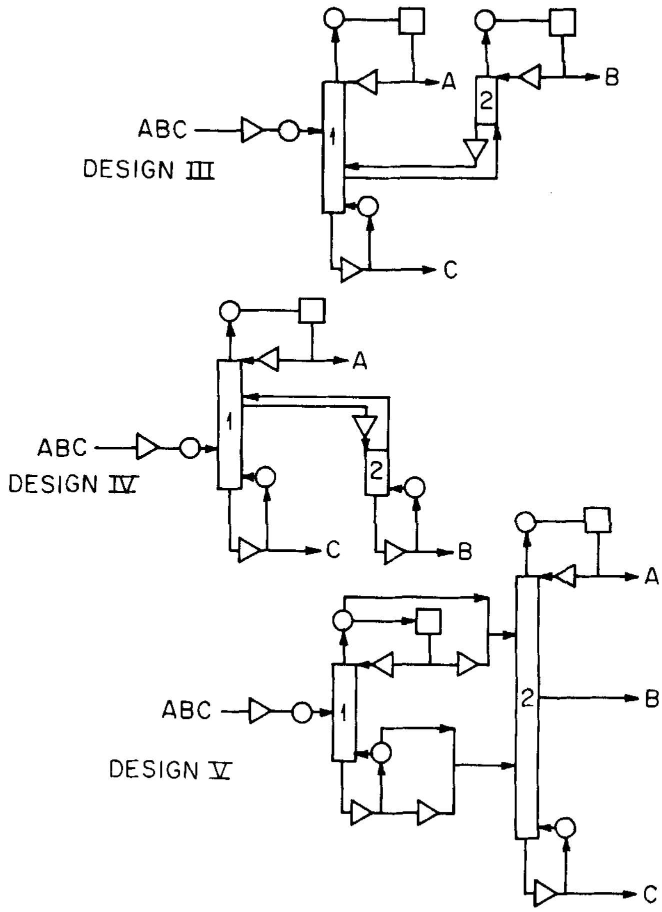


**Fig. 2. Complex designs.**

that considered by Stupin (1970). Although design V is often attractive for other reasons, thermal coupling is an essential elment underlying the advantage perceived for design III, as shown in Figure 6.

The class of designs I through VIII is much larger than that class represented by designs I and II alone, especially as the number of feed constituents increases. When different subsets of the analogues corresponding to designs I through VIII are enumerated as shown in Table 2, the problem magnitude becomes more evident. Heaven (1969) derived a recursion formula giving the results shown for set 1. Similar, but more complex, expressions have been derived for the remaining sets shown in the table [see Tedder, 1975]. Examination of sets 4 and 5 in Table 2 indicates that the number of design alternatives increases tremendously when components are permitted to distribute themselves between the keys. Of course, many of these designs, like VIII, violate the N-1 rule (see Lockhart, 1947), since they require additional towers. Other designs, like V, VI, and VII, require less than N-1 towers to separate N components, and it is not always clear which fraction of these designs, if any, should be excluded from reasonable considerations a priori. The venture cost of a single tower with a large diameter and high reflux rate, for example, can be substantially greater than that associated with three relatively small units. Consequently,

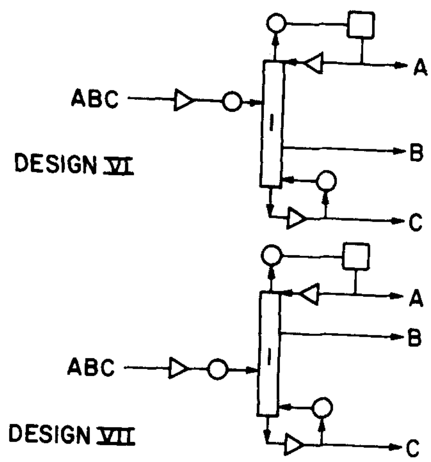


**Fig. 3. Single-tower designs.**

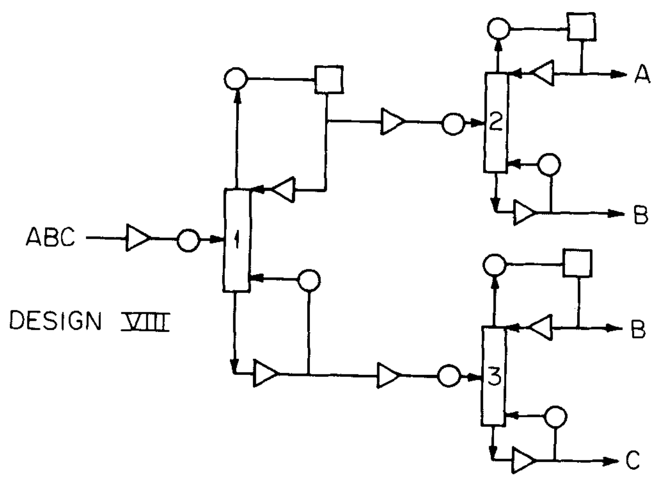


**Fig. 4. Three-tower design.**

TABLE 1. COMPARISON OF DESIGN ALTERNATIVES' CHARACTERISTICS

| Design | Degrees of freedom | Characteristics |
|---|---|---|
| I | 6 | Variable = $(f_1, P_1, V_1, f_2, P_2, V_2)$ |
| II | 6 | Variables = $(f_1, P_1, V_1, f_2, P_2, V_2)$ |
| III | 4 | Variables = $(f_1, P_1, V_1, V_2)$ Lower, dew-point vapor side stream. Thermally coupled. Bubble-point liquid recycle. |
| IV | 4 | Variables = $(f_1, P_1, V_1, V_2)$ Upper, bubble-point liquid side stream. Thermally coupled. Dew-point vapor recycle. |
| V | 7 | Variables = $(f_1, P_1, V_1, g_1, f_2, V_2, f_3)$ Middle product distributed in upstream tower. Does easiest split first. |
| VI | 2 | Variables = $(f_1, P_1)$ Lower, dew-point vapor side draw. $V_1$ is variable when the bottom product rate is very small. |
| VII | 2 | Variables $(f_1, P_1)$ Upper, bubble-point liquid side draw. $V_1$ is variable when the upper product rate is very small. |
| VIII | 10 | Variables = $(f_1, P_1, V_1, g_1, f_2, P_2, V_2, f_3, P_3, V_3)$ Middle product distributed in upstream tower. Does easiest split first. |

State variable optimization legend (subscript refers to $i^{th}$ tower)

$f_i$ = fractional vaporization of tower feed. It may be subcooled or superheated.
$P_i$ = tower operating pressure on top tray.
$V_i$ = molar vapor rate at the tower pinch point.
$g_i$ = fraction of tower feed sent overhead.

rigid adherence to the N-1 rule and simple tower structures may exclude the optimal design, especially when some of the recovered feed constituents are present in only trace amounts or only low product purities are required.

## PARAMETERS VARIED

The minimum venture cost for separating ternary mixtures into three nearly pure product streams was determined for each design after state optimization with the degrees of freedom shown in Table I. Descriptions of the computer design model are given elsewhere (see Tedder and Rudd, 1976; Tedder, 1975). Additional discussion of the product composition estimation method and the design evaluation are given in Part III of this series of papers.

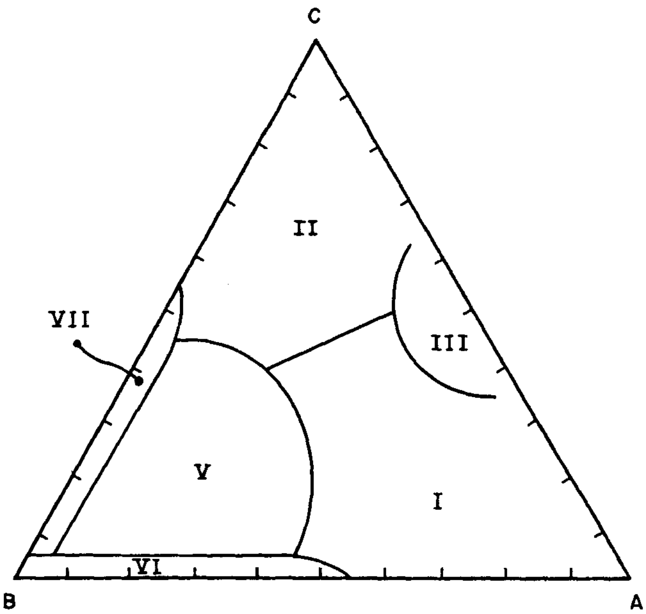


Fig. 5. Expected regions of optimality for ESI < 1.6.

