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A STUDY OF THE OPTIMAL SEQUENCING OF
MULTICOMPONENT DISTILLATION TRAINS

by

Brian David Henry
M.Sc. (New South Wales)

A Doctoral Thesis
submitted in partial fulfilment of the
requirements for the award of
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of the Loughborough University of Technology

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NOMENCLATURE

F	Feedstock flow rate, moles/hour
D	Overhead product flow rate, moles/hour
B	Bottoms product flow rate, moles/hour
$X_{i,F}$	Mole fraction of component 'i' in feedstock
$X_{i,D}$	Mole fraction of component 'i' in overhead product
$X_{i,B}$	Mole fraction of component 'i' in bottoms product
RF_i	Recovery fraction for component 'i'
R_{act}	Operating reflux ratio
R_{min}	Minimum reflux ratio
T_d, T_b	Dew and bubble point temperatures of the overhead and bottoms product, respectively
V	Overhead vapour flow rate, moles/hour
q	Degree of vaporisation of the feed
q_c	Condenser heat load, GJ/hour
q_r	Reboiler heat load, GJ/hour
K_i	Equilibrium vaporisation coefficient or 'K' value of component 'i'
E.S.I	Rudd and Tedder's separation index
H.I	Heaven's separation index
Greek letters -	
α_{ij}	Relative volatility of component 'i' to component 'j'
ϕ	Underwood's parameter
λ	Enthalpy difference between saturated vapour and liquid states of overhead product/mole of overhead product

Δ Measure of difficulty of separation used by
Rudd *et al.*

Δ_{RM} Optimality criterion used by Rod and Marek

Sub-scripts

1D, 2D, 1i, 2i First and second column in direct and
indirect configuration

I N T R O D U C T I O N

INTRODUCTION.

The process design of chemical processes may be divided into two broad phases. One, a synthesis phase, is all activities associated with the selection of the process route or configuration together with the selection of the type of process units required for a given processing function. The other is an analysis phase in which the design and optimisation of each unit within a given configuration or process scheme is established.

Historically, the discipline of chemical engineering has been concerned primarily with the analysis phase of process design; in that it pioneered the concept of breaking down processes into unique processing steps or 'unit operations'. Most of these 'unit operations' have now been developed to a very high degree of sophistication. However, the synthesis phase has not received the same degree of attention. For example, the selection of the optimal process route for a given process function from among a number of possible process routes has been made to a certain extent upon the process designer's experience and/or intuition, there being no formal techniques available to assist in the selection.

Process synthesis has been regarded more or less as an art and consequently it has received very little attention in chemical engineering research.

Since the late 1960's, however, there has been considerable interest in the process synthesis phase in an attempt to provide formal design techniques. The increasing complexity, scale and capital intensiveness of the modern chemical process plant have been among the principal reasons for this interest. More recently, there has been the energy crisis which has been of particular concern

to those processes which are energy intensive.

Of the techniques so far proposed in the field of process synthesis, the use of 'heuristics' is of major concern to this thesis. 'Rules of thumb' and 'guidelines' have been used synonymously in the literature with the term 'heuristics'. The term 'heuristics' is defined by the Oxford Dictionary as 'serving to find out or discover'. However, the use of the term 'heuristics' in the field of process synthesis has been based on the interpretation given in Webster's Dictionary as 'serving to guide, discover or reveal. Valuable for empirical research but unproved or incapable of proof....'.

Heuristics have been proposed as a means of preliminary screening to be used when a large number of process routes is possible for a given processing function. They may also be used as an aid in the design of the processing scheme. The literature shows that heuristics have been applied to the selection of the optimal configuration of the distillation columns required for the separation of multicomponent feedstocks. This type of separation is an example of the attitude existing prior to the recent interest in process synthesis in that the selection of the process route was in most cases made on the basis of the process designer's intuition and experience.

Distillation is the most widely used of all separation processes in the chemical process industries. It is also one of the most energy intensive. Many techniques have been proposed for the reduction of the energy requirements of individual distillation columns. The number of distillation columns required for a given separation of a multicomponent feedstock into relatively pure products is a function of the number of products to be produced. For the separation of multicomponent feedstocks by distillation, the

number of process configurations possible as a function of the number of components may be determined from a relationship developed by Heaven (1969). Table 1 illustrates the results obtained from this relationship. The physical arrangement of all possible configurations for the separation of three, four and five component feedstocks into relatively pure products is included in the Appendix.

TABLE 1. Number of column configurations for separating N components into N products.

Number of Components	Number of column configurations
2	1
3	2
4	5
5	14
6	42
7	132

If such a number of different configurations are possible for a given separation, then it is conceivable that one of these configurations could be optimal in terms of a given objective function. The possibility that one of the configurations will be optimal for a given separation has made multicomponent distillation trains of interest for the application of the techniques being developed in the field of process synthesis. The literature has indicated that considerable energy savings should be possible by the selection of the optimal configuration.

The selection of the optimal configuration from among the number of configurations possible will obviously be a function of a number of process parameters. Some of these will be economic parameters of the environment in which the distillation plant is to operate. Several studies in the area have endeavoured to optimise the distillation columns in terms of these economic parameters. As these parameters are not common to all plants, this study was concerned solely with the effect of non-economic parameters such as the following upon the selection of the optimal configuration for a given separation:-

- (i) feed composition
- (ii) feed component volatility
- (iii) degree of recovery of the components

The literature has shown that several studies have been reported on the development of heuristics for the selection of the optimal configuration of multicomponent systems. This thesis thus initially set out to investigate the validity of these heuristics as it was felt that there may be limitations in the scope of the analysis used. A detailed investigation was then made of the effect of the above parameters upon the selection of the optimal configuration for a range of three, four and five component feedstocks. The results obtained confirmed that considerable energy benefits could be obtained in certain instances. From a study of the proposed heuristics, it was shown that a major obstacle existed which prevented the effective use of the heuristics in process design. This obstacle was the inability to specify the process conditions under which each heuristic would determine the optimal configuration. In particular, conflicts existed between the heuristics in that the heuristics could propose

different configurations for the same process conditions. The conflicts could not be clarified by the design method and thus the feasibility of mathematically modelling a system(s) of multicomponent distillation columns was investigated. This proved not to be feasible principally as a result of the nature of the distillation process. However, an approximation to a mathematical relationship was obtained through the use of the new concept of pseudo-components. These components provided a means by which the interaction between the heuristics could be illustrated.

A review of the previous work will be given in Chapter 1. In Chapter 2, the initial phase of the thesis will be described. This phase was the study of the effect of a range of process parameters upon the selection of the optimal configuration for three, four and five component feedstocks. The results of this study will be given in Chapter 3. In Chapter 4, the feasibility of mathematically modelling multicomponent distillation systems will be discussed. After this investigation showed that it was not feasible to develop suitable mathematical models, Chapter 5 discusses the concept of pseudo-components which were used as an approximation to a mathematical relationship. The results of this study will be given in Chapter 6.

In Chapter 7, all computer programmes developed and used throughout the entire study will be discussed. Listings of the principal programmes will be included in the Appendix.

In Chapter 8, the conclusions reached in this thesis will be given.

CHAPTER 1. - REVIEW OF PREVIOUS WORK

CHAPTER 1. PREVIOUS WORK

1.1 Introduction

Until recently, the study of the optimal sequencing of multicomponent distillation trains has received little attention in the literature. However, interest has arisen in this area as a result of (i) activity in the new field of process synthesis and (ii) increasing energy costs.

Prior to the study of Heaven (1969), there had been very little interest in the study of the optimal sequencing of multicomponent distillation trains. Following Heaven's work, King (1971) also proposed a set of heuristics which has been used in the recent developments in the field of process synthesis. The only papers published prior to this time were the following:- Lockhart (1947), Harbert (1957), Rod and Marek (1959), Petyluk *et al.*, (1965), Nishimura *et al.*, (1971) and Maikov *et al.*, (1972), (1972a).

All of the previous work can be conveniently divided into two areas:-

(i) one in which the study of multicomponent distillation systems has been made in an attempt to generate guidelines for the selection of the optimal arrangement of the columns required for a given separation. Work in this area can be further divided into two areas in which the analysis of the configurations has been made by -

(a) design methods and,

(b) by analytical methods.

(ii) one in which the sequencing of multicomponent distillation systems has been used as an example for the application of the techniques being developed in the field of process synthesis.

1.2 Methods used for the comparison of Multicomponent Distillation Sequences.

1.2.1 Design Methods.

Lockhart (1947), the first reported study in this area, adopted a design approach in which the cost of separation of a feedstock was determined by the design and costing of the distillation plant required for the various configurations. Lockhart considered a small number of feedstocks associated with the processing of natural gasoline. Calculations were made of the size of the distillation columns required for these separations to the extent of determining the number of stages and the reflux ratio by the methods of Fenske and Underwood, respectively. From these investigations, Lockhart proposed that the configuration in which the components are removed in decreasing order of volatility was the optimal configuration. He further suggested that should either the most or least volatile component be present in large amounts, then that component should be removed first. The principal contribution of this study was that it proposed a configuration other than the direct configuration could be considered as the optimum and suggested a feedstock property which would justify this alternative configuration.

Heaven (1969) made a considerable contribution as a result of a systematic design analysis of a number of three component feedstocks in which a range of feed compositions and feed types was studied. The three component feedstocks considered by this author were as follows:-

- (i) iso-butane, n-butane, n-hexane
- (ii) iso-butane, iso-pentane, n-hexane
- (iii) iso-butane, n-pentane, n-hexane
- (iv) n-butane, n-pentane, n-hexane
- (v) iso-butane, n-butane, iso-pentane

The effect of feed composition was studied using one feedstock namely, iso-butane, n-butane and iso-pentane. The range of mole fractions of each component in this feedstock was varied over the range 0.2, 0.3 and 0.4.

A single four and five component feedstock was also considered.

The cost of the separation of all feedstocks into relatively pure products was determined for the possible configurations by a detailed design procedure. The effect of component volatility was considered by using equimolar mixtures of the three component feedstocks. The effect of the presence of a non-key component was considered by the introduction of a small fraction of a fourth component to the equimolar feed, comprising iso-butane, n-butane, and iso-pentane. The fourth component was either ethane, propane, n-pentane or hexane.

The operating pressure in each column was economically optimised for given economic parameters.

The contribution of Heaven's work was that it was the first attempt to propose a set of guidelines or heuristics based on the use of systematic design and economic analysis for a range of process conditions.

Heaven proposed a set of heuristics from this study and these were subsequently reported by King (1971).

The heuristics proposed by these authors were as follows:-

- (I) Separations where the relative volatility of the key components is close to unity should be performed in the absence of non-key components.
- (II) Separations which remove the components one by one in the column overheads should be favoured.
- (III) Sequences which give a more equimolar division of the feed between the distillate and the bottoms products should be favoured.
- (IV) Sequences involving very high specific recoveries should be left until last in the sequence.

However, King developed these heuristics in terms of the thermodynamic net work consumption for the separation of liquid mixtures.

The limitations in Heaven's work will be discussed subsequently in section 1.3. These, it is claimed, were as a result of the small range of feed composition and component volatility used in the study.

Freshwater and Henry (1974), (1975) undertook a similar design and economic evaluation procedure. These authors considered a wider range of both three and four component feedstocks together with a range of five component feedstocks. A range of feed compositions for the five component feedstock was investigated instead of the one composition considered by Heaven. However, the extent of this work will comprise part of the present study and so will not be discussed in detail in this chapter.

The design and economic evaluation methods adopted by Heaven (1969), Freshwater and Henry (1974), (1975) were basically identical in principle. These studies used the 'short cut' techniques for the process design of the distillation columns. In particular, Underwood's (1946) method for the determination of minimum reflux ratio, a modified Fenske (1932) method for total reflux and the Erbar-Maddox correlation (1961) for the number of equilibrium stages at the operating reflux ratio were used. Agreement was found between the results obtained for the number of equilibrium stages, the minimum reflux ratio, together with the condenser and reboiler heat loads. A comparison of these results has been provided in Freshwater and Henry (1974). As this agreement was to be expected, this tabulation will not be included here. However, the engineering design of the columns to determine the diameter and height of the actual number of stages and shell thickness was different in method and detail.

The criterion adopted for the objective function was in fact identical though it differed in the values of the economic parameters used. This criterion was the total annual operating cost, defined as the sum of the annual depreciation charge for the capital investment required for the columns and heat exchangers for each configuration, together with the annual cost of the supply of process cooling water and steam. The significance of the effect of differing values of the economic parameters used was not considered to be of great consequence. Wherever in the initial phase of the study common feedstocks permitted a comparison, the relative differences between configurations derived from both studies followed the same trend.

Absolute comparisons were difficult because Heaven had adopted a policy of determining the economic optimum operating pressure for each column within a configuration. It is felt that when considering feedstocks of a wider composition range than those used by Heaven, this policy may have influenced the conclusions proposed from this study. However, this aspect will be discussed in more detail later. Further difficulties were encountered in the comparison of both results as a result of the interpretation of the recovery fraction of each component adopted by Heaven. Heaven had adopted the definition of recovery fraction of a given component as the amount of that component recovered in terms of the amount of that component in the feed to the column in which it is to be recovered. This policy is in contrast to the policy adopted in this study in which the recovery fraction is related to the amount of the component in the feedstock to the configuration as a whole.

Rudd and Tedder (1975) have used a similar design and economic method for the evaluation of simple serial distillation configurations of the type being considered in this study together with the more complex systems in which sidestreams and multiple feeds are used. However, the section of the work in which the simple systems are considered is of interest to this study.

These authors considered a range of seven, three component feedstocks and seven feed compositions. The feed components used were the alkanes from propane to n-heptane. The objective function used was the minimisation of the venture cost which was expressed as a function of the annual operating cost and the total capital investment.

As in Heaven's study, each column was optimised in regard to operating pressure and degree of vaporisation of the feed.

A criteria, the "Ease of Separation Index", was proposed by these authors. This index was defined as follows:

$$\text{E.S.I.} = \frac{K_A \cdot K_C}{K_B \cdot K_B}$$

The index was proposed to show which separation was the more difficult in a three component feedstock. For values of the E.S.I. less than 1.0., the separation between components A and B would be more difficult than between components B and C. For values greater than 1.0 the reverse case applied. By the use of this index, these authors proposed that distinction could be made between the two configurations for a three component separation. The direct configuration would be optimal for feedstocks having values of the E.S.I. greater than 1.6. The indirect configuration would be optimal for values of the E.S.I. less than 1.1. For values of the index between these two values, the situation was described as doubtful.

The results obtained from Rudd and Tedder's work were compared with the results obtained by Rod and Marek (to be discussed in section 1.3) and disagreements were found between the results of the two studies. These will be discussed in Chapter 6.

In the definition of the E.S.I., a value of 1.0 denotes an equal degree of difficulty or value of the relative volatility between components A and B and between B and C. However, this would be the case if the value of the relative volatility between each pair of components in a feedstock was 1.5 or 4.5. This index does not allow for the different absolute values of the relative volatility. However, this aspect will be discussed in detail in Chapter 6.

It is interesting to note that Heaven also proposed an index which was expressed as:-

$$\text{H.I.} = \frac{\frac{K_B}{K_C} - 1}{\frac{K_A}{K_C} - 1}$$

This index will also be discussed in Chapter 6.

However, Rudd and Tedder's work is principally concerned with development of optimisation techniques for use in the selection of the optimal configuration for a given separation from among all possible simple and complex systems. It is in this area that the contribution of the paper lies.

The current study will discuss what is considered to be limitations in this work. These occur through the definition of the E.S.I. and the small range of component volatilities used.

1.2.2. Analytical Methods.

Harbert (1957) proposed two broad principles for the sequencing of distillation trains based on the concept of minimising the heat utilisation in the configuration. These were:-

- (i) "The advantage of minimum quantities of difficult separation" by which he implied the later use of King's heuristic I.
- (ii) "The advantage of the 50/50 split" by which he implied the use of King's heuristic III.

To overcome any difficulties or conflicts which may arise between the use of these two principles for a given separation, Harbert proposed the minimisation of the following expression as the criterion for column sequencing:-

$$\Sigma \text{ MH.F} \left[\frac{T_h}{T_h - T_l} \right]$$

where MH = moles overhead product times the latent heat of vaporisation

F = a factor to correct for the presence of non-key components

T_h, T_l = boiling points of the heavy and light keys respectively.

This expression was put forward as being proportional to the total heat load of the configuration. Harbert was aware of the possible extent of the variation in heat requirements between the process configurations possible for any separation and was convinced that the cost of supplying heat was the only factor to be considered in selecting the optimal sequence.

Two further studies proposed the use of mathematical models for the prediction of the optimal sequence. These were the studies of Rod and Marek (1959) and Nishimura *et al.*, (1971).

Rod and Marek derived a mathematical model to relate the differences in the sum of the overhead vapour flow from each column in a configuration to the composition and relative volatilities of the feed components. The overhead vapour flow was assumed to be directly proportional to the cost of separation. The criterion was:-

$$\Delta = \Sigma V_d - \Sigma V_i$$

where $\Sigma V_d, \Sigma V_i$ are the sum of the vapour loads from the columns in the direct and indirect configurations respectively, and

$$V = D(1.25R_{\min} + 1)$$

For a three component feedstock being separated into pure components only, the optimality criterion developed was:-

$$\Delta_{RM} = \frac{(\alpha_A + 0.25)x_A - 1.25x_C}{\alpha_A - 1}$$

where α_A = relative volatility referred to the heavy key at the feed conditions

x_a, x_c are the mole fractions of components A and C.

The criterion for the optimal sequence was as follows:- the direct sequence for a positive Δ and the indirect sequence for a negative Δ

The limitations of the model are as follows:-

- (i) Pure products only were considered
- (ii) Relative volatilities were determined at the feed conditions
- (iii) The use of the Robinson and Gilliland method for the determination of the minimum reflux ratio. The reasons for this and the errors caused will be discussed at length in Chapter 2.
- (iv) The model assumed that the cost of all distillation plant is directly proportional to the overhead vapour flow rate.

Nishimura *et al.*, (1959) proposed a mathematical model having an objective function in terms of the tower volume and the reboiler heat load. The objective function was then developed in terms of the minimum number of equilibrium stages and the product specification.

These authors proposed an additional heuristic which was 'that if any component is in excess, than the configuration which favours its early removal from the feed should be favoured'.

In a recent book by Rudd, Powers and Sirola (1973), this heuristic has been included together with those proposed by King (1971) as the group of heuristics to be used in separation process sequencing.

On the other hand, techniques have been reported for the determination of the optimal process route for processing schemes should an analytical relationship be available between the objective function and the process variables. For example, Ichikawa and Fan (1973) have developed a search method called Evolutionary Search for Optimal Structure (ESOS) which has been shown to select the optimal structure or configuration, subject to various constraints. However, the technique does require a continuous function describing the system.

The remaining papers in this area are a group of Russian papers, two by Petyluk *et al.*, (1965), (1966) and two by Maikov *et al.*, (1972), (1972a). These papers are all basically similar in that they develop an optimality criterion for column sequencing using a Thermodynamic Optimality Index which is derived in terms of the net work consumption for the separation of liquid mixtures.

King (1971) had also used this concept in the formulation of his heuristics. For example, King accepted the proposition that the net work consumption for a distillation process is proportional to the product of the interstage vapour flow and the difference between the reciprocals of the reboiler and the condenser temperature. King suggested that column sequences should be arranged in such a way that high values of both the interstage vapour flow and the temperature differential should not occur at the same time in any column. This would indicate that for the separation of a difficult pair of components in the presence of another component, there would be a

high interstage flow because of the difficult separation and there would be a higher temperature differential because of the presence of the third component. This would suggest that the third component be removed first and leave the difficult separation until last in the sequence. Similar principles can be applied to the reason for the removal of components one by one in the overhead product. Additional components in the overhead stream would increase the interstage vapour flow. This was the reasoning for King's heuristics (i) and (ii).

However, this proposition assumes that heat is added to and removed from the columns in a thermodynamically reversible manner. In this study and indeed in most distillation units, the processes are performed above ambient conditions, and process cooling water and process steam are used as the heat transfer media. The temperatures of both these media are constant. With the allowance for the temperature approach required for the heat exchangers, the temperature range over which heat is actually degraded is constant and greater than the difference in temperature over a given column.

In this thesis, the temperature differential over each column in all configurations is the same in thermodynamic terms. The net work consumption would then be a function of the interstage vapour flow only.

Thus the contribution of the Russian work will be discussed later in the thesis when studies have been made on the feasibility of the use of thermodynamic criteria for the selection of the optimal configuration of an industrial distillation plant.

In a recent book, Rudd, Siirola and Powers (1973) have discussed the optimal sequencing of separation processes. These authors incorporated the five heuristics discussed previously in

this review as part of a wider set of heuristics to include other physical separation processes. However, for distillation processes, a very simplified model is proposed for use in the preliminary screening of the possible alternative configurations for a given separation. These authors suggest that as a first approximation, the cost of separation by distillation is directly proportional to the feed rate and inversely proportional to the relative volatility of the light key.

That is:

$$\text{Cost of separation} \propto \frac{F}{\alpha}$$

These authors analyse various separation processes using this criterion. For example, a four component feedstock in which the separation between the second and third components is three times more difficult than between the first and second and between the third and fourth components, is separated into four pure components. The relative volatility between each pair of components is given by:-

$$\alpha_{12} = \alpha_{34} = \alpha \text{ but } \alpha_{23} = \frac{\alpha}{3}$$

The total difficulties for the five possible configurations are then developed and are as follows:

Configuration

Total Difficulty

(refer Figure A1 in Appendix)

1	$\frac{F}{\alpha} (4 + 9 + 2) = 15\frac{F}{\alpha}$
2	$\frac{F}{\alpha} (4 + 6 + 3) = 13\frac{F}{\alpha}$
3	$\frac{F}{\alpha} (2 + 12 + 2) = 16\frac{F}{\alpha}$
4	$\frac{F}{\alpha} (2 + 9 + 4) = 15\frac{F}{\alpha}$
5	$\frac{F}{\alpha} (3 + 6 + 4) = 13\frac{F}{\alpha}$

It will be noted that configuration number three is the most difficult. This is the configuration in which the difficult separation is made first. Configurations two and five are the least difficult. These are the configurations in which the difficult separation is left until last in the sequence.

This approach is extremely approximate and of questionable value. Certainly it does not consider any of the conflicting situations which may occur through the use of the heuristics. The author's comments may be applicable when they state "all things being equal ...".

1.2.3. Process Synthesis Methods.

Reference has been made to the developments in the new field of process synthesis. As a consequence renewed interest in the optimal sequencing of multicomponent distillation trains has been generated.

The field of process synthesis may be said to have developed since the late 1960's and since that time the literature has seen much activity in the many facets of this field.

Reviews of this development have been reported in the literature and, in particular, reference should be made to the paper by Hendry, Rudd and Seader (1973) and the book by Rudd, Siirola and Powers (1973).

Of the papers covered in these reviews, several have been concerned with the sequencing of multicomponent distillation trains, for example:- Hendry, Rudd and Seader (1973), Thompson and King (1972), Rathore, Wormer and Powers (1974), Hendry and Hughes (1972), Powers (1972) and Freshwater and Zigou (1975).

As these are of direct concern to this thesis, they will be reviewed here.

The principal theme in most of the papers listed above has been in the development of computer techniques using the various synthesis techniques of heuristics and dynamic programming. The type of problem of interest has been the application of these techniques to the optimal sequencing of separation processes in which distillation is not the only separation process used.

Quite sophisticated process synthesis programmes have been developed in this field, for example, the programme AIDES (Adaptive Initial Design Synthesis) discussed by Powers (1972) and the programme discussed by Thompson and King (1972). These programmes have been written on the basis that the decisions made within the programme are made using the various algorithms and heuristics previously proposed by the respective authors.

The development of these programmes has reached a high degree of sophistication. This study, however, is concerned solely with the feasibility and accuracy of the heuristics adopted for distillation trains and so these programmes will not be discussed in detail.

However, as previously referred to, one paper considered the optimal sequencing of multicomponent trains using conventional distillation columns. This was the paper by Rathore, Wormer and Powers (1974). These authors considered the five component feedstock used by Heaven (1969). This feedstock was to be separated into pure products only. The design and economic evaluation method used by these authors was the same as that adopted by Heaven. Dynamic Programming, however, was used to determine the optimum sequence.

Some reservations have been made by Rathore *et al.*, (1974) of this method for those processes in which feedback of information occurs. This is contrary to Bellman's Principle of Optimality. For these column sequences in which energy integration is carried out then recycling of information occurs. (This aspect will be discussed in a subsequent section) Rathore *et al.*, noted this difficulty and referred to the limitations of the method of Dynamic Programming in that it requires (a) constant pressures in all columns in those sequences using energy integration and (b) very High recovery fractions.

Hendry and Hughes (1972) also considered the method of Dynamic Programming in a study of a purification system for n-Butylene. As in the other papers in this area, however, separation processes in addition to distillation were considered for each separation process.

Thus far, the available literature on studies of the optimal sequencing of conventional distillation columns and sequences comprised of distillation as well as other separation processes, has been discussed. In the former, each distillation column has had an associated overhead condenser and reboiler, that is, for a three column configuration, six heat exchangers were required.

Recently, several papers have considered modifications to the traditional sequence in an attempt to reduce the energy consumption of the configuration. The modifications are:-

- (a) the concept of energy integration through heat stream matching and
- (b) the concept of thermal coupling.

Three papers are of interest in the former area. These are

Rathore, Wormer and Powers (1974), (1974a) and Freshwater and Zigou (1975), while in the latter, papers by Stupin and Lockhart (1972) and Petyluk *et al.*, (1965), (1966) are relevant. The work of Rudd and Tedder (1975) has been discussed previously.

The concept of energy integration involves the matching or sharing of heat streams wherever possible within a configuration. Thus heat stream matching may be possible between the sensible heat of the feed streams and/or the heat loads of the overhead condenser and reboiler. Work reported to date has considered only the matching of the heat available between the condensation and vaporization heat loads as these are significantly greater than the sensible heat loads of the feed streams. Also these processes take place at constant temperature. The feasibility of heat stream matching depends on the availability of the heat streams, that is, the temperature and heat content. Through this concept it has been claimed, Rathore *et al.*, (1974) that more energy benefits may be realised than through the use of traditional columns. Should there be an imbalance between the heat loads to be matched, then external sources would provide this difference as in the case of traditional columns. In this case, however, the heat requirements would be considerably smaller. Rathore *et al.*, considered the application of the concept of energy integration to the five component feedstock considered by Heaven (1969). This feedstock was used by them for the determination of the optimal sequence of traditional columns. Two cases were considered for heat energy integration:-

- (i) isobaric column operation and
- (ii) variable pressure

In both cases, high recovery fraction of each component was specified. Greater energy savings were realised with energy integration over that obtained in the optimal configuration using traditional columns. It is of interest to this thesis to note that the optimal sequence was different in the three cases.

Rathore *et al.*, have developed a feasibility matrix and a set of rules by which the streams between which energy integration was possible could be determined. These rules are based upon isobaric operation and very high recovery rates. Dynamic programming was also used to determine the optimal configuration. Freshwater and Zigou (1975) have shown that in at least two of the cases considered by them, Rathore's matrix is not obeyed.

Whereas Rathore *et al.*, had considered only one feedstock, Freshwater and Zigou (1975) undertook a study similar to the study of Freshwater and Henry (1974) for traditional column sequences. They examined the effect of a wide range of process variables upon energy integration for a range of four and five component feedstocks. That is, a range of feed compositions, feed components relative volatilities and the degree of recovery for four and five component feedstocks were considered.

These authors were able to show the extent of variation of energy savings through the use of energy integration and how this benefit is affected by the perturbations of the factors considered. However, no formal guidelines were proposed for the prediction of the optimal conditions and these authors felt that considerably more work was required.

The concept of thermal coupling has also been suggested in the literature as providing cost savings for the process of

multicomponent distillation. This concept, which it is believed, was first proposed by Petyluk *et al.*, has also been considered by Stupin and Lockhart (1972). Thermal coupling offers reduction in cost of separation through the reduction in the number of heat exchangers required. For a three component feedstock being separated into three components by distillation, two columns are required but in this instance the function of the overhead condenser and the reboiler of the first column is carried out within the second column. This arrangement eliminates the need for the condenser and reboiler of the first column. The three products are taken in the second column, the intermediate component being taken as a side stream product. Whilst savings may be realised through the reduction in the number of heat exchangers required, no indication has been given in the literature of the additional design features necessary for the second column or the problem of high recovery of the intermediate product.

Petyluk *et al.*, (1965) have put forward a range of such processing schemes for the separation of three, four and more component feedstocks. For these feedstocks, it is proposed that reduction in the number of columns required may be made by taking more than one sidestream.

Stupin and Lockhart considered only a three component separation and indicated that considerable cost benefits were possible by the use of Thermal Coupling.

1.3 Evaluation of Previous Work

The principal areas in which limitations are considered to exist in the literature are the following:-

- (i) limitations in the existing studies which have been used as a basis for the formulation of the heuristics
- (ii) lack of any satisfactory quantitative relationship available by which the prediction of the optimal configuration can be made.

Decision criteria currently being used in the field of process synthesis for the prediction of the optimal sequencing of separation processes are incorporating the heuristics discussed in the preceding Chapter. These heuristics have been derived from two principal areas:-

- (a) The studies of Heaven, Lockhart and others but principally the study of Heaven in which the heuristics were proposed as the result of a study of a limited number of feedstocks and,
- (b) studies of King and Petyluk *et al.*, based on the thermodynamic analysis of a configuration.

The most comprehensive studies reported to date in the literature are the studies of Heaven (1969) and Rudd and Tedder (1975). However, it is claimed here that there are limitations which must be resolved before sound design criteria can be proposed on the basis of these studies.

These limitations were generated through the limited consideration of the following:-

- (i) range of number of component feedstocks
- (ii) range of the relative volatilities of the feed components particularly in regard to difficult separations

- (iii) range of feed compositions, particularly the consideration of components present in excess.
- (iv) the lack of study of the position of the difficult separation within a feedstock.
- (v) range of degrees of recovery.

The definition of the recovery fraction and the use of the optimum economic operating pressure in each column within a configuration may have had a masking effect.

It is thought that the principal properties of the feedstock influencing the optimal configuration would be the feed composition and the component relative volatility. The range of feed component mole fractions was too narrow in Heaven's study. A far wider range of mole fractions should have been considered.

It is claimed that this limitation did not permit adequate consideration of the effect of the presence of a dominant component in a feedstock.

The effect of the presence of very difficult separations was not adequately investigated. For example, the selection of the components for the feedstocks did not really provide a difficult separation; the most difficult separation considered was that between iso-pentane and n-pentane in which the relative volatility is of the order of 1.25. Separations having relative volatilities down to the magnitude of 1.1 or slightly lower, should have been considered. The possible source of conflict between the heuristics as a result of the position of a difficult separation and components present in excess, could not really have been resolved by Heaven's study.

The position of a difficult separation and the position of a dominant component cannot be resolved adequately by the consideration

of three component feedstocks. Further study is required for four component feedstocks in which the extent of a component present in excess could be similarly studied. This aspect could be studied by allowing the feed component mole fraction to vary in the range of say 0.1 - 0.7.

The same consideration could be given to the degree of difficulty of a separation as proposed in the three component feedstocks. Of more significance, is the fact that four component feedstocks provide three positions within the feedstock, in terms of relative volatility, for the position of a difficult separation. In the case of a four component feedstock comprising A, B, C and D feedstocks could be formulated in which a difficult separation occurred either between A and B, B and C, or between C and D. Also the influence of the presence of non-key components could be investigated particularly when the non-key component was present in excess or when one of the key components was present in excess.

From the survey of the previous work, a number of objective functions has been proposed. These were economic, process and thermodynamic parameters. The total annual operating cost has been adopted more widely than other criteria being used for example by Heaven, Rathore *et al.*, and Freshwater and Henry while Rudd and Tedder (1975) have used the venture cost expressed as a function of the total capital investment and the annual operating costs.

Use has also been made of the following:- overhead vapour flow rate, reboiler heat load and the thermodynamic net work consumption as objective functions. All of these parameters will be determined in the evaluation of each configuration and thus their feasibility as objective functions will be determined.

The review has also discussed the limitations of the reported mathematical models. It is felt that the limitations of these models are such as to preclude their use. Consequently, the development of such a mathematical model is still required and this aspect will comprise a major aspect of the thesis.

CHAPTER 2. - APPLICATION OF HEURISTICS

CHAPTER 2. APPLICATION OF HEURISTICS2.1 Introduction

The literature relevant to the proposed field of study has been reviewed. This review has shown that there is need for further investigation into the development of techniques for the prediction of the optimal process route or configuration for a given process when a number of alternate process routes are possible. The process to be considered in this study is the separation of a multicomponent feedstock into its components by the process of distillation. There are two principal reasons for the selection of this one process for the thesis. These are as follows:-

- (i) Limitations in the available literature. While the literature review has revealed that previous studies have been made in this area, it was thought that the results of these studies could not be generally applied in practice with any degree of confidence.
- (ii) The industrial importance of the process of distillation for the separation of multicomponent feedstocks.

In an era of ever increasing energy costs and as the process of distillation is highly energy intensive, the selection of the optimal process route for a given separation may provide a reduction in the energy consumption and hence considerable cost benefits. For example, petroleum refineries currently use approximately 6% of their feedstock as refinery fuel. Of this, at least one half is used for the associated distillation operations.

It has been common practice to separate a multicomponent feedstock into its components by a train of distillation columns, one less in number than the number of products to be produced.

Until recently, the columns have been entirely 'traditional' in that they are supplied with one feedstock and produce two products, one overhead and one bottom. Each column has an associated overhead condenser and reboiler.

It was noted in the literature review that consideration had been given recently to the use of distillation columns in which the concepts of heat stream matching and thermal coupling have been proposed as a means of reducing the energy requirements of the process. From these studies, it has been claimed in the literature that it may be possible to achieve greater energy economies in certain instances than would be the case for the same separation by the use of 'traditional' columns. While it is acknowledged that such possible benefits may be realised by the use of these concepts, they will not form part of this study. It is suggested that in the development of techniques for the prediction of the optimal process configuration incorporating heat stream matching or thermal coupling, the knowledge of multicomponent systems generated from this study of traditional columns would be of use.

This thesis will be concerned with the feasibility of techniques for the prediction of the optimal process configuration of a sequence of distillation columns having a single feedstock and producing two products only.

In this Chapter, the proposed plan of the initial phase of the thesis will be discussed. This phase was the study of the effect of the process configuration upon the separation of multicomponent feedstocks by a design method. It would also provide an opportunity

to assess the existing data and conclusions from the literature.

The design and costing procedure adopted for the evaluation of each configuration will be discussed in this chapter.

2.2. Method of Analysis

The initial phase of the thesis was the generation of qualitative data which would illustrate the effect of column configuration upon the separation of three, four and five component feedstocks. This investigation considered a wide range of feedstocks varying in composition and component volatility. In particular, consideration was given to a far wider range of variables than has been previously considered.

To select the optimal configuration from among a number of possible configurations for a given separation, an objective function was required. In the review, the objective functions used in previous studies were discussed. The criteria to be used in this study will be the total annual operating cost. This cost would comprise the depreciation cost of the total capital investment required for all distillation columns and heat exchangers within a configuration, together with the annual cost of process steam and cooling water required for the reboilers and condensers respectively. Each process unit within a configuration would be designed to the degree which would permit its accurate costing.

The method of analysis of each configuration was identical in all cases. The following specification for a given configuration was made:-

- (i) feed composition
- (ii) operating pressure and hence the degree of vaporisation of the feed

- (iii) ratio of the operating reflux ratio to the minimum reflux ratio
- (iv) the process topology, that is, the interconnection of process streams within the configuration
- (v) the degree of recovery of all components.

The process duty of all distillation columns and heat exchangers in the configuration was then specified. This was carried out by a material balance in which the flowrates, compositions and temperatures of all process streams within the configuration were determined, together with the process design of all columns and the heat loads for the heat exchangers.

Because of the large number of feedstocks to be considered, use was made in the initial phase of this section of a commercially available computer simulation programme to calculate the material balances. The simulation of industrial processes by computer is now a well established design procedure in the industry, particularly for those processes in which recycling of the process streams occur. Many such computer packages are commercially available and consequently will not be discussed here.

While the configurations considered in this study did not incorporate any recycling of process streams, a computer simulation package provided a ready means of effecting the mass balances for the large number of cases to be considered. In addition the package determined the process design of all columns, condensers and reboilers. In the initial phase, access was obtained to one of the commercially available simulation packages in the United Kingdom, where this phase of the study was undertaken by the author whilst on a sabbatical study leave in the Department of Chemical Engineering of the University of Technology, Loughborough, England. The computer package used was that

developed by the Imperial Chemical Industries Ltd. under the name 'Flowpack'. The package used by the author was the Mark 1 version which has been recently updated and issued as the Mark 2 version.

As well as making use of the executive facility within Flowpack for the calculation sequencing, the distillation sub-routine performed all calculations required for the distillation columns. The extent of the design of the columns made by the package was as follows:-

- (i) number of theoretical stages
- (ii) reflux ratio
- (iii) location of feed tray
- (iv) condenser and reboiler heat loads.

2.3 Specification of Variables

The variables which influence the optimal process configuration are the following:-

- (i) feed composition
- (ii) component volatility
- (iii) degree of recovery of all components
- (iv) operating pressure of all columns within the configuration
- (v) thermal condition of the feedstock, that is, the degree of vaporisation
- (vi) type of condenser, total or partial
- (vii) ratio of operating reflux ratio to the minimum reflux ratio.

Several of these variables are subject to the influence of external economic parameters. These variables are the operating pressure in each column of the configuration and the operating reflux ratio. These two variables were not considered in the initial phase of the thesis. It was felt that the optimal process configuration obtained under one set of economic values may not be optimal under

another set. In the review it was noted that in one study, the individual economic optimum operating pressures were used for each column within a configuration. It was suggested that this policy may have obscured the results obtained in the study.

The effect of feed vaporisation was not considered at this stage. The decision was taken to consider all feedstocks at their bubble point temperature for the column pressure.

Thus the variables considered in this phase of the thesis were the following:-

- (i) feed composition
- (ii) feed component volatility
- (iii) degree of recovery of all components.

The remaining variables were considered constant and were given the following values:-

(i) The operating pressure in each column was set at 100 psi. The selection of this pressure was made on the basis of (a) common industrial usage; (b) a pressure at which reliable data is available and in particular (c) several previous studies had used this pressure.

(ii) The ratio of the operating reflux ratio to the minimum reflux ratio was set at a value of 1.25. This value was used because it has been shown from many studies in the literature of the economic optimum reflux ratio that the classical curve illustrating the optimum reflux ratio as a function of total cost exhibits a slow increase above the value of the optimum reflux ratio. The value of 1.25 was considered to be on this slow rising portion of the curve in most instances.

2.4 Design of Distillation Columns

The design of each distillation column was made in the sequence in which it occurred in the configuration so that the input stream to the next column in the configuration could be specified.

The columns were designed as tray columns and the process specification of the columns was made by the use of established 'short-cut' design methods. Fenske's (1932) method was used for the calculation of the minimum number of equilibrium stages, Underwood's (1946) method for the calculation of the minimum reflux ratio and Gilliland and the Erbar-Maddox correlations for the number of equilibrium stages at the operating reflux ratio. The details of the methods will not be described here as these methods are readily available in standard texts on Distillation. However they will be discussed in so far as their use affected the analysis.

It was accepted that the design of the columns by the short-cut methods would be of sufficient accuracy for the thesis. A comparison of the results obtained was made by spot checks with the use of a rigorous method for the analysis of multicomponent columns. The extent of the variation produced in these comparisons was considered to be of little consequence. On the other hand, the agreement was considered to be very good and tended to confirm the results of Van Winkle and Todd (1975). However this aspect will be discussed later in the thesis.

The vapour-liquid equilibrium data used in the design of the columns was initially generated from Antoine constants. The equilibrium vaporisation values for all components were derived as the vapour pressure determined by the Antoine relationship divided by the column pressure. The initial feed components were considered to be ideal and the data generated by the Antoine relationship was considered to be of sufficient accuracy for the low operating pressure within each column. Later in the study, equilibrium values were obtained from Natural Gas Processors' Association data ⁽²²⁾ and the Chao-Souder correlation. ⁽³⁾ All 'K' data and enthalpy data were supplied to the computer programmes in the form of three degree polynomials as a function of temperature.

As stated, all feedstocks were at their bubble point temperature for the column operating pressure. For each feed this temperature was calculated by a bubble point programme described in the Appendix. This programme adopted the Newton-Raphson convergence method.

Subsequent to the mass balances and the process design of all columns and heat exchangers within a configuration being calculated, further computer programmes were written to design the distillation columns and heat exchangers to a degree from which quite accurate cost estimates could be made.

Each column was considered as a valve tray column and designed in accordance with the manual published by Glitsch (8) for the design of this type of column. The description of the computer flow diagram used in the design of each column is supplied in the Appendix. Similarly each heat exchanger was designed to the extent that the heat transfer area was calculated. The design parameters used in these calculations are listed in the Appendix.

Basically each column was designed to the following extent:-

- column diameter
- column height
- shell thickness
- actual number of stages.

Subsequent to this design being made for each column, the capital investment required was calculated by the cost programme developed by the author and included in the Appendix. The total annual operating cost for each column was then determined as the sum of the annual depreciation charge for the capital investment required for each column and heat exchanger and the annual cost for the supply of process steam and cooling water.

The design procedure incorporated in the distillation sub-routine was as follows:-

- (i) Underwood's method for the determination of the minimum reflux ratio
- (ii) a modified Fenske method for the determination of the number of equilibrium stages at total reflux conditions.
- (iii) the distribution of components in the product streams, based upon total reflux conditions.
- (iv) the Erbar-Maddox correlation for the determination of the number of equilibrium stages.

In spite of the limitations in these short-cut methods for the determination of the above conditions, the methods were used in this phase of the study because of their wide acceptance.

2.4.1 Calculation of Minimum Reflux Ratio

Limitations which were of particular concern to this study arose through the use of the Underwood method. These difficulties were as follows:-

- (i) The aim of the study was the development of techniques to be used to predict the optimal process configuration. As will be described later in the study, an aspect of this development was the formulation of mathematical models of a given configuration and indeed the modelling of the differences between all the possible configurations for a given separation. The solution of the Underwood equations required an iterative solution method and this requirement limited the use of the Underwood method in a mathematical model.

In view of this difficulty, a review was made of all other methods available in the literature for the determination of the minimum reflux ratio for multicomponent columns. As it has been noted in the review of previous work, Rod and Marek's (1959) study was the only

reported attempt at a mathematical model for the comparison of process configurations of distillation columns. This model, while of limited use, as discussed in the literature, incorporated the method of Robinson and Gilliland (1950). The required solution did not need an iterative solution. From the review of other methods in the literature, the methods available were either more difficult or cumbersome in their solution or required an iterative solution as in Underwood's method.

A study was made of the use of the Robinson and Gilliland method and a comparison made between the results obtained by this method for a wide range of feedstocks with the method of Underwood. The author was not able to find any reference in the literature to any similar comparison. As a result of the investigation, it was found that reasonable agreement was reached between the two methods for multi-component feedstocks in which the two key components were the major constituents. It was found that quite large discrepancies were evident when feedstocks contained non-key components in substantial amounts. As this study would be considering a wide range of feed compositions as indicated in Table 2.2 and feedstocks in which the position of the two key components were to be varied to suit the particular configuration being considered, then the method of Robinson and Gilliland could not be used.

This difficulty, together with the necessary adoption of the iterative procedure required by Underwood's method, imposed great problems which will be discussed presently.

Further, because of the wide acceptance of the method of Underwood for the determination of minimum reflux ratios within distillation technology throughout the world, it was then decided that

further work in this study would be based upon the use of the Underwood method and that the associated limitations would be accepted.

As the solution of the Underwood equations provides the same number of roots as the number of components in the feed, the selection of the key components is important. However in all configurations considered, the position of the keys was always as adjacent components. There was never the occasion when there was a component(s) existing as a distributing component(s) between the two keys. Thus in the solution of the Underwood equations, only one root was required and that root had a value less than the relative volatility of the light key component.

(ii) Another difficulty with the use of the Underwood equations, though not particular to the Underwood method alone, arose through the interpretation of the value of the relative volatility term in the equations. In the derivation of the Underwood equations, two assumptions are made. These are:-

- (a) the relative volatility of all components is constant over the column length and
- (b) constant molal overflow.

However in regard to the first assumption, there is confusion in the literature as to the appropriate value of the relative volatility to be used. Referring to the original papers of Underwood, no clarification is given. Rather the comment is made that "relative volatilities are assumed constant over the column". In the literature, for example, Smith (1963) uses the cubic mean of the relative volatilities calculated at three temperatures; the feed temperature, the dew point temperature of the overhead product and the bubble point temperature of the bottoms product. King (1971) uses the geometric mean of the dew point temperature

of the overhead product and the bubble point temperature of the bottoms product. References are further made to arithmetic and geometric means in the literature.

A study was made of this aspect, for it was felt that the extent of this variation had to be established. Provision was made in the programme developed by the author and described in Chapter III. This Programme basically replaced the Flowpack package which was not available to this study when the author returned to Australia where the study was continued. By this modification to the programme, the effect of the various interpretations of the relative volatility could be assessed.

It was found that quite considerable variation occurred as a result of the interpretation in the value of the minimum reflux ratio calculated by the method of Underwood. However in this phase of the work, the primary concern was in the generation of qualitative data. Throughout the remainder of this phase of the work, the value of the relative volatility term to be used in the Underwood equations was determined as the geometric mean of the dew point temperature of the overhead product and the bubble point temperature of the bottoms product. It must be noted that from the review of the previous work, this interpretation was the most widely held.

It was noted above, that the Flowpack package had adopted the policy of the value of the relative volatility term as being determined at the bubble point temperature of the feed to each column. This policy was no doubt brought about because of the nature of the calculation procedure adopted in the executive segment of the package. Within simulation packages, process stream conditions, i.e., flowrates pressure and temperature are determined for a given process item, say

a distillation column, by calling a subroutine by which the design of the distillation column would be made. If the overhead product stream from this unit was the feed stream to another process item, the information flow would incorporate the conditions of the overhead stream only as the properties of the feed stream to the next process unit. Thus the Flowpack package could generate results which would be at variance with results obtained by the author's programme in which the geometric mean described above was used.

(iii) A further difficulty arose from the use of the Underwood method for the determination of the minimum reflux ratio by the Flowpack programme. As indicated, later in this study when access was not available to the Flowpack programme, the author developed a programme which would perform, among other functions, the same function as the Flowpack programme. For the solution of the Underwood equations, the author adopted the convergence method of Newton-Raphson whereas Flowpack had adopted a modified Bounded False-Position method. During comparison of the results obtained by both programmes, it was noted at a quite late stage in this phase of the study, that differences existed in the values of the reflux ratio obtained by both programmes under certain circumstances. On investigation, it was found that an error existed in the Flowpack programme through its use of the Bounded-False-Position method. The reason for the error arose through a combination of the nature of the Underwood equation in the vicinity of the roots and the procedure incorporated in the programming of the method in Flowpack in an attempt to force the programme to a quicker convergence.

It was observed that the error was quite significant for only those feeds in which the non-key components were in significant amounts. Unfortunately, as all of the results of this part of the exploratory

phase of the thesis had used Flowpack, it was necessary to re-calculate all of the results thus far.

Fortunately, the error was found to be essentially a constant error and could be said to have little influence on the results at this stage. The aim was to generate data to indicate the extent of the variation to the total operating cost by the different process configurations possible for a given separation. Quantitative data was not being generated from this phase of the work. Rather interest was only in the relative differences in the costs of each configuration.

In all subsequent calculations, the value of the minimum reflux ratio was determined by the Underwood equations incorporating the Newton-Raphson convergence procedure only. All results obtained by the Flowpack programme incorporating the Bounded-False-Position method were re-calculated.