For each feed mixture, the composition is considered at seven points on the surface shown in Figure 7. The composition points are labeled as points Cl through C7 in Table 3, where the triplet $(X_A, X_B, X_C)$ implies that the components are arranged according to decreasing volatility. It is understood that each high purity product con-

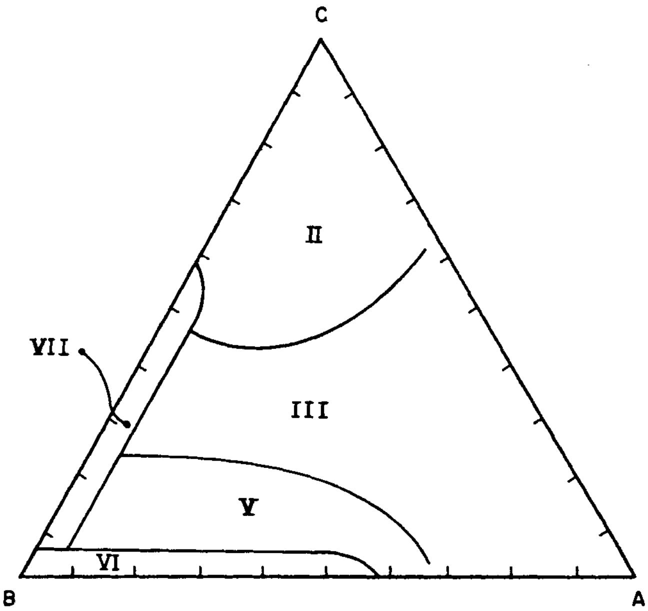


Fig. 6. Expected regions of optimality for ESI ≧ 1.6.

TABLE 2. TOTAL NUMBER OF DISTINGUISHABLE DESIGNS, ACCORDING TO THE NUMBER OF FEED CONSTITUENTS RECOVERED, AND THE TYPES OF COMPLEX AND SIMPLE DESIGNS PERMITTED

| Set number | Design analogues in set | Total distinguishable designs, and number of feed constituents recovered: 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|
| 1 | (I, II) | 2 | 5 | 14 | 42 |
| 2 | (I, II), (III, IV), V | 5 | 22 | 106 | 527 |
| 3 | (I, II), (III, IV), V, (VI, VII) | 7 | 33 | 204 | 1 129 |
| 4 | (I, II), (III, IV), V, (VI, VII), VIII | 8 | 265 | 110 415 | $\sim 1.25 \times 10^{10}$ |
| 5 | (I, II), VIII | 5 | 46 | 2 795 | 8 110 988 |

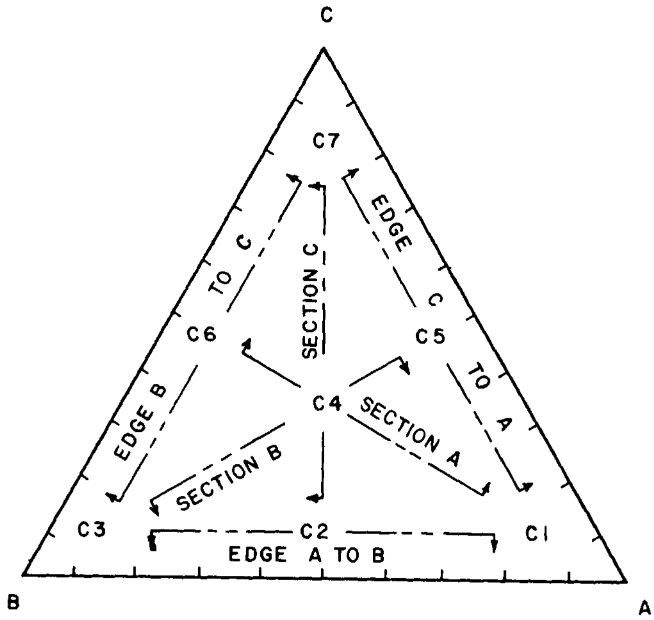

Fig. 7. Definition of composition points, sections, and edges.

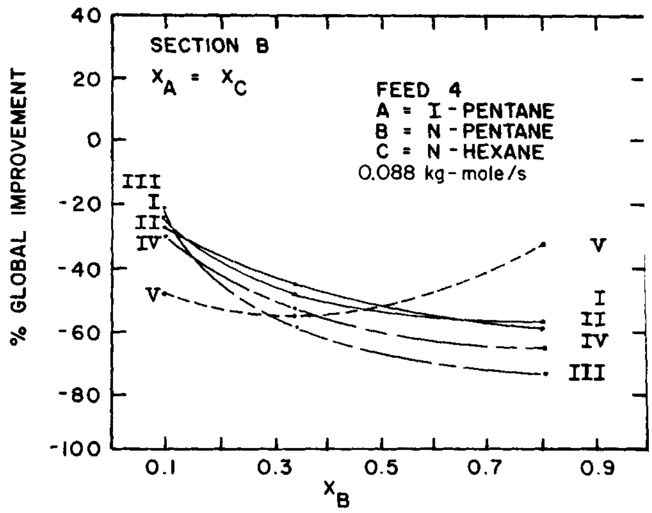

Fig. 8. Typical section B plot.

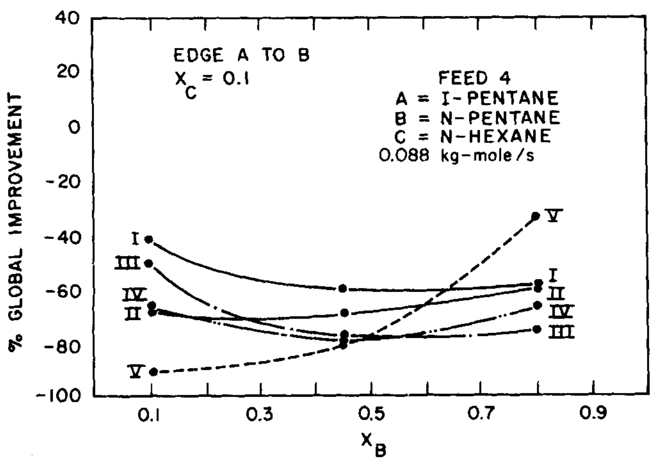

Fig. 9. Typical edge from A to B.

TABLE 3. DEFINITION OF COMPOSITION POINTS

| Label | Composition triplet |
|---|---|
| C1 | (0.8, 0.1, 0.1) |
| C2 | (0.45, 0.45, 0.1) |
| C3 | (0.1, 0.8, 0.1) |
| C4 | (0.333, 0.334, 0.333) |
| C5 | (0.45, 0.1, 0.45) |
| C6 | (0.1, 0.45, 0.45) |
| C7 | (0.1, 0.1, 0.8) |

TABLE 4. DEFINITION OF FINAL PRODUCT COMPOSITIONS

| Final product | Composition triplet |
|---|---|
| Overhead | (0.987,* 0.01, 0.003*) |
| Middle | (0.01, 0.98, 0.01) |
| Bottom | (0.004,* 0.01, 0.986*) |

* Varies with feed species.

TABLE 5. RANGE OF UTILITY COSTS

| | $T$(°K) | Low | High |
|---|---|---|---|
| Steam ($/GJ) | 504 | 1.03 | 10.30 |
| | 442 | 0.77 | 7.70 |
| | 418 | 0.57 | 5.70 |
| | 389 | 0.42 | 4.20 |
| Ammonia ($/GJ) | 274 | 1.65 | 16.50 |
| | 255 | 2.97 | 29.70 |
| | 246 | 3.96 | 39.60 |
| Cooling water (¢/m³) | 297 | 0.66 | 6.60 |

tains from 1 to 2 mole % of impurities (see Table 4).

The seven composition points define three edge and section projections, comprised of three points on each abscissa. A smooth curve is constructed for each design, defined by three points on a projection. Typical plots are shown in Figures 8 and 9. Any surface discontinuities are ignored, although they sometimes occur, since at each point the model employs that utility which minimizes the venture cost and satisfies temperature approach. Table 5 shows the range over which the utility cost rates were permitted to vary, each by the same proportion. Unprimed feed numbers indicate that the lower utility cost rates were used; primed numbers mean that the high rates were used in obtaining a particular figure.

The regions of optimality are defined by the intersection lines for the minimum venture cost surfaces of two different designs. The ordinate for each design is arbitrarily presented as a percentage of $250 000 in annual venture cost, a typical design cost at the low utility rates. The percentage Global Improvement, % GI, is increasingly positive as costs decrease:

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

A venture cost of $297 500, or −19% GI, is equal to a processing cost of about 11¢/kg-mole of feed.

Six ideal ternary mixtures have been examined. The feed species mixtures are shown in Table 6, along with their average volatility properties which varied during the cost analysis. The Ease of Separation Index (ESI) is defined in terms of the component distribution coefficients

$$\text{ESI} = \frac{K_A K_C}{K_B K_B} \qquad (2)$$

It is useful for examining the species heuristic, do the easy separation first. An ESI less than unity indicates that

TABLE 6. DEFINITION OF FEED MIXTURES

| Feed number | | ESI | $K_A/K_B$ | $K_B/K_C$ | $K_A/K_C$ |
|---|---|---|---|---|---|
| 1 | *n*-pentane, *n*-hexane, *n*-heptane | 1.04 | 2.57 | 2.47 | 6.35 |
| 2 | *n*-butane, *i*-pentane, *n*-pentane | 1.86 | 2.38 | 1.28 | 3.05 |
| 3 | *i*-butane, *n*-butane, *n*-hexane | 0.18 | 1.36 | 7.52 | 10.23 |
| 4 | *i*-pentane, *n*-pentane, *n*-hexane | 0.47 | 1.25 | 2.65 | 3.31 |
| 5 | *i*-butane, *n*-butane, *i*-pentane | 0.59 | 1.38 | 2.35 | 3.24 |
| 6 | propane, *i*-butane, *n*-butane | 1.72 | 2.38 | 1.38 | 3.28 |

the *A/B* split is harder than the *B/C* split and conversely for an ESI greater than unity.

## UNCERTAINTIES IN COMPARISONS

Freshwater and Henry (1974) have suggested that significant differences between designs often cannot be discerned. For that portion of a feed composition surface where the venture cost difference between two designs is less than 5% GI (about 4.6 mills/kg-mole of feed), it is probably more realistic to consider that an advantage is nondiscernible. These regions tend to be smaller when the high utility rates are used, but they are larger when the minimum cost surfaces of the designs compared are highly correlated. Consider, for example, section B of the minimum cost surfaces for designs I and II as they appear in Figure 8. Two intersection points lie on this projection, but considerable uncertainty exists as to their exact location. The small advantage perceived for design II at composition point C4 may well be due to errors in the state optimization.* On the other hand, there is little doubt that design I is favored over II along edge A to B as shown in Figure 9. Similarly, the discernible regions are relatively larger when comparing designs II and V as they appear in Figures 8 and 9 because their minimum cost lines are not highly correlated.

Another source of uncertainty in the location of intersection lines between two designs, and affecting the size of nondiscernible regions, results from bias in cost minima, since utilities have been assumed available at discrete, invariant temperatures as shown in Table 5. If we separate feed 3, for example, the observed difference between designs I and II at point C4 is judged significant, being about 17% GI. However, a closer examination of the differences between the two designs at that feed composition indicates that almost all of the additional cost for design I is due to the use of 418 deg steam heat in the upstream reboiler, rather than the 339 deg steam heat used in the downstream reboiler of design II. During the state optimization, the venture costs were calculated for all four stream sources shown in Table 5. Apparently, 418 deg steam is less expensive for design I at that point, but if design II were constrained to also use 418 deg steam, then the economic differences between the designs would be smaller, Usually, however, the various designs will require the same utilities at their optimal states, and economic differences most often exist because of differences in the tower dimensions, reflux requirements, and operating pressures.

Despite these limitations, we believe that the conclusions drawn here are largely applicable to distillation trains

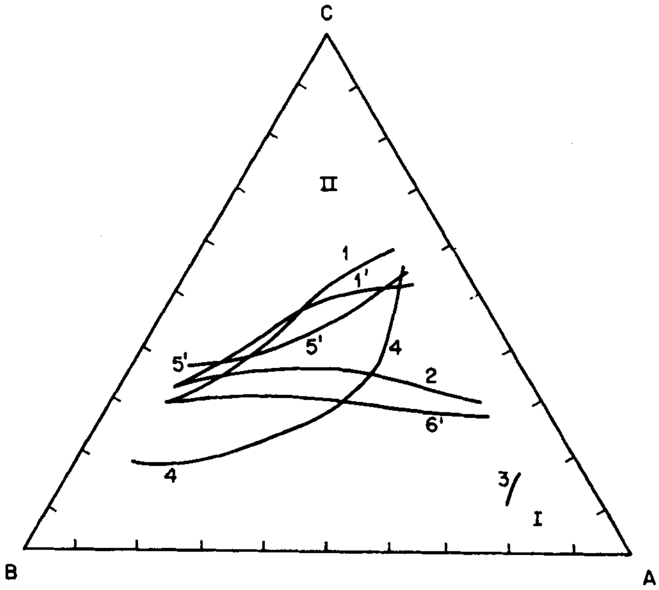


Fig. 10. Intersection lines obtained by comparing designs I and II only.

which are subject to different specific cost rates because the apparent regions of optimality for a design are not greatly changed with the utility cost rates. In fact, the minimum cost surfaces become steeper and are translated downward in percent GI as the utility rates are increased from the low to high cases, but the general appearance of the resulting equal cost contours on the surfaces, and the locations of the surface intersections themselves, usually do not shift significantly. Therefore, we believe that while the actual dollar amounts associated with the designs have limited significance, the intersection line locations and the trends observed in the surface contours are of more general value, since they are less sensitive to the assumed price levels.

## SIMPLE DESIGNS I AND II

Figure 10 indicates the intersection lines which have been found for the minimum venture cost surfaces of designs I and II. No case has been found where one design is preferred over the other for all feed compositions examined, and the differences at point C1 and C7 were always significant. All lines in Figure 10, except that for feed 3, are located fairly closely to section B in Figure 7. The region on the composition surface interior to the lines is smaller than the two regions exterior to them. Thus, while the species volatilities are changing, the intersection lines tend to remain in the central regions of the composition surface. Also, the close proximity of lines 1, 1′, 5′, and lines 2 and 6′, suggests that the apparent regions of optimality are not strongly changed when utility rates are increased by a factor of ten.

Figure 11 illustrates the characteristic effect of ESI

* The minimum annual venture cost was typically 30% or less of that cost calculated at the start of the gradient search over the state response surface. However, the resulting minimum venture cost is a function of the assumed starting point and the specified tolerance for improvement between successive iterations. A better operating state for design I might be found by changing the starting point and reducing the improvement tolerance or by utilizing a different search routine. Multiple starting points are necessary whenever the optimization terminates on a local minimum, an event which did not occur in this example.

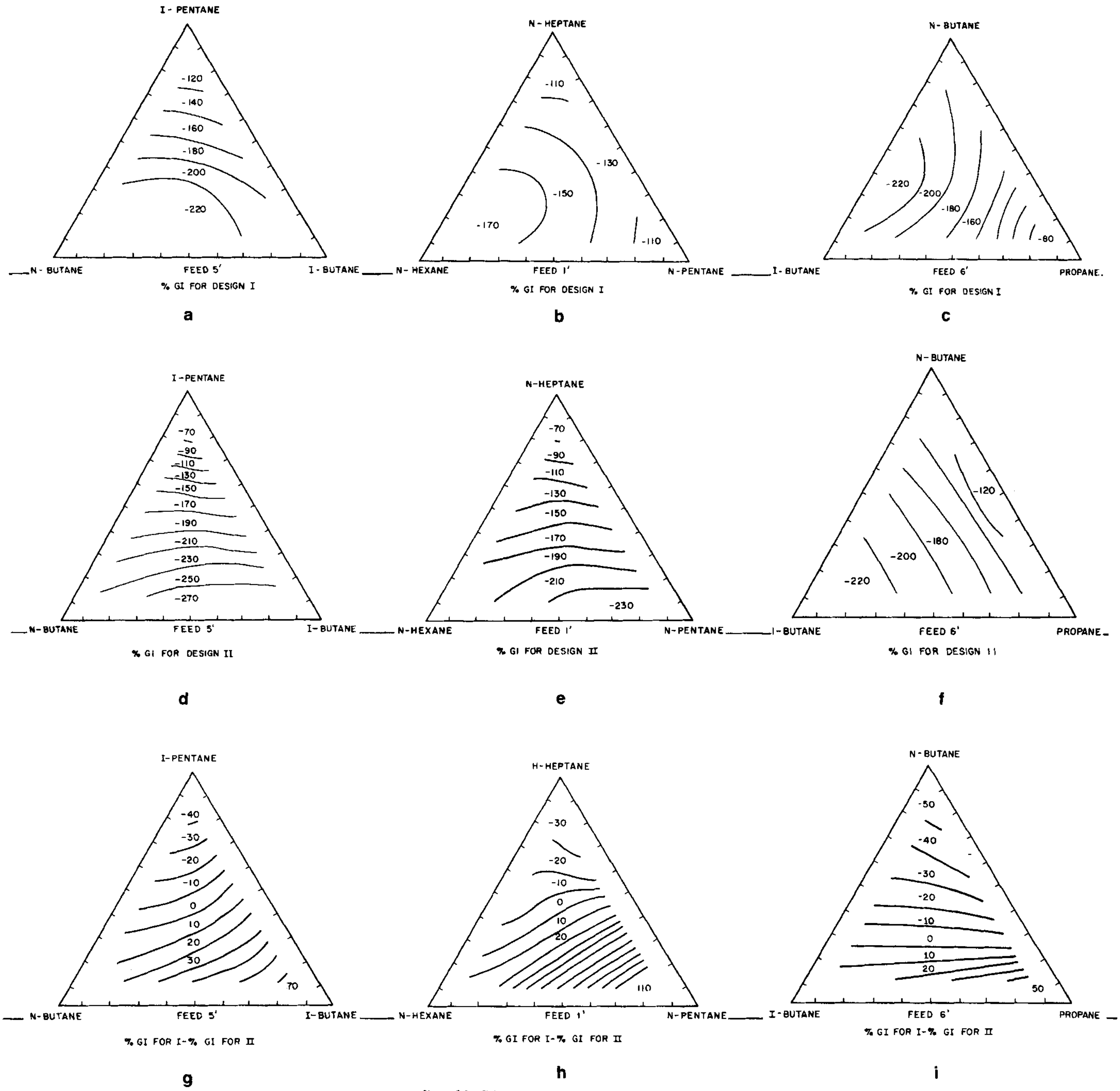


**Fig. 11. Effects of ESI on designs I and II.**

which has been observed on the minimum costs and the cost differences between these two designs. The top row consists of the minimum cost surfaces observed for design I separating feeds 1′, 5′, and 6′. The second row is the same set of surfaces as observed for design II, and the third row consists of the three difference surfaces formed by subtracting the costs in row 2 from those in row 1.