Verification of the fact that the method adopted in Flowpack was in error was confirmed by the Supervisor and later acknowledged by ICI and the solution procedure was modified in the Mark II version of the package. An example illustrating the error will be included in the Appendix.

2.5 Degree of Recovery Specification

For each feed, each feed composition and each process configuration, three values of product recovery were considered. These were identical for each component in the feed and were the following: 90%, 95% and 99%.

The specified degree of recovery which was adopted in this study for each component was defined as the percentage recovery of a given component to the amount of that component in the feed to the configuration. The alternative definition was to refer the amount of

the component recovered to the amount of the component in the feed to the column in which it is to be recovered. Heaven (1969) adopted this definition of recovery in his study. By the use of this definition an additional variable is introduced. For example, for components recovered as products in other than the first column in a configuration, the overall recovery factor specified is composed of two recovery factors which can be varied between two limits. For a three component feed comprising components A, B and C being separated by the direct sequence, then B and C would be recovered in the second column. If the recovery of B was specified to be 95% then the value of the degree of recovery of B in the first column would be within the range of 95.5% and 99% with the corresponding value of the degree of recovery of B in the second column to provide an overall recovery of 95%.

Thus there is an optimal value of the two values of recovery in both columns. While it was realised that this concept had merit, it was not considered at this stage. The concept will however be taken up at a later stage in the thesis.

2.6 Description of Experimental Procedure

The investigation as stated, proposed to study the effect of a number of parameters upon the selection of optimal configurations. Initially, a number of feedstocks were selected which it was felt would allow the effect of feed composition and the degree of recovery to be evaluated. To examine the effect of component volatility a further number of feedstocks were required. This section will discuss the selection of the feedstocks used.

Each feedstock was then analysed in an identical manner by the design method described earlier in this chapter. The results obtained will be given in Chapter 3.

2.6.1 Selection of feedstocks to study the effect of feed composition and component recovery

It was proposed to limit the number of feedstock components to a maximum of five. Two factors influenced this decision. These were:

(i) For the separation of five component feedstocks into pure components, fourteen configurations are possible, whereas for six component feedstocks, forty two configurations are possible. This number of configurations was considered far too large a number for the physical handling of the data and results. Moreover, it is very rare to have distillation plants in practice making more than four or five products.

(ii) Trends evident in four component feedstocks would be expected to be applicable to five or more component feedstocks. With four component feedstocks there was the possibility of considering the influence of the non-key components upon the optimal configuration. For example, by the selection of the key components, a four component feedstock could provide, in terms of volatility, one non-key component on either side of the key components. Further it is possible to have two components as non-keys on either side of the keys. Five component feedstocks could provide two non-keys on either side of the keys together with one non-key on the other. Six component feedstocks would provide at least two components on both sides of the key components. Thus it was felt that the influence of non-keys could be adequately investigated by considering four and five component feedstocks.

The components selected for the three, four and five component feedstocks are given in Table 2.1. These components were selected for the following reasons:

- (i) readily available and accurate data
- (ii) previous studies had used these components
- (iii) these components comprise the greatest tonnage of all materials distilled.

TABLE 2.1 Components used in three, four and five component feedstocks.

Feedstock	Components
Three	n-Butane, iso-Pentane, n-Pentane
Four	iso-Butane, n-Butane, iso-Pentane, n-Pentane
Five	Propane, iso-Butane, n-Butane, iso-Pentane, n-Pentane

As noted previously, all feedstocks were considered to be at their bubble point temperature for the operating pressure used. The range of feed compositions used for each feedstock is given in Table 2.2.

TABLE 2.2 Feed compositions for feedstocks Table 2.1

Component	Feed Type (Compositions in mole fractions)					
	1	2	3	4	5	6
(i) Three component feeds						
A	.33	.8	.1	.1	-	-
B	.33	.1	.8	.1	-	-
C	.34	.1	.1	.8	-	-
(ii) Four component feeds						
A	.25	.7	.1	.1	.1	-
B	.25	.1	.7	.1	.1	-
C	.25	.1	.1	.7	.1	-
D	.25	.1	.1	.1	.7	-
(iii) Five component feeds						
A	.2	.6	.1	.1	.1	.1
B	.2	.1	.6	.1	.1	.1
C	.2	.1	.1	.6	.1	.1
D	.2	.1	.1	.1	.6	.1
E	.2	.1	.1	.1	.1	.6

It should be noted again at this point that of the reported studies in the literature, the most comprehensive in terms of feedstocks considered, was the study of Heaven (1969). This author considered a small number of three component feeds and compositions together with one four and one five component feed.

2.6.2 Selection of feedstocks to study the effect of component volatility

For the study of the effect of component volatility using the design method used so far, certain inherent difficulties existed and these were as follows:-

(i) Low values of relative volatility between an adjacent pair of components in a feedstock compared with the relative volatilities between the remaining adjacent pairs of components in the feedstock would make the former separation more difficult than the latter. The degree of difficulty would of course depend on the absolute value of the relative volatility of the 'difficult' pair.

(ii) Associated with (i), is the possibility, the study of which has not been reported in the literature, that a difficult separation may be dependent upon the actual value of the relative volatility of the other pairs of components in the feedstock. For example, for the separation of a three component feedstock A, B and C in which the relative volatilities for A and B and for B and C are 1.1 and 4.0 respectively, the question arises whether the separation of components A and B will be as difficult when the relative volatility between B and C has a value of say 2.0. This aspect has been considered later in Chapter 7 and will not be considered further at this stage.

(iii) The position of the difficult separation within the feedstock may occur in any of 'n-1' positions in an 'n' component feedstock.

(iv) An additional difficulty and one to which considerable attention will be given later in the study, is the possibility that one of the components of a difficult pair could be the predominant component in the feedstock. In terms of the proposed heuristics, a conflict would exist. On the one hand, one heuristic would suggest the removal of the predominant component early in the sequence while another would suggest that the difficult separation be left until late in the sequence.

Clearly, the study of the effect of relative volatility upon the selection of the optimal configuration could be made easier if a suitable analytical relationship was available. As will be discussed in Chapter 4, the possibility of such a relationship is not feasible and the study must be made using the design method so far used. As a result, a very large number of cases would be required to be analysed in order to obtain meaningful results.

In view of the difficulties described above, it was proposed to investigate the effect of component volatility in the following manner:-

(i) To consider the position of the difficult separation within a feedstock. It was decided to use a four component feedstock as this would provide three positions for the difficult separation. Four component feedstocks were selected in which a difficult separation occurred in each of the three positions. Components were selected which would provide a value of relative volatility which could be considered as difficult. However the absolute value of this figure was not identical in all feedstocks. This was not possible as the result of using actual compounds for the feedstock. Later in the study, use was made of the concept of 'pseudo-components' which are hypothetical components given properties so as to produce values of

the relative volatility of any predetermined value. In all feedstocks, the degree of difficulty of the difficult separation was made to be a value which was considered to be typical of a difficult separation in practice. The value was also considerably less than the relative volatilities between the other adjacent pairs of components in the feedstock. The four component feedstocks selected are given in Table 2.3. Values of the relative volatilities are also included.

TABLE 2.3 Additional four component feedstocks to study the effect of varying position of a difficult separation.

Feed	Components	Relative volatility	
1	iso-Butane	VVV	2.65
	iso-Pentane		2.95
	n-Hexane		2.35
	n-Heptane		
2	1-Butene	VVV	2.58
	1-Pentene		1.17
	n-Pentane		2.45
	n-Hexane		
3	iso-Butane	VVV	1.31
	n-Butane		2.76
	n-Pentane		2.62
	n-Hexane		

(ii) The next phase was to vary the value of the relative volatility of the difficult pair. This investigation was made using three component feedstocks instead of the four components used previously. Only two positions were available for the difficult pair. Five binary feedstocks were selected in which the relative volatility varied from a low value of 1.07 to a high of 2.0. To each binary

feedstock, a third component was added, in one case a lighter component and in the other a heavier component so as to make in all ten three component feedstocks. These feedstocks were formulated as follows:-

<u>Type A</u>	<u>Type B</u>
A	X
B	A
Y	B

where components A and B are the binary feed components and X and Y the lighter and heavier components respectively. The relative volatility between components B and Y and between components X and A was selected to be considerably greater than between components A and B. Table 2.4 gives the ten three component feedstocks formed while Table 2.5 gives the values of the relative volatility.

For each feedstock, a range of feed compositions was used. The ranges are given in Table 2.6.

All of the above feedstocks were treated in the same way as previously. The total annual operating cost and the reboiler heat loads were calculated for each feedstock.

TABLE 2.4 Additional range of three component feedstocks to study possible conflict in heuristics.

Feed		Component	Feed	Component
1a	A	Propane	1b	Trans-2-Butene
	B	Trans-2-Butene		Cis-2-Butene
	C	Cis-2-Butene		Hexane
2a	A	Propane	2b	Iso-Butane
	B	Iso-butane		Iso-Butene
	C	Iso-butene		Hexane
3a	A	Propane	3b	Iso-pentane
	B	Iso-pentane		n-pentane
	C	n-pentane		Heptane
4a	A	Propane	4b	Iso-butane
	B	Iso-butane		n-butane
	C	n-butane		Hexane
5a	A	n-butane	5b	Hexane
	B	Hexane		Benzene
	C	Benzene		Octane

TABLE 2.5 Relative volatilities of feedstocks given in Table 2.4

		Relative Volatilities of Three Components Feeds (Equimolar)	
		Type 'A' Feeds	Type 'B' Feeds
1	A	3.75	1.06
	B		
	C		
2	A	2.65	1.10
	B		
	C		
3	A	7.9	1.18
	B		
	C		
4	A	5.92	1.28
	B		
	C		
5	A	2.65	1.32
	B		
	C		

TABLE 2.6 Range of feed compositions for feedstocks in Table 2.4.

Component	Feed Compositions (mole fraction)					
	(1)	(2)	(3)	(4)	(5)	(6)
A	0.4	0.3	0.2	0.1	0.1	0.8
B	0.4	0.3	0.2	0.1	0.8	0.1
Y	0.2	0.4	0.6	0.8	0.1	0.1
X	0.2	0.4	0.6	0.8	0.1	0.1
A	0.4	0.3	0.2	0.1	0.8	0.1
B	0.4	0.3	0.2	0.1	0.1	0.8

The results obtained from these investigations will be given in the next chapter.

CHAPTER 3. - RESULTS OF DESIGN ANALYSIS

CHAPTER 3. RESULTS OF DESIGN ANALYSIS3.1 Introduction

In chapter 2, the initial phase of the study was described. This phase was the generation of qualitative data which would illustrate the effect of column configuration upon the separation of three, four and five component feedstocks into products of varying purity. The data was to be obtained for a range of values of feed composition, component volatility and component degree of recovery. The results of this phase of the study will be presented in this chapter.

For the comparison of the configurations possible for a given separation, the objective function used was the total annual operating cost for each configuration. The design method used to calculate the objective function has been described in chapter 2. The results, both design and economic, obtained by this method for each configuration were considerable. For example, for each configuration, a mass and energy balance was made and this balance provided the flowrates, compositions and temperatures of all process and product streams. From this information, the design and subsequent costing of all process items and utilities for a configuration were made. All of the results obtained for the large number of cases considered in the study could not be included in the text. Only the values of the objective function, the total annual operating cost, have been reported. A computer printout showing the results obtained for a typical configuration has been included, however, in the Appendix.

3.2 Effect of Process Parameters

The initial phase of the study proposed to consider the effect of the following three parameters upon the selection of the optimal

configuration for a given separation:-

- (i) feed composition
- (ii) feed component volatility
- (iii) degree of recovery of all feed components.

3.2.1 Feed composition

Results which show the effect of feed composition upon the optimal configuration for the three, four and five component feedstocks used, are given in Tables 3.1, 3.2 and 3.3 respectively. The feed compositions used are as given in Table 2.2. The cost for each configuration is given as the total annual operating cost expressed in Pounds Sterling. The percentages given are the difference in the total annual operating cost for a given configuration relative to the corresponding figure for the direct configuration.

TABLE 3.1 Total Annual cost for three component feed comprising:- n-Butane, iso-Pentane and n-Pentane for the two possible configurations.

Configuration	Recovery	Feed Types (refer Table 2.2)			
		1	2	3	4
1	90%	255,011	141,442	332,335	288,368
	95%	281,100	154,654	370,752	315,442
	99%	306,252	164,928	406,225	343,928
2	90%	272,112	198,811	345,991	294,919
	95%	297,374	211,126	384,926	324,820
	99%	313,746	222,440	406,722	339,097
Percentage Cost difference relative to Configuration 1					
2	90%	-6.3	-40.5	-3.8	-2.2
	95%	-5.8	-36.2	-3.7	-2.9
	99%	-2.4	-34.5	-0.2	+1.4

Table 3.1 gives the results for the three component feedstock. Four feed compositions were used and for each feed composition, three degrees of recovery were specified.

TABLE 3.2 Total annual cost for a four component feed comprising:- iso-Butane, n-Butane, iso-Pentane and n-Pentane for five possible configurations.

(Percentage cost difference relative to configuration 1 given in brackets.)

CONFIGURATION AND RECOVERY		FEED TYPES (refer Table 2.2)				
		1	2	3	4	5
1	90%	382,349	307,378	346,848	454,808	401,498
	95%	420,354	335,418	381,075	502,100	429,246
	99%	451,881	354,173	403,663	546,388	476,172
2	90%	399,738 (-4.5)	380,149 (-23.6)	350,839 (-1.2)	465,490 (-2.3)	405,320 (-0.9)
	95%	435,550 (-3.6)	407,169 (-21.4)	385,100 (-1.0)	512,075 (-1.9)	440,100 (-0.2)
	99%	471,214 (-4.3)	436,869 (-23.3)	411,209 (-1.8)	556,623 (-1.8)	479,117 (-0.6)
3	90%	407,345 (-6.5)	366,439 (-19.2)	424,112 (-22.3)	473,038 (-4.0)	399,366 (+0.5)
	95%	442,823 (-5.3)	393,290 (-17.3)	455,494 (-19.5)	520,925 (-3.8)	434,575 (+1.1)
	99%	464,013 (-2.7)	407,749 (-15.2)	478,779 (-18.5)	548,414 (-0.4)	450,632 (+5.4)
4	90%	426,762 (-11.6)	437,660 (-43.3)	426,775 (-23.0)	484,043 (-6.4)	406,125 (-1.15)
	95%	462,030 (-9.9)	464,650 (-38.5)	459,510 (-20.5)	532,706 (-6.09)	441,620 (-0.5)
	99%	486,698 (-7.7)	489,790 (-38.3)	484,538 (-20.1)	559,012 (-2.3)	459,716 (+3.4)
5	90%	403,362 (-5.5)	317,956 (-3.44)	413,325 (-19.2)	475,848 (-4.6)	415,630 (-3.5)
	95%	441,677 (-5.0)	344,838 (-2.9)	447,754 (-17.5)	525,446 (-4.6)	456,920 (-4.0)
	99%	464,558 (-2.8)	359,388 (-1.4)	471,055 (-16.7)	553,897 (-1.37)	477,742 (+0.33)

Table 3.2 gives the results for the four component feedstock. Five feed compositions were used and again for each composition, three degrees of recovery were specified. The results are also given in Figure 3.1.

In all cases in this thesis, the percentage difference between configurations is expressed as follows:-

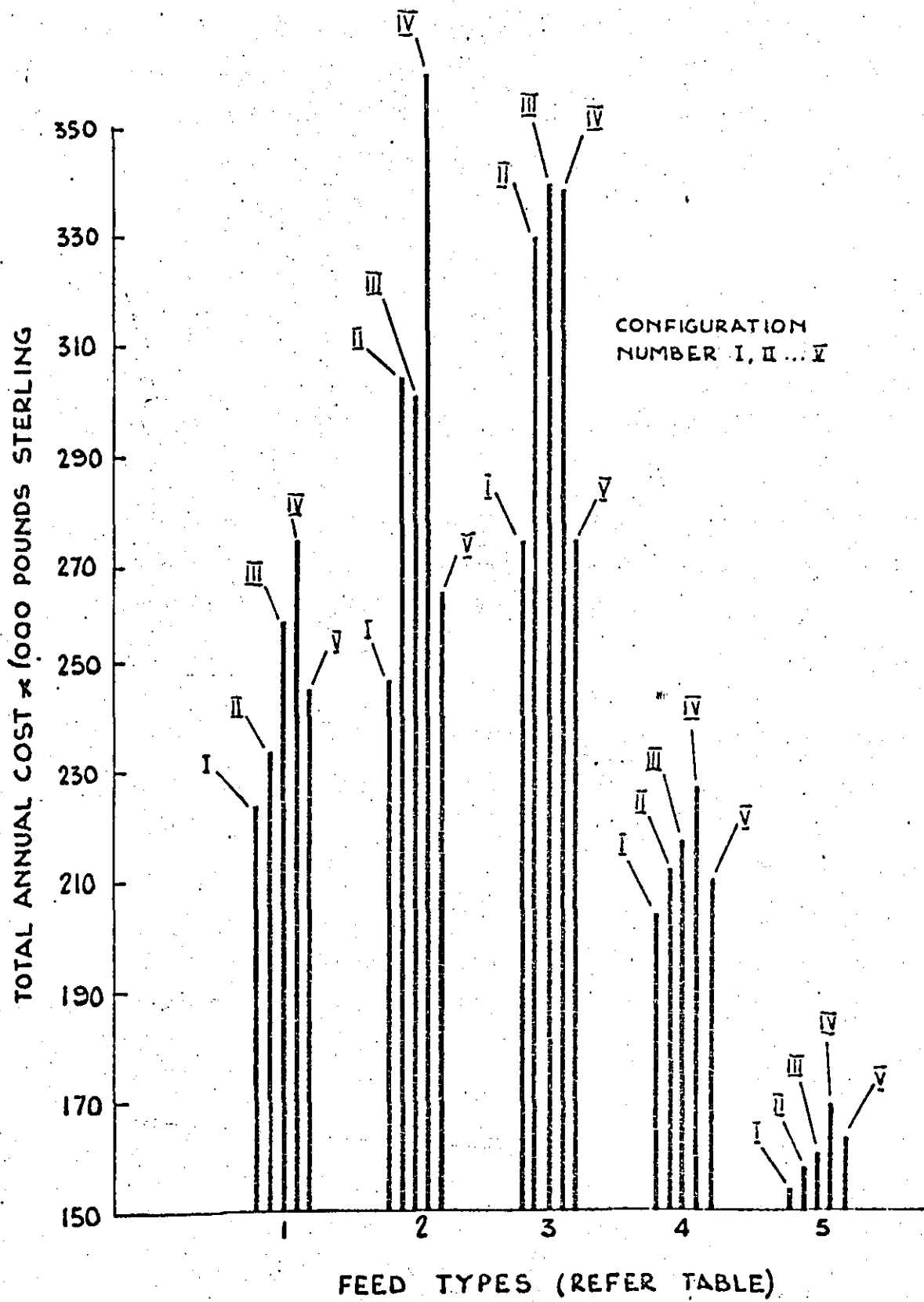
$$\text{Percentage Difference} = \frac{\text{Cost of Direct Configuration} - \text{Cost of Indirect Configuration}}{\text{Cost of Direct Configuration}} \times 100\%$$

It must be noted that the total annual operating costs as a function of feed composition have been given in the form of a 'bar' chart or histogram. This is necessary as the joining of the values of the total annual operating costs to form a curve would imply a function between these variables. The existence of such a function was not considered but will be considered at a later stage in the study.

Table 3.3 gives the results for the five component feedstock. Six feed compositions were used together with the three degrees of recovery. The total annual operating costs are given for the direct configuration only. The costs for the remaining thirteen possible configurations are given as a percentage of the cost of the direct configuration. The results are also given in Figure 3.2.

3.2.2 Effect of the Degree of Recovery of the Components

The three values of the degree of recovery of the feed components were 90, 95 and 99%. As discussed in Chapter 2, the degree of recovery was defined, in this study, as the amount of the component recovered as a percentage of the amount of the component in the feed to the configuration. The alternate definition is to relate the amount of the component recovered to the amount of the component in the feed to the column in which the component is to be recovered.



2.2

FIGURE 3.1 - Total Annual Operating Cost for Four Component Feedstock given in Table 2.1

TABLE 3.3 Total annual cost and percentage difference, relative to configuration 1, for a five component feedstock comprising:- Propane, iso-Butane, n-Butane, iso-Pentane and n-Pentane.

CONFIGURATION AND RECOVERY		FEED TYPES (refer Table 2.2)					
		1	2	3	4	5	6
1	99%	629,589	886,326	630,086	554,439	702,135	630,576
	95%	591,313	795,305	599,136	526,043	650,031	586,250
	90%	540,310	731,822	551,830	484,027	590,636	537,139
2	99%	-5.8	-3.3	-22.0	-15.0	-3.3	-1.4
	95%	-7.6	-9.3	-22.4	-15.5	-6.7	-1.9
	90%	-8.8	-21.0	-24.3	-17.2	-7.1	-2.56
3	99%	-2.7	-1.6	-13.2	-0.6	-1.7	-0.4
	95%	-2.4	-12.5	-12.0	-0.2	-1.9	-0.1
	90%	-3.2	-19.4	-13.5	-0.1	-2.3	-0.8
4	99%	-2.0	-1.1	-1.0	-12.5	-1.3	-0.3
	95%	-3.6	-1.36	-1.9	-13.2	-4.0	-3.2
	90%	-3.8	-1.4	-2.0	-14.1	-3.98	-2.0
5	99%	-2.3	-1.2	-8.3	-13.6	-1.5	-3.2
	95%	-4.2	-0.5	-9.7	-14.4	-4.4	-0.2
	90%	-5.0	-1.0	-10.4	-16.3	-4.7	-0.8
6	99%	-81.8	-76.6	-136.0	-132.0	-40.0	-44.0
	95%	-86.2	-24.7	-142.6	-139.0	-42.7	-48.0
	90%	-88.6	-28.0	-142.8	-143.0	-44.1	-49.0
7	99%	-83.8	-77.7	-137.0	-145.0	-41.3	-45.9
	95%	-89.8	-26.0	-144.0	-152.0	-46.7	-51.0
	90%	-92.5	-29.5	-147.0	-157.0	-48.2	-52.0
8	99%	-59.5	-62.0	-14.0	-2.2	-54.0	-30.9
	95%	-62.5	-41.7	-13.0	-1.5	-58.3	-32.0
	90%	-66.8	-45.6	-15.1	-2.0	-63.5	-35.0
9	99%	-137.0	-139.0	-149.0	-133.0	-89.0	-68.7
	95%	-142.0	-69.0	-151.0	-137.0	-95.0	-72.0
	90%	-149.0	-76.0	-154.0	-138.0	-101.0	-75.7
10	99%	-140.0	-235.0	-159.0	-149.0	-89.6	-63.0
	95%	-147.0	-140.0	-162.0	-154.0	-99.4	-69.0
	90%	-154.0	-151.0	-167.0	-156.0	-104.0	-73.0
11	99%	-2.4	-96.0	-9.0	-14.3	-1.2	+6.0
	95%	-4.5	-69.0	-10.6	-15.3	-4.2	+2.3
	90%	-5.8	-73.0	-12.8	-17.4	-4.7	+1.4
12	99%	-83.0	-173.0	-146.0	-148.0	-41.0	-3.42
	95%	-89.0	-95.0	-154.0	-151.0	-46.7	-40.1
	90%	-93.0	-102.0	-155.0	-162.0	-48.6	-43.4
13	99%	-62.0	-158.0	-24.0	-17.5	-54.8	-24.0
	95%	-67.0	-112.0	-25.0	-18.5	-62.7	-29.0
	90%	-72.0	-120.0	-27.3	-20.4	-66.0	-32.0
14	99%	-6.1	-98.0	-23.0	-15.7	-3.0	+4.0
	95%	-7.9	-68.0	-23.4	-16.3	-6.1	+0.6
	90%	-9.7	-93.0	-35.0	-18.4	-7.1	-0.41

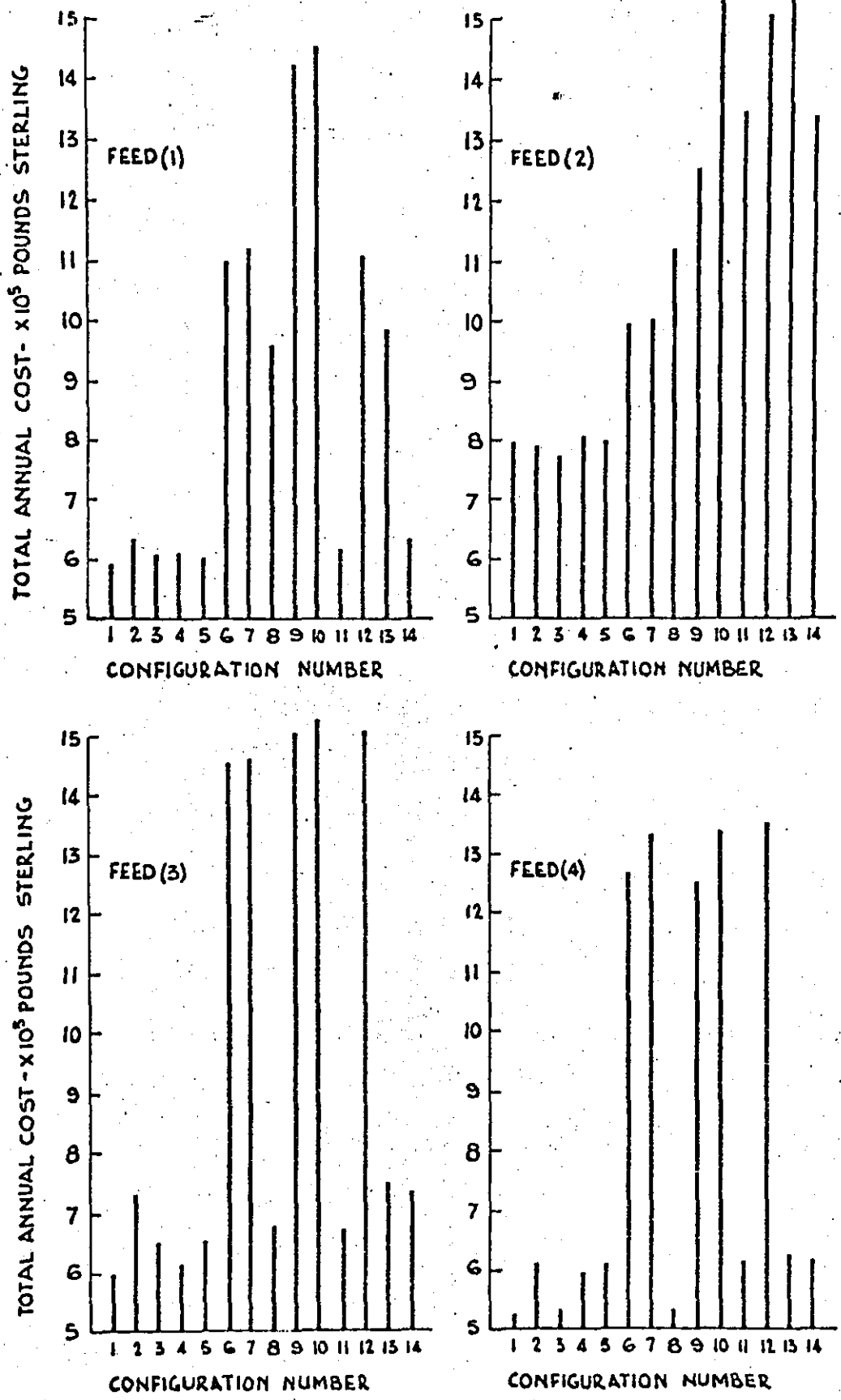


FIGURE 3.2 - Total Annual Operating Cost for Five Component Feedstock given in Table 3.1

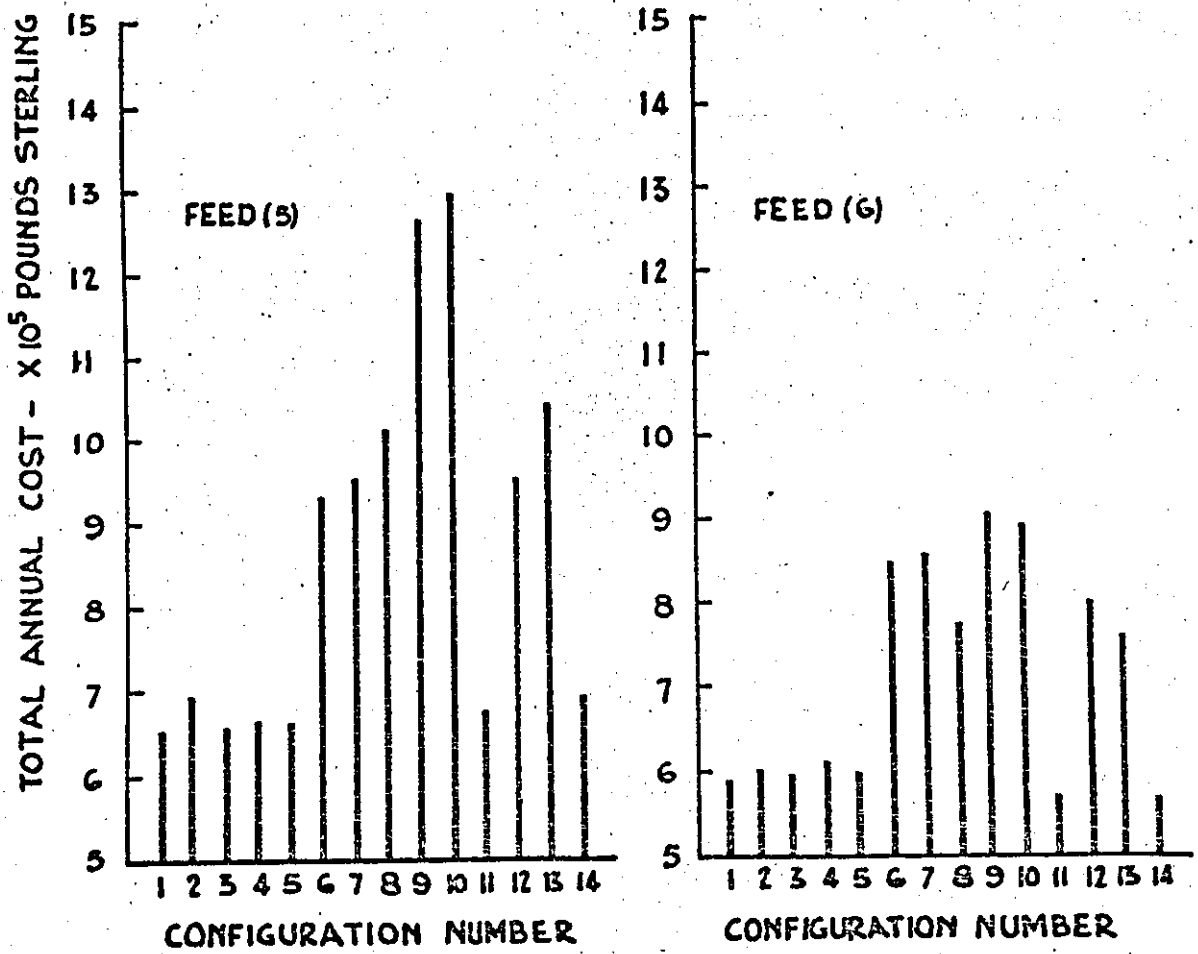


FIGURE 3.2 (Continued)

The effect of the three values of the degree of recovery used can be noted from Figures 3.3 and 3.4 which are the results for the four and five component feedstocks respectively. As to be expected, the results show that the higher the recovery rates, the higher is the cost of the separation. However the results do indicate that higher values of the degree of recovery did not produce, in all cases, a correspondingly higher value of the cost of the separation.

Several runs were made using a 98% component recovery rate in order to compare the results of this study with results of previous studies. Both definitions were used so as to compare the results and also to indicate the effect of the two interpretations of the degree of recovery. The results, when using the same definition, were in agreement. Since this aspect has been discussed in a previous publication by the author (1974) it will not be presented in this study.

As the results obtained were those expected, there appeared to be no justification for considering this aspect further.

3.2.3 Discussion of Results of Section 3.2.1 and 3.2.2

Before considering the effect of the third parameter, component volatility, it is proposed to comment briefly upon the results given in the previous two sections.

Firstly, the results have shown that the physical arrangement of the distillation columns for a given separation into the number of different configurations possible does have an effect upon the cost of the separation. The size of the effect has been shown, for the feedstocks used, to vary from insignificant to differences of the order of 150%.

Secondly, the results have shown that for the feedstocks used, the direct configuration was, in nearly all cases considered, the optimal

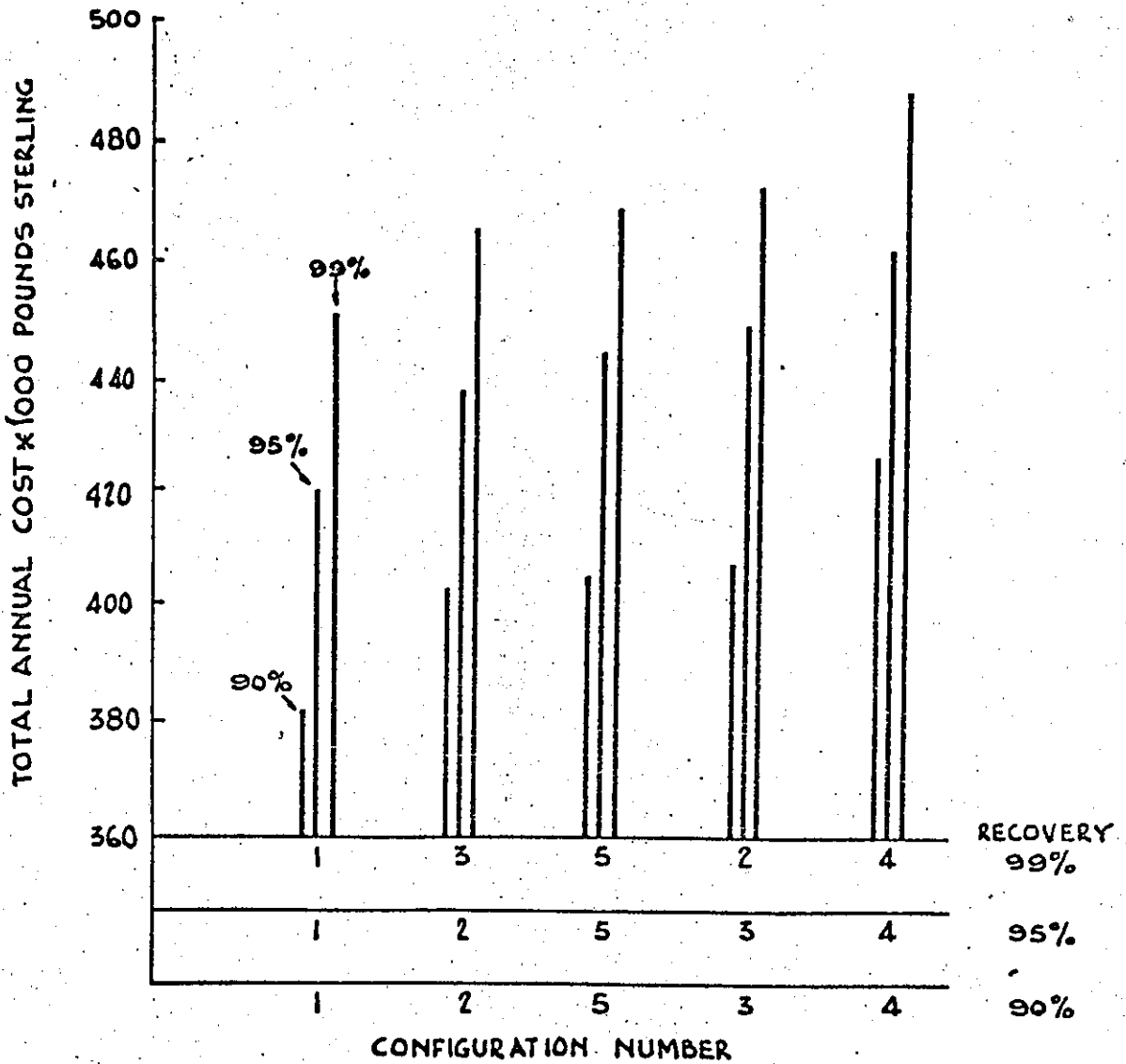


FIGURE 3.3 - Effect of Component Degree of Recovery
on Total Annual Operating Cost for
Four Component Feedstock

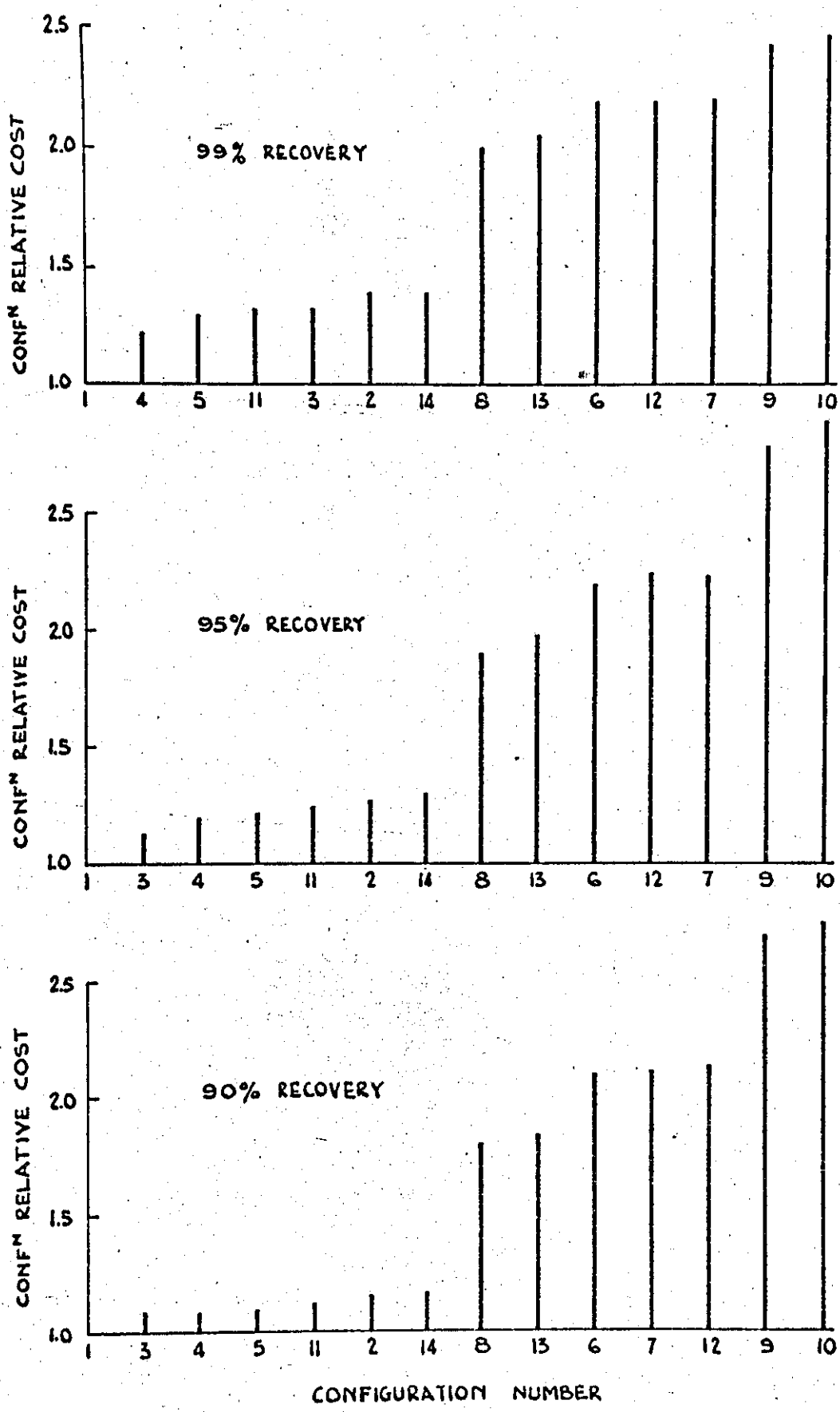


FIGURE 3.4 - Effect of Component Degree of Recovery on Five Component Feedstock

configuration. In the very small number of cases in which this was not the case, the percentage cost difference between the optimal configuration and the direct configuration was very small. However, before any conclusions can be drawn from the fact that the direct configuration was optimal in nearly all cases, it must be stressed that the feedstocks used did not contain a separation which could be considered difficult. This eliminated any consideration of the influence of the presence of a difficult separation upon the selection of the optimal configuration. While the feedstocks did not contain any difficult separations, the values of the relative volatilities between all possible pairs of components were not equal and it is put forward that until the effect of component relative volatility is studied, then no conclusions can be drawn from these results in regard to the effect of the presence of a difficult component.

Thirdly observations which can be made from the results may be summarised as follows:-

(i) There is a considerable variation in the cost differences between the configurations possible for a given separation.

(ii) The greatest cost difference occurred in those feedstocks in which the lightest component was the predominant component.

(iii) The cost of separation was greatest for those feedstocks described in (ii) while the reverse occurred for those feedstocks in which the least volatile component was the predominant component.

(iv) The degree of recovery of the components did not appear to influence the selection of the optimal configuration.

(v) For the separations in which the direct configuration was optimal, the next optimal configuration from those possible was not predictable. There were many cases in which the

optimal configuration, after the direct configuration, could be selected on the basis of one or two of the proposed heuristics, though there were cases in which the heuristic thought to be applicable for a given separation did not apply.

(vi) As a result of the comments in (v) it was felt that no further observations were meaningful until the study was made of the effect of the third parameter.

3.2.4 Study of the Effect of Component Volatility

The four component feedstocks specified in Table 2.3 were treated in the same manner as the previous feedstocks. Only one value of component recovery was specified for each component. The value used was 95%. The results obtained are given in Tables 3.4, 3.5, 3.6 and 3.7. It is to be noted that the reboiler heat load rather than the total annual operating cost has been used as the objective function. In all of these tables, the differences in reboiler heat loads of a configuration have been expressed as a percentage of the reboiler heat load of configuration one. The justification of the use of the reboiler heat load as the objective function will be discussed in the Appendix.

The results are shown graphically in Figures 3.5, 3.6 and 3.7. In Figure 3.5 the three cases denoted by I, II and III provide the cost relative to configuration 1 of the following:-

(i) Bars denoted by (I) indicate the relative cost for an equimolar feedstock in which no difficult separation occurs.

(ii) Bars denoted by (II) indicate the relative cost for an equimolar feedstock in which a difficult separation occurs between components A and B.

(iii) Bars denoted by (III) indicate the relative cost for an equimolar feedstock in which the difficult separation occurs between components B and C.

TABLE 3.4 Reboiler heat duty for each of the five possible configurations for the separation of the following four component feedstock :- iso-Butane, iso-Pentane, n-Hexane and n-Heptane (95% recovery of all components).

CONFIGURATION NUMBER	REBOILER HEAT DUTY, GJ				
	FEED 1	FEED 2	FEED 3	FEED 4	FEED 5
1	4.253 (0.0)	3.386 (0.0)	4.22 (0.0)	5.644 (0.0)	3.955 (0.0)
2	4.39 (-3.2)	4.431 (-30.1)	4.43 (-5.0)	5.581 (+1.2)	3.639 (+7.05)
3	4.944 (-16.2)	6.971 (-105.8)	5.74 (-36.0)	6.383 (-13.1)	3.365 (-14.9)
4	5.201 (-22.3)	8.377 (-147.3)	5.982 (-41.7)	6.351 (-12.5)	4.051 (-2.9)
5	4.589 (-7.91)	3.651 (-7.8)	5.486 (-30.8)	6.024 (-6.7)	3.46 (+12.1)

TABLE 3.5 Reboiler heat duty for each of the five possible configurations for the separation of the following four component feedstock :- 1-Butene, 1-Pentene, n-Pentane, n-Hexane. (95% recovery of all components)

CONFIGURATION NUMBER	REBOILER HEAT DUTY, GJ				
	FEED 1	FEED 2	FEED 3	FEED 4	FEED 5
1	10.025 (0.0)	4.132 (0.0)	13.96 (0.0)	12.73 (0.0)	4.34 (0.0)
2	10.08 (-0.5)	5.022 (-21.5)	12.23 (+12.4)	12.69 (+0.3)	4.82 (-33.9)
3	10.285 (-2.6)	5.265 (-27.4)	13.02 (+6.7)	13.06 (-2.5)	4.45 (-2.6)
4	10.216 (-1.9)	6.13 (-48.3)	13.84 (+0.8)	12.94 (-1.5)	4.46 (-2.6)
5	10.012 (+0.12)	4.252 (-2.9)	15.28 (-9.5)	-	-

TABLE 3.6 Reboiler heat duty for each of the five possible configurations for the separation of the following four component feedstock :- iso-Butane, n-Butane, iso-Pentane and n-Hexane (95% recovery of all components).