Feed 5′ represents a feed where the $A/B$ split is more difficult than the $B/C$; the opposite is true for feed 6′. The middle column represents an intermediate case where neither split is easier, so the effects of relative volatility changes are seen by comparing the columns.

Figures 11*a* and *b* have similar contours, since the middle product feed concentration largely determines the size of both towers in design I, whenever the $A/B$ split is as hard or harder than the $B/C$ split. Otherwise, when the $B/C$ split is harder, the contours are most strongly correlated with the overhead product feed concentration, as shown in Figure 11*c*, since this factor largely determines the size of the more expensive, downstream tower.

Comparison of Figures 11*d* and *e* also shows almost identical contours. The $A/B$ split is either as hard or harder than the $B/C$ split, but the economics of the inverted sequence for these feeds are largely determined by the amount of bottoms product, since this factor controls the required size for the more expensive downstream tower. But if the $B/C$ split is more difficult, as shown in Figure 11*f*, then the minimum cost contours for the inverted sequence are dominated by the amount of middle product in the feed, since this factor controls the required size for the more expensive, upstream tower.

Thus, for an ESI less than or equal to unity, the minimum cost contours for designs I and II appear very similar. Figures 11g and *h* also indicate that the cost differences are relatively unaffected when the $A/B$ split becomes more difficult, since it does not interact strongly with the most important economic factors.

For feed 6′, the equal cost contours show significant changes in correlation for both designs I and II (Figures 11*c* and *f*), since the components which dominate the designs' economics have changed. Similar distortions are observed when feed 2 is separated, and the corresponding difference surface appears similar to Figure 11*i*. The 0% line for feed 2 also appears horizontal and is almost superimposed on the line for feed 6′, as shown in Figure 10. We conclude, therefore, that when the *B/C* split is significantly more difficult than the *A/B*, the region of optimality for design II increases somewhat, and the net interaction is that the cost differences are more strongly correlated with the amount of bottoms component in the feed.

Feeds 5′ and 6′ are similar, although not identical, to the feeds examined by Lockhart (1947). Feed 5′ is comparable to his feed in which he varied the ratio of iso to normal butanes. When the feed contained 44% bottom product (*i*-pentane plus heavier), Lockhart found the inverted sequence preferred for feeds containing less than 17% iso butane. Here it appears that the inverted sequence is preferred whenever more than 25% of the feed goes iso butane for the same bottoms concentration (see Figure 11g). Both studies indicate that the direct sequence is always preferred when only 30% of the feed is bottoms.

Lockhart also examined feeds which were essentially mixtures of propane, iso and normal butanes, like feed 6′. He found that for feeds containing 64% bottom product, the inverted series is preferred when less than 15% is propane. This study finds that the inverted series is favored for all amounts of overhead and middle products with 64% bottoms. From Figure 11*i*, the regions of optimality for feed 6′ are divided by a nearly horizontal line located at rough by 30% normal butane. Lockhart found the direct sequence always preferred for a feed containing only 21% bottoms. This general agreement also suggests that economic differences between designs are relatively insensitive to the underlying, common price structure and the form of the objective function, so long as operating costs and capital investment requirements are both considered.

A closer examination of the designs' states for feeds 2 and 6′ suggests that design II is favored over a larger region partly because the smaller, downstream tower, operated at high pressure in design II, is much less expensive than the larger, upstream tower in design I operated at about the same pressure. We therefore agree with Lockhart in that it is not always best to reduce the pressure level of a distillation system as quickly as possible (as with I), especially when the pinch point for all four possible towers is below the feed tray, and the bottom product rate for the high pressure tower can be significantly reduced (as with II). If a difference greater than about 0.17 $MN/m^2$ (25 $lb/in.^2$) exists between the optimal overhead operating pressures for two towers in a sequence, then it may be more advantageous to perform the high pressure separation last.

Rod and Marek (1959) developed a comparison criterion which considers only the feed composition and the ratio of distribution coefficients $K_A/K_C$ for comparing designs I and II. For ternary systems, their criterion predicts that the direct series is preferred for all composition points below and to the right of section B in Figure 7. Moreover, they predict that as the ratio $K_A/K_C$ is increased from unity, the intersection line separating the regions of optimality rotates from section B toward the edge B to C. They show the line separating the regions nearly parallel to the edge B to C for $K_A/K_C = 10$. However, this study does not support their findings. For feed 3, the inverted series is preferred over nearly all the surface, which strongly suggests that their comparison criterion is inadequate. There does not appear to be any significant trend as they indicate; lines 1, 4, and 3 in Figure 10 suggest a trend in the opposite direction and consistent with the heuristic, do the easy separation first. Intersection lines 5′, 2, and 6′, however, do not appear significantly shifted in accordance with this rule. For these latter cases, the advantage of performing the high pressure separation last favors design II over a larger region.

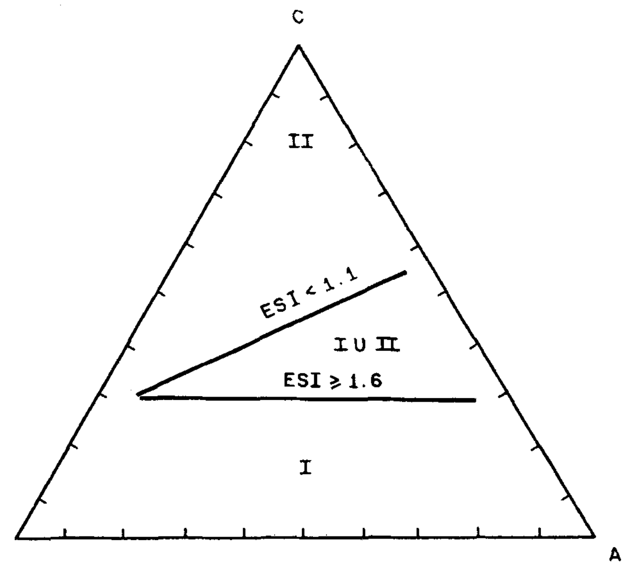


Fig. 12. Expected optimal regions for designs I and II only.

Figure 12 indicates the expected optimal regions when only designs I and II are considered. Design I is favored in the center region for ESI less than 1.6, but the advantage is small. The large advantage perceived for design II separating feed 3 at that point is partly an artifact of the assumed available steam pressures as explained; the intersection line 3 in Figure 10 should perhaps be shifted more closely toward the others. We therefore believe that in this central region the differences between designs I and II are largely nondiscernible, but we also support the heuristic suggested by Nishimura and Hiraizumi (1971) "favor the direct sequence when equimolar amounts are present in the feed, and the relative volatilities are the same."

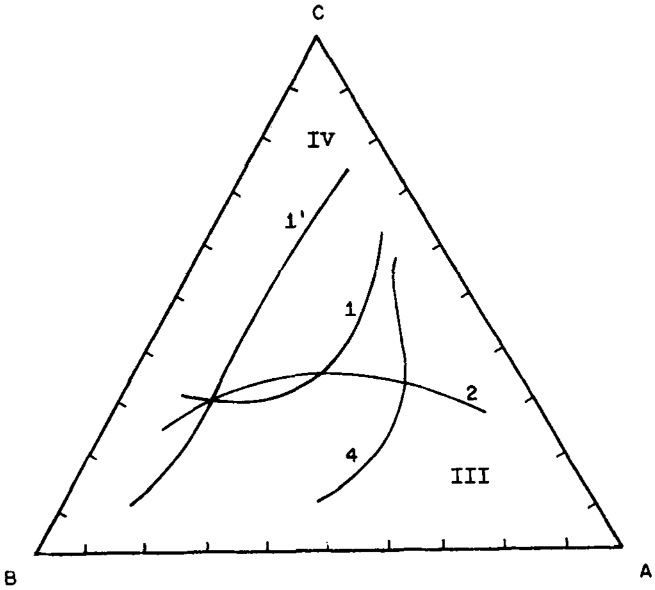


Fig. 13. Intersection lines obtained by comparing designs III and IV only. Design III is favored everywhere separating feed 6′; IV is favored everywhere separating 3.