CONFIGURATION NUMBER	REBOILER HEAT DUTY, GJ				
	FEED 1	FEED 2	FEED 3	FEED 4	FEED 5
1	11.046 (0.0)	8.478 (0.0)	9.574 (0.0)	13.17 (0.0)	12.59 (0.0)
2	10.93 (+1.05)	9.854 (-16.2)	9.636 (-0.6)	12.94 (+1.76)	11.922 (+5.36)
3	10.56 (+4.39)	9.215 (-8.6)	10.78 (-12.6)	13.5 (-2.5)	11.24 (+10.8)
4	10.68 (+3.24)	10.61 (-20.1)	10.82 (-13.6)	13.31 (-1.04)	11.19 (+11.4)
5	10.87 (+1.59)	8.403 (+0.7)	10.56 (-10.2)	13.69 (-3.9)	12.04 (+4.4)

TABLE 3.7 Reboiler heat duty for each of the five possible configurations for the separation of the following four component feedstock :- iso-Butane, n-Butane, n-Pentane and n-Hexane

CONFIGURATION NUMBER	REBOILER HEAT DUTY, GJ				
	FEED 1	FEED 2	FEED 3	FEED 4	FEED 5
1	7.03 (0.0)	7.301 (0.0)	8.28 (0.0)	6.47 (0.0)	5.29 (0.0)
2	6.9 (+1.8)	8.54 (-16.1)	8.3 (-0.2)	6.26 (-3.26)	4.73 (-10.1)
3	7.533 (-7.2)	8.65 (-18.4)	9.68 (-16.9)	7.03 (-8.6)	4.99 (+5.7)
4	7.63 (-8.5)	9.86 (-35.4)	9.742 (-17.6)	6.89 (-6.5)	4.99 (+5.6)
5	7.34 (-4.5)	7.48 (-2.3)	9.49 (-14.6)	6.84 (-5.7)	5.33 (-0.6)

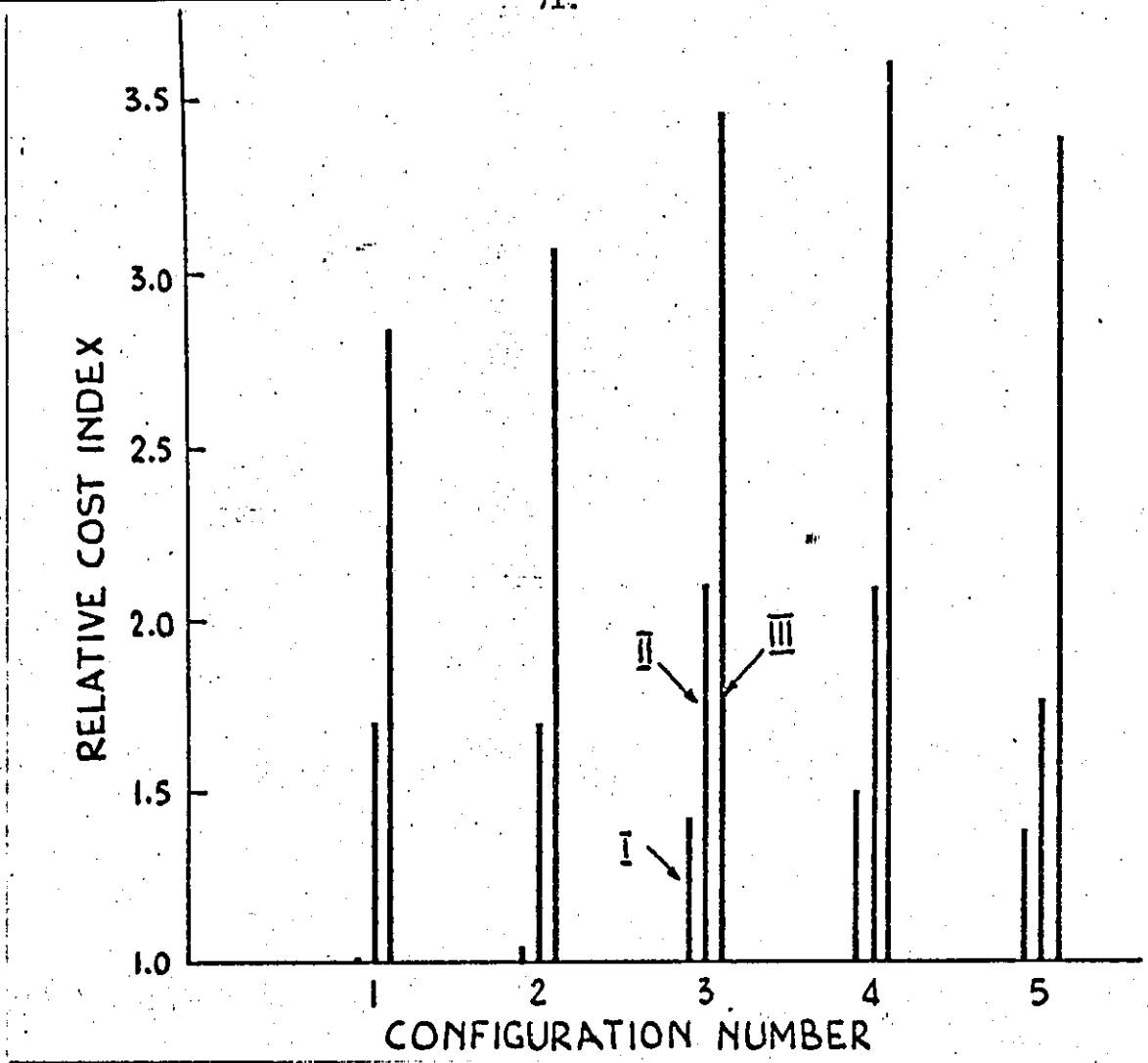


FIGURE 3.5 - Effect of Position of Difficult Separation in an Equimolar Feedstock

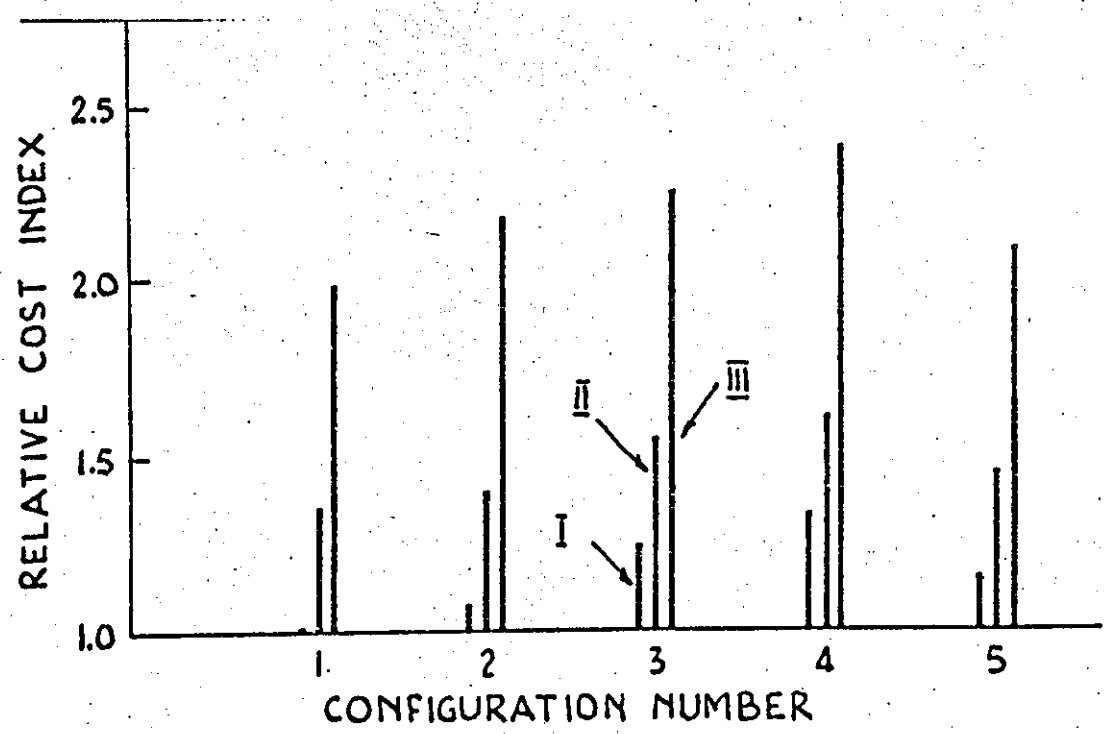


FIGURE 3.6 - Effect of Position of Difficult Separation in a Feedstock in which Component A is dominant

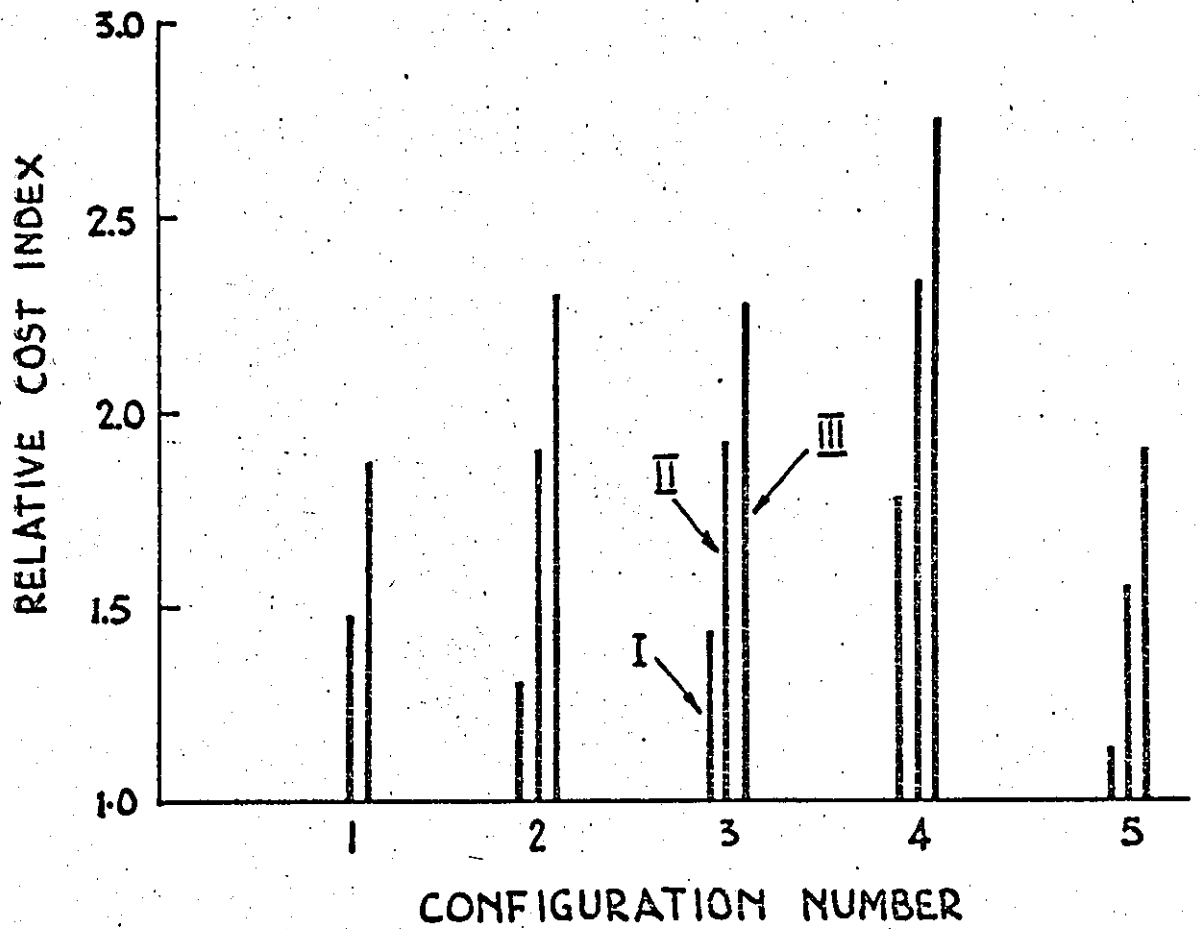


FIGURE 3.7 - Effect of Position of Difficult Separation
in a Feedstock in which Component B is
dominant

In Figures 3.6 and 3.7 the bars I, II and III denote the same feed types as in Figure 3.5. However in Figures 3.6 and 3.7, component A and B are predominant respectively.

With reference to Figure 3.5, (I) indicates that the direct sequence is optimal. (II) indicates that after configuration one, configuration two is optimal. This implies that the separation of components C and D is made first to leave the separation of the difficult separation between A and B until last in the sequence or in the absence of other components. (III) denotes that again after configuration one, configuration five is optimal. This implies that components A and D should be removed early, leaving the difficult separation between B and C to be carried out in the absence of other components.

The effect of a predominant component is illustrated in Figures 3.5 and 3.6. In Figure 3.5 after configuration one, which is again optimal, configuration five is optimal, thus suggesting the removal of the predominant component first. In Figure 3.6, configuration two is optimal, which suggests that the removal of the predominant first should be made first even though the predominant component is one of the difficult pair.

Conclusions which may be drawn from this phase of the investigation of the four component feedstocks would confirm that the reason for a given configuration being optimal can be explained in terms of one of the proposed heuristics, in particular heuristics I and II of Heaven and King and the heuristic proposed by Nishimura et al. The fact that configuration 1, which is Heaven's heuristic I, was optimal in all cases was felt to be a result of the particular value of the relative volatility used in the 'difficult' separation. If the selection of compounds as components of the difficult pair had provided a lower value,

then possibly different results would have been obtained. The principal result from this section of the study is that it is not possible to indicate under what values of feed composition and component volatility each heuristic will dictate the selection of optimal configurations.

3.2.5 Study of the Effect of Component Volatility using three component feedstocks

The three component feedstocks described in Tables 2.4 and 2.6 were treated in an identical manner to the four component feedstocks. The results obtained are given in Table 3.8. For each feed the result obtained has been expressed in terms of percentage difference in the reboiler heat load and the overhead vapour flow rate. These latter figures were included in this table to illustrate the similarity between the two criteria for the type 'B' feedstocks. These figures indicate that for feedstocks in which the difficult separation is between the two lightest components, the overhead vapour rate could appear to be a valid criterion for comparison of the two configurations. This aspect will be discussed, however, in detail in chapter 6.

A study of the results given in Table 3.8 would suggest that there is little significance which can be placed upon them. There are isolated cases in the table where the expected results do not occur; for example, for feedstock 1B having a feed composition of 0.1,0.1,0.8 it would be expected that the indirect configuration would be optimal. It must be concluded from these results that they tend to confirm the results obtained in the previous section of the thesis. It is necessary then that there must be clarification of the conditions at which a particular heuristic will dictate the selection of the optimal configuration.

TABLE 3.8 Percentage difference in reboiler heat load (q_r) and overhead vapour rate (v) for various feed composition.

Feed Number	Basis for Comparison	FEED COMPOSITION (MOLE FRACTION)												
		A		B		A		B		A		B		
		A	B	A	B	A	B	A	B	A	B			
		0.2	0.4	0.33	0.34	0.6	0.2	0.8	0.1	0.1	0.1	0.1	0.1	0.8
		0.4	0.4	0.33	0.33	0.2	0.2	0.1	0.1	0.8	0.8	0.1	0.1	
		0.4	0.2	0.34	0.33	0.2	0.6	0.1	0.8	0.1	0.1	0.8	0.1	
1A	v	1.67		3.27		-7.89		-4.53		-1.78		5.04		
	q_r	-1.8		-3.85		6.01		5.6		-4.42		-8.39		
1B	v	3.44		7.21		10.5		-14.78		2.95		2.54		
	q_r	3.66		7.61		11.26		-14.68		2.97		2.68		
2A	v	2.96		2.46		-2.14		-18.48		1.67		9.19		
	q_r	1.63		-3.83		2.32		-11.93		-2.92		-8.39		
2B	v	3.31		9.44		15.22		10.02		2.81		0.75		
	q_r	3.27		9.31		14.99		9.54		2.83		1.81		
3A	v	1.16		0.83		-3.51		-20.68		-2.46		6.48		
	q_r	-11.6		-11.54		-6.23		-1.92		-12.64		-3.98		
3B	v	-2.73		1.22		3.32		5.55		1.04		-8.36		
	q_r	-2.86		1.05		3.09		4.08		1.15		-8.37		
4A	v	0.88		-5.33		-16.9		-39.0		-2.93		11.58		
	q_r	-0.6		-10.39		-13.42		-34.7		-4.17		-3.6		
4B	v	-6.62		-2.57		1.93		5.00		-0.02		-14.92		
	q_r	-6.65		-2.62		1.91		4.14		-0.06		-14.9		
5A	v	0.08		-2.56		-10.02		-30.62		-3.01		6.88		
	q_r	-15.57		-10.09		-5.73		-16.87		-13.41		-8.42		
5B	v	-8.6		-7.2		7.95		-8.4		-2.17		-24.3		
	q_r	-8.24		-7.65		8.06		-8.75		-2.41		-25.3		

The results of the study of the application of heuristics presented in this chapter have provided data on the effect of the number of process configurations possible for the separation of a multicomponent feedstock comprised of the simple hydrocarbons used. Feedstocks containing up to five components have been studied. For feedstocks comprised of these components, then the results obtained should assist in the selection of the optimal configuration for the range of feed compositions, degrees of recovery and the values of the process parameters used in the analysis.

This study has also shown that the selection of the optimal configuration for a given separation can be explained in terms of the heuristics. However the study has not shown how to determine, under given process conditions, which heuristic will decide the optimal configuration.

The study will now consider the feasibility of the development of mathematical models for the prediction of the optimal configuration as this would appear to be the only way in which differentiation will be obtained between the heuristics.

CHAPTER 4. - DEVELOPMENT OF MATHEMATICAL MODELS

CHAPTER 4. MATHEMATICAL MODELS4.1 Introduction

The review of the previous work has shown that the comparison of configurations possible for a given separation has been made by two methods:-

(i) The design method which required the evaluation of an economic objective function obtained by the detail design and costing of all process items within the configuration. This method was used in this study.

(ii) Analytical methods in which a mathematical model of the configuration is used to determine the optimal configuration. The review has shown that only two such relationships or models of multicomponent distillation systems have been reported. These were the models of Rod and Marek (1951) and Nishimura et al. (1971).

The feasibility of mathematically modelling a system of multicomponent distillation columns was investigated. The aim was to develop a model in the form of a mathematical relationship between a dependent variable which would be directly related to the total annual operating cost of the configuration and independent variables which would specify the given separation. Should it be possible to develop such a model, then that model could be used in the study instead of the more tedious and time consuming method which has been used so far.

This chapter will describe the results of this investigation.

4.2 Selection of the Objective Function for the Model

The total annual operating cost calculated by the design method of chapter 2 could not be analytically related to the variables specified in section 2.1 other than, possibly, by multivariable regression analysis. This possibility was not considered because as discussed in chapter 1, the actual value of the total annual operating cost for a given separation

is dependent on the values of the various economic parameters used throughout the design and costing of each configuration. It was thought to be more appropriate to use a parameter from within the configuration(s). This parameter would be required to be directly related to the total annual operating cost and also to be related analytically to the required process variables specifying the separation.

From the literature and confirmed by this study (see Appendix) the reboiler heat load can be taken as a direct indication of the total annual operating cost of a distillation unit, comprising column, condenser and reboiler. Also for feedstocks at or near their bubble point temperature, the reboiler heat load is approximately equal to the condenser heat load.

Thus two process parameters, the reboiler and condenser heat loads, can be shown to be directly related to the total annual operating cost within the limits of accuracy required for the study. (The accuracy of this assumption will be discussed in chapter 7.) Either parameter can be used as the objective function. The choice of which parameter is more suited to this study is decided by which parameter can be more readily related to the variables describing the given separation.

The reboiler heat load of a distillation column is determined from an energy balance over the column, once the enthalpies of the feed and product streams and the condenser heat load are known. The reboiler heat load is then calculated from equation (4.1):

$$q_r = Dh_D + Bh_B + q_c - Fh_f \quad . . . \quad (4.1)$$

The calculation of the reboiler heat load requires prior knowledge of the condenser heat load. Further, the condenser heat load is related to the following:-

(i) overhead product flow rate
 (ii) operating reflux ratio
 (iii) enthalpy difference between the saturated vapour and liquid states of the overhead product per mole of overhead product, as follows:-

$$q_c = V \Delta H$$

$$= D(R + 1) \Delta H \quad \dots (4.2)$$

where ΔH is the enthalpy difference described above. A total condenser has been used throughout the study.

Thus for the development of the mathematical model, the assumption will be made that the cost of distillation plant processing feedstocks at or near its bubble point temperature can be taken as directly proportional to the overhead condenser heat load. The soundness of this assumption will be discussed in the light of the conclusions made from the study in chapter 7.

The development of an analytical relationship between the overhead condenser heat load and the variables describing separation will now be discussed.

4.3 Selection of Process Variables

The process variables which must be considered for inclusion in such a model are as follows:-

- (i) Feedstock variables comprising (a) the feed composition, (b) the feed component relative volatilities and (c) the physical state of the feedstock, i.e., the degree of vaporisation.
- (ii) The product specification or degree of recovery of all product components.
- (iii) The configurations of the columns.
- (iv) The operating pressure for each distillation column.
- (v) The value of the ratio of the operating reflux ratio to the minimum reflux ratio.

Only the variables under heads (i), (ii) and (iii) were considered. As discussed in Chapter 2, the values of the optimum reflux ratio and the operating pressure are influenced by the values of the economic parameters used in the design analysis. It had been decided that the effect of economic parameters which are influenced by external conditions should not be included in such a model. Consequently a constant operating pressure and a constant ratio of the operating reflux ratio to the minimum reflux ratio, as used in chapter 2, was accepted for each column in every configuration.

The mathematical model was therefore required to relate the overhead condenser heat load to the following variables only:-

- (i) Feed composition
- (ii) Feed component relative volatilities
- (iii) Product recovery specifications.

4.4 Development of Mathematical Models

The basic aim in the development of the model was to express the three variables in equation 4.2, i.e. overhead product flow rate, the operating reflux ratio and the overhead product enthalpy difference in terms of the variables described above.

Unfortunately this was not entirely feasible and the limitations in doing this will now be described. These limitations were in the determination of the following:-

- (i) the distribution of non-key components
- (ii) the relative volatility of components in the second and subsequent columns within a configuration
- (iii) the determination of the enthalpy difference between the saturated and liquid states of the overhead product.

4.4.1 Distribution of non-key components

In order to determine the flowrate of the overhead product from a distillation column, it is necessary to know the composition of that product stream. In the case of a binary feedstock this calculation is simple. For multicomponent feedstocks, however, this is not the case, because of the possibility of the distribution of components other than the light and heavy key components into both the overhead and bottoms product streams. Thus to determine the composition of an overhead product stream from a multicomponent column, the distribution of all components other than the two key components must be known. This is of real concern in columns in which the key components are not adjacent components. In this case there may be one or two 'distributing' components between the two key components. In all cases the extent of the distribution of non-key components in the product streams is a function of the composition and relative volatility of the components. In certain instances the accurate evaluation of the distribution of components may not be essential. However in this work the key components are not necessarily at all times those components which are predominant in the feedstock because of the range of configurations being considered.

Consider for example, the separation of an equimolar four component feedstock comprising components A, B, C and D to be separated by configuration number 2 (refer Appendix A). In this configuration, the components B and C are the light and heavy keys respectively. There is no distributing key and components A and D are the two non-key components. These two non-key components are for this feed composition present in a considerable amount. They will considerably affect the composition of both products. The extent to which this will occur depends upon their concentrations in the feedstock and their relative volatilities.

Thus the consideration of the distribution of the non-key components is of vital concern to this study.

In this study, as relatively pure products were specified, the separation was always made between adjacent components in the feedstock. The light and heavy keys were always adjacent components. Consequently as there was not a component between the two key components, the existence of a 'distributing' component between the two keys did not arise. However as all feedstocks contained three or more components, the distribution of the non-key components had to be calculated so that the composition of both products could be found.

In the preceding sections of this study, the distribution of non-key components in the overhead product streams was calculated at total reflux conditions. The question of the determination of the distribution of non-key components at conditions other than total reflux or minimum reflux conditions has not been adequately resolved since the original work of Geddes (1958), Hengstebeck (1961) and recently King (1971). It has been shown in this latter study however, that for columns operating with reflux ratios of the order considered in this study, the determination of the distribution of non-key components at total reflux conditions is sufficiently accurate. In all preceding calculations, distribution of non-key components has been made at total reflux conditions.

However in a mathematical model it is not feasible to have prior knowledge of the extent of the distribution of non-key components. This is particularly so for columns other than the first column in a configuration. As in the methods discussed above, the calculation of both product compositions from a column requires the knowledge of the relative volatility of the components in the column. This is obtained from a knowledge of the temperatures over the column, that is, the dew point

and bubble point temperatures of the overhead and bottoms product respectively. It also requires a knowledge of the feed stream to the column and the degree of recovery of the key components. This means, for example, that in the direct sequence for the separation of a three component feedstock, the flowrate and composition of the bottoms product from the first column is required. Obviously prior knowledge of these values is not feasible in a model.

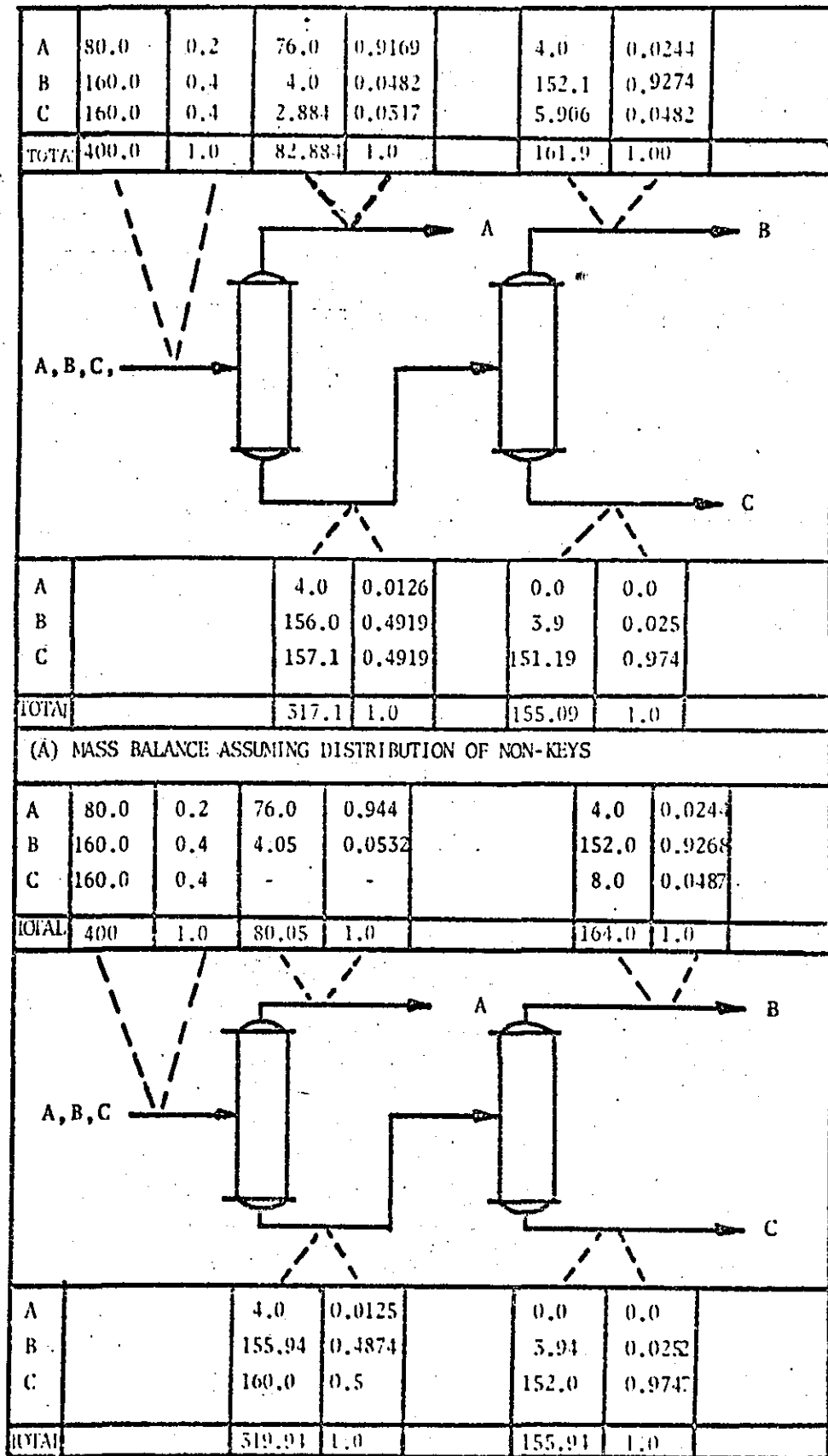
For the model, it can only be feasible to assume that non-key components do not distribute, i.e. all heavy non-key components will only be present in bottoms product streams and all light non-key components will appear in the overhead product streams. This procedure has been used in the subsequent development of the model.

As an example, consider the separation shown in figure 4.1. Here a three component feedstock is being separated by the direct sequence with product recovery specifications on each component of 95%. Note that the recovery specification for component B in the first column is 95%.

In Figure 4.1(a), the product compositions are based on the non-key components distributing and calculated at total reflux conditions. In Figure 4.1(b), the product compositions are calculated on the basis of the non-distribution of non-keys. That is, all of component C will appear in the bottoms product from column 1. Molar flow rates and mole fractions of components are given in Figure 4.1. The effect of the non-distribution of non-keys can be readily noted.

4.4.2 Relative volatility of components

The design methods used throughout this thesis for the determination of the total reflux and minimum reflux conditions have been the Fenske and Underwood's methods respectively. The reasons for



(B) MASS BALANCE ASSUMING NON-DISTRIBUTION OF NON-KEYS.

FIGURE 4.1.

this policy have been discussed in chapter 2. Both of these methods assume constant relative volatility of all components over the entire column.

It was resolved in chapter 2 that the correct interpretation and the policy to be adopted throughout this work would be the relative volatility of each component to be calculated as the geometric mean of the relative volatility at the dew point temperature of the overhead product and the bubble point temperature of the bottoms product.

However, difficulties can be experienced in applying this interpretation of component relative volatility to the mathematical model. This is again because in a simulation of a distillation configuration, the temperatures within the configuration are not known initially. For a three component distillation being carried out by the direct sequence, the temperature of the bottoms product from the first column is not known. The only conditions at which the relative volatilities can be determined in a model are (i) at the feed temperature to the configuration and (ii) at an average value of the relative volatilities of the lightest and heaviest components determined at the pure component boiling points. This policy was proposed principally because it would eliminate the need to determine product compositions, particularly the product compositions of the interconnecting stream within a configuration. The only error introduced could be the difference between the values of relative volatilities at either the dew or bubble point temperature and the values at the pure component boiling points. This aspect has been considered and the errors introduced are quite insignificant and will remain so while high purity products are being specified.

In the simulation which follows, the two volatility conditions mentioned above were considered and results compared with those obtained

by the use of the interpretation of relative volatility accepted for this study.

4.4.3 Enthalpy Difference between Saturated Vapour and Liquid State of Overhead Product

The evaluation of this parameter requires knowledge of the following:-

- (i) the correct composition of the overhead stream, and
- (ii) the vapour and liquid enthalpies as a function of temperature and the dew point and bubble point temperature of the overhead product.

Obviously the determination of the overhead stream enthalpies cannot be determined within a model. The only possibility would be to assume average values to include this value as a separate parameter.

Table 4.1 summarises the differences in the design method and the mathematical model.

Thus the preceding discussion would suggest that the results of any mathematical model of a sequence of multicomponent distillation columns can never reproduce the corresponding results obtained from the design method of the type used in the initial phase of the work. The use of a mathematical model to select the optimal configuration for a given separation can only be feasible if the differences which must occur between the model's results and the corresponding results obtained from the design analysis can be correlated.

4.5 Models Developed

Accepting the limitations imposed by the preceding discussion, it was proposed to develop a mathematical relationship between the overhead vapour rate and the following variables:-

TABLE 4.1 Summary of Differences in Design Method and Mathematical Model.

	Design Method	Mathematical Model
Distribution of non-key components	Calculated at total reflux conditions for each column	Calculated on the basis that non-key components do not distribute
Relative volatilities	Calculated for each column as the geometric mean of the volatilities at the dew point temperature of the overhead product and the bubble point temperature of the bottoms product	Calculated on two bases: (i) at the bubble point temperature of the feed to the first column in the configuration (ii) as the geometric mean at the boiling points of the lightest and heaviest component of the feedstock
Condenser heat load/mole of overhead product	Calculated from the actual product composition, liquid and vapour enthalpy correlations	Calculated only as a constant average figure.

(i) feed composition

(ii) feed component relative volatilities

(iii) specified degree of recovery of each component.

Once the models have been developed, an analysis will be made of the differences between the model's results and the results obtained using the design method for the same feedstocks.

Models were developed for two cases:-

- (I) the comparison of the two configurations possible for the separation of a three component feedstock into three components.
- (II) the comparison of the five configurations possible for the separation of a four component feedstock into four components.

For the development of the models for cases (I) and (II) the objective function was developed in terms of the difference between the sum of the overhead vapour flowrates of each configuration. For case (I) the objective function was developed as the difference of vapour flowrates for the two configurations per mole of feedstock to the configurations, i.e.

$$\frac{\Delta V}{F} = (V_1 + V_2)_D - (V_1 + V_2)_I \dots \dots \dots (4.3)$$

In case (II), this objective function could only be developed between any two of the possible five configurations, i.e.

$$\frac{\Delta V}{F} = (V_1 + V_2 + V_3)_D - (V_1 + V_2 + V_3)_i \dots (4.4)$$

For three component feedstocks, the expression developed is given by equation (4.5). The derivation of this expression has been included in the Appendix.

$$\begin{aligned} \frac{\Delta V}{F} = 1.25 \left[\right. & \chi_{AF} (C_1^1 - d_1 + RF_A (C_1 - d_1^1 - C_1 + 0.2) \\ & + \chi_{BF} (C_2 - 0.2 + RF_B \{C_2^1 + d_2^1 - 0.1\} \\ & + RF_B^{1/2} \{0.6 - d_2 - C_2 - d_2^1\}) \\ & \left. + \chi_{CF} (1 - RF_C) (C_3^1 - d_3) \right] \dots \dots (4.5) \end{aligned}$$

$$\text{where } C_1 = \left[\frac{\alpha_{AB}}{\alpha_{AB} - \phi_1} \right]_{ID}$$

$$C_2 = \left[\frac{1}{1 - \phi_1} \right]_{ID}$$

$$c_1^1 = \left[\frac{\alpha_{AC}}{\alpha_{AC} - \phi_2} \right]_{2D}$$

$$c_2^1 = \left[\frac{\alpha_{BC}}{\alpha_{BC} - \phi_2} \right]_{2D}$$

$$c_3^1 = \left[\frac{1}{1 - \phi_2} \right]_{2D}$$

$$d_1 = \left[\frac{\alpha_{AC}}{\alpha_{AC} - \phi_3} \right]_{1i}$$

$$d_2 = \left[\frac{\alpha_{BC}}{\alpha_{BC} - \phi_3} \right]_{1i}$$

$$d_3 = \left[\frac{1}{1 - \phi_3} \right]_{1i}$$

$$d_1^1 = \left[\frac{\alpha_{AB}}{\alpha_{AB} - \phi_4} \right]_{2i}$$

$$d_2^1 = \left[\frac{1}{1 - \phi_4} \right]_{2i}$$

The model includes only those terms specified and does not include any variables which are not known as input data for the separation. Unfortunately the expression includes the Underwood parameter ϕ . It will be seen that four values of this parameter are required, one for each column in the two configurations being compared. Considerable effort was made to delete the Underwood parameters from the model but this was not possible.

For a four component feedstock, an expression can be derived, relating the process variables to an objective function. In this case, the objective function was the percentage difference in the total vapour flows of each configuration for two of the five possible configurations. It is only possible to compare one of the four other possible configurations

at one time with, say, the direct configuration. As for the three component model, prior determined values of the Underwood parameter are required. In this case, six values are required, one for each column in the two configurations.

However the complexity of the derived expression, together with the requirement of the values of the Underwood parameter, makes the model of little practical use.

The model derived for the three component feedstocks given by equation 4.5 was confirmed using data obtained by the design method. The values of the objective function obtained by the model are in fact identical with the corresponding values obtained by the design method. However in obtaining the model's values for a given separation, four values of the Underwood's parameter, one for each column, are required. These values cannot be obtained through the model and the values used in the model were the four values obtained by the design method for the given separation.

In the derivations of the models, the degree of recovery of the key components in each column was specified, as discussed in chapter 2, on the basis of the amount of the component recovered in the product stream as a percentage of the component in the feedstock. However for the separation of a three component feedstock say A, B and C in which component A is being recovered in the overhead product from column one, components A and B are the light and heavy keys respectively. The question arises as to what degree of recovery is to be specified for the heavy key in the bottoms product from column one. As the degree of recovery is based on the amount of component B recovered in one product, in this case, as the overhead product from column two, then obviously a greater recovery must be specified for component B in the bottoms product from

column one. For example, for a 95% recovery of component B, the recovery fraction of B in the first column must be greater. In fact the value of the recovery of B can vary between two limits, say, from 95.5% to 99.0%. Throughout this study the value of $(95\%)^{\frac{1}{2}}$ has been used for the recovery fraction. This has been applied to all separations unless a component to be recovered in a subsequent column as the principal product is a key in a previous column in the configuration.

The possibility that a range of recoveries for the component B exists in the first column, as discussed above, suggests that an optimal recovery rate could exist for each column. A low recovery specification for component B, being the heavy key in column one, would require a high recovery specification for component B in the second column. The degree of recovery overall would still be based on the amount of component B recovered in the overhead product of column two relative to the amount of component B in the feedstock. Provided this overall degree of recovery was obtained, use could be made of the range of recoveries possible within the two columns for a three component separation so as to find the economic optimum recovery rate for each column.

In this study however, it has been assumed that the split is equally shared. For a recovery rate of 95% of component B in column two the recovery rate for component B in column one is $(95\%)^{\frac{1}{2}}$ or 97.46%.

4.6 Limitations of the Models

It has been shown that on the basis of certain assumptions, which have been discussed previously, it is possible to relate an objective function in terms of feed composition, component relative volatility and the degree of recovery. For three component feedstocks, the equation developed has been presented. As stated, its use is limited by the presence of four values of the Underwood parameter which must be

known. If this were not the case, then it is conceivable that a more useful relationship could be developed. For reasons already discussed, the use of the Underwood's method for the determination of the minimum reflux ratio was considered essential.

If the required values of the Underwood parameter for each column in the configuration could be supplied to the model, the results obtained from the model would be expected to be different from the design method results because of the assumptions and the limitations in the model.

To investigate this aspect, the range of three component feedstocks considered in chapter 3 was used. In this instance, for each of these feedstocks, the comparison of the two possible configurations was made in terms of the overhead condenser heat load. The results obtained are those which a model would be required to provide if the model were satisfactory for use in the determination of the optimal configuration for a given separation. For the same three component feedstocks, the comparison of the two possible configurations was made, but incorporating in the evaluation the assumptions made in the development of the model. These were:-

- (i) non-distribution of non-key components.
- (ii) relative volatilities calculated at the following conditions:
 - (a) at the feed temperature to the configuration
 - and (b) as the geometric mean of the relative volatilities at the boiling points of the pure components A and C.

These calculations were made by the programme 'Optconf' described in chapter 6.

The results obtained are given in Table 4.2. The feedstocks used for the analysis are those described in Tables 2.5 and 2.6 in

TABLE 4.2 Comparison of Model's Results with Design Method's Results.

Feed No.	Compn. No.	TYPE 'A' FEEDS			TYPE 'B' FEEDS		
		Actual Cost	Simulation		Actual Cost	Simulation	
			Case I	Case II		Case I	Case II
1	1	-1.8	9.25	-0.9	3.66	1.67	-1.21
	2	3.85	13.8	-2.7	7.61	5.51	-0.92
	3	9.01	13.55	-5.9	11.26	9.61	-0.47
	4	6.6	2.1	-15.1	14.68	13.31	0.54
	6	2.39	7.52	2.00	2.68	3.166	-4.16
2	1	1.63	8.65	-0.5	3.27	-0.02	-2.36
	2	3.83	10.17	-4.49	9.31	5.12	-2.02
	3	2.32	3.5	-10.85	14.99	11.86	-1.49
	4	-11.93	-14.52	-27.16	19.54	20.31	-0.039
	6	8.39	10.76	5.53	1.81	-6.8	-6.0
3	1	-11.66	14.38	-2.61	-2.56	-3.37	-5.76
	2	-1.54	16.3	-6.9	1.05	1.27	-4.76
	3	6.23	8.11	-14.7	5.09	6.74	-2.93
	4	-1.92	-19.46	-33.3	10.08	13.36	1.82
	6	-3.98	13.79	2.21	-8.37	-12.55	-12.6
4	1	-0.6	4.24	-1.36	-6.65	-7.96	-8.91
	2	-4.39	-0.73	-9.05	-2.62	-3.79	-7.82
	3	-13.42	-12.98	-21.52	1.91	1.72	-5.85
	4	-34.69	-37.24	-42.5	8.14	9.68	-0.8
	6	10.47	13.48	9.51	-14.9	-16.2	-2.1
5	1	-15.57	8.61	-2.65	-8.24	-	-
	2	-10.09	7.81	-8.38	-7.65	-	-
	3	-5.73	-1.98	-18.2	-8.06	-	-
	4	-16.87	-29.2	-39.0	-8.75	-	-
	6	-8.42	11.54	3.65	-25.3	-	-

chapter 2. The column headed 'Actual cost' is the value of the percentage difference in the condenser heat loads of the direct and indirect configurations calculated by the design method. These figures would be the figures which the model would be required to give if the model was to be feasible. The two headings 'Case I' and 'Case II' are the results obtained from the model using the two interpretations of the relative volatility. Case I is based on the relative volatilities calculated at the feed temperature to the first column and Case II is based on the relative volatilities calculated as the geometric mean at the boiling points of the pure components. Both Cases I and II assume non-distribution of non-key components.

It will be noted that large discrepancies exist in these results to the extent which would make the proposed model not feasible. This, together with the necessary prior knowledge of the Underwood parameters, would certainly make this mathematical model of no use in the prediction of optimal configurations.

No consideration was given to the development of another model as it was felt that the same problems would be met.

CHAPTER 5. - PSEUDO-COMPONENT ANALYSIS

CHAPTER 5. USE OF PSEUDO-COMPONENTS5.1 Introduction

Results obtained in chapter 4 have shown that it is not feasible to develop a suitable mathematical model or relationship for use in the prediction of optimal configurations. Consequently the only source of data upon which any design guidelines can be based is data generated by a design method of the type used throughout this study.

The study has shown that the use of heuristics as a design tool is limited until clarification is made of the conditions under which each heuristic would decide the selection of the optimal configuration.

The results given in chapter 3 have indicated that three of the heuristics have been dominant in the selection of optimal configurations. These heuristics are:-

- (i) the removal of components in decreasing order of volatility
- (ii) the early separation of a predominant component and
- (iii) the separation of difficult separations late in the sequence.

However the results have shown that conflicts do exist under certain circumstances between the heuristics for the feedstocks used in this study. For these heuristics to be of use in design, it is essential to show under what conditions each heuristic will dictate the selection of the optimal configuration.

Consequently it was decided that the only way in which the conflicts could be resolved would be by the generation of a considerable volume of data illustrating the variation in configuration cost differentials for the case in which the relative volatility and feed

compositions for three component feedstocks are varied by predetermined small amounts. Thus an approximation could be made to a mathematical relationship between the relative volatilities and the composition of a three component feedstock if a sufficiently large amount of data were generated. The graphical representation of this data could well be the only way in which the conflicting influences could be illustrated.

In all previous studies, including this study so far, actual compounds have been used in formulating feedstocks. The absolute value of the relative volatility between adjacent components has not been specified in the selection of these compounds. Rather the component has been selected on the basis of providing a relative volatility between adjacent components which was at least higher or lower than between another pair of adjacent components in the feedstock. The values of the relative volatility obtained were not necessarily simple rational numbers. It was felt that the components comprising the feedstocks could have physical properties which would provide such numbers. More importantly, if predetermined values of the relative volatility could be obtained, then perhaps a way may be provided for studying the interaction between the conflicting heuristics.

This chapter will describe the use of the concept of hypothetical or pseudo-components by the use of which feedstocks can be formulated having predetermined values of relative volatilities. It is claimed that this approach is unique and no previous work incorporating this concept has been reported in the literature.

5.2 Generation of Pseudo-Components

It is not possible to select actual compounds as components which would provide feedstocks having the desired relative volatility. On the other hand, by the use of pseudo-components it should be possible

to formulate feedstocks in which the relative volatilities between the two pairs of components in a three component feedstock have the following predetermined values, say, 1.05, 1.1, 1.25, 2.0, 2.5, To do this, components would have to be generated such that 'K' values would give the required relative volatilities. A set of alkanes given in Table 5.1 was selected as the 'grid' from which the pseudo-components could be generated.

TABLE 5.1 Range of Alkanes used in generating Pseudo-Components.

Propane
 iso-Butane
 n-Butane
 iso-Pentane
 n-Pentane
 n-Hexane
 n-Heptane

The grid was formed in the computer programme 'Pslids' by calculating and storing the 'K' values of the reference compounds as a function of temperature over the required temperature range. The 'K' data used was that previously used in the study, that is, NGPA K values for an operating pressure of 100 psi and a convergence pressure of 2000 psi.

The reasons for the selection of these compounds have been given previously but in addition to those reasons is the fact that a recent study by Rudd and Tedder (1976) had used these compounds. As this study would be comparing their results, the same feedstocks were used.

The least volatile component, n-Heptane, was selected as the base component or in the case of a three component feedstock, this

compound would be the component 'C'. If a pseudo-component to be component B was required to have a relative volatility of, say, 1.25 then the 'K' value of this component would be the value of 1.25 multiplied by the 'K' value of n-Heptane at a given temperature reference point. As in all previous work in this thesis, all feedstocks were taken to be at the bubble point temperature for the column pressure. Hence for the generation of the pseudo-components, the reference temperature was the bubble point temperature for the given feed composition.

The bubble point temperature is the temperature at which the following expression is valid:- $\sum K_i \chi_i = 1.0$

or in terms of the relative volatility between components A and B and between B and C, then this expression can be rewritten as:-

$$\chi_1 (\alpha_{AB} \cdot \alpha_{BC}^{-1}) + \chi_2 (\alpha_{BC}^{-1}) + 1 = \frac{1}{K_C}$$

If $K_C = a + bT + cT^2 + dT^3$ is substituted in the expression, then the value of T which makes the expression valid is the bubble point temperature. The solution was found using the Newton-Raphson Iteration method.

If the value of the 'K' value calculated for the pseudo-component was less than the 'K' value of the next lightest compound, Hexane, at the bubble point temperature, then the 'K' values for the pseudo-component would lie between the 'K' values for n-Heptane and n-Hexane. The following ratio: $R = \frac{K_{sc} - K_R}{K_{R-1} - K_R}$ where K_{sr} , K_R

K_{R-1} are the 'K' values of the pseudo-component, reference compound and next lightest reference compound respectively, was then calculated.

Using this ratio, the 'K' values of the pseudo-component were calculated by generating values in the same proportion between the two reference components over the specified temperature range. The procedure is illustrated in Figure 5.1.

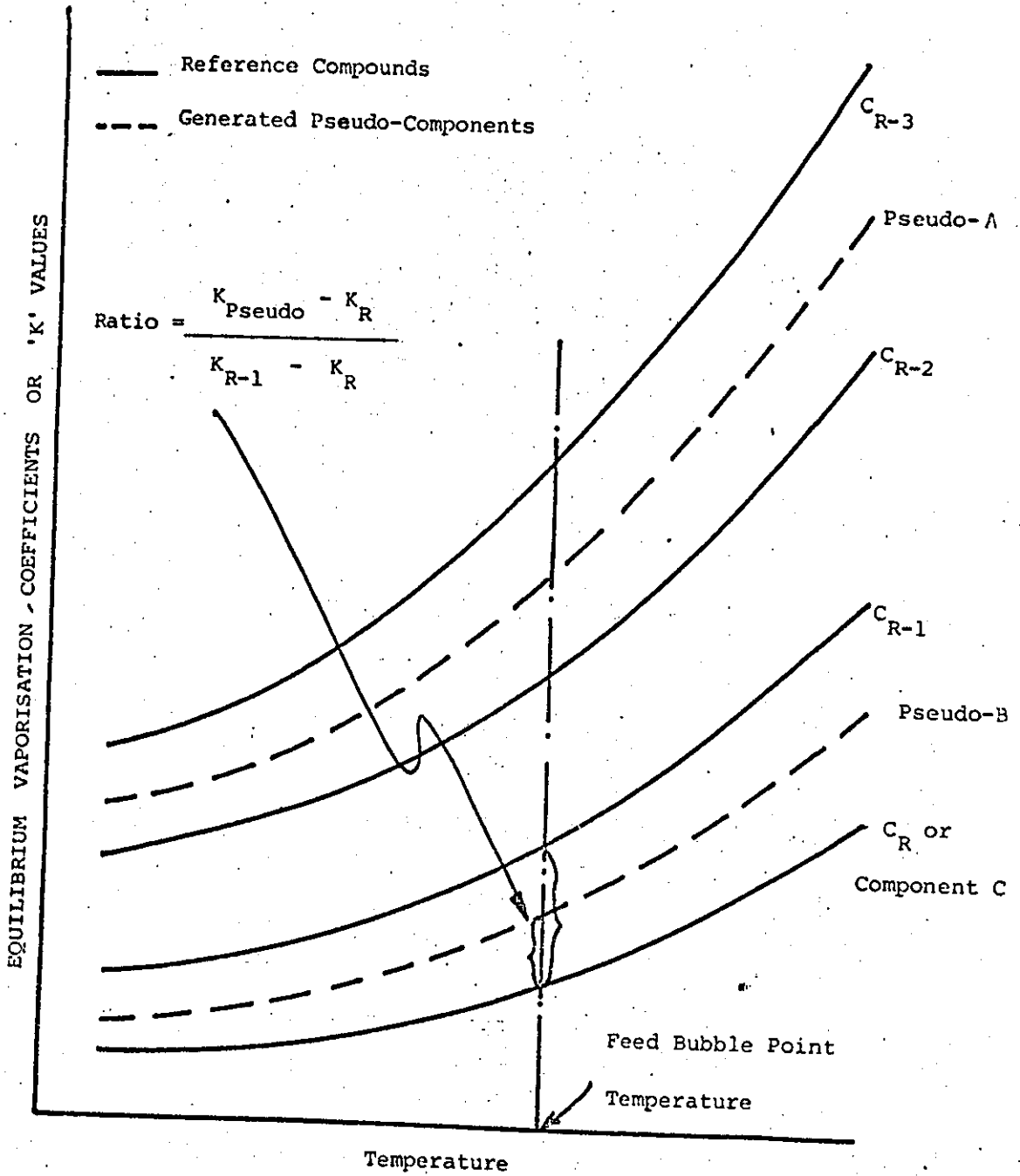


FIGURE 5.1 - Generation of Pseudo-Components

The 'K' values obtained were then fitted by the regression analysis subroutine in 'Pslids' and the coefficients used subsequently in the Programme.

If the required relative volatility value gave a 'K' value for the pseudo-component greater than the 'K' value of n-Hexane then the 'K' values for the pseudo-component would lie between the next pair of compounds, that is, n-Hexane and iso-Pentane. The same procedure would then be followed to generate the required 'K' values.

The same procedure was followed in generating component A in which the reference 'K' value for this component would be calculated by multiplying the required relative volatility by the 'K' value of component B at the reference temperature point. This procedure was used to generate two pseudo-components which together with n-Heptane formed a three component feedstock.

In this study it will be noticed that both relative volatilities are not relative to the one component, say, component C. Instead relative volatilities are expressed as the relative volatility of component A to component B and the relative volatility of component B to component C.

The liquid and vapour enthalpies for the pseudo-components were generated in the same manner. The enthalpies were generated within a reference grid comprised of the enthalpies of the reference compounds.

The same ratio which was used in the derivation of the 'K' values was applied to the two adjacent component enthalpy curves to calculate the required enthalpy for the pseudo-component. The values obtained were then fitted by the regression analysis programme.

The generation of the 'K' value and enthalpy coefficients was made by the programme 'Pslids' which will be briefly described in section 5.3.

5.3 Computational Procedure

It was proposed to consider a very wide range of three component feedstocks. For each feed composition, the range of component relative volatilities used was as follows:

The relative volatilities of 'A' to 'B' and 'B' to 'C' were each set initially at a lower limit of 1.1. The relative volatility of 'A' to 'B' was increased while holding the relative volatility of 'B' to 'C' constant. The range of values used for the relative volatility of 'A' to 'B' were as given in Table 5.2.

TABLE 5.2 Range of Relative Volatilities Used.

1.1
1.2
1.3
1.4
1.5
1.75
2.0
2.5
3.0
3.5
4.0
4.5
5.0

That is, thirteen values of the relative volatility of 'A' to 'B' were used. For each set of relative volatility values, the programme 'Pslids' calculated the percentage cost difference between the two configurations. When the thirteen values had been considered, the value of the relative volatility of 'B' to 'C' was increased to the next value, that is 1.2 and again the thirteen values of the relative volatility of 'A' to 'B' were used. This procedure provided $13 \times 13 = 169$ feedstocks.

However, for each feedstock, ten feed compositions were used. The values of the feed compositions used are given in Table 5.3. In the recent study of Rudd and Tedder (1976), seven of these feed compositions had been used. These authors did not consider the feed compositions, numbers 4, 5 and 6 in Table 5.3.

TABLE 5.3 Feed Compositions Used.

Feed No.	Feed Composition (Mole fraction)		
	Component		
	A	B	C
1	0.333	0.333	0.334
2	0.8	0.1	0.1
3	0.1	0.8	0.1
4	0.1	0.1	0.8
5	0.6	0.2	0.2
6	0.2	0.6	0.2
7	0.2	0.2	0.6
8	0.45	0.45	0.1
9	0.45	0.1	0.45
10	0.1	0.45	0.45

This investigation was able to consider 1690 feedstocks.

It should be noted before comparing the results obtained from this study with results relevant from the study of Rudd and Tedder, that these authors considered only seven feedstocks. The feedstocks used by these authors together with values of both indices, that is Heaven's and Rudd and Tedder's are given in Table 5.4.

The computer programme 'Pslids', discussed in chapter 7 then provided the following data for each feedstock:-

- (A) For each column in the direct and indirect configurations
- (i) product compositions - based on the distribution of non-key components at total reflux conditions.

TABLE 5.4 Feedstocks used by Rudd & Tedder.

Feed Number	Components	K_A/K_C	HI	ESI
1	n-pentane, n-hexane, n-heptane	6.35	0.27	1.04
2	n-butane, i-pentane, n-pentane	3.04	0.14	1.86
3	i-butane, n-butane, n-hexane	10.22	0.71	0.18
4	i-pentane, n-pentane, n-hexane	3.32	0.71	0.47
5	i-butane, n-butane, i-pentane	3.26	0.60	0.59
6	propane, i-butane, n-butane	3.30	0.17	1.72

(ii) minimum and operating reflux ratio

(iii) overhead vapour flow rate

(iv) heat balance providing the heat loads for the overhead condenser and reboiler. The enthalpy of the feed to the second column in both configurations was taken as the enthalpy of the relevant product stream from the first column.

(v) the thermodynamic net work function.

(B) For the comparison of the two possible configurations for three component feedstocks the programme provided the following as percentage differences:

(i) reboiler heat load

(ii) condenser heat load

(iii) overhead vapour flow rate

(iv) thermodynamic net work consumption.

As previously, several runs were made incorporating the full design and costing programmes and the results obtained confirmed the reboiler heat load and the total operating cost provided identical percentage figures. Thus the reboiler heat load was used as the objective function throughout this phase of the study.

The results obtained from this analysis indicated that there were regions on the ternary composition diagram in which more data was required. Ten additional feed compositions are given in Table 5.5.

TABLE 5.5 Additional Three Component Feedstocks.

Feed No.	Feed Composition (Mole fraction)		
	A	Component B	C
11	0.7	0.15	0.15
12	0.5	0.25	0.25
13	0.3	0.2	0.5
14	0.1	0.1	0.6
15	0.2	0.5	0.3
16	0.2	0.3	0.5
17	0.2	0.1	0.7
18	0.1	0.6	0.3
19	0.1	0.3	0.6
20	0.1	0.2	0.7
21	0.4	0.2	0.4
22	0.55	0.1	0.35

By this computational method it was possible to generate over 4000 data points by the use of which clarification of the conflict between the heuristics should be obtained.

CHAPTER 6. - RESULTS OF PSEUDO-COMPONENT ANALYSIS

CHAPTER 6. RESULTS OF PSEUDO-COMPONENT ANALYSIS6.1 Introduction

In Chapter 5, the use of the concept of pseudo-components as an alternative to the use of a mathematical relationship between the cost of separation and feed composition, component volatility and degree of recovery was discussed. The results of the analysis using the concept of pseudo-components and described in that chapter will now be given.

6.2 Presentation of Results

The results obtained are presented in the following manner. For each feed composition, the calculated percentage difference between the two configurations for each pair of relative volatilities was plotted. The relative volatilities for each pair were in the range of 1.1 to 5.0. When all values of the percentage difference for each feed composition had been plotted, contour lines representing constant percentage differences between configurations were then drawn for values of the percentage difference of, say, -5,0,5,10% The graphs obtained are given in Figures 6.1 to 6.22. The original graphs were plotted on graph paper 45 cms by 45 cms so that accuracy could be obtained in the generation of the contours. Each graph is given in reduced form so that the graphs can be included in the text.

In figure 6.23 the results for the twenty-two feed compositions have been plotted on triangular co-ordinates showing (a) compositions for which only the direct configuration is optimal, and (b) compositions for which both configurations can be optimal. In the composition region indicated by the open circles, the direct configuration is always optimal. In the composition region indicated by the full circles, both the direct and indirect configuration can be optimal depending upon the values of the relative volatilities of the feedstock.

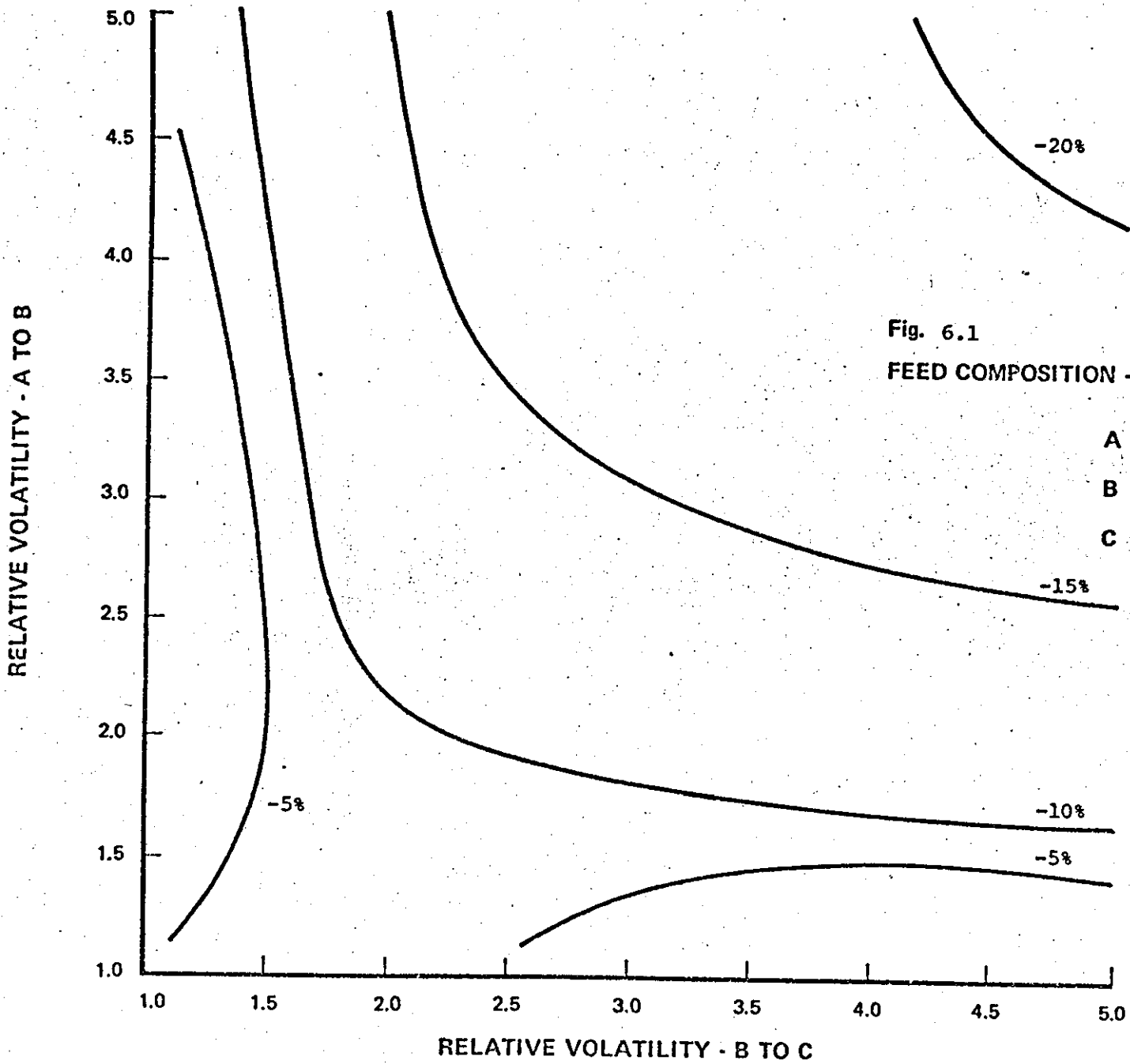
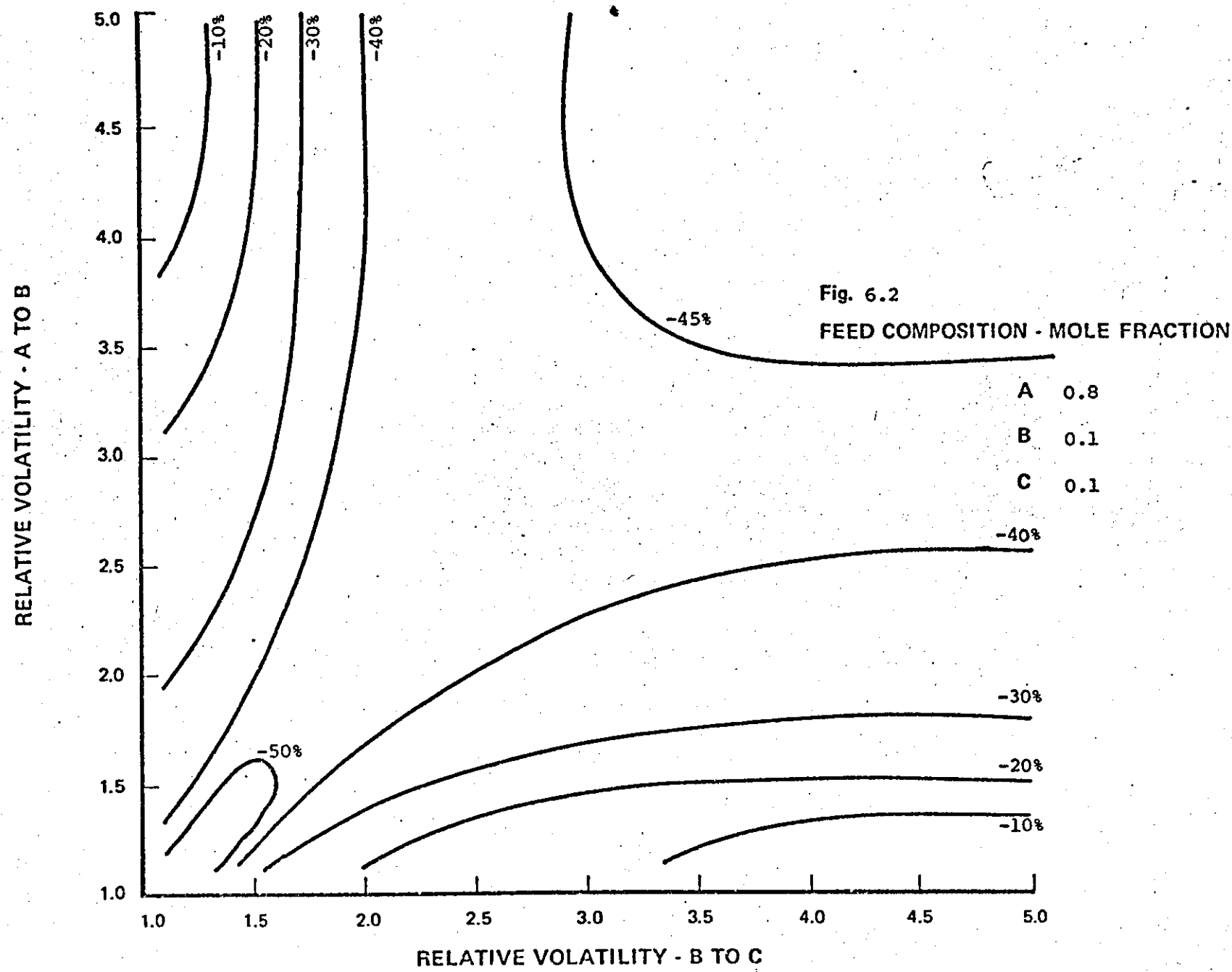
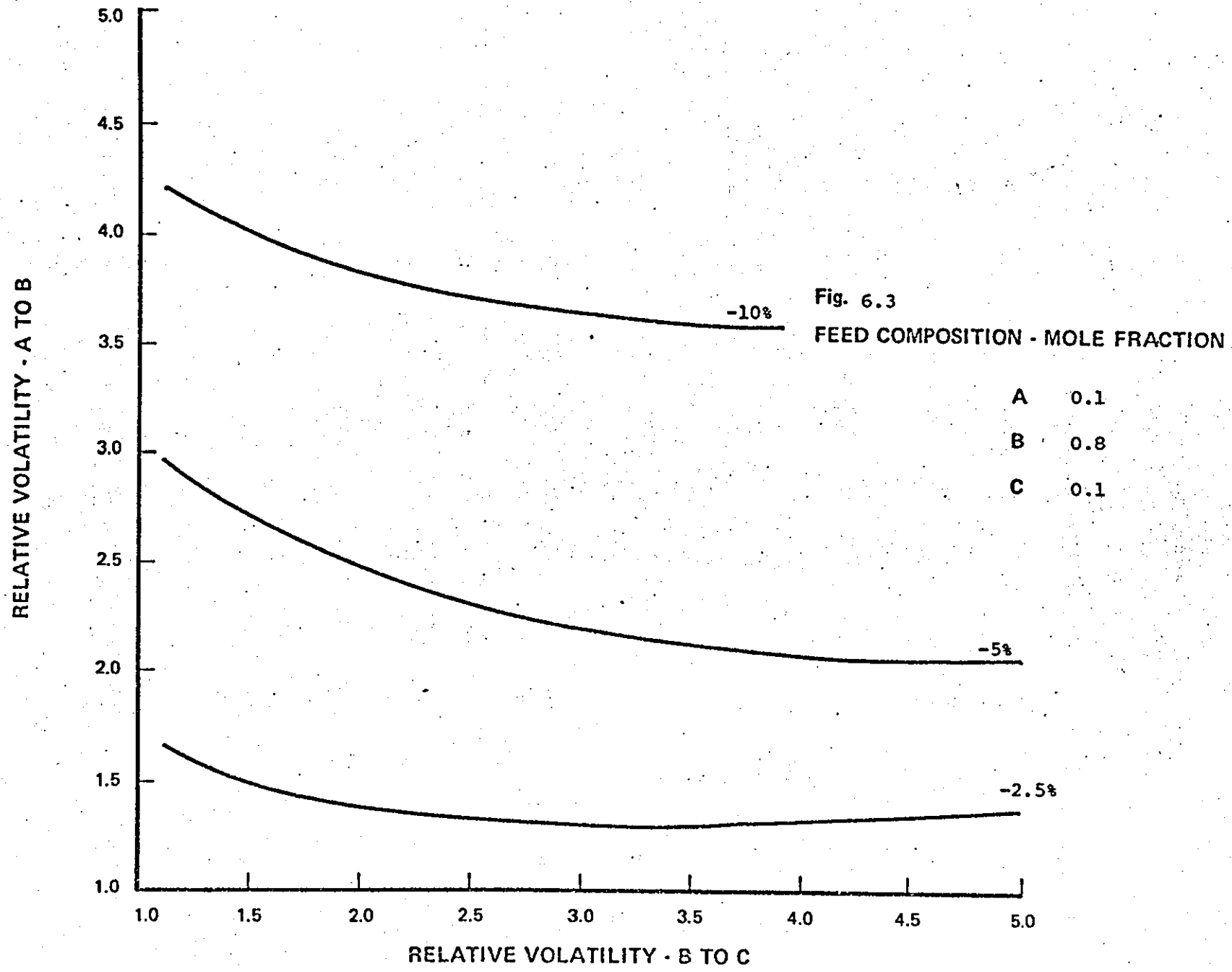


Fig. 6.1
 FEED COMPOSITION - MOLE FRACTION

- A 0.33
- B 0.33
- C 0.34





RELATIVE VOLATILITY - A TO B

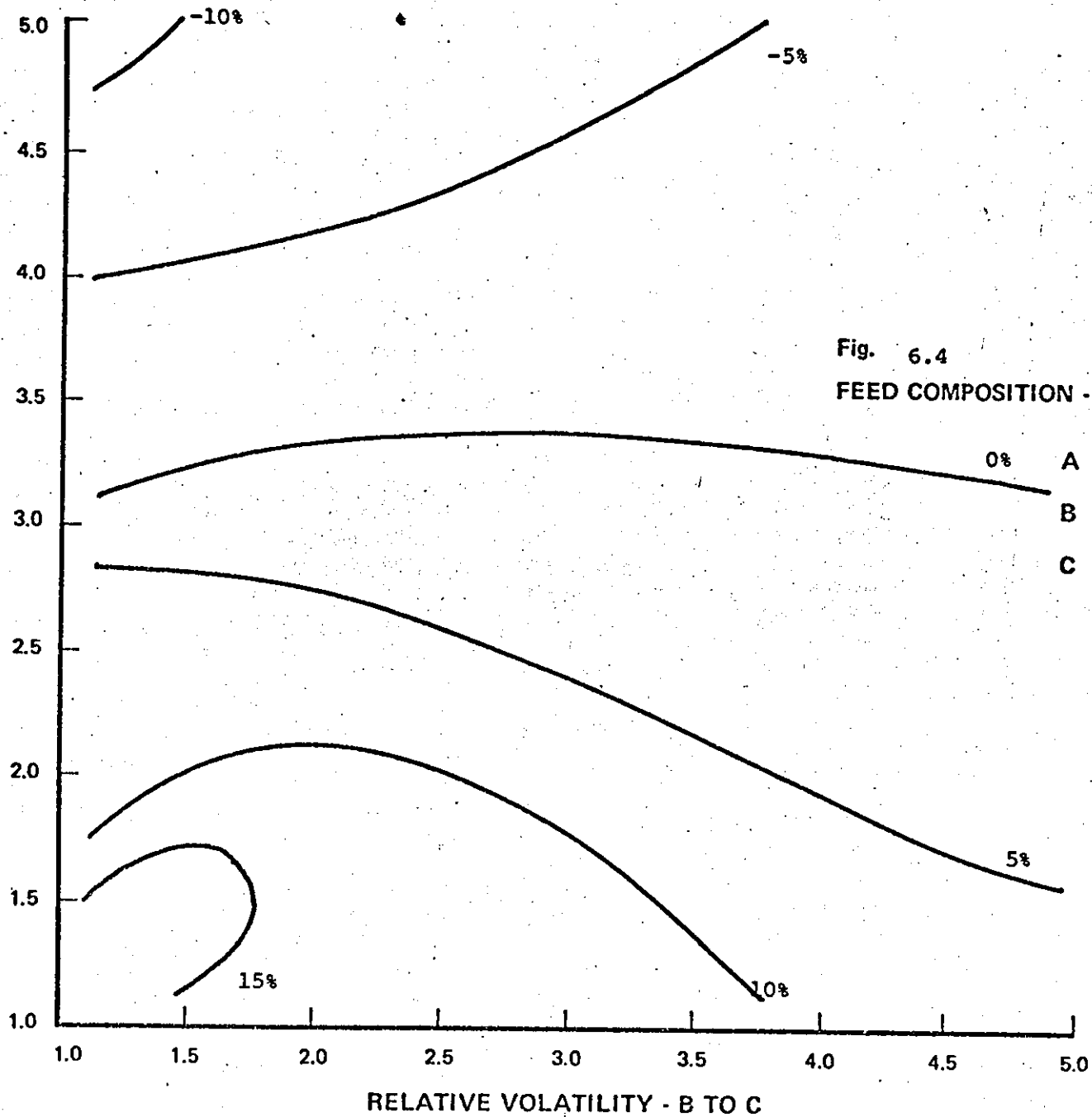
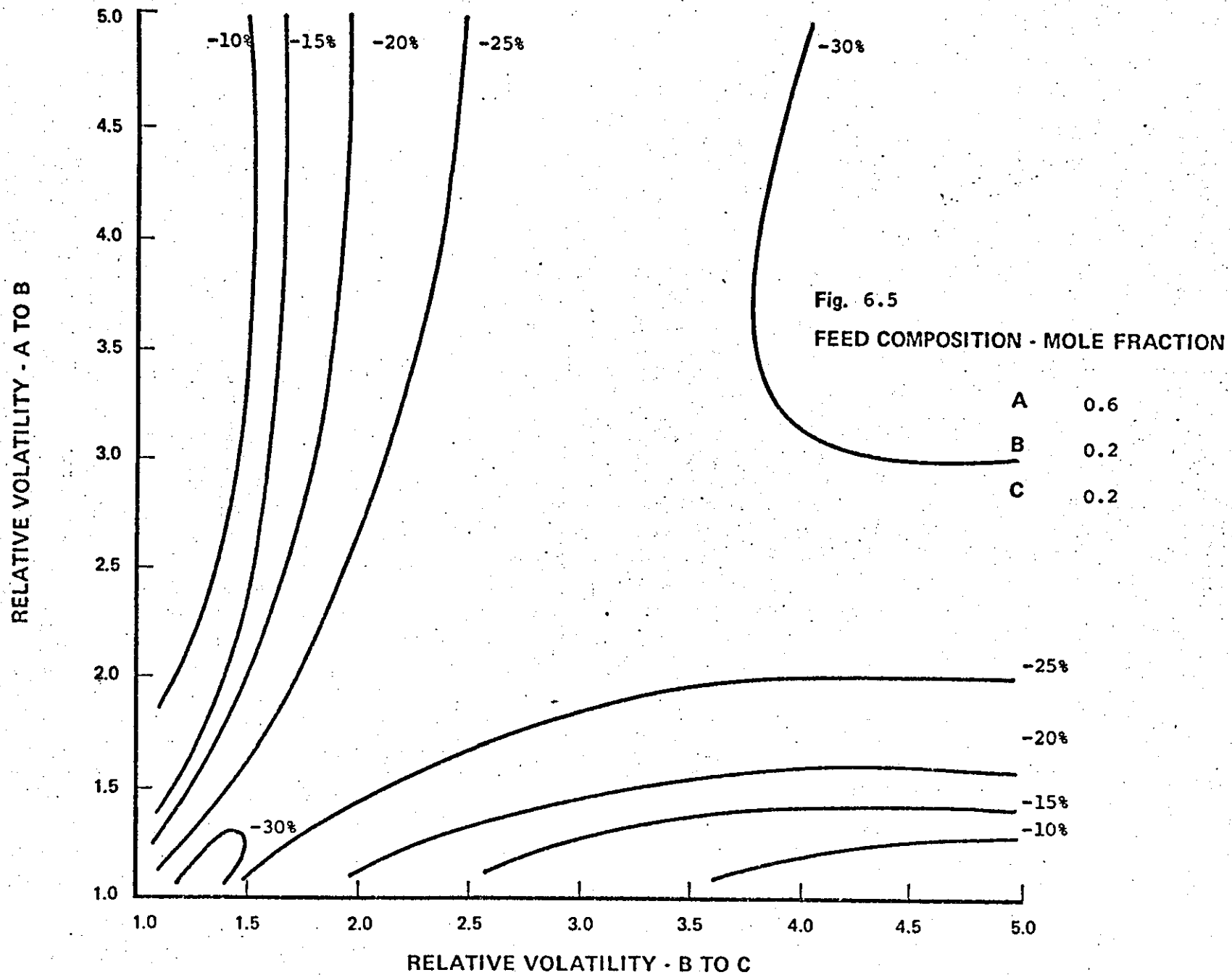


Fig. 6.4
FEED COMPOSITION - MOLE FRACTION

A	0.1
B	0.1
C	0.8



RELATIVE VOLATILITY - A TO B

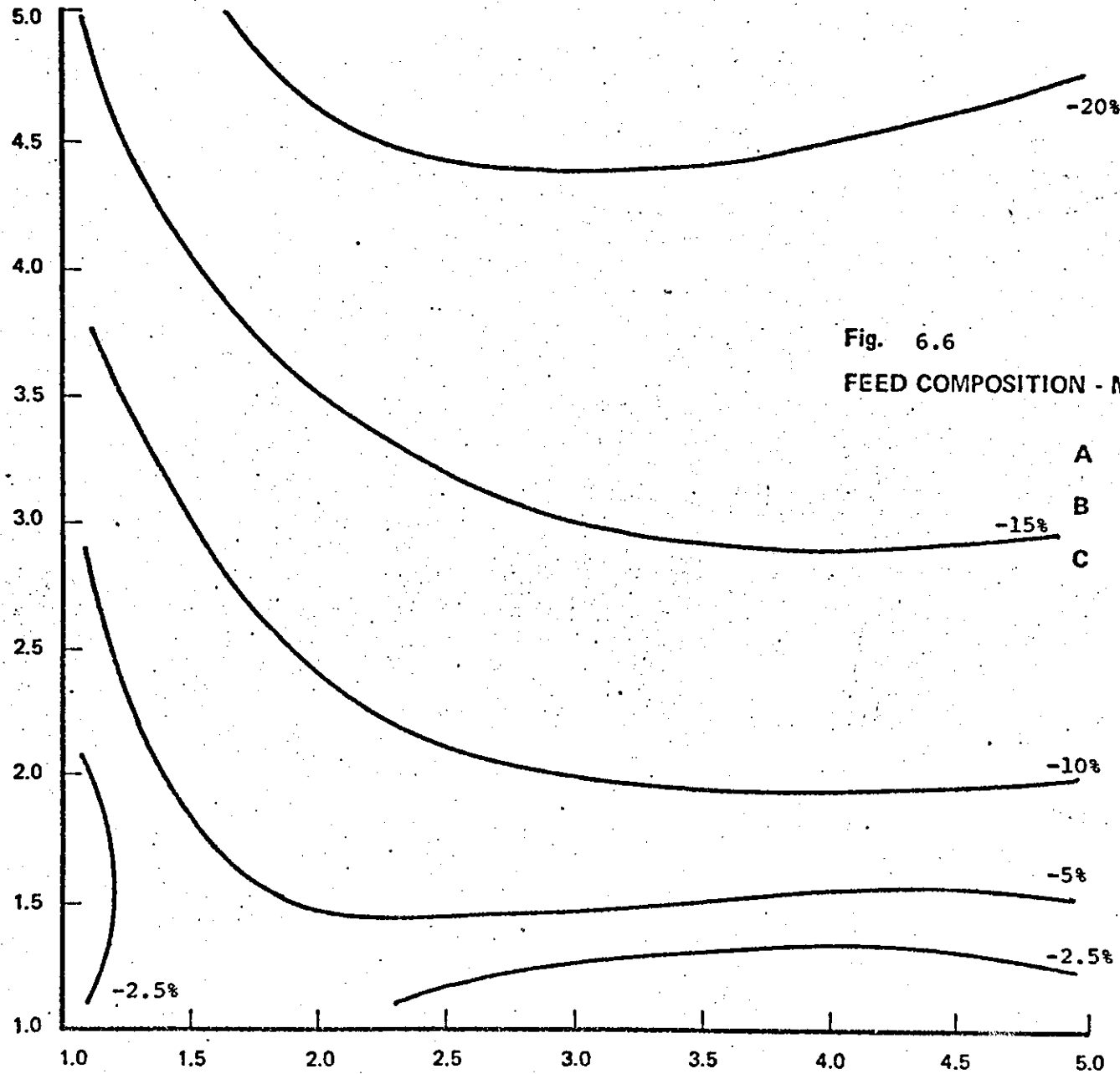
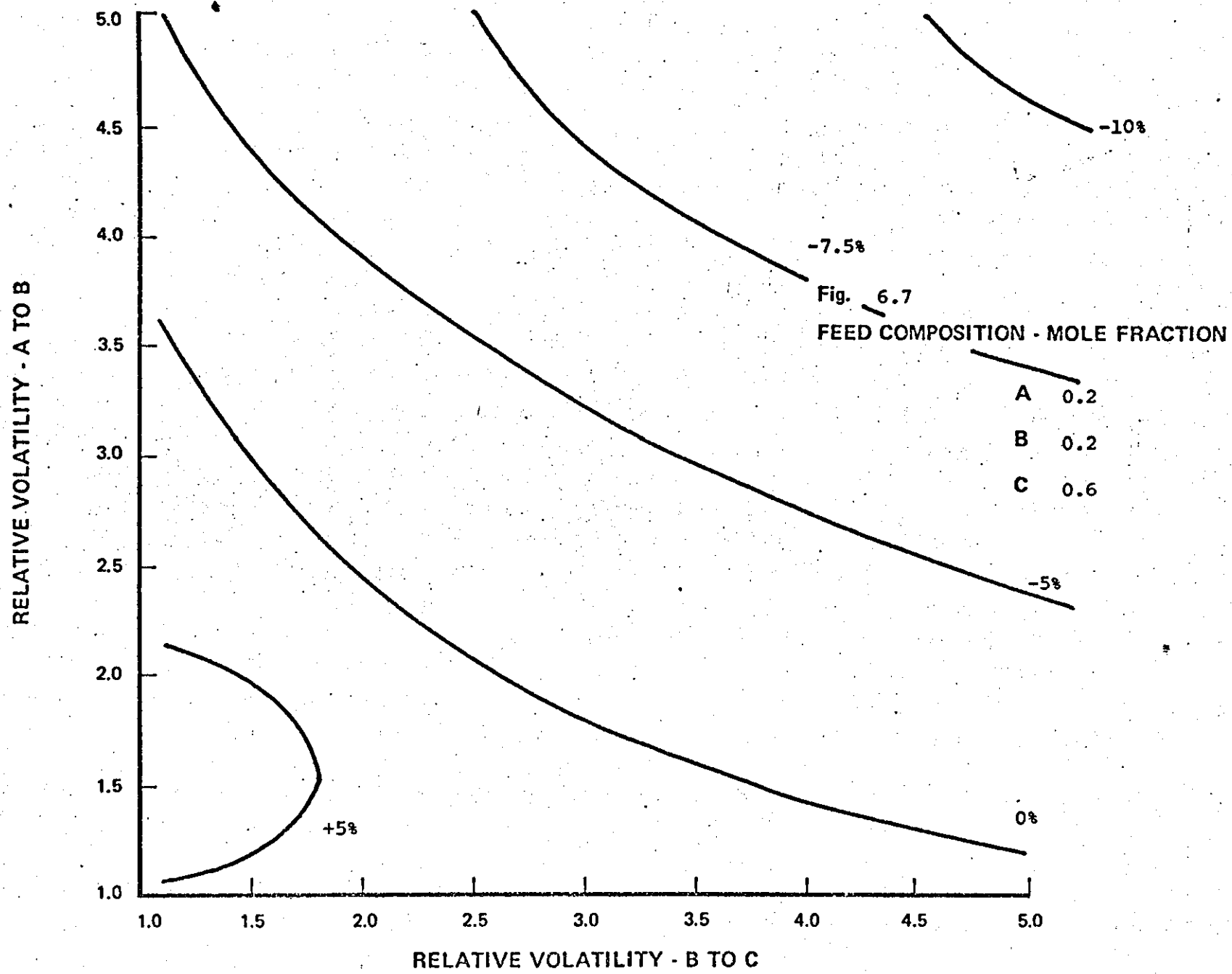