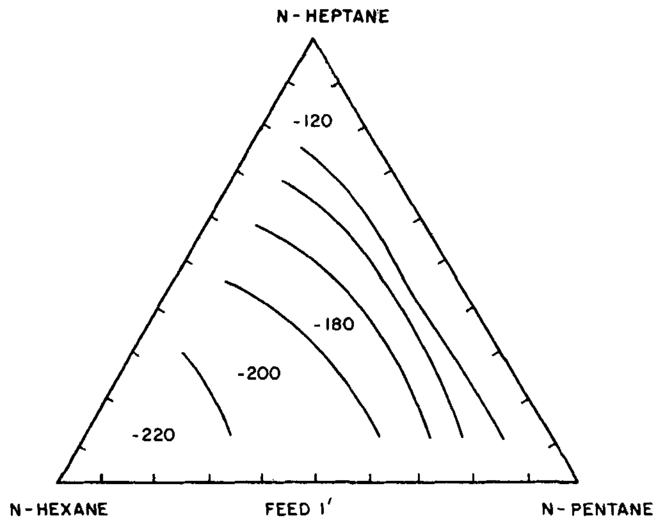


Fig. 14. Percent GI for design III separating feed 1′.

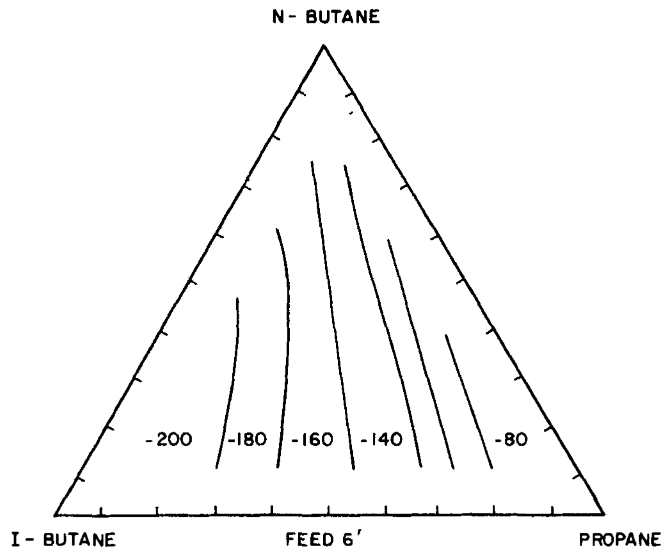


Fig. 15. Percent GI for design III separating feed 6′.

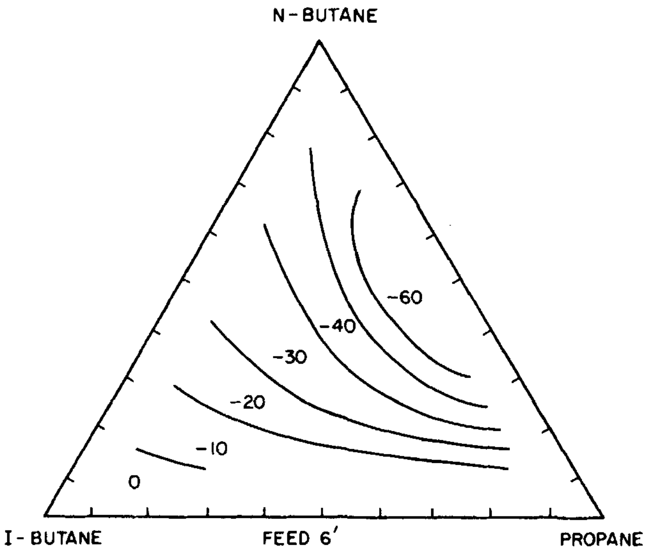


Fig. 16. Difference surface defined by the percent GI for I minus the percent GI for III.

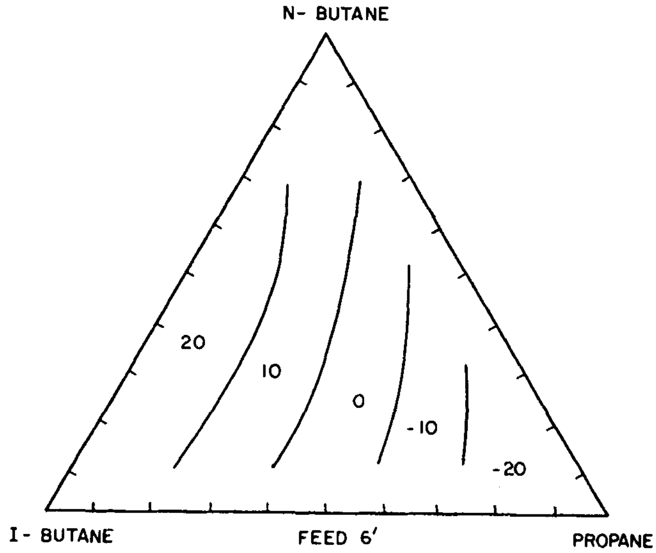


Fig. 17. Difference surface defined by the percent GI for II minus the percent GI for IV.

## THERMALLY COUPLED DESIGNS III AND IV

Figure 13 indicates the intersection lines which have been found for the minimum venture cost surfaces of designs III and IV. Comparison with Figure 10 suggests the behavioral similarities which exist between designs I and III, and between designs II and IV. In fact, the difference surfaces obtained by subtracting the percent GI for design IV from that for design III appear almost identical to Figures 11*g*, *h*, and *i*. So the relative costs of designs III and IV are largely determined by the same factors which lead to differences between designs I and II.

However, the costs of designs III and IV are more strongly controlled by the amount of middle product than is the case for either design I or II. Figure 14 shows the minimum cost surface obtained for design III separating feed 1′, and this surface is also representative of the contours obtained by separating feeds 1, 3, and 4. It is similar to Figure 11*b* but somewhat steeper, as is often the case. The minimum cost contours for design IV separating feeds with ESI less than or equal to unity also appear similar to Figure 14, but when the ESI is much less than unity, as with feeds 3 and 4, the contours for design IV are also more strongly correlated with the amount of bottoms product taken, like Figures 11*d* and *e*. However, designs III and IV are always most attractive along the edge from *C* to *A*, whenever the downstream tower can be made small.

For feeds 2 and 6′, the minimum cost contours for designs III and IV are more nearly independent of the bottoms rate, as shown in Figure 15, because the vapor rate in the bottom section of the upstream tower is largely established by the relative amounts of overhead and middle products. Under these conditions, the vapor rate in the bottom section of the upstream tower greatly exceeds the minimum required to produce the bottoms product, so the contours appear more nearly parallel to section *C*.

The effects of thermally coupling two towers can be seen from Figures 16 and 17, which represent the difference surfaces for designs I and III and designs II and IV, respectively. The differences shown change in sign and magnitude with the species separated, but the appearance of the difference contours are largely unchanged for all feeds examined. If design III is favored over I at all, the greatest advantage always exists at

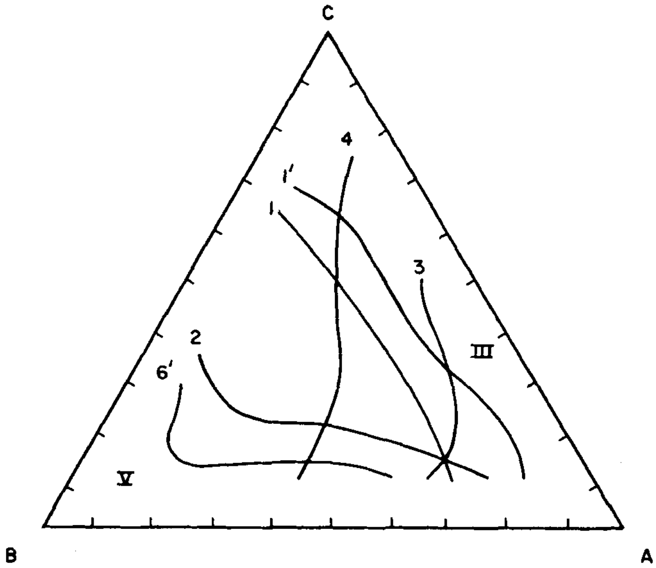


**Fig. 18. Intersection lines obtained by comparing designs III and V only.**

feed composition C5. At composition C5, both towers in design I must be large, whereas the downstream tower in III may be small. Similarly, design IV always appears most attractive, relative to design II, at composition C1. The difference contours between designs IV and II are always correlated with the overhead product rate, since IV recovers the $A$ component only once as overheads, whereas II recovers the $A$ component twice as overheads.