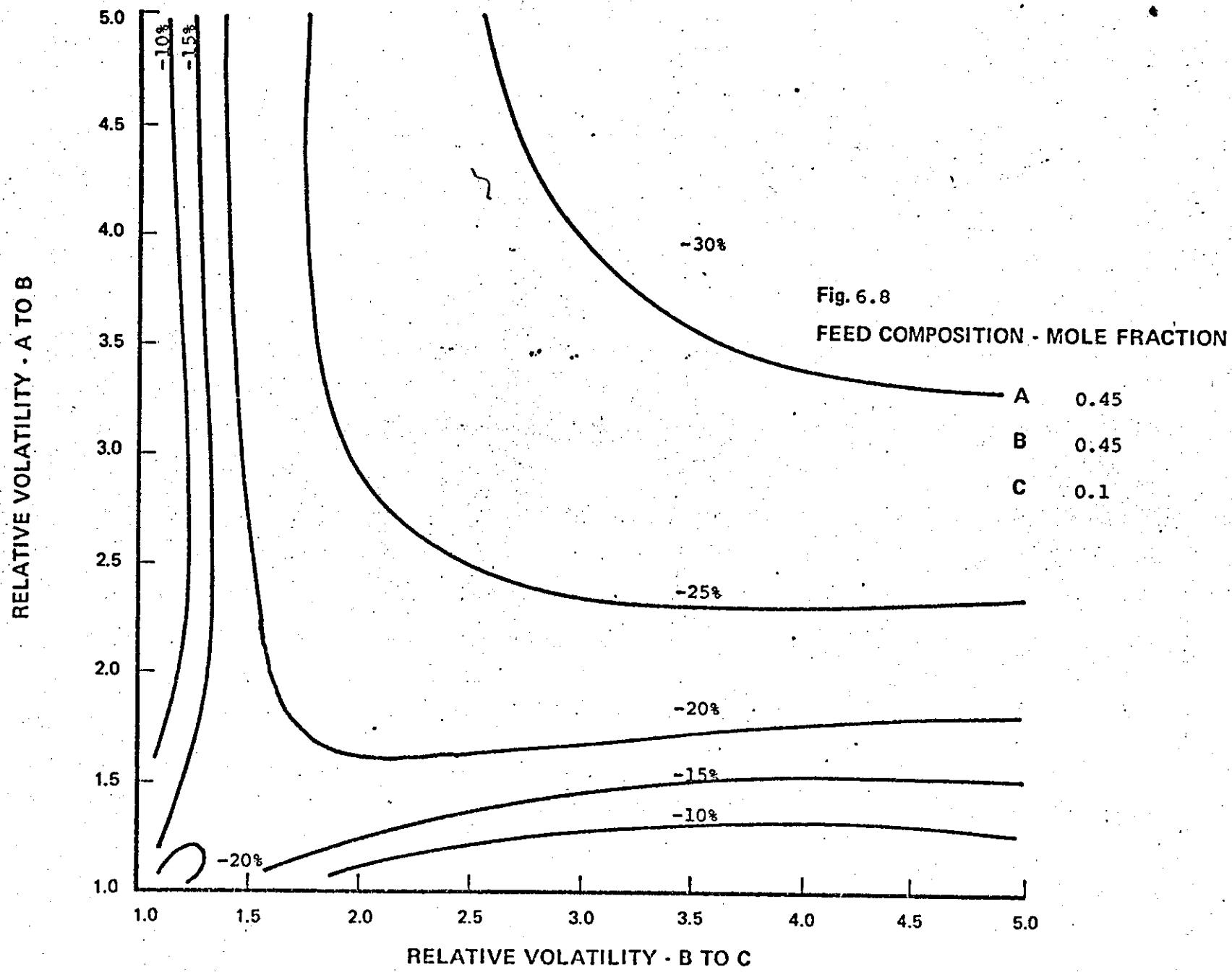
Fig. 6.6

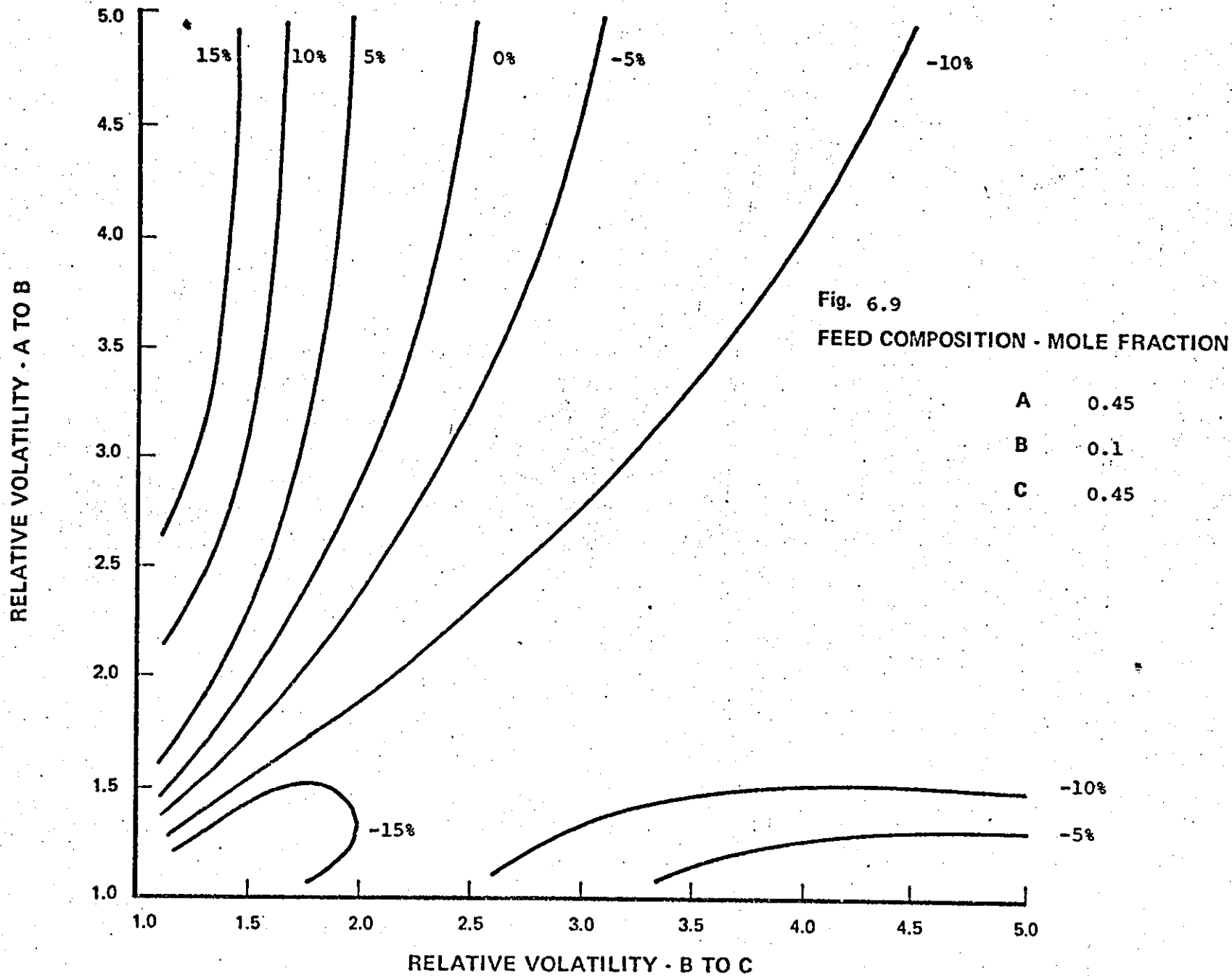
FEED COMPOSITION - MOLE FRACTION

A	0.2
B	0.6
C	0.2

RELATIVE VOLATILITY - B TO C







RELATIVE VOLATILITY - A TO B

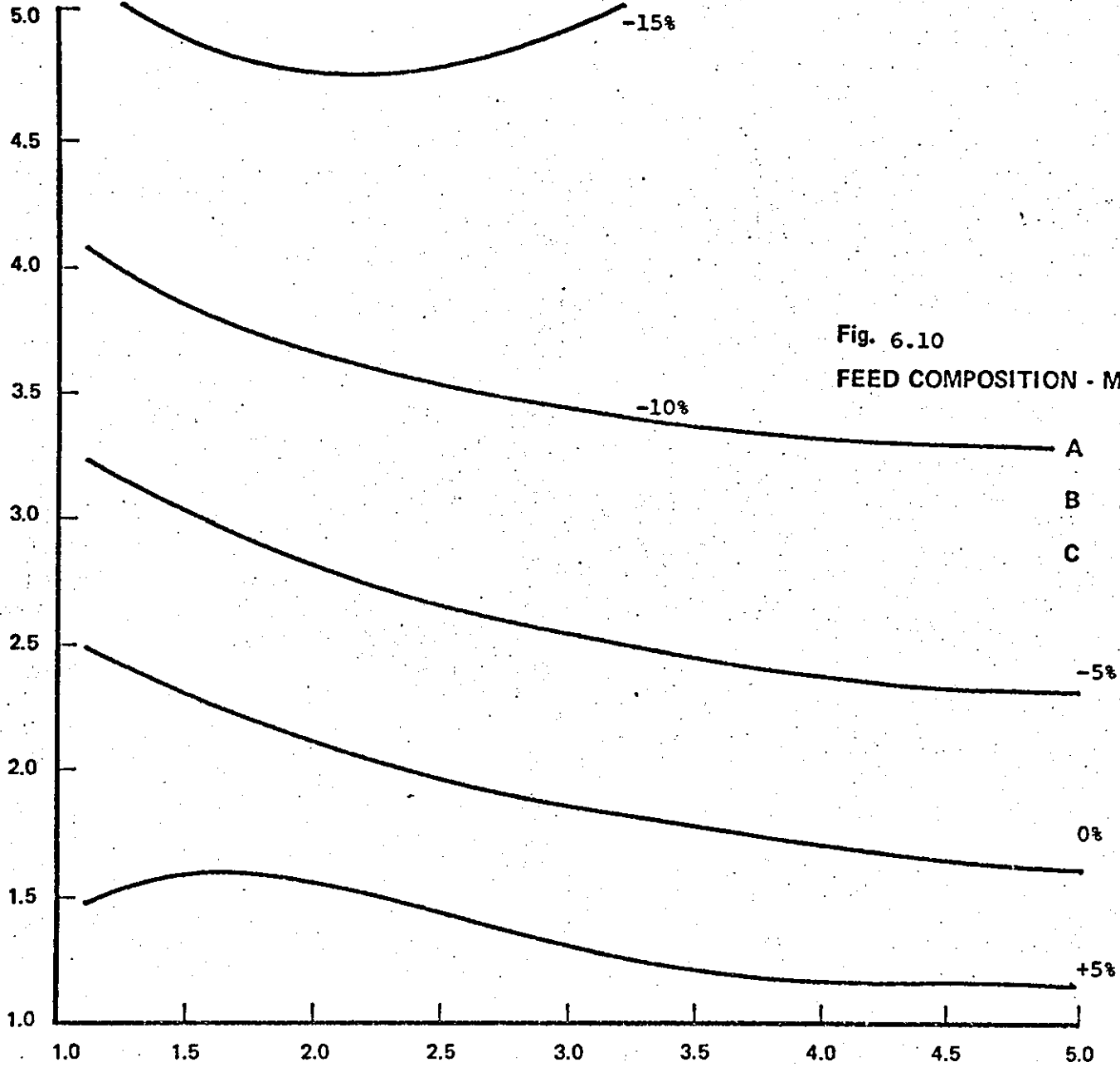


Fig. 6.10

FEED COMPOSITION - MOLE FRACTION

A 0.1
B 0.45
C 0.45

RELATIVE VOLATILITY - A TO B

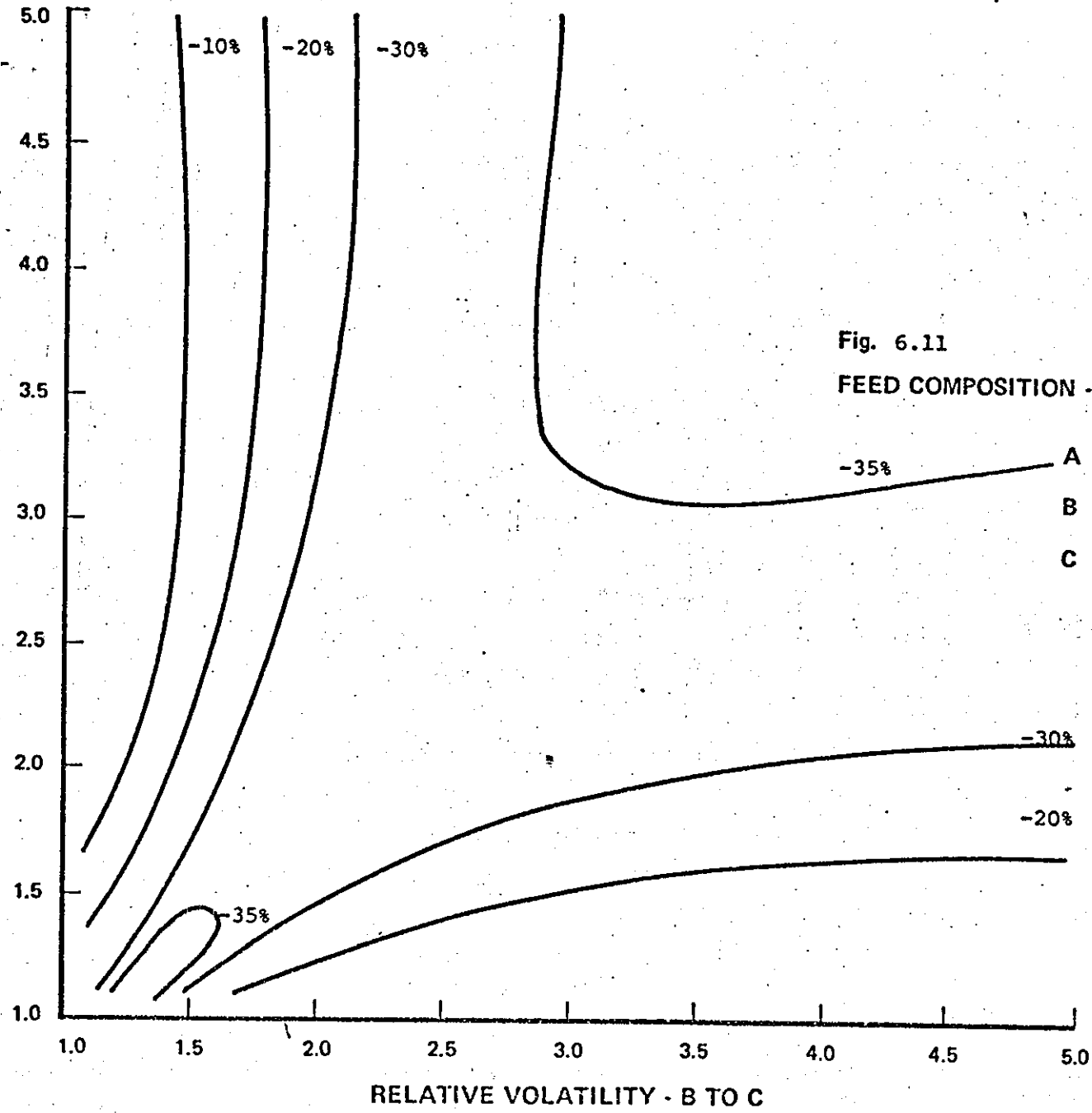


Fig. 6.11

FEED COMPOSITION - MOLE FRACTION

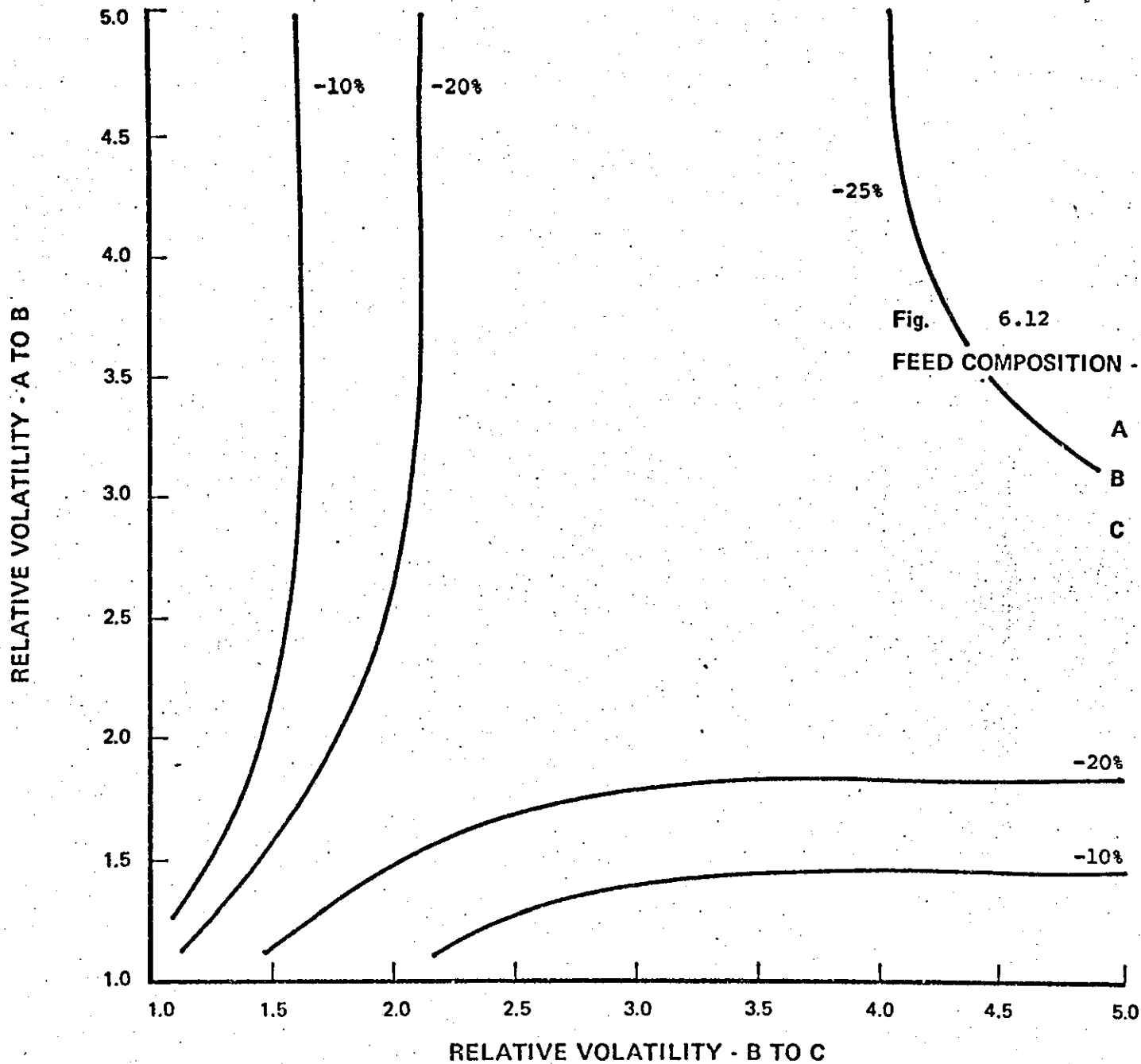


Fig. 6.12
FEED COMPOSITION - MOLE FRACTION

A 0.5
B 0.25
C 0.25

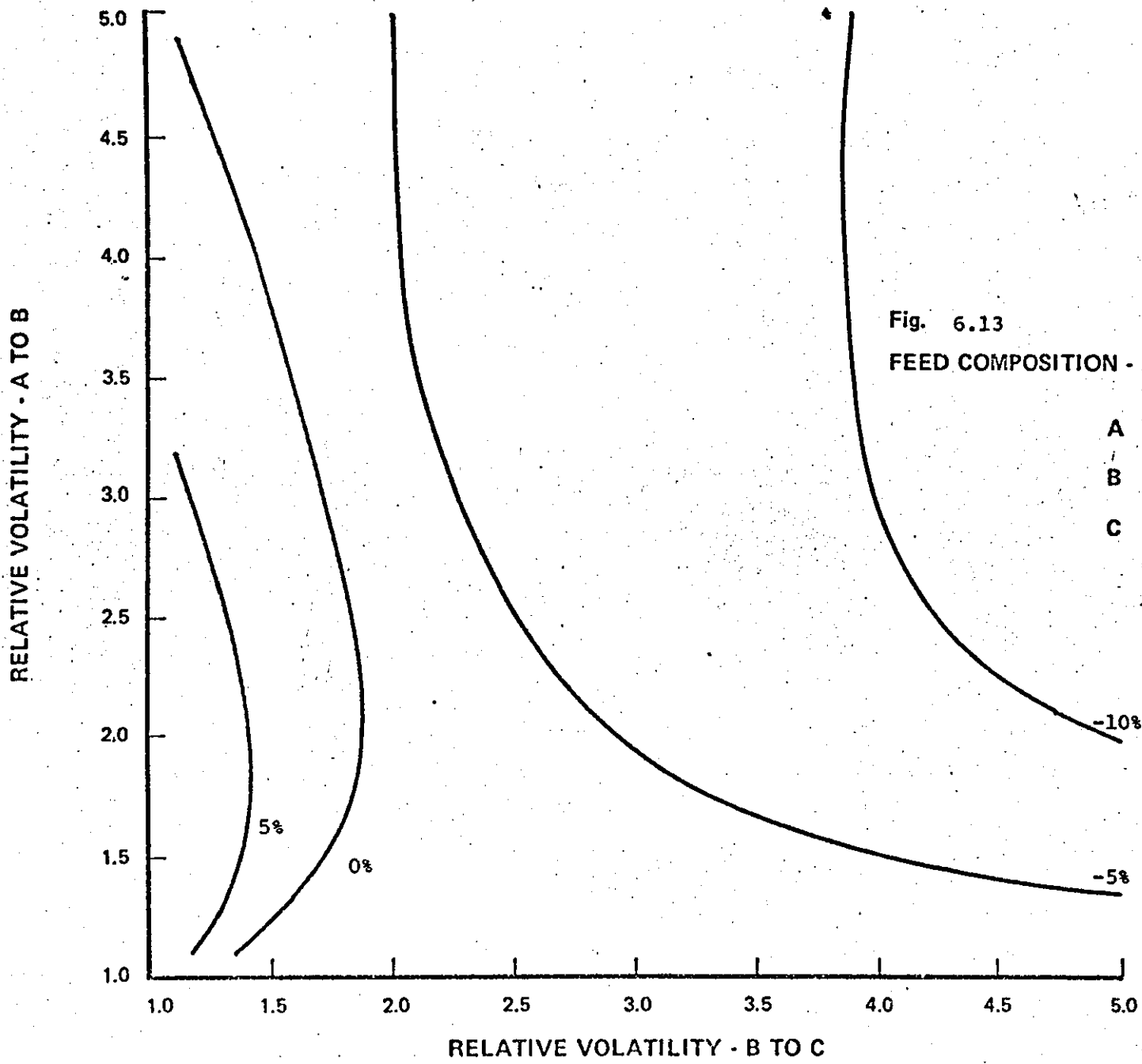


Fig. 6.13

FEED COMPOSITION - MOLE FRACTION

A	0.3
B	0.2
C	0.5

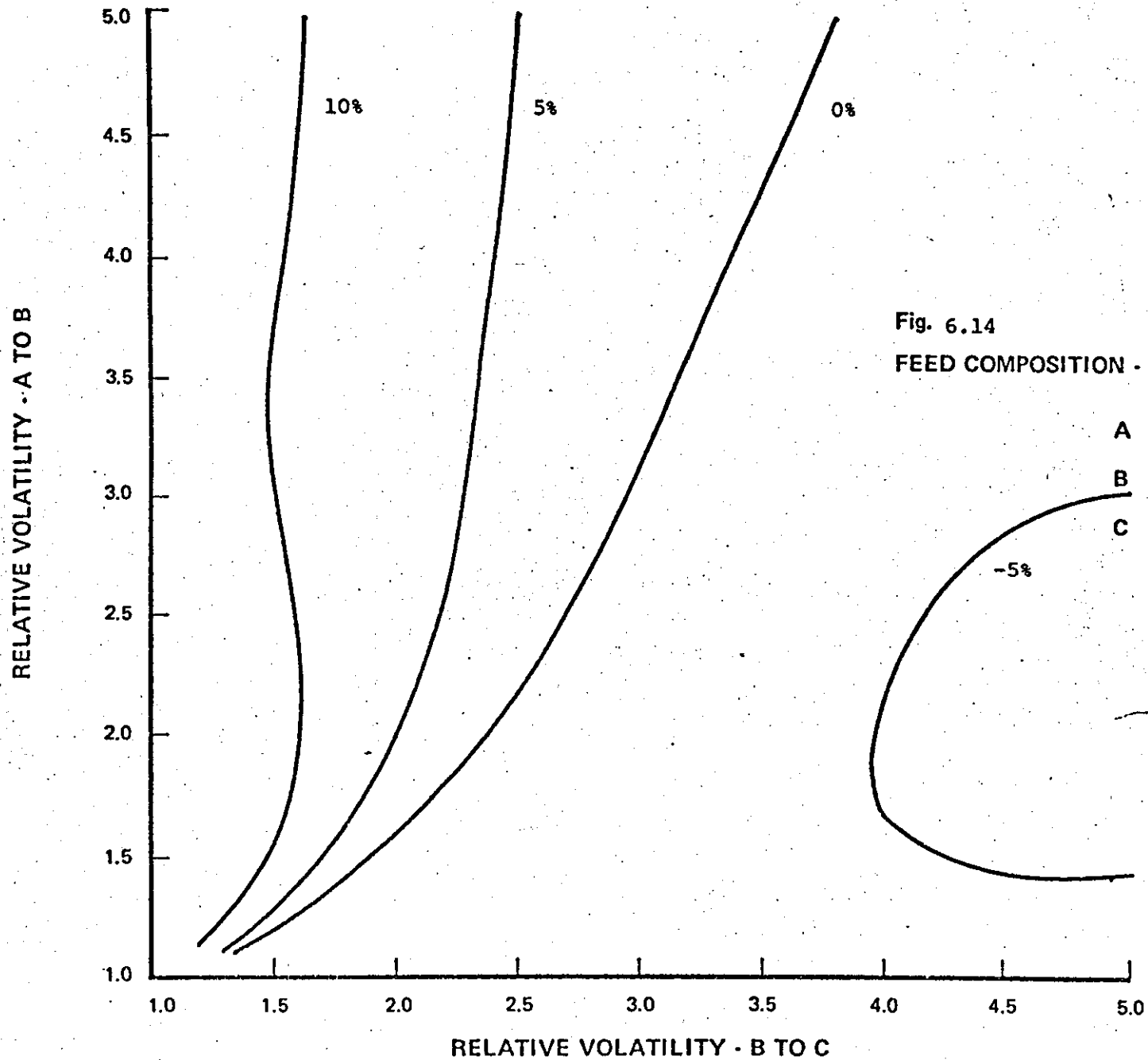


Fig. 6.14
 FEED COMPOSITION - MOLE FRACTION

A	0.3
B	0.1
C	0.6

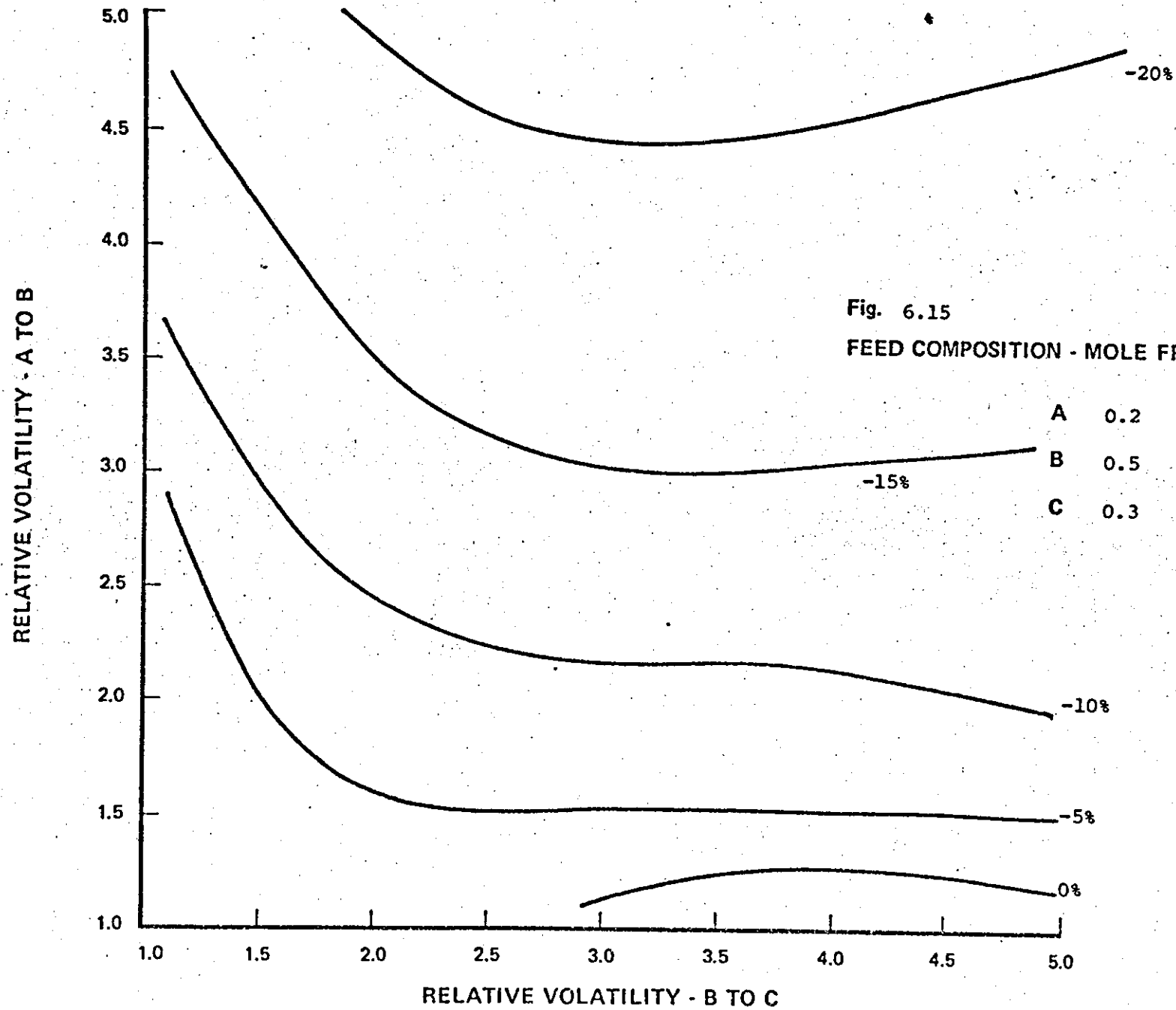
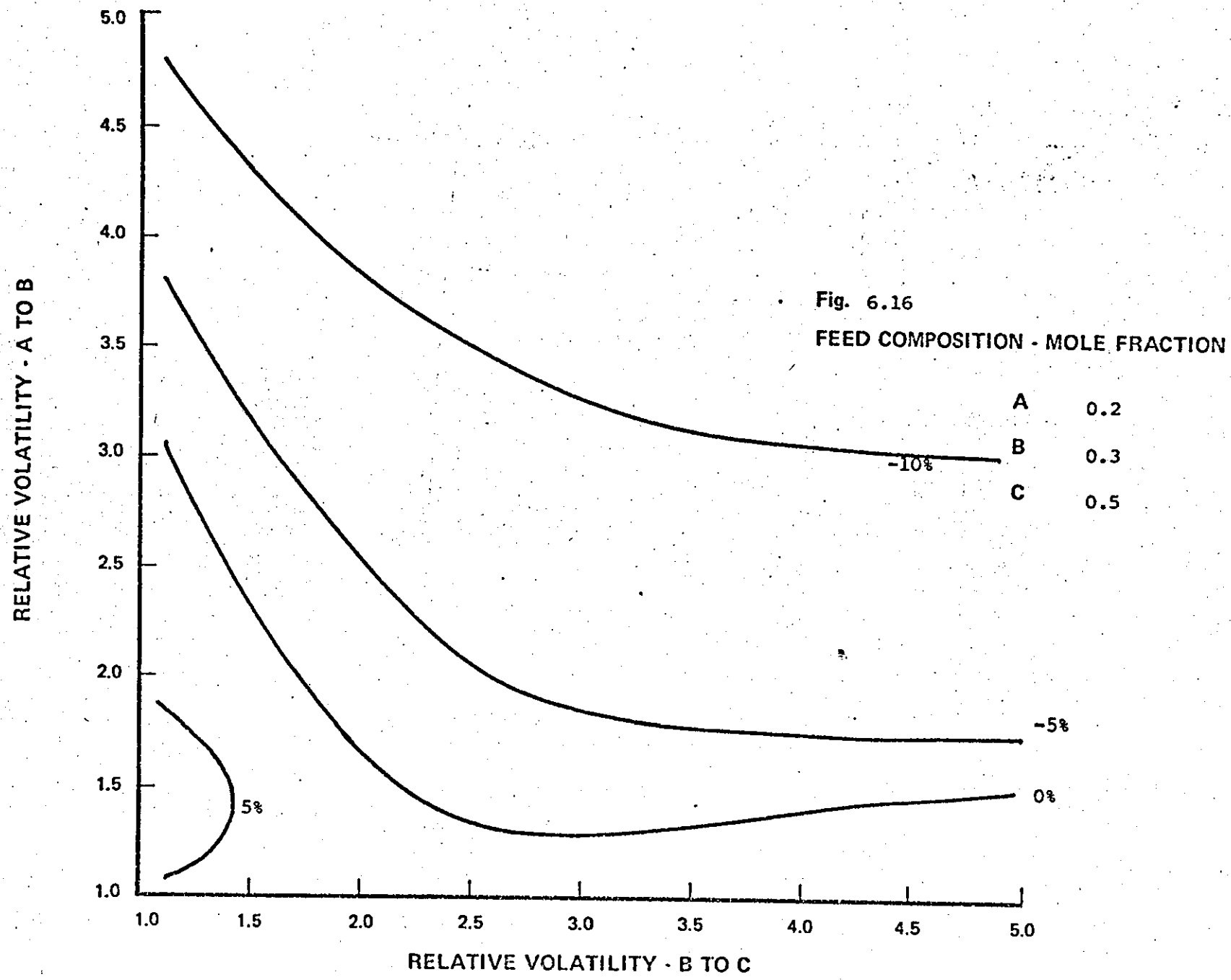


Fig. 6.15

FEED COMPOSITION - MOLE FRACTION

- A 0.2
- B 0.5
- C 0.3



RELATIVE VOLATILITY - A TO B

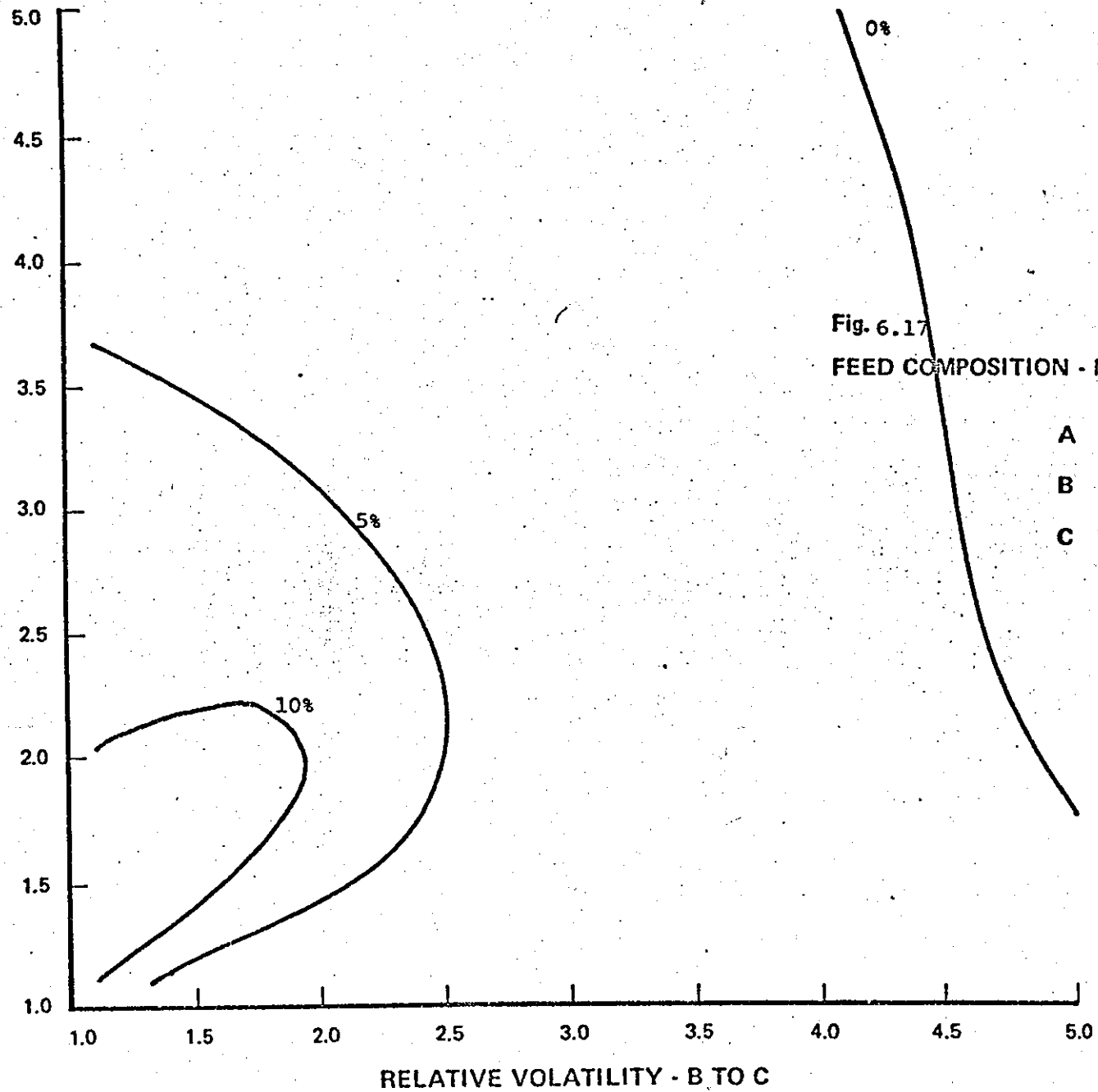


Fig. 6.17

FEED COMPOSITION - MOLE FRACTION

A	0.2
B	0.1
C	0.7

RELATIVE VOLATILITY - A TO B

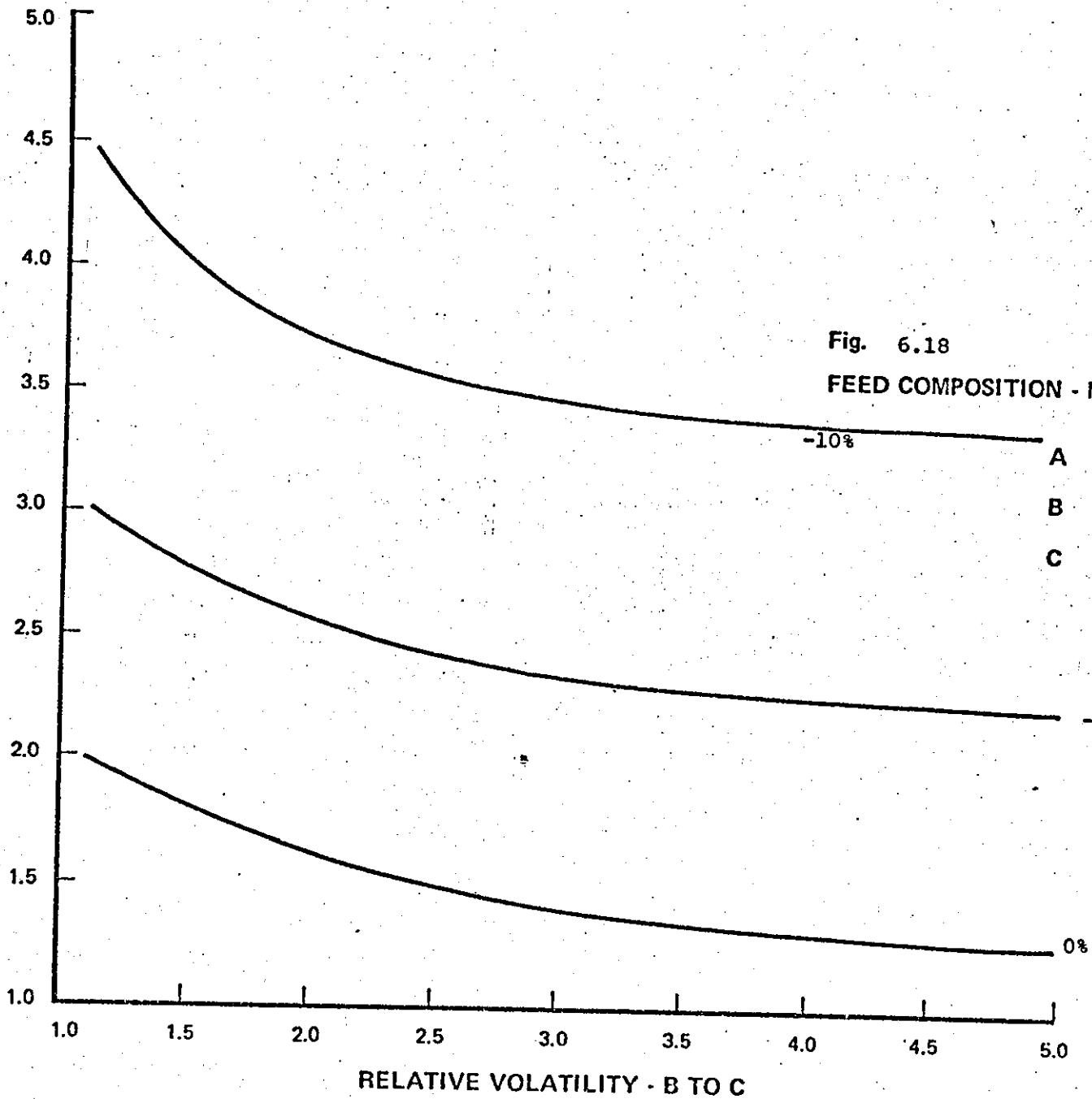


Fig. 6.18

FEED COMPOSITION - MOLE FRACTION

A 0.1
B 0.6
C 0.3

RELATIVE VOLATILITY - A TO B

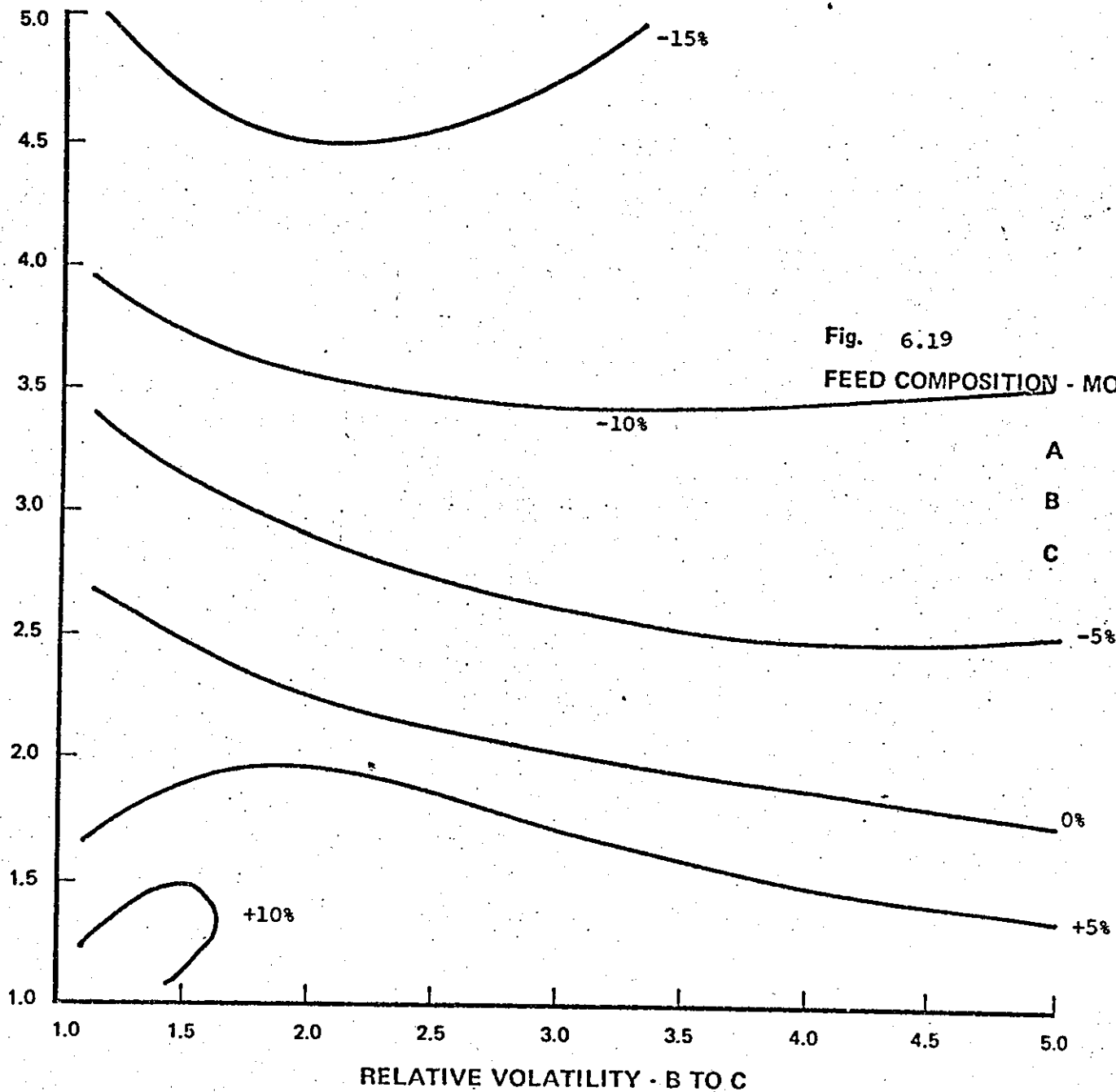


Fig. 6.19

FEED COMPOSITION - MOLE FRACTION

A 0.1
B 0.3
C 0.6

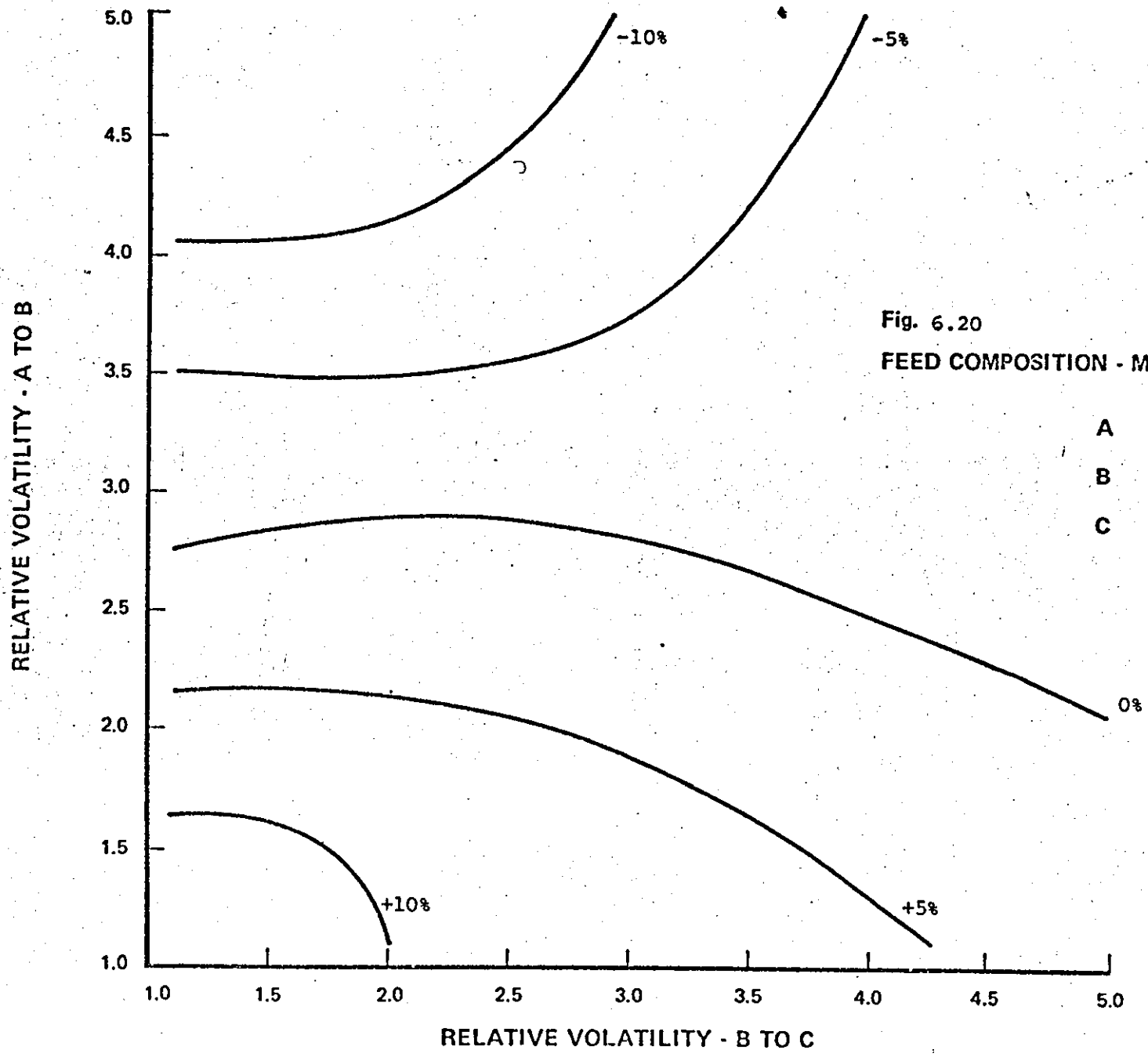


Fig. 6.20
 FEED COMPOSITION - MOLE FRACTION

A	0.1
B	0.2
C	0.7

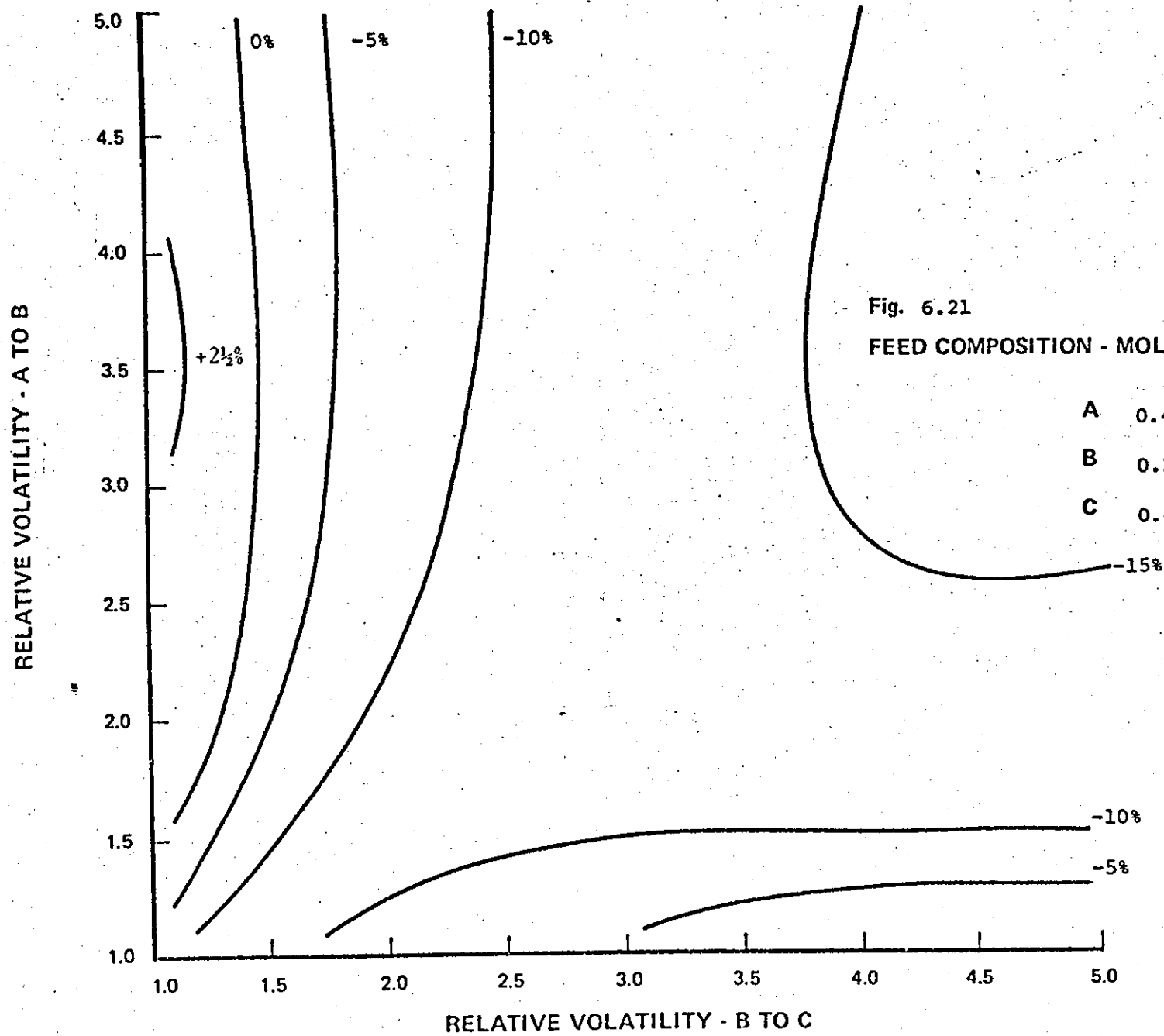


Fig. 6.21
 FEED COMPOSITION - MOLE FRACTION

A	0.4
B	0.2
C	0.4

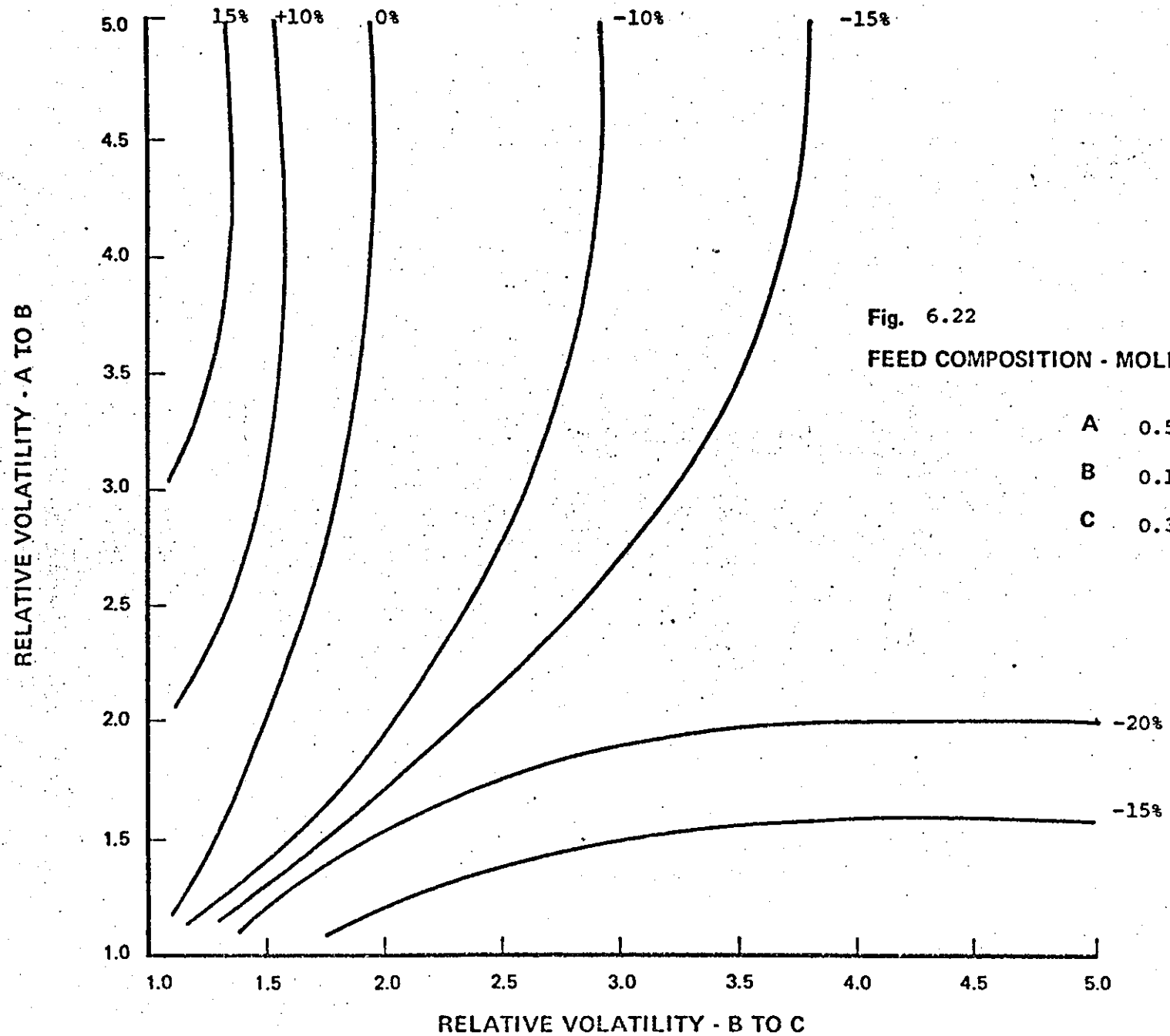


Fig. 6.22

FEED COMPOSITION - MOLE FRACTION

- A 0.55
- B 0.1
- C 0.35

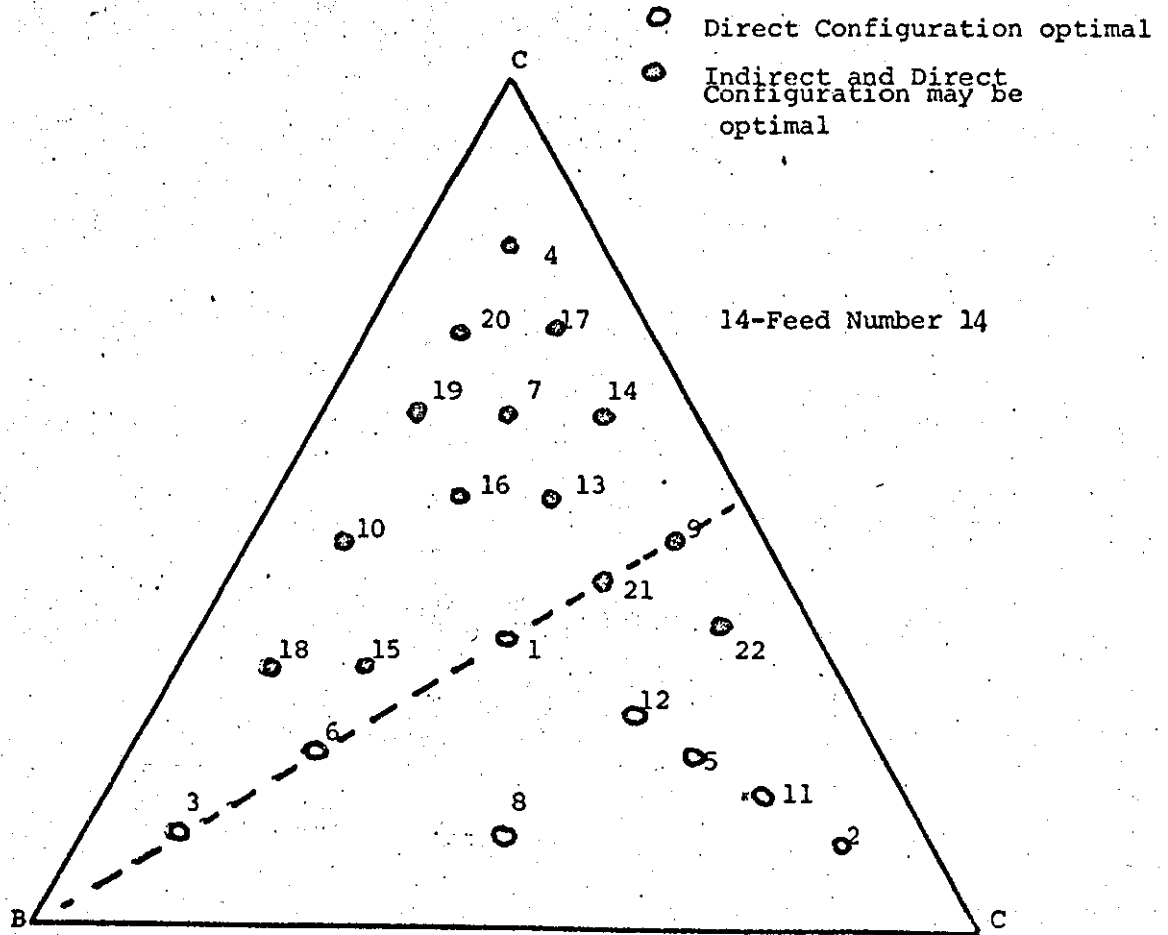
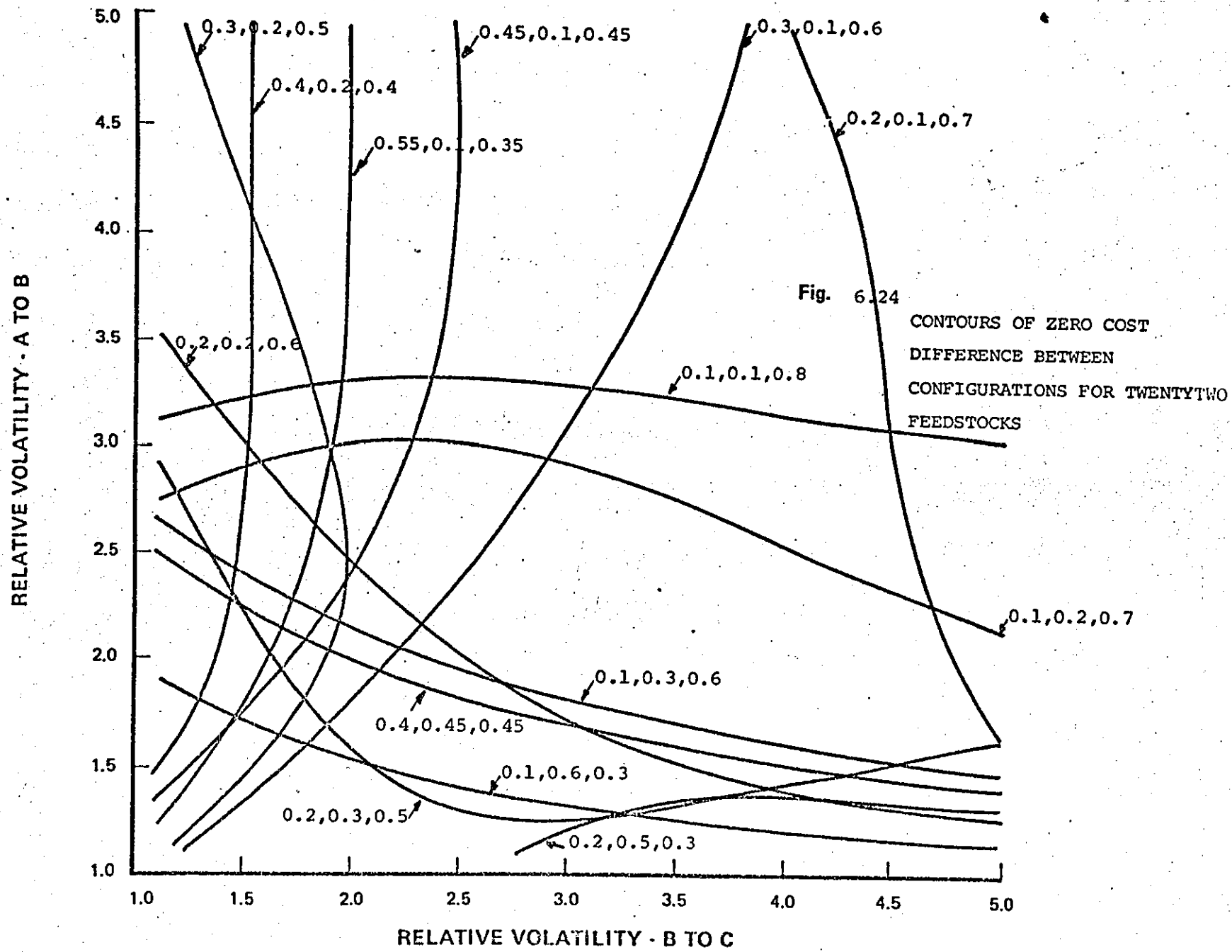


FIGURE 6.23 - Regions in which each configuration is optimal



It is noted that the indirect configuration can be optimal in the region below the line through the composition points (0.1,0.8,0.1) and (0.45,0.1,0.45) as indicated by the broken line in Figure 6.23. Rod and Marek's results indicated that the indirect configuration was not optimal below this line. The results of this thesis have shown that at the point (0.45,0.1,0.45) (refer Figure 6.9) the indirect configuration can be optimal depending upon the values of the relative volatilities of the feedstock. The two feedstocks given by feed numbers 21 and 22 also show that the indirect configuration can be optimal in the region below this line.

In Figure 6.24, contours of zero percentage difference between configurations are drawn for those feed compositions in which either the direct or indirect configuration can be optimal. The region in which the indirect configuration is optimal is below the contour of zero percentage difference in all cases except for contours representing the feed compositions (0.3,0.2,0.5), (0.45,0.1,0.45), (0.3,0.1,0.6) and (0.2,0.1,0.7) in which case the indirect configuration is optimal in the region to the left of the zero percentage difference contour.

The Figures 6.1 to 6.22 together with 6.23 or 6.24 provide a new method by which the selection of the optimal configuration for three component feedstocks can be predicted. The method is applicable to feedstocks having relative volatilities between the two pair of components in the range of 1.1 to 5.0. The method requires reading of two charts:- firstly reference to Figure 6.23 or 6.24 shows, for the given feed composition and component volatilities, whether the direct or indirect configuration will be optimal. Secondly, the size of the percentage difference between the two configurations and hence the benefit to be realised by the selection of the optimal configuration

can be obtained from the figure within the series of graphs 6.1 to 6.22, corresponding to the given feed composition.

The charts provide the required illustration of the interaction of the influence of relative volatility and feed composition. That is, they provide quantitative data of the values of the concentration of a component and the relative volatility of a difficult separation at which either will decide the optimal configuration. Consequently they resolve the conflict in the choice of the heuristics when one component of a difficult pair of components is the dominant component in the feedstock.

Further observations which can be made from the figures are:-

(i) Equimolar feedstocks always gave the direct configuration as the optimal configuration. The trends of the values of the percentage difference when plotted, did however indicate that at very low values of relative volatility, that is, below 1.1, the difference between configurations was negligible. They also indicate that the contour of zero percentage difference might occur in this region. In fact, values indicated that in these regions the indirect configuration could be slightly optimal.

(ii) For a feed containing 0.8 mole fraction of the lightest component, the early removal of this component was confirmed.

In no instance was the indirect configuration optimal. The lowering of the value of relative volatility between either pairs of components lowered the percentage difference between configurations but not sufficiently to make the indirect configuration optimal. Figure 6.25 has been included to show the effect of varying the amounts of the lightest component in a feedstock in which the relative volatilities between each pair of components are equal, thus neglecting the effect of component volatility. Components B and C were present in equal amounts in these feedstocks.

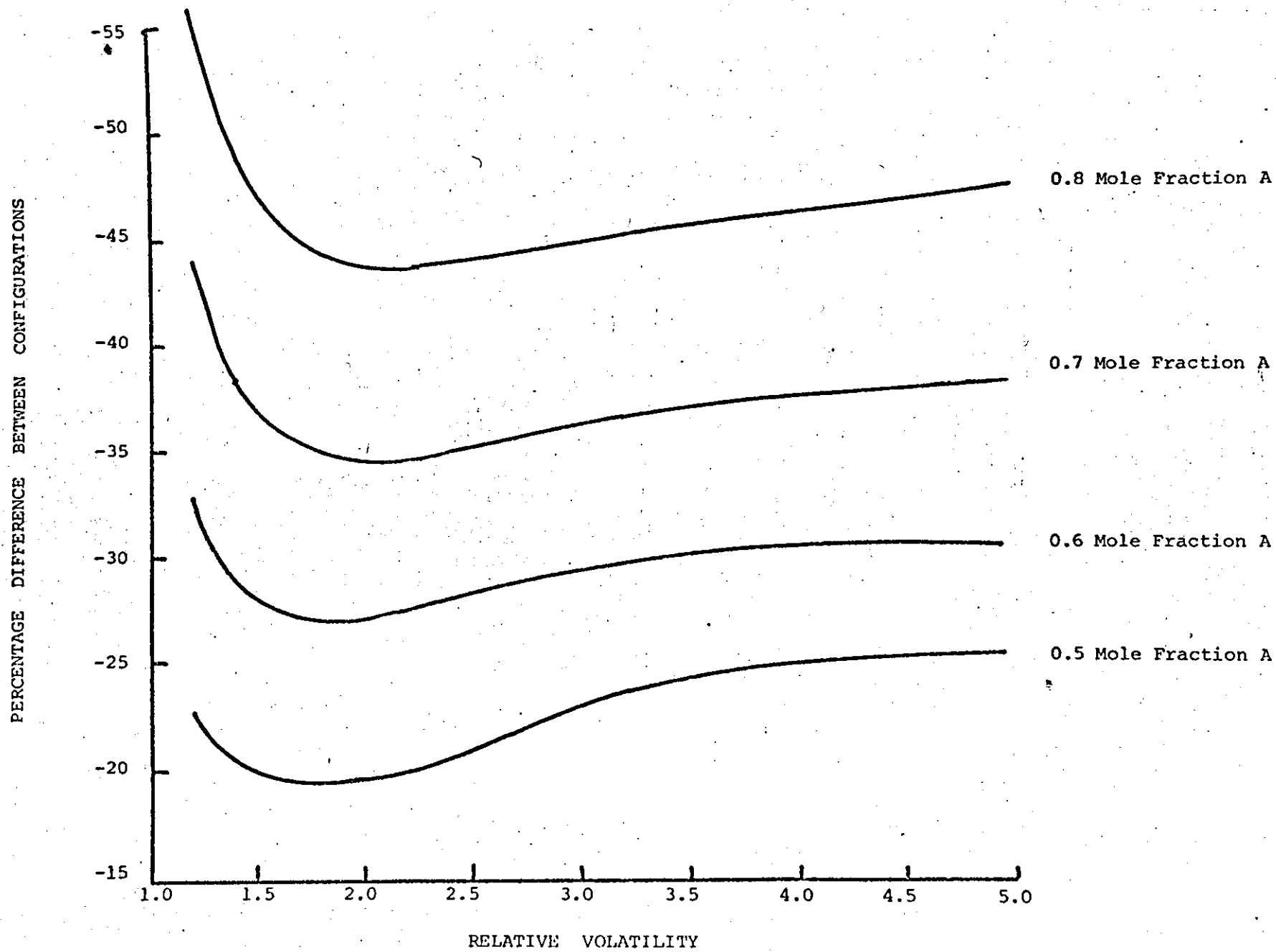


FIGURE 6.25 - Effect of Varying Amounts of Component A

In the case of the heaviest component being the predominant component in the feedstock, it is noted that its early removal is only valid when the relative volatility between the two lightest components is below a particular value. For example, Figure 6.4 shows that for a feed composition in which the heaviest component has a mole fraction of 0.8, then the relative volatility between Component B and C does not influence the selection of the optimal configuration. However in Figure 6.7 in which the mole fraction of component C is 0.6 both relative volatilities influence the selection of the optimal configuration.

6.3 Use of Indices for the Prediction of Optimal Configurations

Two indices have been proposed in the literature for the prediction of the optimal configuration for three component feedstocks. Both indices are expressed only in terms of the two relative volatilities, that is between components A and B and between B and C.

Rudd and Tedder's index, as discussed in Chapter 1, gave a measure of the relative difficulty of the two separations, that is, between A and B and between B and C. A value less than 1.0 indicates that the separation between A and B is more difficult and a value greater than 1.0 indicates that the separation between B and C is more difficult. As discussed previously, the index does not consider the actual value of the relative volatility. This aspect was investigated in this thesis by considering a range of three component feedstocks each having equal volatilities between A and B and between B and C of the following values:- 1.1, 1.35, 1.5, 1.75, 2.0, 2.5, 3.0, 3.5, 4.0, 4.5, 5.0. The percentage difference between the two configurations calculated for each feed is given in Figure 6.26. From this figure it will be noted that the percentage difference between the two configurations increases as the value of the

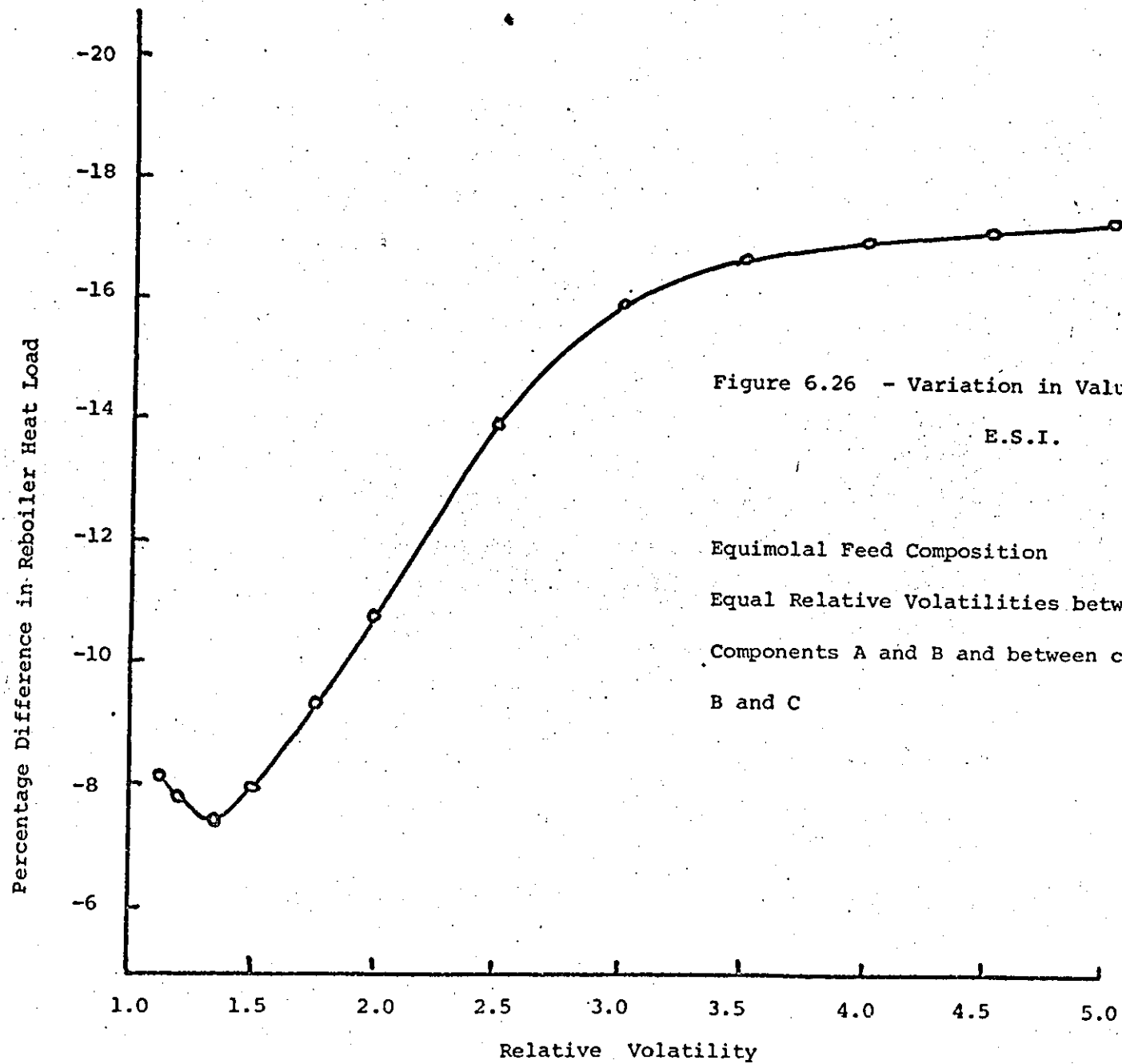


Figure 6.26 - Variation in Value of
E.S.I.

Equimolal Feed Composition
Equal Relative Volatilities between
Components A and B and between components
B and C

relative volatility increases. The contours of zero percentage difference for a number of values of the relative volatility used are plotted on triangular co-ordinates in Figure 6.27.

Figure 6.27 shows that for feedstocks having equal relative volatilities between each pair of components or an E.S.I of 1.0, then as the value of the relative volatility between each pair of components increases, the region in which the direct configuration is optimal increases. For example, for feedstocks having equal relative volatilities of 3.0, the indirect configuration is optimal only for feed numbers 4 and 17. These results would therefore confirm the inadequacy of indices of the type proposed by Rudd and Tedder.

The value of Heaven's index obtained for the feedstocks used by Rudd and Tedder have been included in Table 6.2. As this index too is based only upon relative volatility terms, it is claimed that this index has limitations similar to the index proposed by Rudd and Tedder.

The development of an index was considered in this thesis. A large number of indices were proposed containing the two relative volatility values together with at least two composition values for a three component feedstock. Despite the large number of combinations considered, it was not possible to develop an index which could predict the regions on a triangular composition diagram in which either configuration would be optimal.

6.4 Effect of Component Degree of Recovery

The effect of component degree of recovery was also considered in this study of pseudo-components. This was done by considering a range of values of the degree of recovery of 90, 92.5, 95, 97.5 and 99% for all components. The equimolar feedstock was used and the percentage

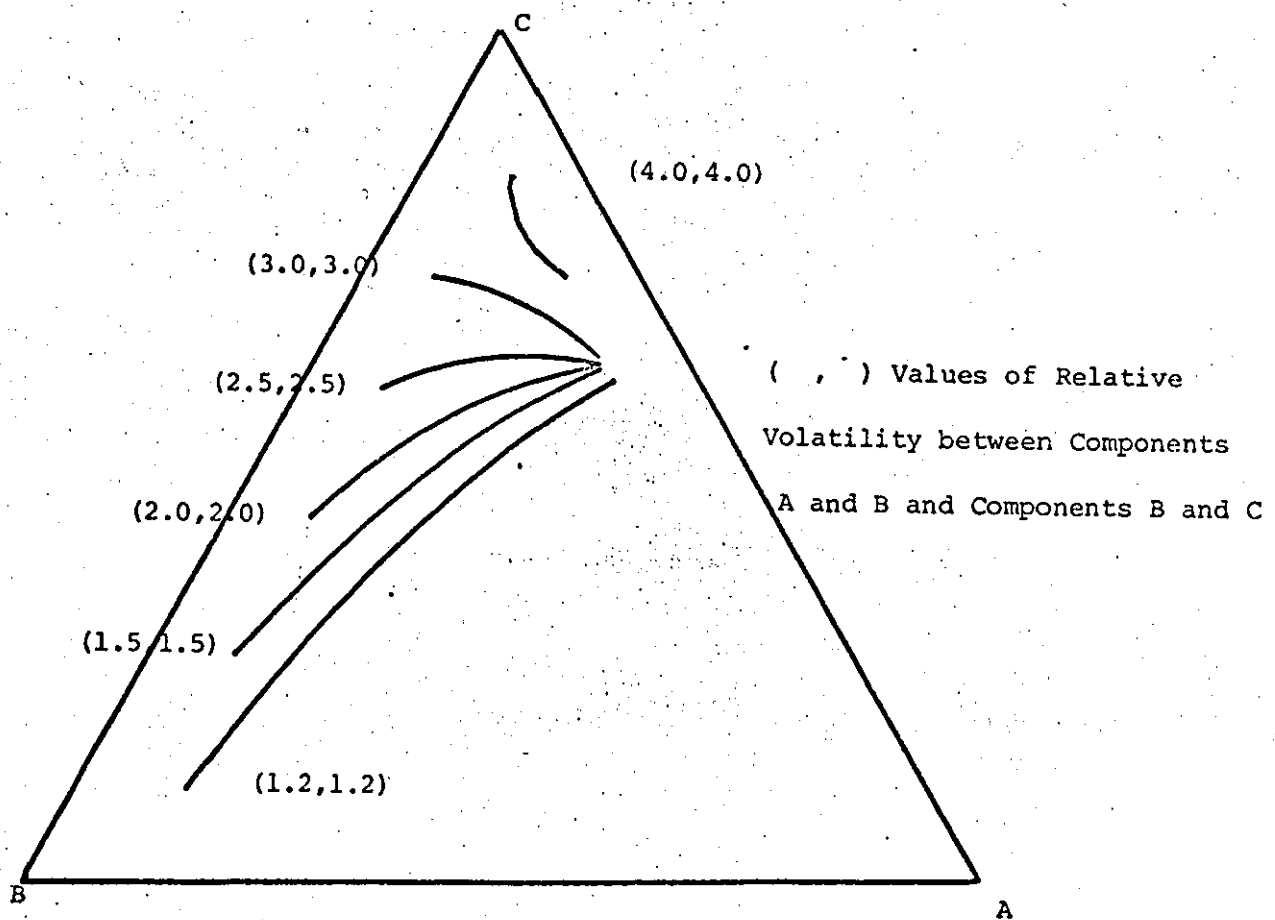


FIGURE 6.27 - Zero Percentage Difference Contours
for Feedstocks having Equal Relative
Volatilities between both pairs of
Components

difference in the configurations calculated for the range of relative volatilities of 1.1 to 5.0.

The results obtained were in accordance with the previous conclusions reached in Chapter 3. The higher the component degree of recovery, the higher the cost of the separation. The percentage difference between configurations did not increase proportionately with the increase in the degree of recovery. However, the shape of the zero percentage difference contours was identical to the results given in Figure 6.1 which were based on a 95% degree of recovery of all components.

6.5 Comparison of Results

Before comparing the results of Rudd and Tedder and the results of this thesis, the effect of different data used in each study was considered. It was only possible to consider the effect of different 'K' value data. The corresponding values of the E.S.I, Heaven's Index and K_A/K_C using the 'K' data used in this thesis are given in Table 6.1. The agreement between both sets of results for the values of E.S.I and H.I are considered satisfactory.

TABLE 6.1 Values of Indices for Feedstocks used by Rudd and Tedder.

Feed No.	Components	K_A/K_C		H.I.		E.S.I	
		Tedder	Henry	Tedder	Henry	Tedder	Henry
1	nC5,nC6,nC7	6.35	3.56	0.27	0.33	1.04	1.02
2	nC4,ic5,nC5	3.04	2.34	0.14	0.12	1.86	1.71
3	ic4,nC4,nC6	10.22	7.92	0.71	0.73	0.18	0.22
4	ic5,nC5,nC6	3.32	2.78	0.71	0.8	0.47	0.55
5	ic4,nC4,ic5	3.26	2.78	0.6	0.62	0.59	0.63
6	C3,ic4,nC4	3.3	3.01	0.17	0.18	1.72	1.59

TABLE 6.2 Percentage Difference in Configurations for Feedstocks used by Rudd and Tedder calculated by this study.

Feed No.	Compn. No.	ESI	HI	α AB	α BC	Percentage Difference
1	1	1.0156	0.341	1.09	1.87	-13.6
	2	1.0284	0.323	2.04	1.99	-46.8
	3	1.0133	0.345	1.87	1.85	- 4.5
	4	1.0053	0.359	1.77	1.76	+ 9.9
	8	1.0206	0.33	1.96	1.92	-31.4
	9	1.0168	0.34	1.92	1.88	- 8.79
	10	1.0094	0.35	1.83	1.81	- 0.12
2	1	1.712	0.126	2.0	1.17	- 4.68
	2	1.734	0.135	2.09	1.21	-27.2
	3	1.698	0.122	1.96	1.15	- 3.98
	4	1.69	0.12	1.94	1.15	5.07
	8	1.72	0.129	2.03	1.18	-14.3
	9	1.72	0.128	2.02	1.18	4.9
	10	1.69	0.121	1.95	1.15	0.24
3	1	0.217	0.73	1.31	6.05	- 4.33
	2	0.184	0.72	1.34	7.29	-15.76
	3	0.204	0.72	1.32	6.48	- 0.64
	4	0.29	0.75	1.25	4.31	7.88
	8	0.194	0.72	1.33	6.88	- 9.06
	9	0.224	0.73	1.305	5.82	- 6.1
	10	0.24	0.74	1.29	5.42	3.29
4	1	0.552	0.8	1.13	2.04	- 0.8
	2	0.537	0.78	1.14	2.13	-11.42
	3	0.545	0.79	1.13	2.08	0.37
	4	0.576	0.82	1.1	1.92	13.69
	8	0.54	0.79	1.14	2.1	- 6.46
	9	0.55	0.8	1.12	2.02	- 3.28
	10	0.56	0.807	1.12	2.0	7.02
5	1	0.63	0.62	1.32	2.1	- 5.24
	2	0.62	0.61	1.35	2.18	-24.5
	3	0.63	0.62	1.33	2.11	- 0.79
	4	0.64	0.63	1.29	1.99	16.22
	8	0.62	0.61	1.33	2.15	-12.01
	9	0.63	0.62	1.32	2.09	- 9.3
	10	0.63	0.63	1.31	2.06	5.51
6	1	1.59	0.19	2.18	1.38	-11.77
	2	1.65	0.18	2.35	1.43	-41.2
	3	1.56	0.19	2.12	1.37	- 5.64
	4	1.53	0.19	2.05	1.34	4.57
	8	1.61	0.18	2.24	1.4	-39.3
	9	1.6	0.18	2.22	1.39	- 3.78
	10	1.54	0.19	2.09	1.36	- 0.5

It must be noted, of course, that Rudd and Tedder had optimised their columns in terms of the degrees of freedom available. Consequently differences would be expected between the results.

The feedstocks used by Rudd and Tedder were then analysed using the computer programme used in this study and the results obtained are given in Table 6.2. The relative volatilities between A and B and between B and C were also calculated for the feedstocks used. This permitted the comparison of Rudd and Tedder's results on the corresponding figure within Figures 6.1 and 6.22. The results again were considered satisfactory.

In Figure 6.28, the zero percentage difference contours are drawn for these feedstocks. Agreement was shown for the feedstock numbers 1, 2, 4 and 5, but disagreement was found with feedstock numbers 3 and 6.

In Figure 6.29 the zero percentage difference contours are plotted for a range of feed volatilities given in Table 6.3.

TABLE 6.3 Range of Feedstocks used to investigate Concept of E.S.I

Feed Number	α_{AB}	α_{BC}	ESI
1	1.2	1.2	1.0
2	1.2	2.0	0.6
3	1.2	3.0	0.4
4	1.2	4.0	0.3
5	1.2	5.0	0.24
6	2.0	1.2	1.67
7	3.0	1.2	2.5
8	4.0	1.2	3.3
9	5.0	1.2	4.17

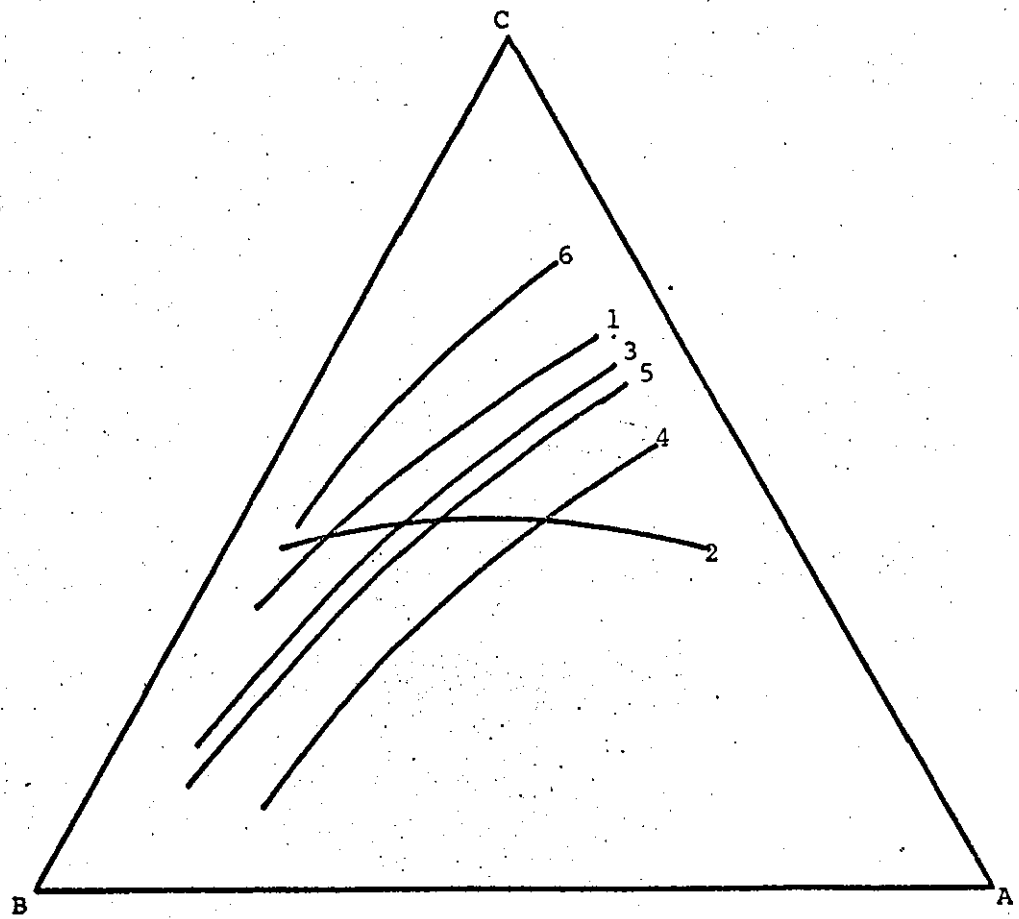


Figure 6.28 - Zero Percentage Difference Contours for
Feedstocks used by Rudd and Tedder

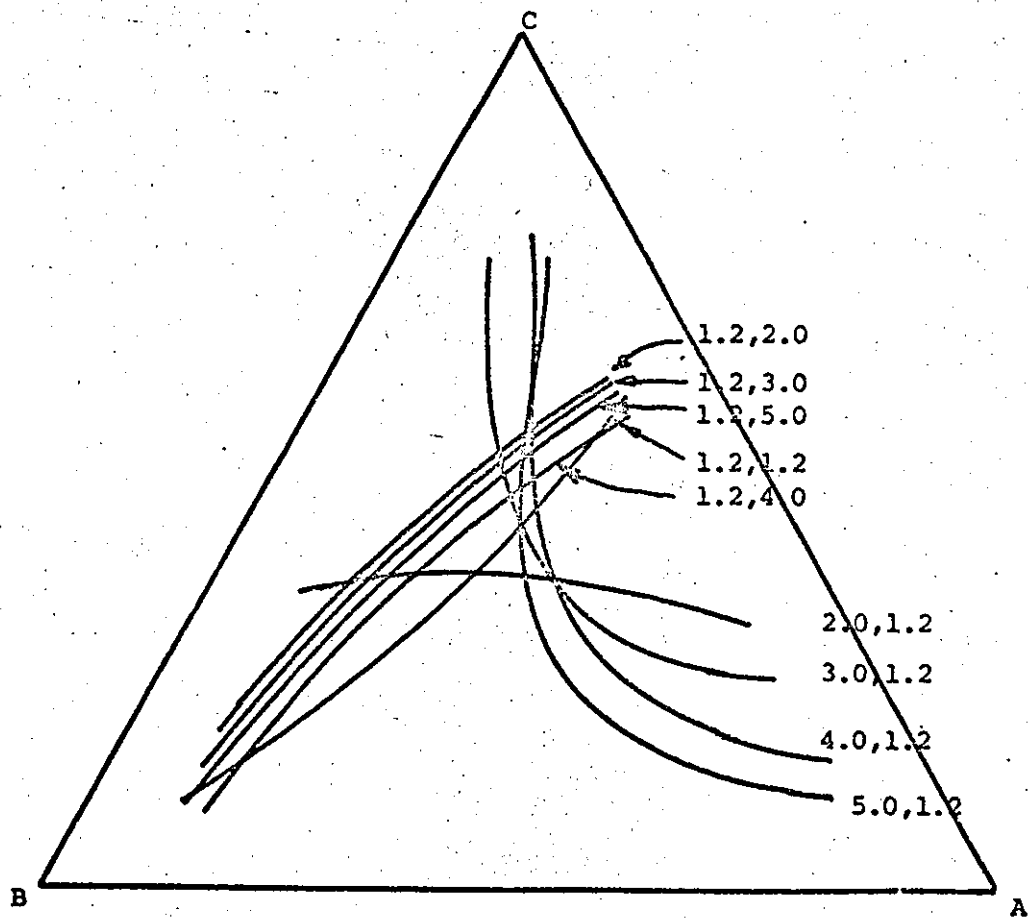


FIGURE 6.29 - Zero Percentage Difference Contours
for various Relative Volatilities

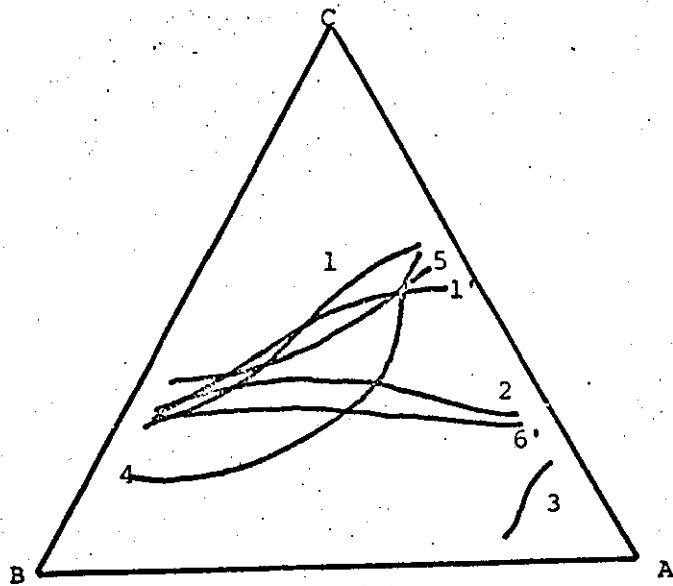
It is noted from the figure, that for ESI values less than 1.0, the zero percentage cost contours are in the same region as the results of Rudd and Tedder. However for values greater than 1.6 the results do not agree. For feed number 2 having an ESI of 1.71 there is agreement. However for feed numbers 7, 8 and 9 for which the ESI is greater than 1.6, the zero percentage difference contour swings completely away from the results given by Rudd and Tedder. These feedstocks are those in which the difficult separation is between the least two volatile components, that is, components B and C. Approximate agreement is only found for those feedstocks in which the difficult separation is between components A and B. Rudd and Tedder's proposals have been included for reference in Figure 6.30.

6.5.1 Comments on Rod and Marek's Results

The criterion used by Rod and Marek has been discussed in Chapter 1. The expression proposed was:

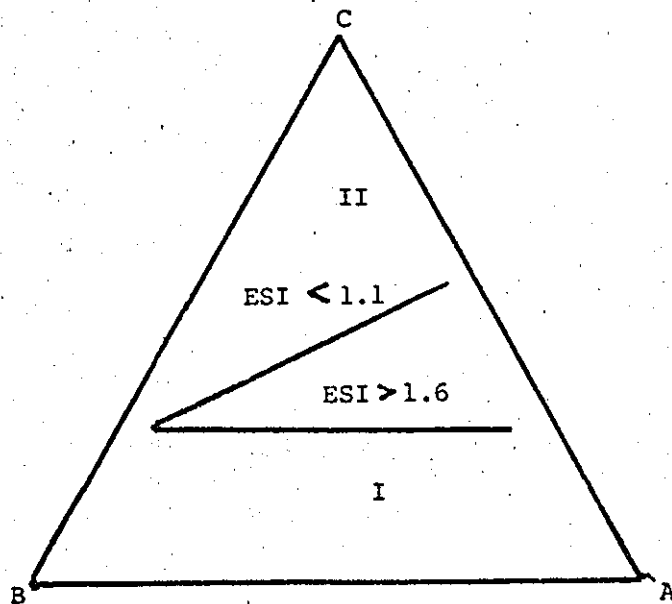
$$\Delta_{RM} = \frac{(\alpha_A + 1.25) x_4 - 1.25x_c}{\alpha_A - 1}$$

Positive values of Δ_{RM} suggested the direct configuration was optimal while negative values suggested the indirect configuration was optimal. Results derived from the pseudo-component analysis were applied to this expression. However it was found that the definition of the relative volatility of component A in which the volatility is calculated relative to component C limits the use of this expression. For example, a relative volatility of 6.0 for A to C could be obtained by (a) a relative volatility of A to B of 4.0 and for B to C of 1.5 and (b) a relative volatility of A to B of 1.5 and for B to C of 4.0. Referring to Figure 6.10, for example, relative volatilities of 4.0 and 1.5 for A to B and for B to C respectively would indicate that the indirect configuration was optimal by approximately 12%. On the other hand, relative volatilities of 1.5



Lines defining Optimal Regions

for Designs I and II only



Expected Optimal Regions for

Designs I and II only

FIGURE 6.30 - Rudd and Tedder's Expected Optimal

Regions. (From Rudd and Tedder (1976))

and 4.0 for A to B and for B to C respectively would give the direct configuration being optimal by approximately 10%. The model does not include the effect of the volatility of the component B and this, together with (a) the use of the overhead vapour rate as the objective function and (b) the use of Robinson and Gilliland's method for the determination of the minimum reflux ratio, are the reasons suggested for the inaccuracies in this model.

6.6 The Effect of the Choice of Component 'C' in the Formulation of Three Component Feedstocks

In the formulation of all three component feedstocks, the component 'C' was n-Heptane. Components 'A' and 'B' were pseudo-components generated to provide the required relative volatilities between components. The three component feedstocks could also be formulated having either of the compounds i-Pentane, n-Pentane or n-Hexane as the component 'C'. In either case, the pseudo-components 'A' and 'B' could be similarly generated to provide the same values of relative volatility between components as the feedstock having n-Heptane as component 'C'.

Thus it would be possible to have four feedstocks in which the relative volatilities between components had the same values. These feedstocks would be progressively lighter depending upon whether component 'C' was either n-Heptane, n-Hexane, n-Pentane or i-Pentane. The range of relative volatilities available would also be least when the compound i-Pentane was component 'C'.

To determine whether the choice of component 'C' could influence the percentage difference between configurations, feedstocks were formulated in which component 'C' was either n-Heptane, n-Hexane, n-Pentane or i-Pentane. Pseudo-components 'A' and 'B' were generated so that the relative volatility between 'A' and 'B' in all feedstocks was

the same value and similarly for components 'B' and 'C'. The twenty-two feed compositions used previously were considered together with the range of relative volatilities possible.

The results showed that for the equimolar feedstock and feedstocks in which the component 'A' was predominant, the choice of component 'C' was significant. For these feed compositions, given by numbers 1, 2 and 5 in Table 5.3, the difference in percentage difference between configurations varied considerably from a maximum for n-Heptane to a minimum for i-Pentane. The decrease in the percentage difference was proportional to the relative volatility between the compound used for component 'C' and n-Heptane. For all other feed compositions, the percentage difference between configurations was approximately constant.

However for those feedstocks in which the effect was significant, the direct configuration would normally be selected as the indirect configuration was never optimal. Thus the effect of the choice of a compound as component 'C' was considered insignificant.

CHAPTER 7. - COMPUTER PROGRAMMES

CHAPTER 7. DEVELOPMENT OF COMPUTER PROGRAMMES7.1 Introduction

A number of computer programmes were developed for the calculations required for this study. All were written in Fortran IV and performed on an ICL 1904A operating under the George III system, both in the United Kingdom and in Australia.

The development of these programmes will be discussed in this chapter. As most of the programmes are quite large, it is proposed to present only a description of the essential features of the principal programmes in this chapter. Description of the data input, typical printout details and the listing of these programmes will be included in the Appendix.

For the initial phase of the study, the size of the calculations needed for each configuration has been discussed in preceding chapters. The calculation of the mass balances together with the process design of the distillation columns and heat exchangers was made using the ICI simulation programme 'Flowpack'. Details of this programme will not be included in the study as this programme is available commercially in the United Kingdom.

Subsequent to the author's return to Australia, when access was not available to 'Flowpack', a programme 'Flowdist' was developed by the author. This programme performed those functions of 'Flowpack' of interest to this study. The only limitation in the programme was that recycle streams could not be considered. The distillation subroutine was essentially the same as that incorporated in 'Flowpack'.

The calculation of the engineering design of the columns and heat exchangers to the extent described in Chapter 2, together with the calculation of the total annual operating cost for each configuration was performed by the programme 'Cost' developed by the author.

Two further programmes were subsequently developed to examine many aspects which arose from the results generated by use of the previous programmes. The major programme 'Optconf' was developed to consider three component feedstocks only since it was felt that a number of aspects needing clarification could be resolved by consideration of these feedstocks.

Finally, programme 'Pslids' was developed to study the comparison of three component feedstocks in which the feed components were considered as pseudo-components.

Two regression analysis programmes, 'Mulreg' and 'Polreg' were used for the statistical analysis of the results throughout the many aspects of the study. These programmes were standard packages and were checked against standard solutions before use.

7.2 Programme 'Flowpack'

The method of presentation of data to the 'Flowpack' programme is given in the Appendix. The distillation subroutine included in this programme required the following input for each distillation column.

a. physical property data

This included the vapour-liquid equilibrium data as well as the vapour-liquid enthalpy data for each feed component.

Initially the vapour-liquid equilibrium data was generated by the use of Antoine Coefficients but later in the study Natural Gas Processors Association data⁽²²⁾ was used.

Enthalpy data was obtained by the method of Yen and Alexander⁽⁴⁴⁾ and A.P.I.⁽¹⁾ data.

All equilibrium and enthalpy data was supplied to the programme as regression analysis coefficients expressed as a three degree polynomial as a function of temperature.

b. feed temperature and pressure

- c. number and composition of feed components
- d. specification of the light and heavy keys
- e. recovery specification of the light key in the overhead product and the heavy key in the bottoms product
- f. reflux ratio as a function of the minimum reflux ratio
- g. pressure drop per plate
- h. type of overhead condenser
- i. process topology, that is, the arrangement of the distillation columns within the configuration.

The printout obtained from 'Flowpack' provided the following information:

- a. mass balance for each configuration
- b. number of equilibrium stages above and below the feed plate for each distillation column in the configuration
- c. reflux ratio for each column
- d. condenser temperature, pressure and heat load
- e. reboiler temperature, pressure and heat load.

An example of the format of the printout from this programme is included in the Appendix.

7.3 Programme 'Flowdist'

This programme was developed to replace the 'Flowpack' programme when 'Flowpack' became unavailable to the author.

This programme was developed as a general purpose mass balance programme capable of handling a maximum number of ten process units. The topology of the given process was read in as data as in the case of 'Flowpack'. The programme incorporated a master segment in which the overall mass balancing and sequencing of calculations was determined. The programme was principally used for the sequencing of distillation trains by the calling up of a distillation sub-routine within the

programme. It is a general purpose programme in that other separation processes may be incorporated as sub-routines.

'Flowdist' incorporates as a subroutine the programme 'Cost' for the design and costing of each column and heat exchangers as in 'Flowpack'.

7.4 Programme 'Cost'

This programme provided the design of all distillation columns and heat exchangers to the degree required to determine the total annual operating cost. This cost was also calculated by the programme.

The printout for the programme provided the cost of each equipment item in the configuration, the cost of process cooling water and process steam and the total annual operating cost. The economic life for all equipment for depreciation was taken as 10 years. An installation cost of three times the major equipment cost was used.

A flow chart of the programme is given in the Appendix together with a detailed description of the programme.

One of the difficulties of the use of an objective function such as the one adopted in this study is the necessary decision to base the analysis on one type of column, a given design procedure and assumed values of the economic parameters. It is not proposed to consider in depth in this study the current state of knowledge in regard to, for example, tray hydraulics for tray distillation columns. Rather the decision was made to base the design of the columns, heat exchangers and cost data on current technology and practice. Consequently the columns were designed as ballast tray towers and the design method followed was in accordance with a currently available commercial design manual, in this case, the Glitsch Ballast Tray Design Manual.⁽⁸⁾ Similarly, values of heat transfer coefficients and temperature approach for the heat exchangers were also taken as typical of current practice.

Cost data was taken from a recent publication by the Institution of Chemical Engineers. (14)

The principal assumptions made in the design and costing of the columns and heat exchangers were as follows:-

- a. tray spacing constant at 61 cms
- b. tray efficiencies maintained constant in all cases at 60%
- c. heat transfer coefficients in the condenser and reboiler maintained constant at values of 568 and 710 $W/m^2 \text{ } ^\circ K$.
- d. temperature approach in all heat exchangers at 10 centigrade degrees
- e. distillation tower diameters based upon the vapour rate at the top of the column
- f. a depreciation period of 10 years for all equipment.

While the above are typical of current practice, the decision to maintain a constant value of the overall tray efficiency for each column in every configuration requires further comment. In the objective function used in the study, the fixed investment required for the column, condenser and reboiler are included as a yearly depreciation amount based on a ten year depreciation period. Thus the contribution of the cost of the column only to the total annual operating cost is not significant. It was shown from the calculations that the contribution of the column to the total annual operating cost was never greater than 2.5%. Further a 2.5% variation in the overall tray efficiency does not produce the corresponding variation in the total column cost. Consequently it was considered that the amount of calculation required to determine a more accurate overall tray efficiency for each column was not warranted.

The cost of individual columns and heat exchangers was calculated from the basic capacity and cost by the following:-

$$\text{Cost of A} = \text{Cost of B} \left(\frac{\text{Size of A}}{\text{Size of B}} \right) \times \text{Slope of Cost Curve}$$

All costs were updated to present day values by the use of the Process Engineering Cost Indices. ⁽¹⁴⁾ The values of utilities were taken from Blackhurst and Harker (1973).

7.5 Programme 'Optconf'

The initial phase of this study has been the investigation of the effects of the various possible configurations for the separation of three, four and five component feedstocks. From the results obtained from these investigations, conclusions were made as to the area in which further work should be done and these have been discussed. However, it was felt that these areas could be investigated by considering three component feedstocks only.

Consequently a computer programme was developed in which the following calculations for three component feedstocks could be carried out -

- a. mass balances for the direct and indirect configurations
- b. process design of the distillation columns for each configuration, together with the heat loads for the heat exchangers
- c. the overhead vapour flowrate from the expression

$$V_i = D_i (R_i + 1)$$

- for each column and the determination of the percentage difference between the total overhead vapour flow rate between both configurations

- d. the condenser heat load calculated from the expression

$$q_{c,i} = V_i \lambda_i$$

- for each column and the percentage difference between both configurations
- e. the thermodynamic net work consumption for each column and the percentage difference for both configurations. The thermodynamic net work consumption was obtained from the following expression

$$\text{T.N.W.C.} = V_i \left[\frac{1}{T_D} - \frac{1}{T_B} \right]$$

where T_D , T_B are the dew point and bubble point temperatures of the overhead and bottoms product respectively

- f. the vapour flowrate difference for the configurations calculated by the use of the mathematical model developed in this study and discussed in Chapter 4.

In addition, the extent of the variation caused in the value of certain parameters by the various interpretations of the relative volatility term in the Underwood equations has been discussed. This variation has been investigated by the use of this programme. Provision was made in the programme for the calculation of the relative volatilities to be used in the determination of the minimum reflux ratio to be made at the following conditions:

- (i) feed temperature to the column
- (ii) geometric mean of the dew point temperature of the overhead product and the bubble point temperature of the bottoms product
- (iii) cubic mean of the following temperatures -
 - (a) the feed temperature and (b) and (c) being the two temperatures in (ii)
- (iv) geometric mean of the boiling point of pure components A and C.

The effect of the assumption of non-distribution of the non-key components was also investigated in this programme. All of the above calculations were repeated for each feed on the assumption that the non-key components did not distribute.

7.6. Programme 'Pslids'

Programme 'Pslids' was developed to incorporate the concept of pseudo-components to generate components having specified relative

volatilities. By the use of this programme, three component feedstocks could be formulated in which the volatility of the components would be as predetermined simple multiples and not the values obtained by the use of actual components. This concept has been discussed in Chapter 5. A flowchart and listing of this programme will be included in the Appendix.

7.7 Programme 'Bubble'

Prior to the development of 'Optconf', the data for input for 'Flowpack' and 'Flowdist' required the temperature of each feed to be specified. As all feeds were at their bubble point temperature at the operating pressure, the bubble point temperature was calculated by this programme.

The basic calculation of the programme was to find the temperature at which the expression $\sum_i K_i x_i = 1.0$ was valid. The tolerance set in all cases was 0.001. The Newton-Raphson convergence procedure was used to solve the expression. A listing of this programme is included in the programme 'Pslids'.

CHAPTER 8.

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CONCLUSION

CHAPTER 8. CONCLUSION

The thesis has considered the possibility that of the number of process configurations possible to separate a multicomponent feedstock by the process of distillation into relatively pure components, one of these configurations should be optimal and predictable. The distillation columns considered were columns supplied with a single feedstock and producing two products, one overhead and one bottoms. From the previous work, a set of guidelines or heuristics had been proposed by the use of which it was claimed the optimal configuration could be predicted.