Significant differences can exist between I and III, and designs II and IV, so that III may be better where I on would normally be favored, and IV may be better where II might be favored. Figure 16 indicates a case where III is significantly better than I at composition Cl, where design I is normally preferred. This advantage for III results from thermal coupling and the ability to operate the upstream tower in III in a manner which reduces the vapor requirements of the downstream tower. In particular, by subcooling the feed 6′ and increasing the vapor and overflow traffic in the middle and bottom sections of the upstream tower, the vapor draw becomes sufficiently enriched in middle product that less reflux is required in the downstream tower. This effect cannot occur with design I, because subcooling the feed to the downstream tower in that case only increases the minimum vapor requirements (see Underwood, 1948) for the bottom half of the tower where the pinch point is located. With design III, however, the bottom section of the upstream tower also serves as the bottom section of the downstream tower, and, therefore, the size of the downstream tower is independent of the bottom section requirements. So, by thermal coupling, the vapor in the downstream tower is controlled by the smaller, middle product rate, rather than the bottom product rate as with design I. In addition, although the Underwood minimum vapor rate for the bottom section of the upstream tower in design III is greater than the minimum vapor required in the middle section, the pinch point is in the middle section because the total vapor in the bottom section greatly exceeds the minimum. So, subcooling the feed to the upstream tower in design III decreases the vapor rates, whereas in design I the vapor rates in the downstream tower are minimized when the feed is near its bubble point.

The comparative costs of design I and III, for example, in separating feed 6′ at composition Cl are as follows: the upstream tower in III costs 5.8% more than the upstream tower in I, the downstream tower in III costs 72.3% less than the downstream tower in I, and design III costs 5.8% less than I overall, a savings of 10.9% GI. So, for ESI $\geqq$ 1.6, the required cost increase for the upstream tower is small, while the savings in downstream tower costs are large.

The results shown in Figure 16 have been verified by simulating design III with an equivalent equilibrium stage model, operated at the optimum conditions found by the design model. Based on these independent calculations, it appears that the Underwood equations used in the design model correctly predict behavior. All equilibrium stage calculations have verified the Underwood rating method, including its applicability to complex designs III, IV, and V.

Although thermal coupling in designs III and IV is important in lending optimality, the full significance and importance of these designs cannot be realized without the ability to optimize the operating state. With these designs, subcooling and superheating the feeds to the upstream towers play important roles in minimizing costs. For design III to be favored over I for a wide range of feed compositions, it must be true that the ESI is sufficiently greater than unity that the more difficult $B/C$ split dominates the cost. Then, the total design costs can be greatly reduced by subcooling the feed and minimizing the vapor requirements to the downstream rectifying section. For design IV to be favored over II for a wide range of feed compositions, it must be true that the ESI is sufficiently less than unity that the more difficult $A/B$ split dominates the cost. Then, the total design costs can be reduced by superheating the feed and minimizing the overflow requirements to the downstream stripping section.

The main advantages perceived for designs III and IV through the Underwood equations are due to shifts in the pinch points and the additional flexibility in minimizing total vapor requirements. However, a more important advantage, the middle product enrichment in the upstream tower, is not explicitly considered in the design model. So, the economic advantage for either design III or IV over I or II may be generally greater than indicated here. The fact that these designs are favored at all is significant. Certainly, if less than half the feed is middle product, then designs III and IV should be carefully examined as alternatives. In addition, it should be recognized that the optimal regions for III and IV will increase as the middle product purity specifications are relaxed. Although the magnitude of this effect has not been examined, we believe that it is large.

## COMPLEX DESIGNS III, V, AND VIII

Figure 18 indicates the intersection lines which have been found for the minimum cost surfaces of designs III and V. These lines are generally perpendicular to those shown in Figure 10 because the cost differences between III and V are dominated by the amount of middle product in the feed, rather than the amount of overheads or bottoms. Design III is often favored along the edge from $C$ to $A$, but design V has been found optimal at composition C3 for all seven observations.

The minimum cost contours which have been observed for design V are generally different from those observed for designs I and II. When the ESI is near unity, the minimum cost contours for V appear largely uncorrelated as in Figure 19. Although it is usually less expensive to operate this design at composition C3 than at C5 (see Figures 8 and 9), the design is relatively attractive at C3 primarily because the other designs cannot economically produce large quantities of middle product.

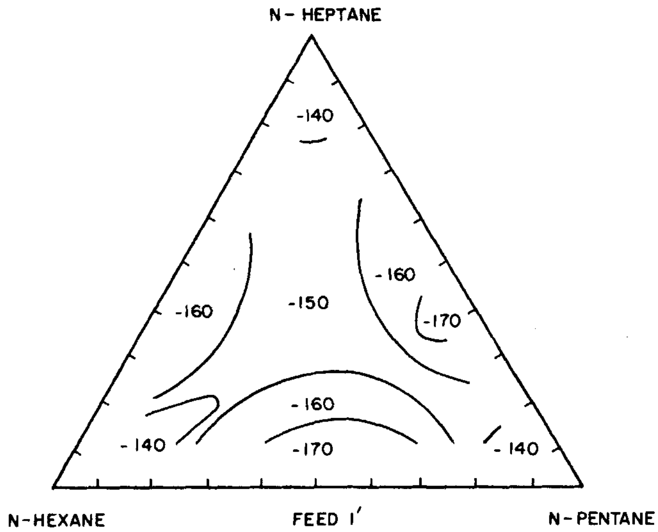


Fig. 19. Percent GI for design V separating feed 1'.

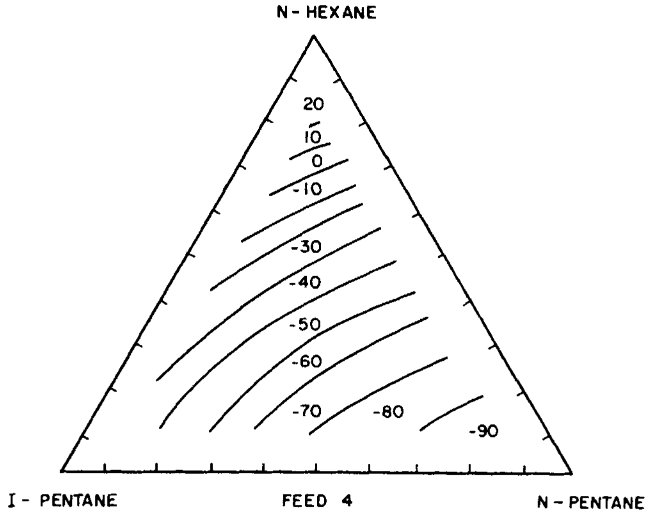


Fig. 20. Percent GI for design V separating feed 4.

So, the cost surface for V is often flatter than the surfaces observed for the other designs, and it is this feature which makes V characteristically optimal at composition C3.

The contours of the minimum cost surface for design V suggest that its costs are less strongly a function of the middle product rate than for the other designs. For ESI not near unity, the cost contours are nearly parallel to section B and therefore are nearly independent of the middle product rate as shown in Figure 20. For ESI less than unity, the observed direction of steepest descent in percent GI is toward point C1. It is then more expensive to produce overhead product than bottoms. For ESI greater than unity, the converse is true; it is then less expensive to produce overheads than bottoms using design V. But for all feeds examined, the minimum cost for V is essentially fixed by the overheads to bottoms ratio, regardless of the middle product rate.

This behavior for design V contrasts with that for design VIII which also tends to cost less than either designs I or II at C3 but is much more expensive than either I or II at C4. If the feed is mostly middle product, then towers 2 and 3 in design VIII can be relatively small. But if large amounts of either overheads or bottoms must be produced, then the total cost of VIII increases drastically compared to the other designs. Although VIII may be less expensive than I or II at C3, it should definitely be avoided whenever economic insensitivity to changes in feed composition is required.

Design V also has unusual control features. The upstream tower does not produce a final product, and this characteristic could be used to introduce lead time into a control algorithm. There is also an additional degree of freedom in that the overhead product rate from the upstream tower in V can be used as a control variable to meet target specifications for the downstream tower.

Designs V and VIII are also favored at composition C3 because of a flexibility which the other designs do not possess. The optimization range over which the overhead rate can be varied increases with the middle product rate, so that the optimum split at composition C3 is usually closer to fifty-fifty than it could be for designs I or II, for example. Designs V and VIII can therefore obey the rule suggested by Harbart (1957), "favor equimolar splits." In addition, they perform the easiest $A/C$ split first, rather than the more difficult $A/B$ or $B/C$ splits.