These heuristics were studied by considering a very wide range of feedstocks of varying feed composition formulated from simple hydrocarbons from Propane through to n-Heptane. These feedstocks contained up to a maximum of five components. To compare all configurations possible for a given separation, a detailed design and economic evaluation method was developed. In its development, the method used various design and economic parameters. The values of these parameters were taken as those typical of current industrial practice. Other process parameters were considered constant, for example the column operating pressure and the ratio of the operating to the minimum reflux ratio. These were maintained constant because the thesis adopted a policy of not considering 'external' economic parameters because a configuration could be optimal under one set of economic parameters and not be optimal under another set. Further, several reported studies had considered each column to be economically optimised in regard to the operating pressure of the column and the degree of vaporisation of the feedstock. This thesis was concerned with the development of techniques which could predict the optimal process configuration as a function of those process parameters which specify the separation. These were:-

- (i) feed composition
- (ii) component volatility
- (iii) degree of recovery of the components.

The objective function used initially to compare each configuration was the total annual operating cost. As it was subsequently shown that the reboiler heat load provided identical percentage differences between configurations, this parameter was used as the objective function throughout the remainder of the thesis.

The results obtained from the analysis of the three, four and five component feedstocks provided an illustration of the variation in cost of the separation by the use of the configurations possible. It also showed the effect of feed composition, degree of recovery and the component volatility upon the cost of the separation.

The study of these feedstocks also showed that while the individual heuristics could be shown to be valid, it was not possible to predict under what process conditions each heuristic would dictate the selection of the optimal configuration. Further it was shown that there were conflicts between the heuristics arising from the interaction of the influence of the feed composition and the component volatility.

The only manner in which this aspect could be resolved was by the use of a mathematical model relating the cost difference between configurations and the component volatility, feed composition and the degree of recovery of the components.

The thesis examined the use of indices proposed in the literature as a guide to the prediction of optimal configurations. It was shown that these indices could not adequately predict the optimal configuration. The thesis found that the development of such indices for the prediction of optimal configurations of distillation trains was not feasible.

A mathematical model was developed relating the overhead condenser heat load to the process variables described previously. As all feedstocks were taken to be at their bubble point temperature for the column pressure, the condenser heat load was used as the objective function.

It was shown that there were two major difficulties which prevented the use of this model for the prediction of optimal configurations. These were:-

(i) The adoption of the Underwood method for the determination of the Minimum reflux ratio. In the solution of the two equations in the Underwood method, an iterative solution is necessary for the calculation of the value of the Underwood parameter, ϕ . While the mathematical model developed contained the known variables, that is, feed composition, component volatility and the component degree of recovery, it also contained the Underwood parameter. This parameter occurred in the model as many times as the number of columns in the configurations being compared. The values of these parameters must also be known before solution of the model.

(ii) The nature of the distillation process itself. The model required the knowledge of the actual product compositions. This required the determination of the distribution of the non-key components into both products for all columns. As this knowledge was not possible without prior calculation, the model had to assume that non-key components did not distribute. The value of the relative volatility used in the sizing of the columns was calculated in this thesis as the geometric mean of the relative volatilities calculated at the dew point of the overhead temperature and the bubble point temperature of the bottoms product. As these temperatures could not also be known without prior calculation, the values of the relative volatility for use in the model could only be

calculated at known conditions which were either at the feed temperature to the configuration or a mean of the relative volatilities calculated at the boiling point of the pure lightest and heaviest components.

It was shown that even if the values of the Underwood parameter were known, the results of the model could not be satisfactorily correlated with the actual results obtained by use of the design method.

However, an alternative to a mathematical relationship was proposed by the use of a new concept of pseudo-components. These were hypothetical compounds given physical properties so that they could provide relative volatilities of any desired value. These properties were derived from known compounds, the alkanes from Propane through to n-Heptane. By formulating feedstocks in which small incremental changes in the value of relative volatility were made and analysing a sufficiently large number of feedstocks, it was possible to develop graphical illustrations of the relationship between the cost of a separation and the feed composition and component volatility. It also provided illustration of the interaction between feed composition and component volatility.

The use of the concept of pseudo-components thus enabled a new design method to be developed for the selection of the optimal configuration. This method is applicable to feedstocks formulated from the components used in this thesis and the process conditions specified.

For feedstocks having relative volatilities between the two pairs of components in a three component feedstock in the range of 1.1 to 5.0 the method requires the reading of two charts. One chart indicates whether the optimal configuration will be either the direct or indirect configuration and the other provides the size of the difference between the two configurations.

While the method has been based on a given range of alkanes, it is the first study to illustrate the interaction between the two principal process parameters influencing the selection of the optimal configuration and restricting the use of the proposed heuristics. The study has shown that the method appears to be the only way the interaction can be shown.

As the analysis has been based on the use of non-economic process parameters, it is believed that the results will be of considerable benefit in similar studies of other distillation systems.

The use of a constant value for R/R_{\min} .

For all columns considered in the thesis the following arguments apply.

1. The classical curve illustrating the total annual cost as a function of reflux ratio shows very steeply rising costs at values of R below 1.1 to 1.2 times R_{\min} but rises only very slowly above 1.2 times R_{\min} . Thus it is usual to take an operating optimum value for continuous fractionation of 1.25 times R_{\min} . King (1971) states that by designing columns to operate with a R.R. of 1.2 to 1.3 times R_{\min} , the total annual operating costs will only be 2-6% greater than the cost of the optimum reflux ratio. The results from this study indicated that this figure was high, a maximum value of 4.5% being obtained.
2. Further King suggests the desirable design policy should be to set the operating reflux ratio at 1.2 to 1.3 times R_{\min} and not to go through an optimization calculation for each column. Bolles (1977) has also confirmed this policy. Previous studies, for example that by Robb and Merrick (1969), had used a value of 1.25 and thus comparison was possible with these results.
3. Heaven (1969) considered over 70 distillations in which the operating reflux ratio and column pressure were economically optimised for each column. The optimum reflux ratio was found to be within the range 1.1 to 1.25 times R_{\min} in all cases.
4. Using a constant value of 1.25 for each column, the percentage cost difference between two configurations would of course be slightly different from the value obtained with a constant ratio than if the economic optimum was used. However, as economic parameters vary from design to design, and as the extent of the difference on total annual variable cost is very small, then it is considered more appropriate to base the study on a constant value of the ratio operating to minimum reflux.

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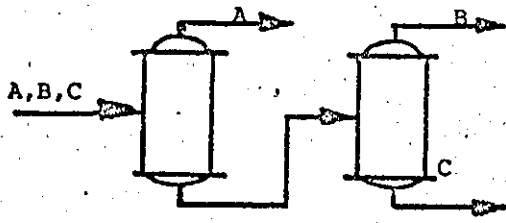
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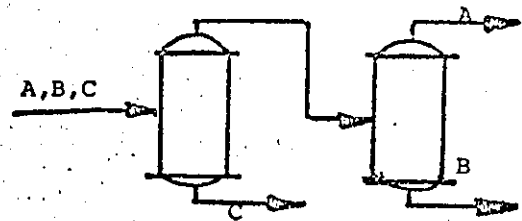
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APPENDICES

APPENDIX A1: Physical Arrangement of all possible configurations for three, four and five component feedstocks.

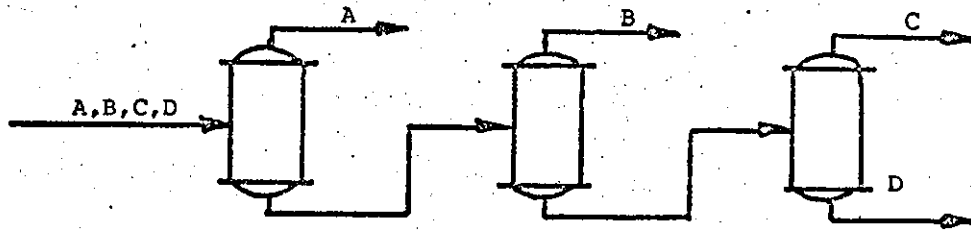


CONFIGURATION 1.

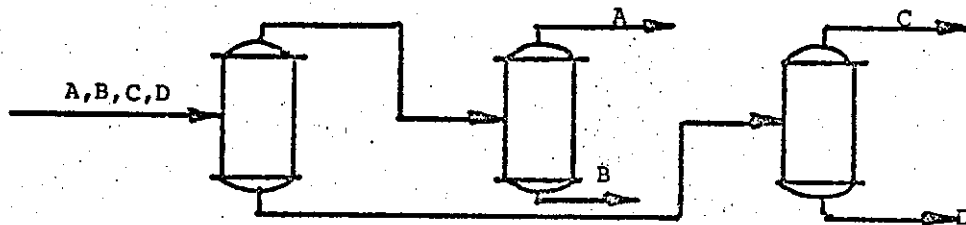


CONFIGURATION 2

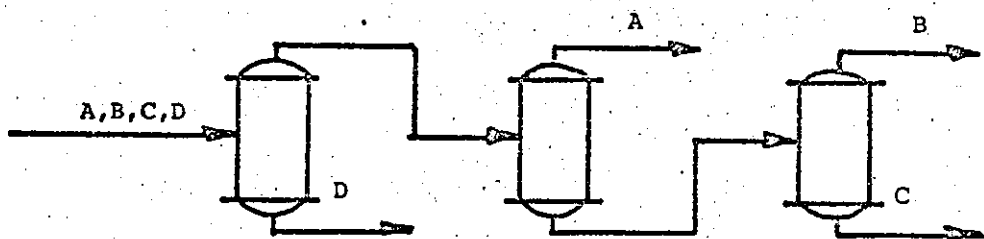
THREE COMPONENT CONFIGURATIONS



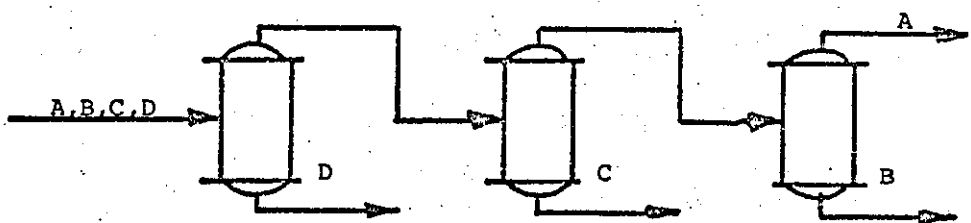
CONFIGURATION 1



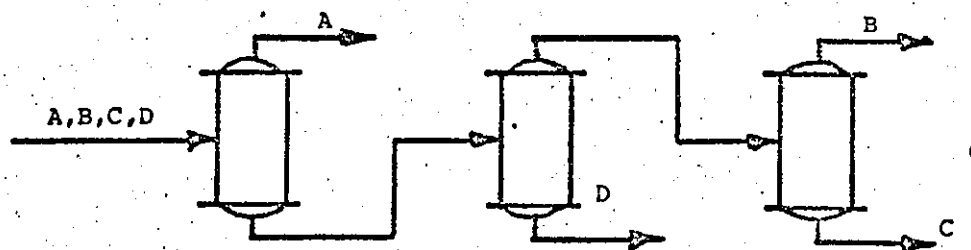
CONFIGURATION 2



CONFIGURATION 3



CONFIGURATION 4



CONFIGURATION 5

FOUR COMPONENT CONFIGURATIONS

FIGURE A1.

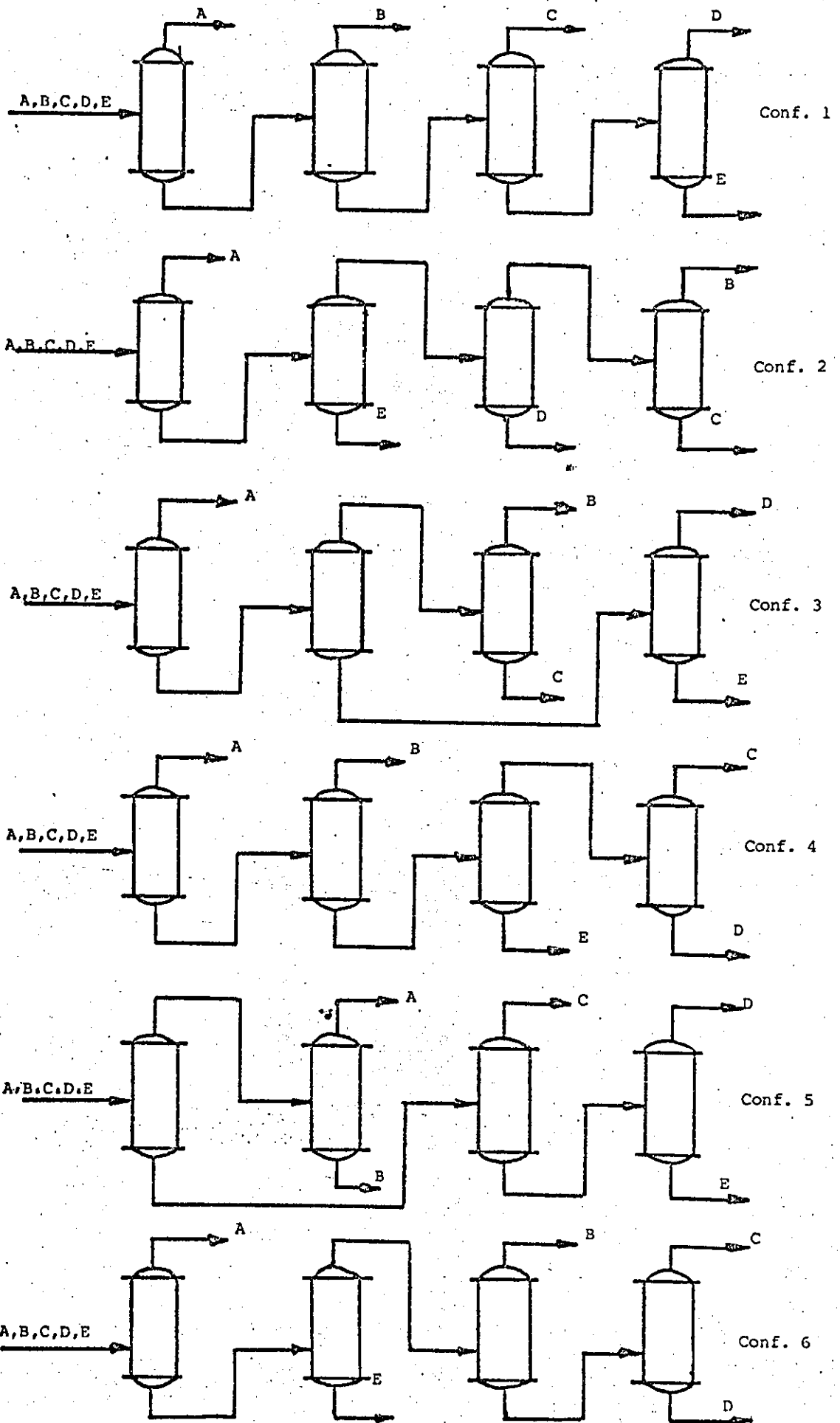


FIGURE A1 (Contd.)

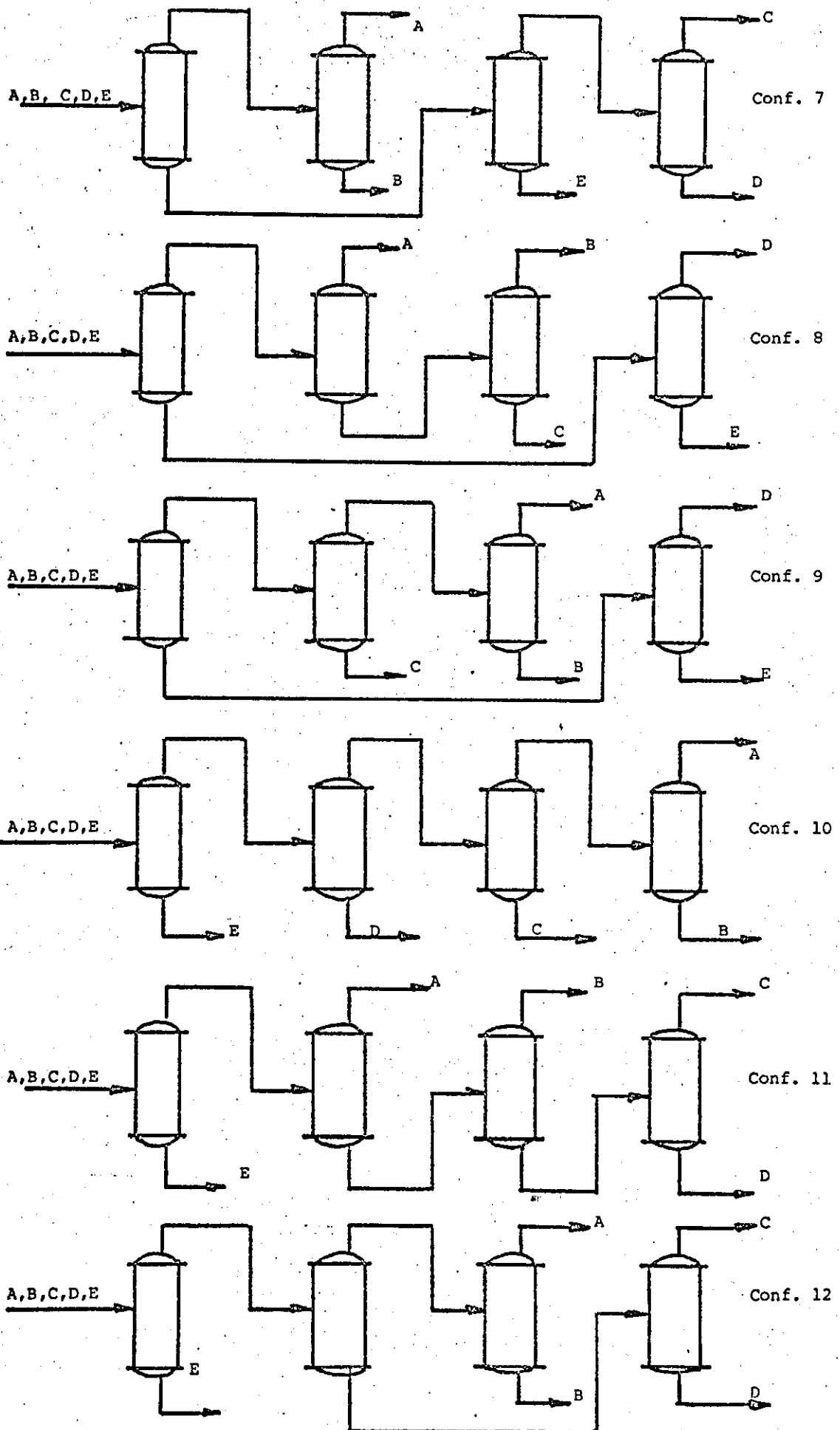
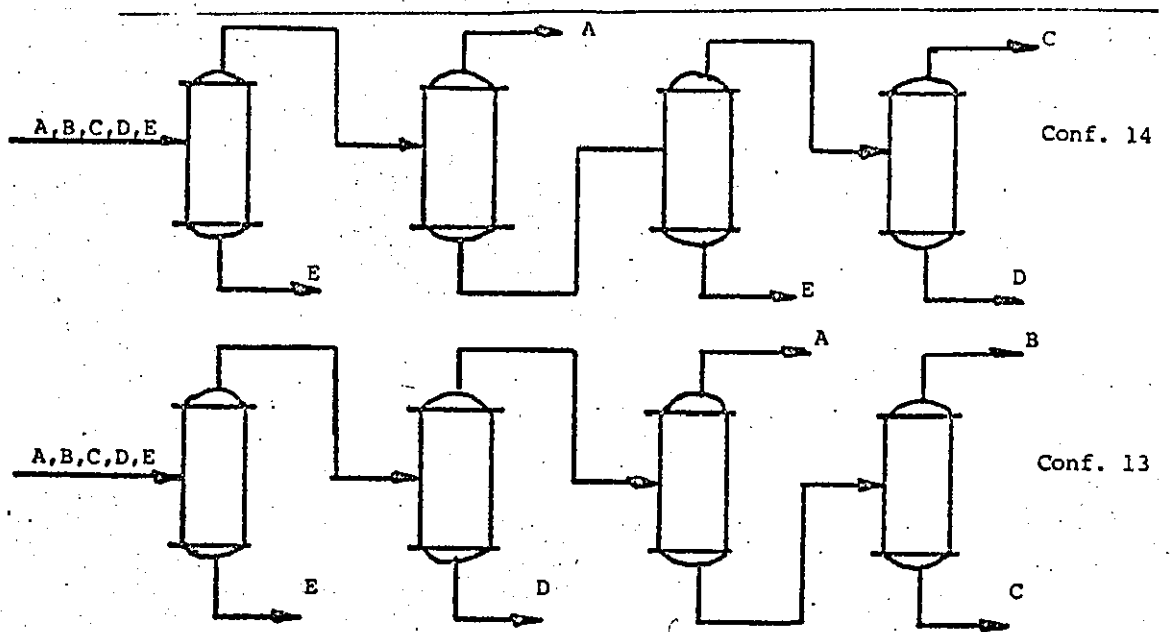


FIGURE A1 (Contd.)



FIVE COMPONENT CONFIGURATIONS

FIGURE A1 (Contd)

APPENDIX A2: Evaluation of Objective Functions.

- A2.1 Reboiler Heat Load
- A2.2 Condenser Heat Load
- A2.3 Overhead Vapour Flowrate
- A2.4 Thermodynamic Criteria as Objective Functions

APPENDIX A2 - Comparison of Objective Functions

The various objective functions used in the previous studies and reported in the literature were discussed in Chapter 2. In the initial phase of this thesis, the objective function used was the total annual operating cost. The calculation of the value of this objective function required the detailed design and costing of all process items in each configuration. Because of the very large number of cases to be considered in the thesis, other parameters were examined for use as the objective function.

Process parameters used in previous studies were the following:

- (i) Reboiler Heat Load
- (ii) Overhead Vapour Flowrate
- (iii) Thermodynamic Net Work Consumption.

During this study, the validity of each of these parameters as objective functions was examined.

A2.1 - Reboiler Heat Load

It was found that the reboiler heat load gave an excellent correlation with the total annual operating cost for all feedstocks used. The percentage differences in configurations based on the total annual operating cost and the reboiler heat load were identical. The reboiler heat load was used as the alternative objective function, as the literature had also shown that the reboiler heat load can be used as an indication of the cost of distillation. Regression Analysis of the results from this study confirmed this selection.

TABLE A1. Comparison of Total Annual Operating Cost and the Reboiler Heat Load as Objective Functions for Feedstock Given in Table 3.7.

Configuration Number	Feed No.	Percentage Difference between Configurations in terms of:-	
		Reboiler Heat Load	Total Annual Operating Cost
1	1	-	-
	2	-	-
	3	-	-
	4	-	-
	5	-	-
2	1	+ 1.781	+ 1.779
	2	-16.94	-16.97
	3	- 0.18	- 0.181
	4	+ 3.185	+ 3.19
	5	+10.52	+10.56
3	1	- 7.327	- 7.329
	2	-18.518	-18.5
	3	-16.88	-16.9
	4	-17.65	-17.65
	5	-14.6	-14.61
4	1	- 8.54	- 8.51
	2	+ 3.25	+ 3.245
	3	- 8.66	- 8.65
	4	- 6.52	6.49
	5	5.71	5.718
5	1	- 4.46	- 4.409
	2	- 2.47	- 2.452
	3	-14.6	-14.61
	4	- 5.72	- 5.718
	5	- 0.76	- 0.756

A comparison of the percentage difference between configurations expressed in terms of the total annual operating cost and the reboiler heat load for the feedstock given previously in Table 3.7 is given in Table A1.

A2.2 - Condenser Heat Load

As discussed in the text, all feedstocks were considered to be at their bubble point temperature for the column operating pressure. Under these conditions, the condenser heat load should be approximately equal to the reboiler heat load. The value of the condenser heat load was determined, together with the reboiler heat load for each configuration and the difference in the configurations was also calculated in terms of the condenser heat load. The results obtained from this study confirmed the suitability of the condenser heat load as an objective function. The percentage difference between the differences in the configurations, expressed in terms of the reboiler heat load and the condenser heat load differed by no more than 4 - 5% for all the cases studied.

A2.3 - Overhead Vapour Flowrate

This parameter had been used in previous studies, in particular, the study of Rod and Marek (1959). A study was made of the feasibility of this parameter for an objective function. In Chapter 3, Table 3.8 it was noted that a good correlation occurred between the overhead vapour flowrate and the reboiler heat load for the type 'B' feeds considered in the Table. These feedstocks were those in which the separation between components A and B was more difficult than between components B and C. For the type 'A'

feedstocks, the correlation was poor and so a study was made of this parameter.

From the results of Chapter 5, using pseudo-components, it was possible to study the relationship between the overhead vapour load and the reboiler heat load. Table A.2 provides a typical illustration of the two parameters for two values of the relative volatilities for the twenty feed compositions used in that Chapter. Two volatilities are considered. In one feedstock, the separation between A and B is more difficult than between B and C while the opposite is the case in the other feedstock. It will be noted from the table that a good correlation occurs for the feedstock in which the difficult separation is between the two most volatile components, while a very poor correlation exists for the other feedstock. Good correlation only occurred in those feedstocks in Chapter 5 in which the separation of the two lighter components was difficult. As a result, it can be concluded that the use of the overhead vapour flow as an indication of the cost of distillation is not advisable.

A2.4 - Thermodynamic Criteria as Objective Functions

In Chapter 1, the use of thermodynamic criteria by King and Petyluk et al has been discussed. Throughout this thesis, the comparisons of the configurations have also been expressed in terms of the thermodynamic net work consumption as defined by King. By this definition, the thermodynamic net work consumption is proportional to the product of the interstage vapour flowrate and the difference in the reciprocals of the overhead and bottoms temperature. As discussed in Chapter 1, the temperature difference over each column in this study was constant in thermodynamic terms, whereas in King's interpretation, the temperature difference varies over each column. Consequently this parameter would be expected to give quite different results.

The results obtained showed no relationship between the other parameters used in this thesis and the thermodynamic net work consumption. As an example, Table A2 provides a comparison between the results given by the three parameters: the overhead vapour flowrate, reboiler heat load and the thermodynamic net work consumption.

TABLE A2. Comparison of Objective FunctionsV - Vapour Flow, q_r - Reboiler Heat Load

T.N.W.C. - Thermodynamic Net Work Consumption.

Feed Number	Percentage Difference Between Configurations					
	$\alpha_{AB} = 4.0, \alpha_{BC} = 1.15$			$\alpha_{AB} = 1.15, \alpha_{BC} = 4.0$		
	V	q_r	T.N.W.C.	V	q_r	T.N.W.C.
1	2.77	- 5.05	-115.0	1.38	1.42	47.9
2	-13.7	- 0.4	-104.9	- 5.76	- 5.57	44.8
3	- 0.9	- 9.2	- 45.1	0.4	0.41	21.8
4	6.81	- 7.13	-120.3	8.17	7.92	51.0
5	- 0.45	4.37	-125.4	- 2.79	- 2.59	45.8
6	- 0.19	-11.8	- 74.65	0.82	0.83	34.3
7	6.2	- 4.19	-119.6	3.83	3.74	54.7
8	3.3	- 9.72	-117.3	- 4.3	- 4.21	21.7
9	10.01	16.88	-143.2	0.87	0.96	52.3
10	1.77	- 9.87	- 49.8	5.89	5.65	52.0
11	- 4.7	4.72	-117.1	- 4.2	- 4.01	45.3
12	1.74	1.66	-128.1	- 1.26	- 1.1	46.3
13	6.63	1.28	-133.4	2.45	2.48	53.5
14	10.28	11.27	-160.3	1.16	1.61	50.4
15	1.06	-11.04	- 79.2	2.55	2.51	43.4
16	4.1	- 7.8	- 98.7	4.23	4.09	53.5
17	9.2	3.8	-157.0	3.34	3.69	49.97
18	0.53	- 9.45	- 44.6	4.03	3.93	43.49
19	3.21	-10.35	- 62.5	6.65	6.26	56.23

APPENDIX A3: Development of Mathematical Model.

APPENDIX A3: Derivation of an analytical relationship to be used for the comparison of the two possible configurations i.e., direct and indirect for the separation of three component feedstocks.

Vapour flow from the top of a distillation column is given by

$$V = D(R+1)$$

$$\text{if } R = 1.25 R_{\min}$$

$$\text{then } V = D (1.25 R_{\min} + 1) \quad \dots\dots\dots (A1)$$

R_{\min} will be determined using Underwood's method, i.e. R_{\min} will be calculated from the following:

$$\frac{\alpha_A}{\alpha_{A-\phi}} \cdot x_{AD} + \frac{\alpha_B}{\alpha_{B-\phi}} \cdot x_{BD} + \frac{\alpha_C}{\alpha_{C-\phi}} \cdot x_{CD} = R_{\min} + 1 \quad \dots\dots\dots (A2)$$

where ϕ is calculated from the following:

$$\frac{\alpha_A}{\alpha_{A-\phi}} \cdot x_{AF} + \frac{\alpha_B}{\alpha_{B-\phi}} \cdot x_{BF} + \frac{\alpha_C}{\alpha_{C-\phi}} \cdot x_{CF} = 1 - q \quad \dots\dots\dots (A3)$$

as all feeds will be at their bubble point temperature, then

$q = 1$ and eqn (3) becomes

$$\frac{\alpha_A}{\alpha_{A-\phi}} \cdot x_{AF} + \frac{\alpha_B}{\alpha_{B-\phi}} \cdot x_{BF} + \frac{\alpha_C}{\alpha_{C-\phi}} \cdot x_{CF} = 0 \quad \dots\dots\dots (A4)$$

Putting the left hand side of eqn. (A2) = Y

$$\text{i.e. } Y = R_{\min} + 1$$

then it can be shown that

$$V_i = D_i [1.25 Y_i - 0.25] \quad \dots\dots\dots (A5)$$

Thus for two columns in a given configuration, the sum of the vapour loads from each column would then be

$$\begin{aligned}
 &= V_1 + V_2 \\
 &= D_1 [1.25Y_1 - 0.25] + D_2 [1.25Y_2 - 0.25] \\
 &= 1.25[D_1 Y_1 + D_2 Y_2] - 0.25[D_1 + D_2] \quad \dots\dots\dots (A6)
 \end{aligned}$$

For the comparison of the two possible configurations for the separation of three component feeds, an expression relating the difference between the total vapour load from each configuration would be as follows:

$$\begin{aligned}
 (V_1 + V_2)_D - (V_1 + V_2)_i &= 1.25[(D_1 Y_1 + D_2 Y_2)_D - (D_1 Y_1 + D_2 Y_2)_i] \\
 &\quad - 0.25[(D_1 + D_2)_D - (D_1 + D_2)_i]
 \end{aligned}$$

$$\begin{aligned}
 \text{or say } \frac{\Delta V}{F} &= \frac{1.25}{F} [(D_1 Y_1 + D_2 Y_2)_D - (D_1 Y_1 + D_2 Y_2)_i] \\
 &\quad - \frac{0.25}{F} [(D_1 + D_2)_D - (D_1 + D_2)_i] \quad \dots\dots\dots (A7)
 \end{aligned}$$

This expression will now be re-written in terms of variables which describe the state of the feed and the degree of recovery specified for each component.

i.e. in terms of the following:

- (1) Feed composition; x_{AF} , x_{BF} , x_{CF}
- (2) Relative volatility of feed components; α_A , α_B , α_C , and
- (3) The degree of recovery of each component, RF_A , RF_B , RF_C .

(I) Calculation of Distillate flow rates from each column in both configurations in terms of variables specified above

(i) Direct configuration - Column One

Number of moles of D_1 = moles of A + moles of B

(Component C has been assumed not to distribute to this product)

$$\therefore D_{1,D} = x_{AF} \cdot F \cdot RF_A + x_{BF} \cdot F \cdot (1 - RF_B)^{0.5} \quad \dots\dots\dots (A8)$$

(ii) Direct Configuration - Column Two

Number of moles of D_2 = moles of A + moles of B
+ moles of C

G

$$\therefore D_{2,D} = x_{AF} \cdot F \cdot (1 - RF_A) + x_{BF} \cdot F \cdot RF_B + x_{CF} \cdot F \cdot (1 - RF_C) \quad \dots\dots\dots (A9)$$

$$\therefore D_{1,D} + D_{2,D} = x_{AF} \cdot F + x_{BF} \cdot F \cdot (1 + RF_B - RF_B^{0.5}) + x_{CF} \cdot F \cdot (1 - RF_C) \quad \dots\dots\dots (A10)$$

Indirect Configuration - Column One

Number of moles of D_1 = moles of A + moles of B + moles of C

$$D_{1,i} = x_{AF} \cdot F + x_{BF} \cdot F \cdot RF_B^{0.5} + x_{CF} \cdot F \cdot (1 - RF_C) \quad \dots\dots\dots (A11)$$

Indirect Configuration - Column Two

Number of moles of D_2 = moles of A + moles of B

$$\therefore D_{2,i} = x_{AF} \cdot F \cdot RF_A + x_{BF} \cdot F \cdot (RF_B^{0.5} - RF_B) \quad \dots\dots\dots (A11a)$$

$$\therefore D_{1,i} + D_{2,i} = x_{AF} \cdot F \cdot (1 + RF_A) + x_{BF} \cdot F \cdot (2RF_B^{0.5} - RF_B) + x_{CF} \cdot F \cdot (1 - RF_C) \quad \dots\dots\dots (A12)$$

$$\therefore (D_{1,D} + D_{2,D}) - (D_{1,i} + D_{2,i}) = x_{AF} \cdot F + x_{BF} \cdot F \cdot (1 + RF_B - RF_B^{0.5})$$

$$+ x_{CF} \cdot F \cdot (1 - RF_C) - x_{AF} \cdot F \cdot (1 + RF_A) - x_{BF} \cdot F \cdot (2RF_B^{0.5} - RF_B) - x_{CF} \cdot F \cdot (1 - RF_C)$$

$$\text{or } \frac{\Delta D}{F} = x_{BF} (1 + 2RF_B - 3RF_B^{0.5}) - x_{AF} \cdot RF_A \quad \dots\dots\dots (A13)$$

Equation (A13) will be used as the second term in equation (A7).

(II) Development of expressions for the 'Y' terms in Equation (A7)

Underwood's equation for R_{\min} was previously written as

Eqn. (A2)

$$Y = \frac{\alpha_A \cdot x_{AD}}{\alpha_A - \phi} + \frac{\alpha_B \cdot x_{BD}}{\alpha_B - \phi} + \frac{\alpha_C \cdot x_{CD}}{\alpha_C - \phi}$$

or say $Y = C_1 \cdot x_{AD} + C_2 \cdot x_{BD} + C_3 \cdot x_{CD}$

or $Y = C_1 \cdot x_{AD} + C_2 \cdot x_{BD} + C_3 (1 - x_{AD} - x_{BD})$

$$Y = (C_1 - C_3) x_{AD} + (C_2 - C_3) x_{BD} + C_3$$

For column 1 - Direct and Column 2 - Indirect

$$x_{CD} = 0.0$$

then $Y = C_1 x_{AD} + C_2 x_{BD}$

or $Y = x_{AD} (C_1 - C_2) + C_2 \quad \dots\dots\dots (A13a)$

The Y functions will now be derived for each column.

(a) Direct Configuration - Column One

Equation will be of the form:

$$Y = x_{AD} (C_1 - C_2) + C_2$$

$$\begin{aligned} \text{now } x_{AD} &= \frac{\text{number of moles of A in } D_1}{\text{number of moles of } D_1} \\ &= \frac{x_{AF} \cdot F \cdot RF_A}{D_1} \end{aligned}$$

$$\therefore Y_{1,D} = \frac{x_{AF} \cdot F \cdot RF_A}{D_{1,D}} (C_1 - C_2) + C_2$$

$$\text{where } C_1 = \frac{\alpha_{AB}}{\alpha_{AB} - \phi_1}$$

$$\text{and } C_2 = \frac{1}{1 - \phi_1}$$

$$Y_{1,D} = \frac{F}{D_{1,D}} \left[x_{AF} \cdot RF_A (C_1 - C_2) + \frac{C_2 D_{1,D}}{F} \right]$$

$$\text{or } Y_{1,D} = \frac{F}{D_{1,D}} \left[x_{AF} \cdot RF_A (C_1 - C_2) + C_2 (x_{AF} \cdot RF_A + x_{BF} \cdot (1 - RF_B)^{0.5}) \right]$$

..... (A14)

by substituting for $D_{1,D}$ from equation (A8)

(b) Direct Configuration - Column Two

$$x_{AD2} = \frac{x_{AF} \cdot F \cdot (1 - RF_A)}{D_{2,D}}$$

$$x_{BD2} = \frac{x_{BF} \cdot F \cdot RF_B}{D_{2,D}}$$

Substituting in Equation (A13a)

$$Y_{2,D} = (C'_1 - C'_3) x_{AD2} + (C'_2 - C'_3) x_{BD2} + C'_3$$

$$\therefore Y_{2,D} = \frac{F}{D_{2,D}} \left[(C'_1 - C'_3) x_{AF} (1 - RF_A) + (C'_2 - C'_3) x_{BF} \cdot RF_B + \frac{C'_3 D_{2,D}}{F} \right]$$

Substituting for $D_{2,D}$ from Equation (A9)

$$Y_{2,D} = \frac{F}{D_{2,D}} \left[(C'_1 - C'_3) x_{AF} \cdot (1 - RF_A) + (C'_2 - C'_3) x_{BF} \cdot RF_B \right. \\ \left. + C'_3 (x_{AF} [1 - RF_A] + x_{BF} \cdot RF_B + x_{CF} [1 - RF_C]) \right]$$

$$\text{or } Y_{2,D} = \frac{F}{D_{2,D}} [C_{B1} \cdot x_{AF} (1-RF_A) + C_{B2} \cdot x_{BF} \cdot RF_B + C'_3 (x_{AF} \cdot [1-RF_A] + x_{BF} \cdot RF_B + x_{CF} [1-RF_C])] \dots\dots\dots (A15)$$

$$\text{where } C_{B1} = C'_1 - C'_3$$

$$= \frac{\alpha_{AC'}}{\alpha_{AC'} - \phi_2} - \frac{1}{1-\phi_2}$$

$$\text{and } C_{B2} = C'_2 - C'_3$$

$$= \frac{\alpha_{BC'}}{\alpha_{BC'} - \phi_2} - \frac{1}{1-\phi_2}$$

(c) Indirect Configuration - Column 1

Equation is of the form

$$Y_{1,i} = \frac{\alpha_{AC''}}{\alpha_{AC''} - \phi_3} x_{AD} + \frac{\alpha_{BC''}}{\alpha_{BC''} - \phi_3} \cdot x_{BD} + \frac{1}{1-\phi_3} \cdot x_{CD}$$

$$\text{or } Y_{1,i} = x_{AD} (d_1 - d_3) + (d_2 - d_3) x_{BD} + d_3$$

$$\text{where } d_1 - d_3 = \frac{\alpha_{AC''}}{\alpha_{AC''} - \phi_3} - \frac{1}{1-\phi_3}$$

$$\text{and } d_2 - d_3 = \frac{\alpha_{BC''}}{\alpha_{BC''} - \phi_3} - \frac{1}{1-\phi_3}$$

$$\text{Now } x_{AD1} = \frac{x_{AF} \cdot F}{D_{1,i}}$$

$$\text{and } x_{BD1} = \frac{x_{BF} \cdot F \cdot RF_B^{0.5}}{D_{1,i}}$$

$$\therefore Y_{1,i} = \frac{F}{D_{1,i}} [(d_1 - d_3) x_{AF} + (d_2 - d_3) x_{BF} \cdot RF_B^{0.5}] + \frac{d_3 D_{1,i}}{F}$$

substituting for $D_{1,i}$ from Equation (All)

$$Y_{1,i} = \frac{F}{D_{1,i}} [(d_1 - d_3) x_{AF} + (d_2 - d_3) x_{BF} \cdot RF_B^{0.5} + d_3 (x_{AF} + x_{BF} \cdot RF_B^{0.5} + x_{CF} (1 - RF_C))] \dots\dots\dots (A16)$$

(d) Indirect Configuration - Column Two

Equation is of form

$$Y_{2,i} = x_{AD} (d'_1 - d'_2) + d'_2$$

$$\text{Now } x_{AD} = \frac{x_{AF} \cdot F \cdot RF_A}{D_{2i}}$$

$$\begin{aligned} \therefore Y_{2,i} &= (d'_1 - d'_2) \frac{x_{AF} \cdot F \cdot RF_A}{D_{2i}} + d'_2 \\ &= \frac{F}{D_{2i}} [(d'_1 - d'_2) x_{AF} \cdot RF_A + \frac{d'_2 D_{2i}}{F}] \end{aligned}$$

substituting for D_{2i} from Equation (Alla)

$$Y_{2i} = \frac{F}{D_{2i}} [d_B \cdot x_{AF} \cdot RF_A + d'_2 (x_{AF} \cdot RF_A + x_{BF} [RF_B^{0.5} - RF_B])] \dots\dots\dots (A17)$$

$$\text{where } d_B = d'_1 - d'_2$$

$$d_B = \frac{\alpha_{AB''}}{\alpha_{AB''} - \phi_4} - \frac{1}{1 - \phi_4}$$

$$d'_2 = \frac{1}{1 - \phi_4}$$

(III) Development of objective function (Equation A7) in final form

The objective function was previously derived as Equation (A7)

$$\text{i.e. } \frac{\Delta V}{F} = \frac{1.25}{F} [(D_{1D} Y_{1D} + D_{2D} Y_{2D}) - (D_{1i} Y_{1i} + D_{2i} Y_{2i})]$$

$$- \frac{0.25}{F} [(D_{1D} + D_{2D}) - (D_{1,i} + D_{2i})]$$

now substituting as follows:

for Y_{1D}	equation (A14a)
Y_{2D}	equation (A15)
Y_{1i}	equation (A16)
Y_{2i}	equation (A17)

together with equation (A13).

The equation so obtained can be simplified to yield the following expression:

$$\frac{\Delta V}{F} = 1.25 x_{AF} (C_{B1} + C'_3 - d_{A1} - d_3) + 1.25 x_{AF} \cdot RF_A (C_A + C_2 - C_{B1} - C'_3)$$

$$+ 1.25 x_{BF} (C_2 - 0.2) + 1.25 x_{BF} \cdot RF_B (C_{B2} + C'_3 + d'_2 - 0.4)$$

$$+ 1.25 x_{BF} \cdot RF_B^{0.5} (0.75 - C_2 - d_{A2} - d_3 - d'_2) + 1.25 x_{CF} (1 - RF_C) (C'_3 - d_3)$$

The expressions in brackets can be further simplified by expanding the volatility terms and then cancelling.

$$\therefore \frac{\Delta V}{F} = 1.25 [x_{AF} (C'_1 - d_1 + RF_A (C_1 - d'_1 - C'_1 + 0.2))]$$

$$\begin{aligned}
 & + x_{BF}(C_2 - 0.2 + RF_B[C_2 + d_2' - 0.4] + RF_B^{0.5} [0.6 - d_2 - C_2 - d_2']) \\
 & + x_{CF}(1 - RF_C)(C_3' - d_3) \quad \dots\dots\dots(A18)
 \end{aligned}$$

$$\text{where } C_1 = \left[\frac{\alpha_{AB}}{\alpha_{AB} - \phi_1} \right]_{1D}$$

$$C_2 = \left[\frac{1}{1 - \phi_1} \right]_{1D}$$

$$C_1' = \left[\frac{\alpha_{AC}}{\alpha_{AC} - \phi_2} \right]_{2D}$$

$$C_2' = \left[\frac{\alpha_{BC}}{\alpha_{BC} - \phi_2} \right]_{2D}$$

$$C_3' = \left[\frac{1}{1 - \phi_2} \right]_{2D}$$

$$d_1 = \left[\frac{\alpha_{AC}}{\alpha_{AC} - \phi_3} \right]_{1i}$$

$$d_2 = \left[\frac{\alpha_{BC}}{\alpha_{BC} - \phi_3} \right]_{1i}$$

$$d_3 = \left[\frac{1}{1 - \phi_3} \right]_{1i}$$

$$d_1' = \left[\frac{\alpha_{AB}}{\alpha_{AB} - \phi_4} \right]_{2i}$$

$$d_2' = \left[\frac{1}{1 - \phi_4} \right]_{2i}$$

Thus Equation (A18) is a mathematical model relating the difference in

overhead vapour flow per mole of feed to the feed composition, component relative volatilities and the degree of recovery.

The model unfortunately contains four values of the Underwood parameter ϕ .

APPENDIX A4: Error in Flowpack Simulation Package.

APPENDIX A4: Error in Flow Pack Programme

Reference has been made in the text to the error which was discovered by the author in the distillation sub-routine of the programme 'Flowpack'. An example of this error is included to illustrate a difficulty encountered with the use of the Underwood method for the determination of the minimum reflux ratio.

As an example consider a three component feedstock having the following composition:

$$x_A = 0.2$$

$$x_B = 0.4$$

$$x_C = 0.4$$

and having component relative volatilities referred to component B as the heavy key as follows:

$$\alpha_{AB} = 7.2707$$

$$\alpha_{BB} = 1.0$$

$$\alpha_{CB} = 0.7944$$

For this feed at its bubble point, the value of 'q' in the Underwood equations will have a value of 1. Thus an iterative solution procedure is required to solve the following equation:

$$\frac{\alpha_{AB} \cdot x_A}{\alpha_{AB} - \phi} + \frac{\alpha_{BB} \cdot x_B}{\alpha_{BB} - \phi} + \frac{\alpha_{BC} \cdot x_C}{\alpha_{BC} - \phi} = 0$$

Using the Newton-Raphson method, the roots of the equation are found by use of the expression

$$\phi^1 = \phi - \frac{f(\phi)}{f'(\phi)}$$

where ϕ^1 is an improved value of the root. By use of this method, a value of ϕ of 3.0143 is obtained. In this case, interest is only centred on

the value of ϕ lying between the value of the relative volatility of the light key component, i.e. 7.2707 and 1.0. Confirmation of this value of the root can be made by calculating the value of the expression over the range of values of α . Figure A3 provides a computer printout illustrating the solution. The tolerance imposed on the solution by the Newton-Raphson method was 0.001.

For the solution by the method of the Bounded-False-Position, the previous equation of Underwood is modified to the following:-

$$\left[\begin{array}{ccc} \frac{\alpha_{AB} x_{\phi}}{\alpha_{AB} - \phi} + \frac{\alpha_{BB} x_B}{\alpha_{BB} - \phi} & + & \frac{\alpha_{CB} x_C}{\alpha_{CB} - \phi} \end{array} \right] \times \left[\frac{(\alpha_{AB} - \phi)(\alpha_{CB} - \phi)}{E} \right] = \text{error}$$

where the value of E was originally set at a value of 0.00001.

The method of Bounded-False-Position involves the determination of the value of the above expression at values marginally less than and greater than 7.2707 and 1.0 respectively. (By the nature of the Underwood's equations, the expression is infinite at the values of 7.2707 and 1.0). When the value of the expression is determined at these two values, the line joining the two values of the expression provides the improved value of the root by its intersection of the ϕ axis. This value is then used as the upper value to replace the previous upper value of 7.2707. However, in the programming of the method, the value of E was in effect multiplied by 100. A convergence limit of 0.1 was also set. As a result of this, a value of 2.3528 was obtained for ϕ .