The dominant factor, especially favoring V, appears to be the Underwood equations themselves. During the state optimization, product compositions from the upstream tower vary with the overhead rate. The fractional vaporization, and therefore the Underwood roots, of both feeds sent to the downstream tower also change with the state. Consequently, with designs V and VIII, the feed compositions to the downstream tower(s) can be op-

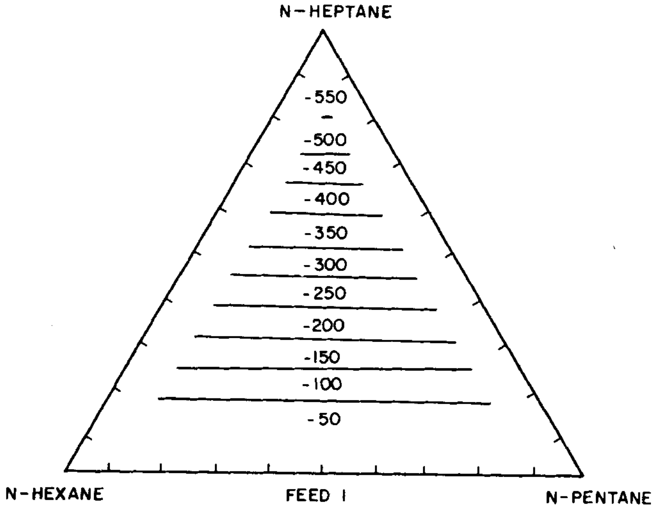


Fig. 21. Percent GI for design VI separating feed 1.

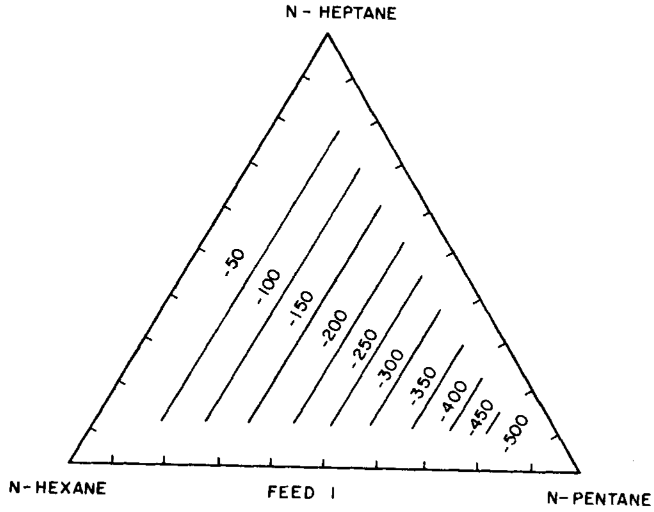


Fig. 22. Percent GI for design VII separating feed 1.

timized so as to minimize the minimum vapor requirements. This variability is a significant contributing factor in minimizing the total vapor flows through the systems. Moreover, the feasibility of the resulting optimal state using design V has been repeatedly confirmed with equivalent, equilibrium stage models.

## SINGLE-TOWER DESIGNS VI AND VII

It has always been observed that designs VI and VII are much more expensive than the other designs for separating feeds whose composition falls within the triangle defined by points C1, C3, and C7 in Figure 7. This result is due to the fact that the single tower must meet high purity specifications for all three products, and the middle product requirements greatly increase the necessary vapor rates in these designs. This constraint is built into the model for design VI by Equation (3), obtained by writing overall and component balances for component C around the bottom section and by neglecting the losses of the bottom component to the vapor at the side draw tray:

$$V' = P_C(X_C/X'_C - 1) \tag{3}$$

The vapor rate calculated from the Underwood equations is characteristically much smaller within the triangle C1, C3, and C7, and it is Equation (3) which makes the minimum cost surface for design VI (see Figure 21) essentially planar, very steep, and correlated with the bottom product rate.

Similarly, the cost of design VII is controlled by the purity requirements of the upper side draw, and this constraint is incorporated into the design model using Equation (4):

$$V' = P_A X_A / K'_A X'_A \tag{4}$$

This expression is derived by writing a material balance for component A around the top section of design VII and by neglecting the losses of the overheads component to the overflow liquid at the side draw tray. It is Equation (4) which makes the minimum cost surface for design VII (see Figure 22) very planar and steep and correlated with the overhead product rate.

Because of Equations (3) and (4), the vapor rates in these designs are often fixed. Then, the state optimization can only be carried out with two degrees of freedom, as shown in Table 1. If the bottom product rate in design VI, or the overhead product rate in design VII, is very small, then the required minimum vapor rates by the Underwood equations become larger than the rates required by Equations (3) and (4). The vapor rate is then treated as a state optimization variable.

Comparison of optimal states for designs VI and VII with equivalent equilibrium stage models indicates that Equations (3) and (4) generally overestimate the vapor requirements somewhat, at least when high purity products are required. These equations also suggest that a lower side draw should always be taken as a vapor, an upper side draw should always be a liquid, and vapor requirements for both designs decrease with the product purity specifications. If product purity requirements are reduced, then the expected regions of optimality should be greater than shown in Figures 5 and 6. However, for the assumptions made here, the regions of optimality for these designs are small, and the minimum cost surfaces are much steeper than for the other designs as shown in Figure 23. It is also clear, however, that for some feed compositions substantial savings can be achieved with these designs. They should not be excluded from consideration too hastily, especially in the vicinity of the expected optimal regions.

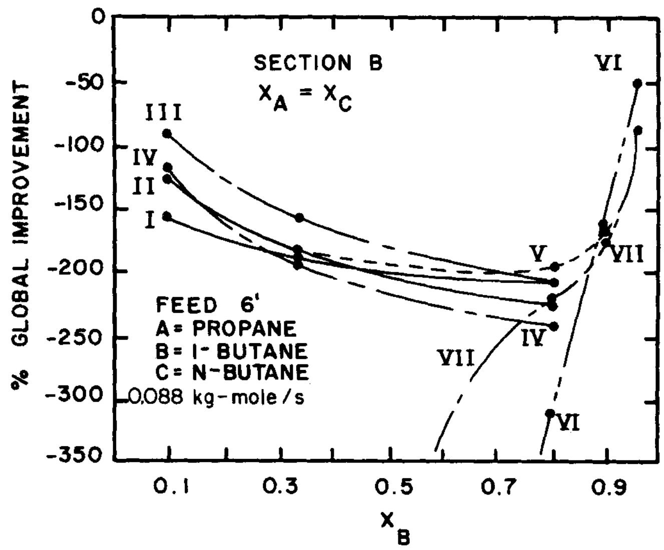


**Fig. 23. Section B plot showing relative steepness of minimum cost surfaces for designs VI and VII.**

## RANGE OF MINIMUM VENTURE COSTS

The minimum venture cost surface reflects the best possible economic behavior of a design to changes in the feed composition. Each design has been state optimized at the seven points on its surface. All the design parameters, the tower dimensions, the utility requirements, operating pressures, etc., are slightly different at each point.

Suppose, however, that a design is actualy constructed using its optimal conditions at point C4 in Figure 7. If, during the subsequent plant operation, the feed composition changes from point C4, then the operating state will have to be adjusted in order to keep the process on line. But the new operating state is no longer the optimal one, since the tower dimensions could not be changed to their new optimal size. Instead, the utilities had to be increased nonoptimally to make up the difference. Consequently, the optimal cost surfaces shown represent lower bounds on the costs of actual operation.

Since they bound the actual venture cost for existing designs with the same economics, the minimum cost surfaces are useful for analyzing the relative design sensitivities to subsequent changes in the feed composition. A flat surface means the design is more economically flexible toward feed changes than a design whose surface is steep. If uncertainty in the feed composition exists, a design with a flat surface should perhaps be preferred, even if it is not optimal at that point.

A measure of the relative flexibility of the various designs to economically separate a feed with any composition is given by the observed range in the minimum venture cost for a design separating a feed for each of the seven composition points shown in Figure 7. The following inequalities have been generally found to relate the ranges of minimum venture costs:

$$R_V < R_I < R_{III}, R_{IV} < R_{II} << R_{VI}, R_{VII}, R_{VIII} \tag{5}$$

So, design V is usually more flexible than the others, but design I may be the preferred configuration for many general purpose applications. The fact that the observed ranges for designs III and IV are often less than for design II indicates the additional flexibility built into these designs by thermal coupling. The large increase in ranges for designs VI and VII, relative to the others, should be smaller with relaxed product purity specifications; reduction in middle product purity specifications

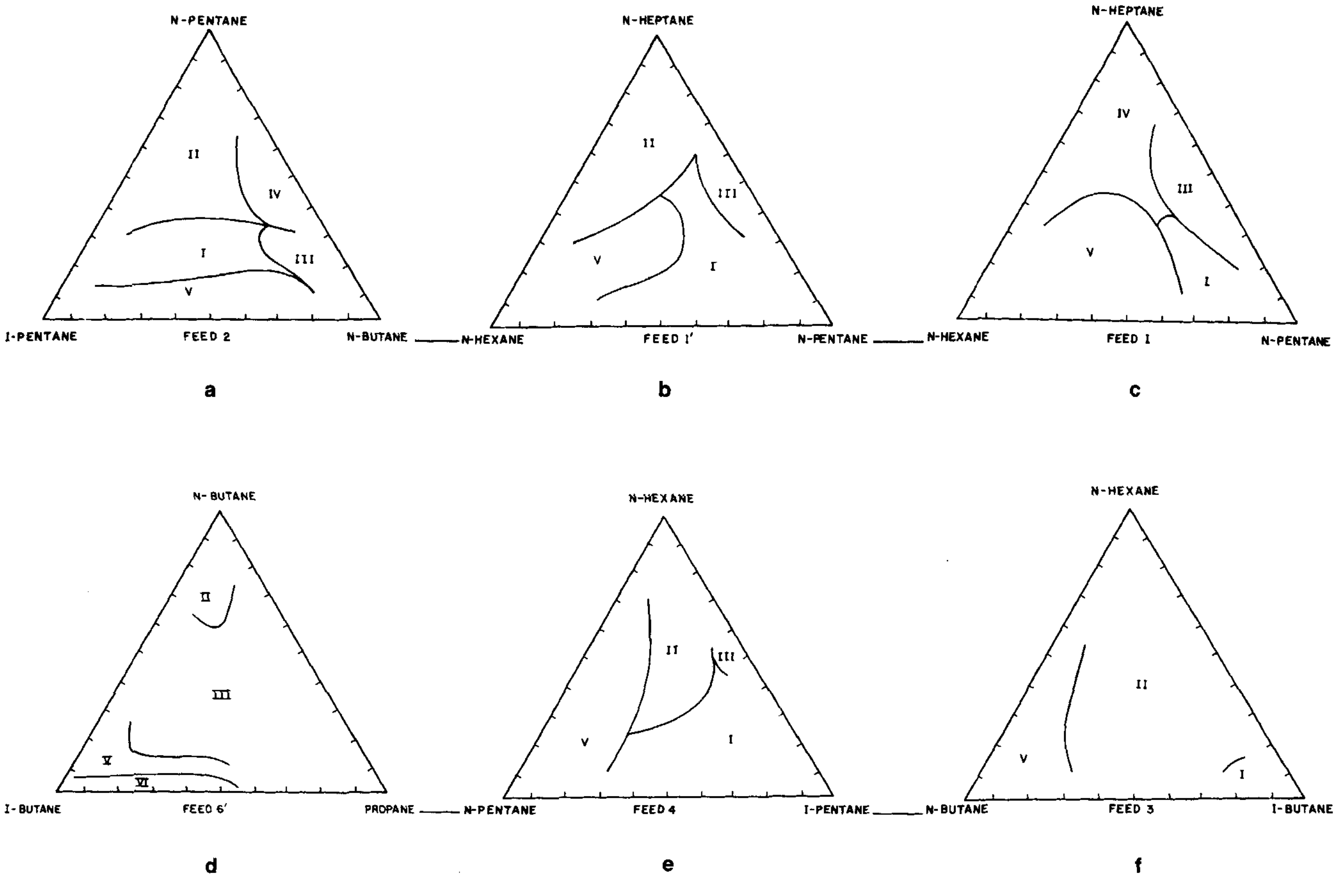


Fig. 24. Observed regions of optimality.

should also further decrease the range of designs III and IV. However, designs VI, VII, and VIII are all much less flexible than design II.

## REGIONS OF OPTIMALITY

Figure 24 shows the regions of optimality which have actually been observed. The expected regions, shown as Figures 5 and 6, were drawn from the optimal regions in Figure 24 but with consideration for the overall trends as well. An optimal region for design VI has only been defined for one feed, shown as Figure 24*f*. So, the expected regions shown for designs VI and VII are based more on Figures 21, 22, and 23.

Comparison of Figures 24*a* and *b* exaggerates any real effects from increasing utility rates. The advantage perceived for design IV in Figure 24*a*, rather than design II, is not significant. The similarity between Figures 24*a*, *b*, and *e* is more important overall, since it reflects the general trends shown in Figures 10 and 18. Figures 24*c* and *f* also indicate that either design III or IV may be important along the edge from *C* to *A*. Design V is always optimal at composition C3. If design II is best at all, then it is best at composition C7. If design I is favored anywhere, then it is at composition C1.

This study supports the general trends observed by Petlyuk et al. (1965) for designs V and VIII, so the regions of optimality perceived for design V in Figure 24 are not unexpected. However, we do not find that design V is less expensive than I or II for all composition points along section B. In addition, the region of optimality is distorted by the ESI as can be seen.

The fact that either design III or IV ever appears better than I or II, however, was not expected. Therefore, we believe that more attention should be given to these designs, especially as alternatives to designs I and II.

## SYNTHESIS EXAMPLE

Figures 5 and 6 can be used to synthesize networks comprised of aggregates of designs I through VII in the following manner. Consider a feed mixture consisting of components A through I, each present in equimolar amounts. Suppose that it is desired to separate this mixture into nine essentially pure streams, and it is required to identify two or three networks as likely, optimal candidates for further, detailed process simulation and economic evaluation. The normal, pure component boiling points for the nine feed species can be readily obtained and arranged in ascending order for the feed species A through I. Suppose, also, that the boiling point temperature differences between adjacent pairs are reasonably well described by classifying adjacent splits as either easy, medium, or hard, as shown in Figure 25. Then, applying the rule, do the easy split first, the nine-component mixture can be treated as a pseudoternary mixture comprised of species A, B-F, and G-I with composition (0.11, 0.55, 0.33) and ESI $< 1.6$, since the $A/B$ and $F/G$ splits only are easy. From Figure 5, design V is preferred to produce overheads product *A*, middle fraction B-F, and ternary mixture GHI as bottoms. Since the $H/I$ split is hard and the $G/H$ is medium, assume the ESI $\geqq 1.6$ for the GHI mixture. From Figure 6, design III should be used to recover pure products G, H, and I.

Since three of the required four splits needed to process the middle fraction are of medium difficulty, three alternatives exist, as shown in Figure 25. One could then perform the $B/C$ and $C/D$ splits, or the $C/D$ and $E/F$ splits, or the $B/C$ and $E/F$ splits; each is shown with its corresponding pseudo ternary feed composition, resulting ESI, and the preferred design from either Figures 5 or 6.

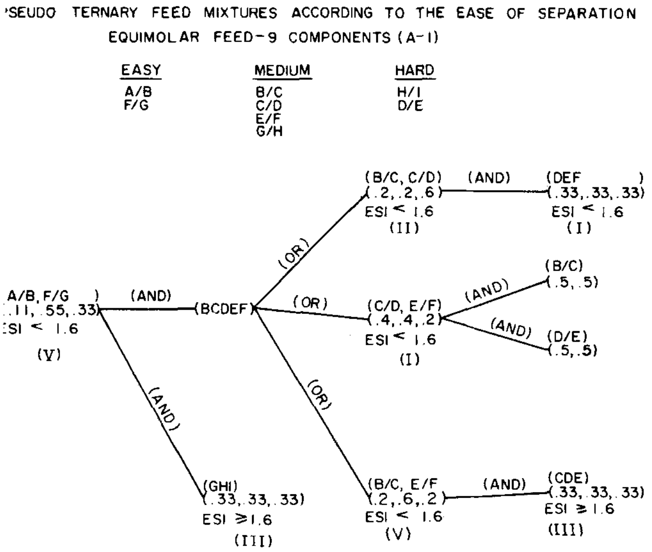


**Fig. 25. Synthesis tree for nine component separation example.**

From this simple analysis, three networks are quickly arrived at for more detailed consideration. It should be realized, however, that this approach excludes a great many design alternatives a priori. One class excluded is that of all designs utilizing a single tower which produces two or more sidestreams; moreover, this class should not be hastily excluded if two or more of the feed components are present in only small amounts compared to other species, or only low product purifies are required. Design analogues of V, consisting of two or three interacting towers, producing four or more streams, are also excluded. Any network combinations, like design VIII, leading to more product streams than components are not considered. Since all three networks shown in Figure 25 require two or more complex designs, they could not be synthesized from consideration of designs like I and II alone. In this manner, heuristic process synthesis is extended to consideration of a wider class of designs but still does not consider all feasible alternatives.

## SUMMARY

The regions of optimality for various designs depend upon the species separated, but changes in feed composition have characteristic effects on the relative costs. These characteristic effects can be used to generate heuristics in the form of expected regions of optimality, based on composition and simple physical properties. The expected effects, however, are somewhat uncertain, because the costs of designs depend upon many variables in a complex way. Of all factors considered, the vapor requirements for a tower are perhaps the most important, but the tower operating pressure and the required tower should also be considered. In addition, complex designs III, IV, and V exhibit economic interactions with the feed fractional vaporization which can often lead to significant savings over simple designs I and II.

## ACKNOWLEDGMENT

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## NOTATION

$A$ = overhead product
$B$ = middle product
$C$ = bottom product
$K$ = average distribution coefficient
$K'$ = distribution coefficient at side draw tray
$P$ = product molar draw rate
$V'$ = internal molar vapor rate at side draw tray
$VC$ = venture cost of a design, defined as 29.96% of the required capital investment plus 52% of the annual operating costs, (see Rudd and Watson, 1968)
$X$ = mole fraction in liquid product
$X'$ = mole fraction in liquid overflow at side draw tray

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