It will be noted from Figure A2 which is a computer output for the iterative solution, that the value of 2.3528 is the first iteration value obtained. This value provides a value of the expression inside the tolerance set by the Bounded-False-Position method as programmed. With the tolerance set by the Newton-Raphson solution, a

```

RUN
DRBT 14:05 13-AUG-75
-9118.32 7.27063
2508.36 1.00001
1356.46 2.35284
-1966.29 3.94591
23.9118 3.00319
.289259 3.01451
-.255539E-3 3.01465
3.01465
    
```

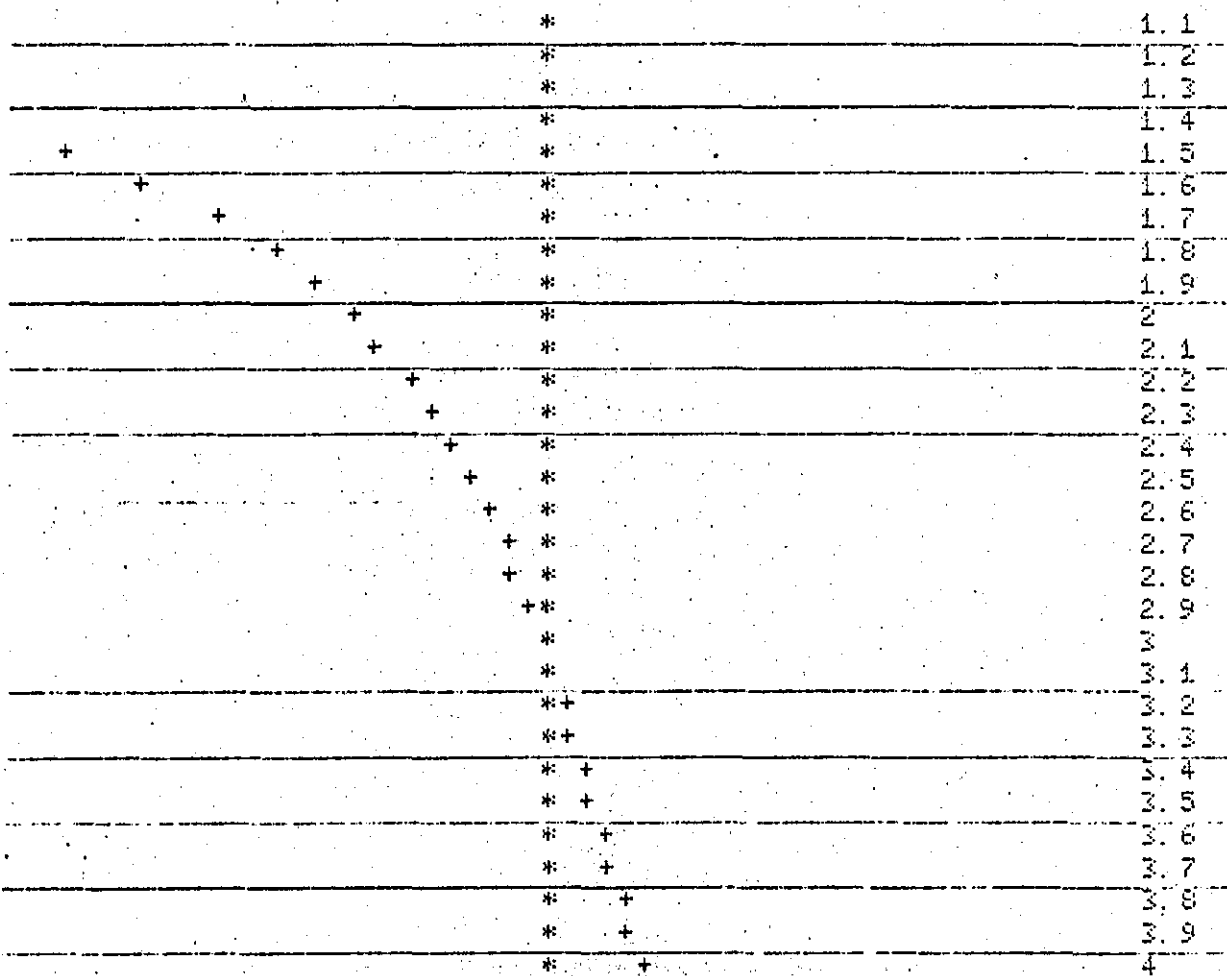
READY

OLD UGH

READY

```

RUN
UGH 14:06 13-AUG-75
Y -AXIS: FROM -1 TO 1 IN STEPS OF .04
    
```



°C

READY

FIGURE A2

value of 3.01465 was obtained four iterations later.

To illustrate the effect of the error in the values of the minimum reflux ratio, an example is given in Table A.3. This table gives the value of the minimum reflux ratio calculated by (a) the Underwood method incorporating the Bounded-False-Position method as incorrectly programmed and (b) the Newton-Raphson method. The feedstock used in the example is a four component feedstock in which components B and C are the light and heavy keys respectively.

When the dominant component is one of the keys, then the difference in values obtained by the two methods is not significant. However, when the dominant component is not one of the keys, the error is highly significant.

TABLE A3. Comparison of Values of R_{\min} Calculated by Incorrect Flowpack Programme and the Correct Values Given by Newton-Raphson.

Com- ponent	Feed Composition	Value of R_{\min}	
		Bounded False Position	Newton-Raphson
A	0.25		
B	0.25	1.5018	1.4096
C	0.25		
D	0.25		
A	0.7		
B	0.1	1.0646	0.6799
C	0.1		
D	0.1		
A	0.1		
B	0.7	1.0079	1.0214
C	0.1		
D	0.1		
A	0.1		
B	0.1	5.2338	4.2334
C	0.7		
D	0.1		
A	0.1		
B	0.1	1.6377	3.4794
C	0.1		
D	0.7		

APPENDIX A5: Papers published by Author in
Field of Study.

APPENDIX A5 - Published Papers

The author has published three papers in the field of study.

These are as follows:

- (i) Freshwater, D.C., and Henry, B.D. "Optimal Configuration of Multicomponent Distillation Systems". Paper presented to the Seventy-Sixth National Conference of the American Institute of Chemical Engineers, Tulsa, Oklahoma, March 1974.
- (ii) Freshwater, D.C., and Henry, B.D. "The Optimal Configuration of Multicomponent Distillation Trains". *The Chemical Engineer*, No. 301, 533-536, September, 1975.
- (iii) Henry, B.D. "Selection of Economic Process Routes for the Separation of Multicomponent Feedstocks by Distillation". *The Institution of Engineers, Australia. Fourth National Conference on Chemical Engineering: The Effective Use of Hydrocarbons Resources, Adelaide, August 1976. Preprints of Papers pp.46-50 (The Institution of Engineers, Australia National Conference Publication No. 76/6).*

APPENDIX A6:

- A6.1 Flowpack - Input Data
- A6.2 Flowdist - Input Data and typical Output
- A6.3 Cost - Description of Programme and
Flow Chart
- A6.4 Pslids - Flowchart
- A6.5 Example of 'Flowpack' Output

APPENDIX A6.1 - Flowpack Programme - Input Specification

For this programme, the cards which constituted the data were:

- CARD 1 This contains the word "DATA TITLE" beginning in column 2.
- CARD 2 The title of the program.
- CARD 3 The number of components. This is punched as number beginning in column 2. A maximum of 25 components is allowed.
- CARD 4 The key word "NAMES". This is given only if the names of the components are to be supplied.
- CARD 5 The component names are now given each on a separate card. Each name may be of up to sixteen characters.
- CARD 6 The key word "YES". This indicates that physical property data will be supplied.
- CARD 7 The key word "ANTOINE" or "NGPA". This indicates whether Antoine coefficients or NGPA data is to be used for K value determination.
- CARD 8 The constants A, B and C are now given, the values for each component being on a separate card. The Antoine constants supplied should fit the equation

$$\log_e P = A + \frac{B}{C + T} \quad \dots\dots\dots (7)$$

where P is the pressure in mm. Hg and T is the temperature in degrees centigrade.

K values determined by NGPA data are given as

$$K(i) = A(i) + B(i).T + C(i).T^2 + D(i).T^3$$

- CARD 9 The key word "NOMOLWT". This indicates that no molecular weights are supplied.
- CARD 10 The key word "HEAT". This indicates that enthalpy coefficients are to be supplied.
- CARD 11 The molar enthalpy coefficients for both liquid and vapor phases are now given, the data for each component being on a separate card.

All eight coefficients for each component must be on the same card the liquid phase coefficients being given first.

The coefficients should fit the equations

$$HL = L_1 + L_2T + L_3T^2 + L_4T^3 \quad \dots\dots (8)$$

$$HV = V_1 + V_2T + V_3T^2 + V_4T^3 \quad \dots\dots (9)$$

where HL and HV are the enthalpies of the liquid and vapor phase in kJ/kg mole; T is the temperature in degrees kelvin; L_1 , L_2 , L_3 and L_4 are the coefficients for the liquid phase and V_1 , V_2 , V_3 and V_4 are the coefficients for the vapor phase.

- CARD 12 The key word "END". This indicates the end of the physical property data.
- CARD 13 The number of external streams to the process.
- CARD 14 This contains the unit number to which the external stream goes and the input number for the stream to the unit in that order.
- CARD 15 The total number of process units. The maximum number of distillation columns (units) is 10.

CARD 16

This card contains the unit number, the unit type, the number of inputs to the unit, the number of outputs from the unit, the destination of output 1 in terms of the unit number it is going to and the input number for the stream, and the destination of Output 2 in the same form as Output 1, in that order.

The unit numbers for distillation columns range from 1 to 10 and the units should be numbered in the order in which the calculation is to be performed.

The unit type number for a distillation column is 7.

The number of inputs to a distillation column unit = 1.

The number of outputs from a distillation column unit = 2.

Output 1 is the top product from the distillation column and Output 2 is the bottom product from the column.

From each output stream the unit number and input number of the unit to which it is joined must be specified.

There is only one input to the distillation columns so the input number is always 1. If the output is to the environment the unit number is put equal to zero.

A card of this type should be provided for each process unit.

CARD 17

This contains the unit parameter data for the distillation column. A card of this type is required for each unit.

The order of the data on the card is as follows:

- (1) Unit number
- (2) Light key component number
- (3) Heavy key component number
- (4) Fractional recovery of light key in the distillate
- (5) Fractional recovery of heavy key in the residue

- (6) Pressure drop per plate
- (7) Reflux ratio as multiple of minimum reflux
- (8) Condenser indicator. The value is 1 for a total condenser and 2 for a partial condenser.

CARD 18 The key word "MOLE". This indicates that the flow rates are to be given as molar flows/hr.

CARD 19 The number of streams to be initialised. "initialisation" means the specification of the temperature, pressure, composition, of the feed stream. As there is only one feed to each configuration, the value for the number of streams to be initialised is 1.

CARD 20 This card contains the data for the feed stream in the following order:

- (1) Unit Number - the feed is from the environment, so the value is zero.
- (2) Output number - as the feed is from environment, the value is one.
- (3) Temperature of the Feed in degrees kelvin.
- (4) Pressure of the feed in N/m^2 .
- (5) The amount in Kg moles/hour of each component in the feed. The amounts are given in the order of the component numbers, the amount of component 1 being first.

CARD 21 This card contains the data for the calculation requirements.

The order of the data on the card is as follows:

- (1) Method of solution - there are six methods for solving the equations in the program and the details of each are available in the FLOWPACK manual. (20) As there are no recycles in the

configurations we are considering, simple repeated substitution is the best method, so a value of 1 should be given.

- (2) Accuracy required - a value for this of 0.001 was given.
- (3) Maximum number of iterations - as there are no recycle streams, only one iteration is needed, but the value is set equal to 20.
- (4) Intermediate Print Parameter - this controls the output of the results from the program. There are four parameters in use. The value 3 is given. This prints out the values of the temperatures, pressure and component molar flow rates.
- (5) Final Print Parameter. The value is 1. This gives a print-out of molar flow rates and mole fractions.

CARD 22 The key word "PARAM". The data for one calculation is complete when Card 21 is supplied. PARAM indicates that a new section of data is going to be provided in which the unit parameters for the units have been changed.

CARD 23 Number of units with parameter changes.

CARD 24 The new unit parameters for each unit are now given. These cards are of the same type as Card 17.

In the project the initial unit parameters gave 99% recovery of all components, and the new parameters give 95% recovery of all components in the feed.

CARD 25 Card 22 is repeated.

CARD 26 Card 23 is repeated.

- CARD 27 This contains the new values of the unit parameters for 90% recovery of all components. One card for each unit must be given and the card is of the same type as Card 17.
- CARD 28 The key word "YES". This indicates that new values are going to be supplied for the unit parameters and for the feed stream specifications.
- CARD 29 Card 23 is repeated.
- CARD 30 Card 17 is repeated.
- CARD 31 Number of streams to be changed. The value for this is 1.
- CARD 32 The new data for the feed stream is provided. The card is of the same type as Card 20.
- CARD 33 Card 22 is repeated.
- CARD 34 Card 23 is repeated.
- CARD 35 Card 24 is repeated.
- CARD 36 Card 22 is repeated.
- CARD 37 Card 23 is repeated.
- CARD 38 Card 27 is repeated.

The calculation for all three cases of recovery for the new feed stream, the data for which was provided in Card 32 has now been completed.

For every new feed stream, Cards 28 to 38 are repeated, the new data for the feed stream being given in Card 32.

If no more new feed streams are to be considered, the program is terminated by giving the key word "NO" instead of "YES" in Card 28.

APPENDIX A6.2:FLOW DIST PROGRAMME - INPUT SPECIFICATION

The data is read in using "Free Format (F.O.O)".

The arrangement of data for this program is as follows:

- CARD 1 The title of the program. Any title of up to 72 characters can be given beginning in column 1.
- CARD 2 The number of components. A maximum of 25 components is allowed. The format is I2.
- CARD 3 The component names are now given, each on a separate card and beginning in column 1. Each name may be of up to sixteen characters.
- CARD 4 Depending on whether Antoine coefficients or NGPA data was being used for the generation of the K values, the constants A, B and C to be read in represented the following:

- (a) Antoine Coefficients. These coefficients fitted the equation:

$$\ln P = A(i) + \frac{B(i)}{C(i) + T}$$

where P is the pressure in mm.Hg. and T is the temperature in degrees centigrade.

- (b) NGPA data. The coefficients fitted the equation:

$$K(i) = A(i) + B(i) \times T + C(i) \times T^2 + D(i) \times T^3$$

- CARD 5 The molar enthalpy coefficients for both liquid and vapour phases are now given, the data for each component being on a separate card. All eight coefficients for each component must be on the same card, the liquid phase coefficients being given first. The coefficients should fit the equations:

$$HL = L_1 + L_2 + L_3 T^2 + L_4 T^3$$

$$HV = V_1 + V_2 T + V_3 T^2 + V_4 T^3$$

where HL and HV are the enthalpies of the liquid and vapour phase in J/Kg; T is the temperature in degrees kelvin; L_1 , L_2 , L_3 and L_4 are the coefficients for the liquid phase and V_1 , V_2 , V_3 and V_4 are the coefficients for the vapour phase (Free Format).

- CARD 6 The costing parameter is now given. If costing is not required read in a value of zero otherwise read in a value of 1 (Format I2). If costing is not required the next data card will be CARD 15.
- CARD 7 The molecular weights of the components, each one being given on a separate card (Free Format).
- CARD 8 The liquid density coefficients for the components. All four coefficients D_1 , D_2 , D_3 , and D_4 are punched on the same card and a separate card is required for each component (Free Format).
- The coefficients should fit the equation:
- $$DL = D_1 + D_2 T + D_3 T^2 + D_4 T^3$$
- where DL is the density of the liquid in Kg/m^3 and T is the temperature in degrees kelvin.
- CARD 9 The values for the Flood Factor and System Factor are read in (Free Format). (The values normally used are 0.7 and 1.0 respectively).
- CARD 10 The service life of equipment in years (Format I2).
- CARD 11 The two coefficients for the vapour capacity factor equation and the two coefficients for the vapour capacity factor limit

point equation are given on the same card with the vapour capacity factor equation coefficients being given first (Free Format).

(The vapour capacity factor equation coefficients are:

$$F1 = 0.46000 \qquad F2 = -0.01500$$

The vapour capacity factor limit point equation coefficients are:

$$F5 = 0.60809 \qquad F6 = -0.06182$$

CARD 12 The overall heat transfer coefficients for the condenser and reboiler, in $W/m^2 \cdot K$ in that order (Free format).

CARD 13 This contains the cost data in the following order (Free format):

(1) The cost of a distillation column with dimension parameter of 100.

(2) The cost of a tray with an area of 9.29 m^2 .

(3) The cost of a heat exchanger with surface area of 92.9 m^2 .

(4) The cost of 4546 litres of cooling water.

(5) The cost of 453.5 Kg of steam.

(6) The cost of 4546 litres of chilled water.

CARD 14 This contains the slopes of the cost curves in the following order (Free format):

(1) Slope of dimension parameter Vs. column cost curve

(2) Slope of tray area Vs. cost curve

(3) Slope of heat exchanger surface area Vs. cost curve.

CARD 15 The total number of process units (Format I2).

CARD 16 This contains the unit numbers to which the distillate and bottoms streams go. The destination of the distillate stream is given first (Format 2I2).

If the distillate stream is a product stream, the unit number is put equal to zero, i.e. $LT(I)=0$.

If the bottoms stream is a product stream, the unit number is put equal to zero, i.e. $LB(I)=0$.

CARD 17 This card contains the data for the feed stream to unit number 1 in the following order (Free Format):

- (1) Temperature of the feed in degrees centigrade
- (2) Pressure in N/m^2 .
- (3) The amounts in Kg. moles/hour of each component in the feed. The amounts are given in the order of the component numbers, the amount of component 1 being first.

CARD 18 This contains part of the unit parameter data for the distillation column. A card of this type is required for each unit. The order of the data on the card is as follows (Format 3I2):

- (1) Light key component number
- (2) Heavy key component number
- (3) Condenser indicator. The value is 1 for a total condenser and 2 for a partial condenser.

CARD 19 The rest of the unit parameter data for the distillation column is given on this card. A card of this type is required for each unit. The order of the data is as follows (Free Format):

- (1) Fractional recovery of light key in the distillate
- (2) Fractional recovery of heavy key in the bottoms
- (3) Pressure drop per plate
- (4) Reflux Ratio as multiple of minimum reflux.

CARDS 18 & 19 are repeated for each unit as follows:

Card 18 for unit 1
Card 19 for unit 1
Card 18 for unit 2
Card 19 for unit 2 and so on.

CARD 20 The value of the parameter KEY is now given. This is a parameter for the reading in of further data (Format I2)

(1) KEY = 0

 No further data to be read in - Program stops

(2) KEY = 1

 New unit parameters are to be read in.

 Data cards 18, 19 and 20 are repeated.

(3) KEY = 2

 New unit stream is to be initialised.

 Data cards 17, 18, 19 and 20 are repeated.

(4) KEY = 3

 New process topology is to be read in

 Data cards from CARD 15 to CARD 20 (both inclusive)
 are repeated.

APPENDIX A6.3 - The Program "Cost"

The program COST, was used to carry out the costing calculations for a distillation column, condenser and reboiler.

All the costs are in pounds sterling. The program COST is in three parts, the master program COST and the subroutines DATAR 1 and COSCA 1.

MASTER COST

This reads in the data which is common for all the runs to be made. The data which is read in is as follows:

- (1) the number of components in the feed to the distillation column.
- (2) The molecular weight of each component in the feed.
- (3) The liquid density coefficients for each component in the feed.
- (4) The coefficients for the vapour capacity factor equation.
- (5) The coefficients for the vapour capacity factor limit point equation.
- (6) The flood factor.
- (7) The system factor.
- (8) The cost of a distillation column with dimension parameter of 100.
- (9) The cost of a distillation column tray with an area of 9.29 m^2 .
- (1) The cost of a 92.9 m^2 surface area heat exchanger.
- (11) The cost of a 4546 litres of cooling water.
- (12) The cost of a 453 Kg of 690 kN/m^2 steam.
- (13) The cost of a 4546 litres of chilled water.
- (14) The slope of the column dimension parameter vs cost curve.
- (15) The slope of the tray area vs cost curve.

- (16) The slope of heat exchanger surface area vs cost curve.
- (17) The overall heat transfer coefficients for the condenser and reboiler.
- (18) The service life of the equipment in years.

It also reads in the number of runs which are to be made and for each run the two subroutines DATAR 1 and COSCA 1 are called up in turn.

SUBROUTINE DATAR 1

This subroutine reads in the data for each run. The following data is required for this subroutine:

- (1) The feed to the distillation column in Kg Moles/hour.
- (2) The top product from the column in Kg Moles/hour.
- (3) The bottom product from the column in Kg Moles/hour.
- (4) The reflux ratio.
- (5) The mole fraction of each component in the bottoms product.
- (6) The number of theoretical plates in the column.
- (7) The top temperature of the column in degrees kelvin.
- (8) The bottom temperature of the column in degrees kelvin.
- (9) The column pressure in N/m^2 .
- (10) The condenser heat load in GJ/hour.
- (11) The reboiler heat load in GJ/hour.

SUBROUTINE COSCA 1

This subroutine performs all the calculations for the cost of equipment, steam and water. The costs for the equipment are summed to give the total major equipment cost and the total yearly operating cost is also calculated.

The assumptions made in this subroutine are:

- 1. The vapour obeys the ideal gas laws.

2. Constant molal overflow is assumed in the column.
3. The diameter of the column is based on the vapour flow at the top of the column.
4. Tray efficiency is 60%.
5. Tray spacing is 61 cms.
6. The tray area is 85% of column area.
7. It is assumed that the equipment is operated all the year.
8. All equipment is considered to be carbon steel.

The design procedure adopted for the design of the columns is in accordance with the Glitsch Ballast Tray Design Manual and will not be described in this Thesis.

Calculation of the cost of the distillation column

The diameter of the column is multiplied by the height to give the dimension parameter VT. The cross sectional area of the column is calculated and the tray area TA is taken to be 85% of it. The cost of the column is now calculated using the equation

$$CT = C_1 \times \frac{(VT)^{E_1}}{(100)} + \left(C_2 \frac{(TA)^{E_2}}{(100)} \times M \right) \dots\dots (15)$$

The cost data provided for the cost of equipment is the cost in 1969, so this is multiplied by 1.505 which is the ratio of the Process Engineering Cost Indices for 1969 and 1973.

The overall heat transfer coefficient, U, for the condenser has been taken as 567 W/m² °K. The surface area of the condenser, A, is then calculated using the formula

$$A = \frac{Q}{U \times TD}$$

If the surface area of the condenser comes out to be greater than 929 m² the area is divided by two and the cost is calculated

for the heat exchangers with the new area and multiplied by two.

The cost equation used for the condenser is of the same type as used for the column, that is

$$CC = C3 \left(\frac{A}{1000} \right)^{E_3}$$

The cost is updated by multiplying by 1.505.

Calculation for the cost of the Reboiler

690 kN/m² steam is used as the heating medium in the reboiler and its temperature is 170°C. The log mean temperature difference in this case is calculated by the equation

$$TB = 170 - T$$

The rest of the method is similar to that used for the costing of the condenser.

Calculation of cooling water cost

The cooling water cost per year is calculated using the equation

$$CW = \frac{24 \times 365 \times C4 \times HC}{1000 \times DT \times 8.33}$$

The cost of chilled water is presented as cooling water cost and is calculated by a similar equation, the only difference being that C4 is replaced by C6.

Calculation of Steam cost

The cost of steam per year is calculated using the equation

$$CS = \frac{24 \times 365 \times C5 \times HR}{1000 \times 1000}$$

Calculation of Total Major Equipment Cost and Total
Yearly Operating Cost

The costs for the distillation column, condenser and reboiler were summed up to give the total major equipment cost, CE.

The installation cost for the equipment was taken to be equal to 3 times the major equipment cost, therefore the total cost of equipment and installation is equal to four times the major equipment cost. The equipment was assumed to be depreciated in 10 years and the total yearly operating cost was then calculated by summing the depreciation cost per year, cooling water and steam costs. The equation for total yearly operating cost is

$$CO = \frac{(4 \times CE)}{(Z)} + CS + CW$$

ARRANGEMENT OF DATA CARDS

All the data is punched out on cards and free format has been used for the data except in cases where some other format is mentioned.

CARD 1 The number of components in the feed mixture to the configuration. The format is I2.

CARD 2 The molecular weight for the component.

CARD 3 The liquid density coefficients for the component.

All four coefficients are punched on the same card.

Cards 2 and 3 are repeated for each component in the feed.

CARD 4 The two coefficients for the vapour capacity factor equation.

CARD 5 The two coefficients for the vapour capacity factor limit point equation.

CARD 6 The flood factor and the system factor.

CARD 7 This contains the cost data in the following order:

- (1) The cost of a distillation column with dimension parameter of 100.
- (2) The cost of a tray with an area of 9.29 m^2 .
- (3) The cost of a heat exchanger with surface area of 92.9 m^2 .
- (4) The cost of 4546 litres of cooling water.
- (5) The cost of 453.5 Kg of steam.
- (6) The cost of 4546 litres of chilled water.

CARD 8 This contains the slopes of the cost curves in the following order:

- (1) Slope of dimension parameter vs column cost curve.
- (2) Slope of tray area vs cost curve.
- (3) Slope of heat exchanger surface area vs cost curve.

CARD 9 The overall heat transfer coefficients for the condenser and reboiler, in $\text{W/m}^2\text{°K}$, in that order.

CARD 10 The service life of equipment in years. The format is I3.

CARD 11 The number of runs to be made. The format is I3.

CARD 12 This contains the values of the feed, distillate and bottoms flow rate and the reflux ratio for the column in that order. All flow rates are in Kg Moles/hour.

CARD 13 This contains the mole fraction of all components in the bottom product from the column in the same order as the molecular weights have been given.

CARD 14 The number of theoretical plates in the column, the temperature of the bottoms and the top product in degrees centigrade, and the pressure in N/m^2 are set out in that order.

CARD 15 The condenser and reboiler heat loads, in GJ/W hour in that order.

Cards 12 to 15 are repeated for each run to be made.

A print-out of the programme is given in the Appendix.

Flood Factor = 0.7

System Factor = 1.0

Cost Data:

Cost of distillation column - dimension

parameter of 100 = £ 1200.0000

Cost of a 9.29 m² tray = £ 270.0000

Cost of a 92.9 m² heat exchanger = £ 2625.0000

Cost of 4546 litres of cooling water = £ 0.0900

Cost of 4546 litres of chilled water = £ 0.1800

Cost of 453.5 of steam = £ 0.5000

Slope of column dimension parameter

vs cost curve = 0.4310

Slope of tray area vs cost curve = 0.9230

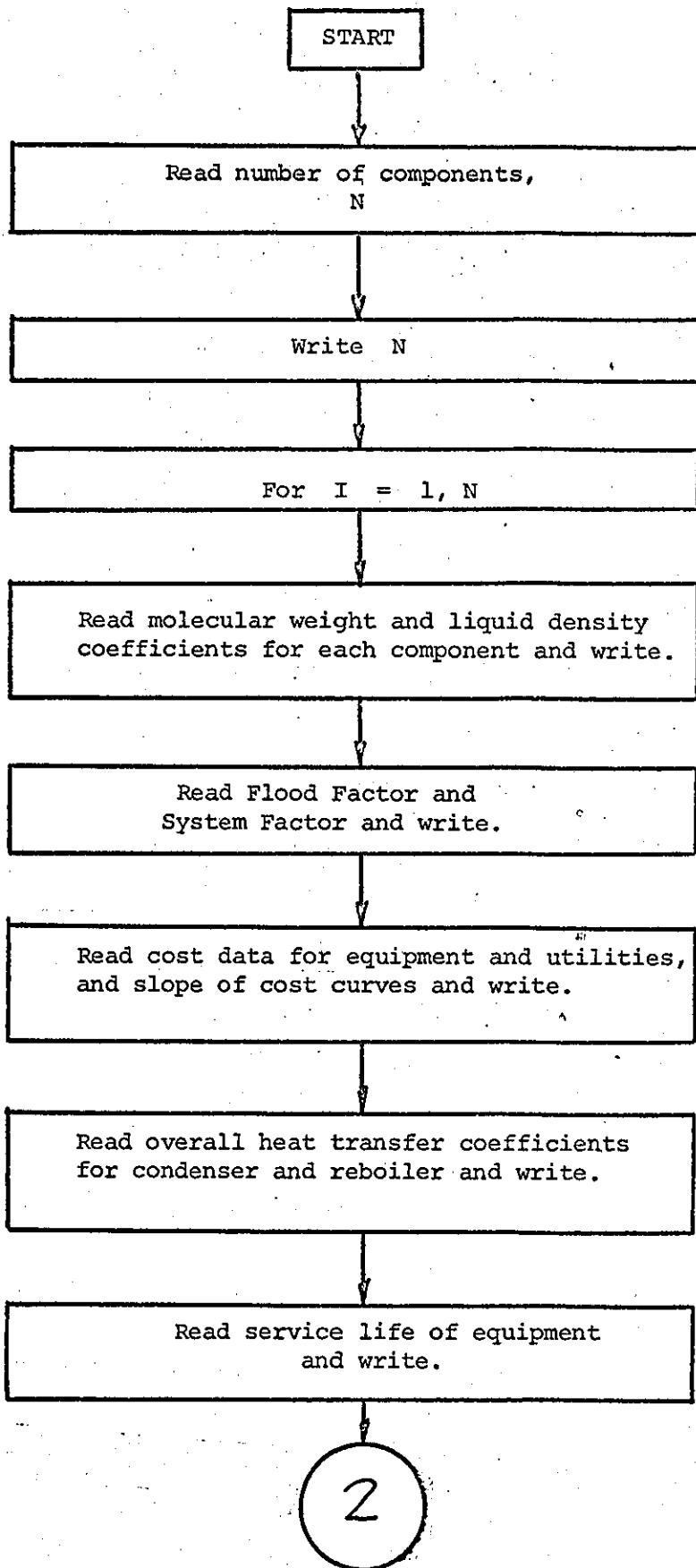
Slope of heat transfer area vs cost curve = 0.6330

Overall Heat Transfer Coefficients

For Condenser: 567.8 W/m²°K

For Reboiler: 709 W/m²°K

Service life of equipment = 10 years

MASTER COST



Read number of runs, III

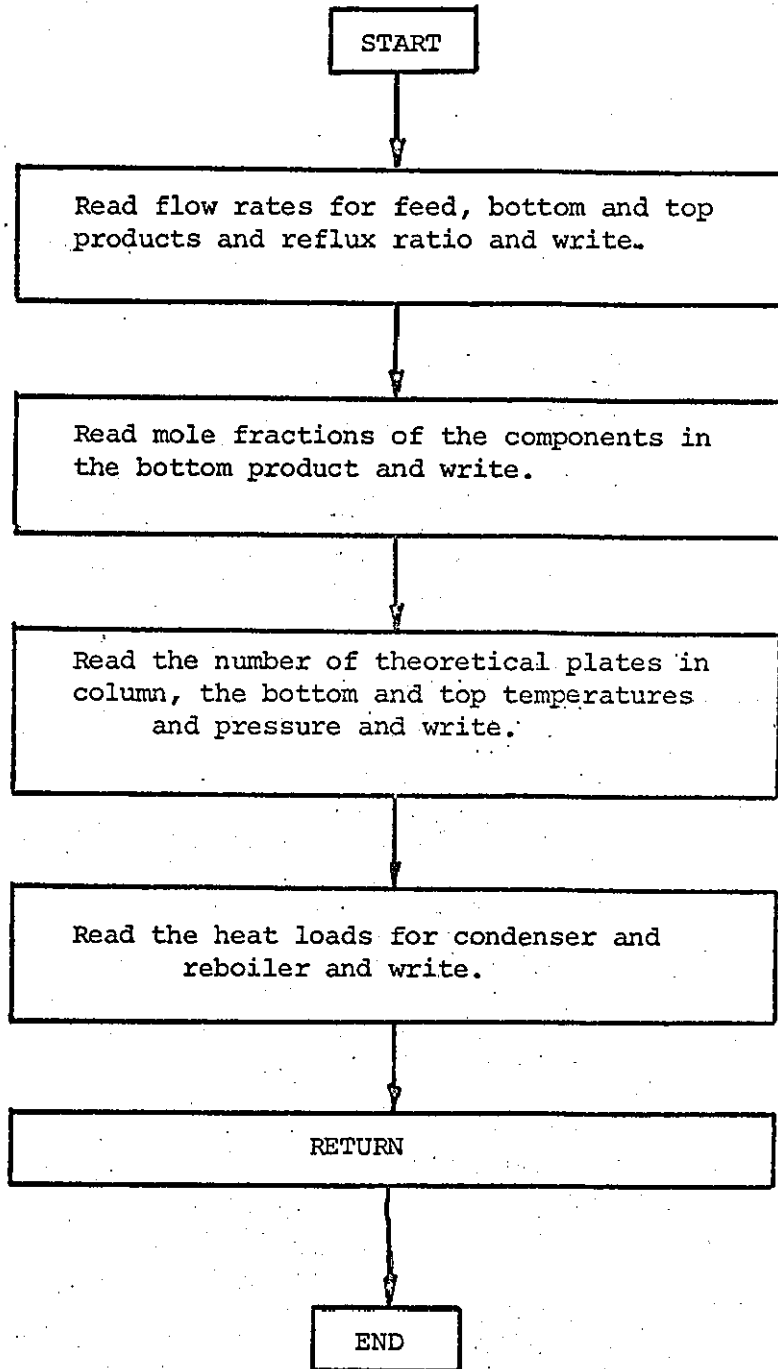
For II = 1, III

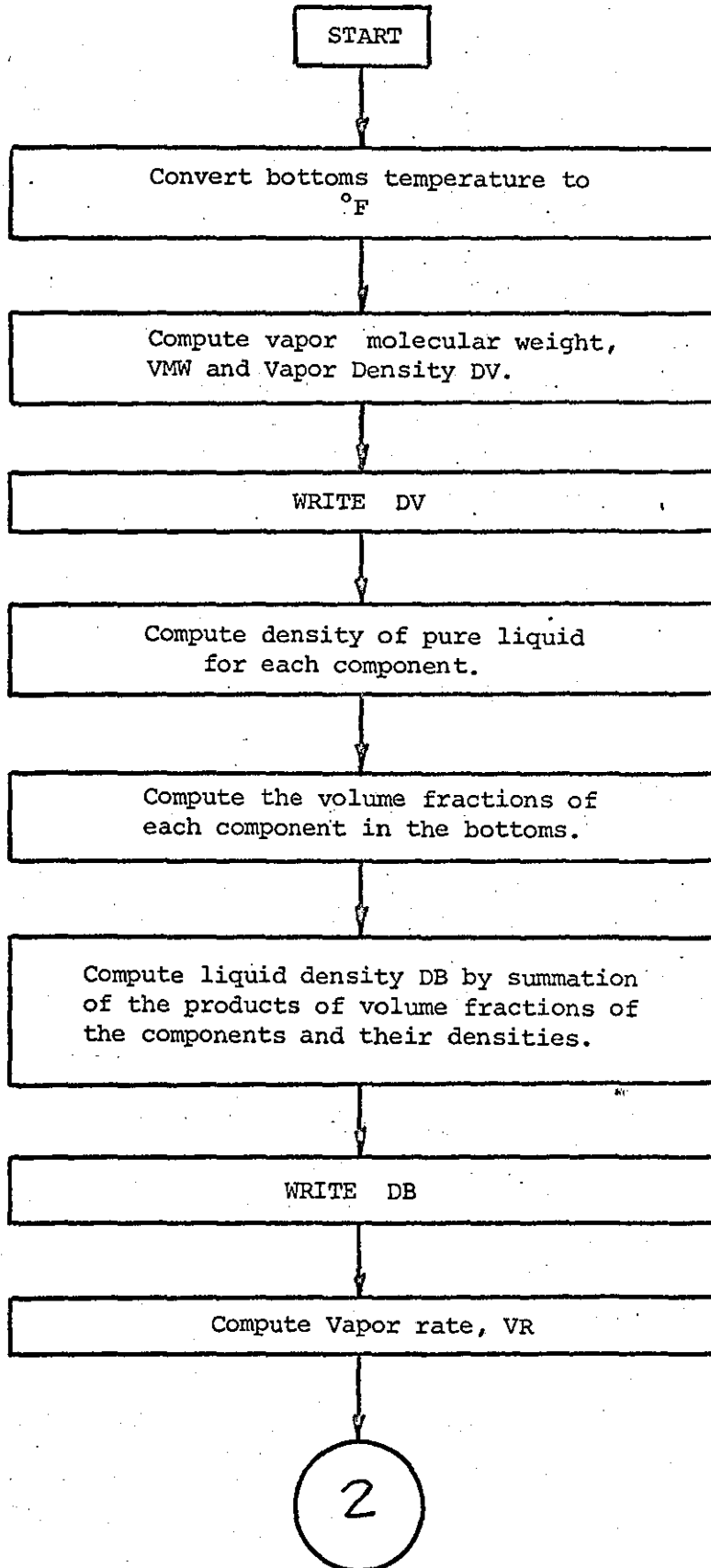
Call DATAR 1

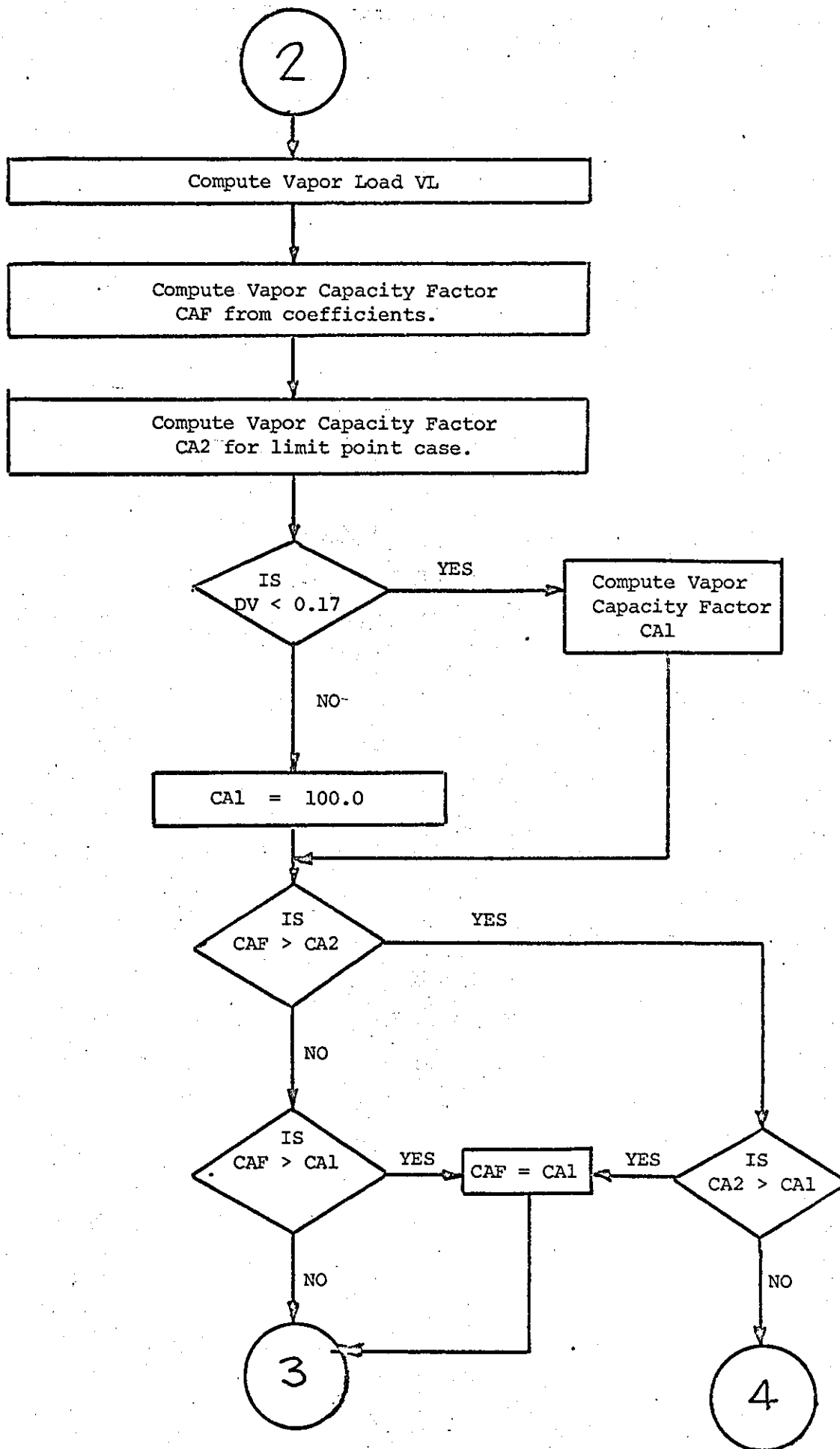
Call COSCA 1

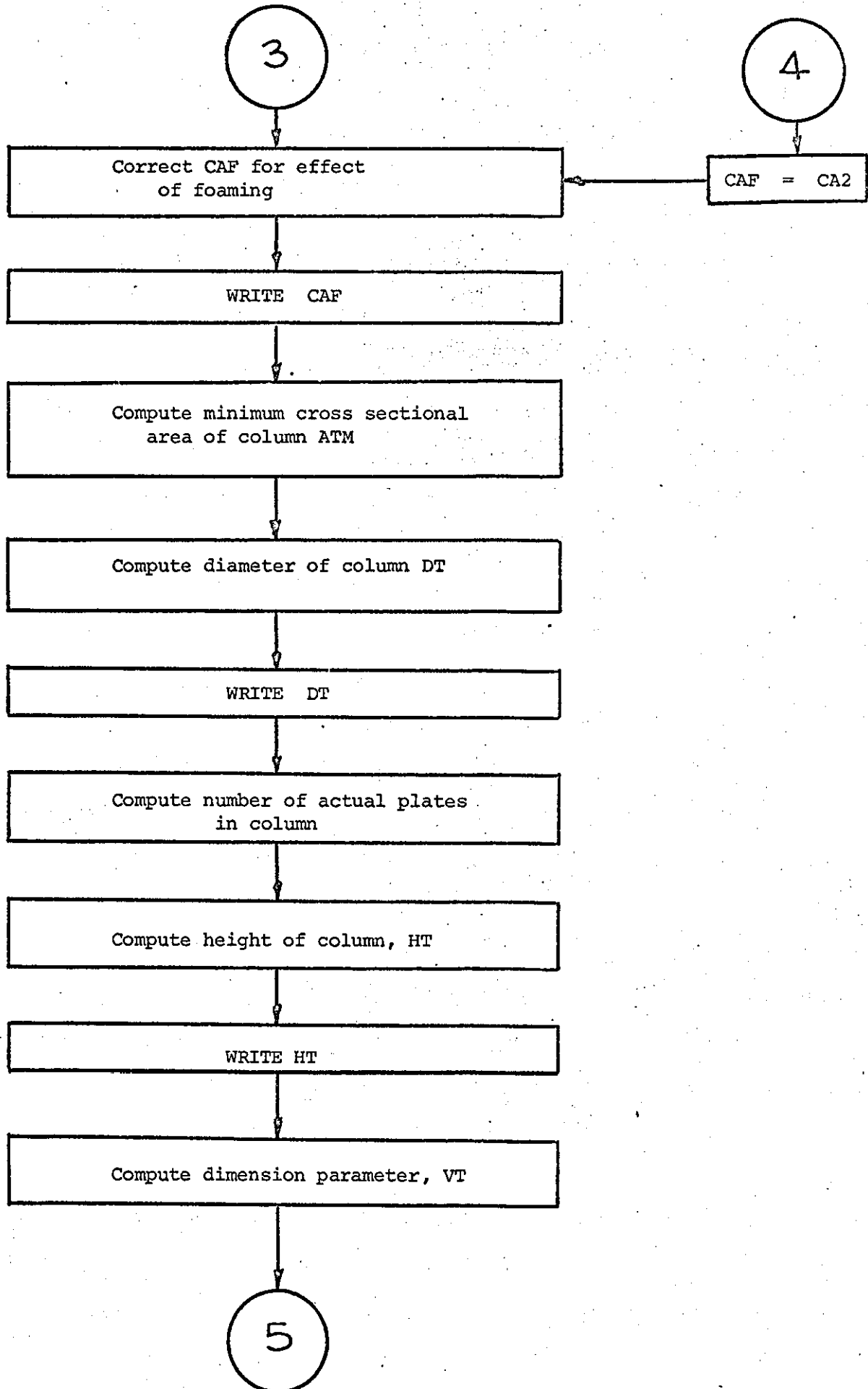
CONTINUE

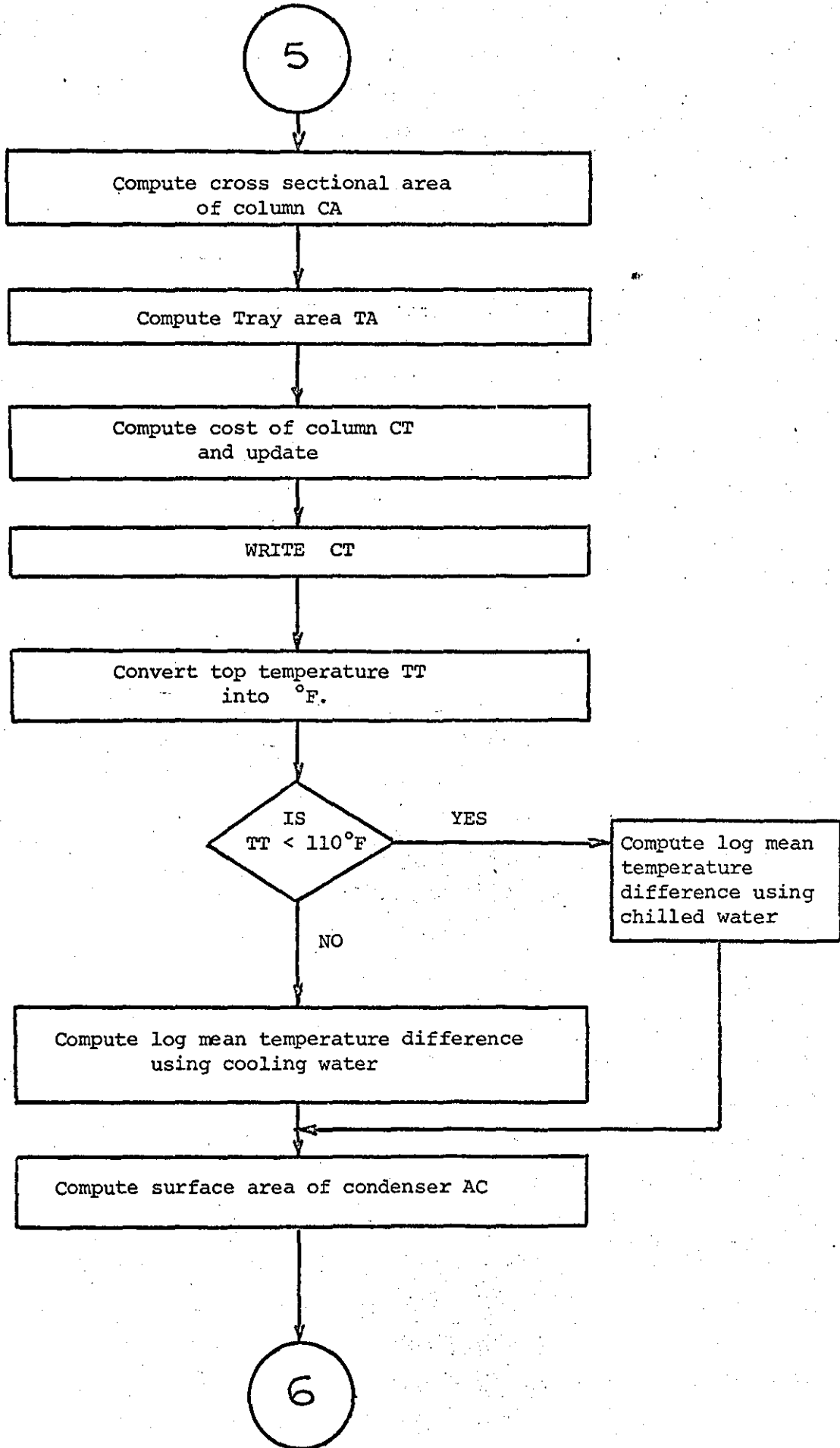
END

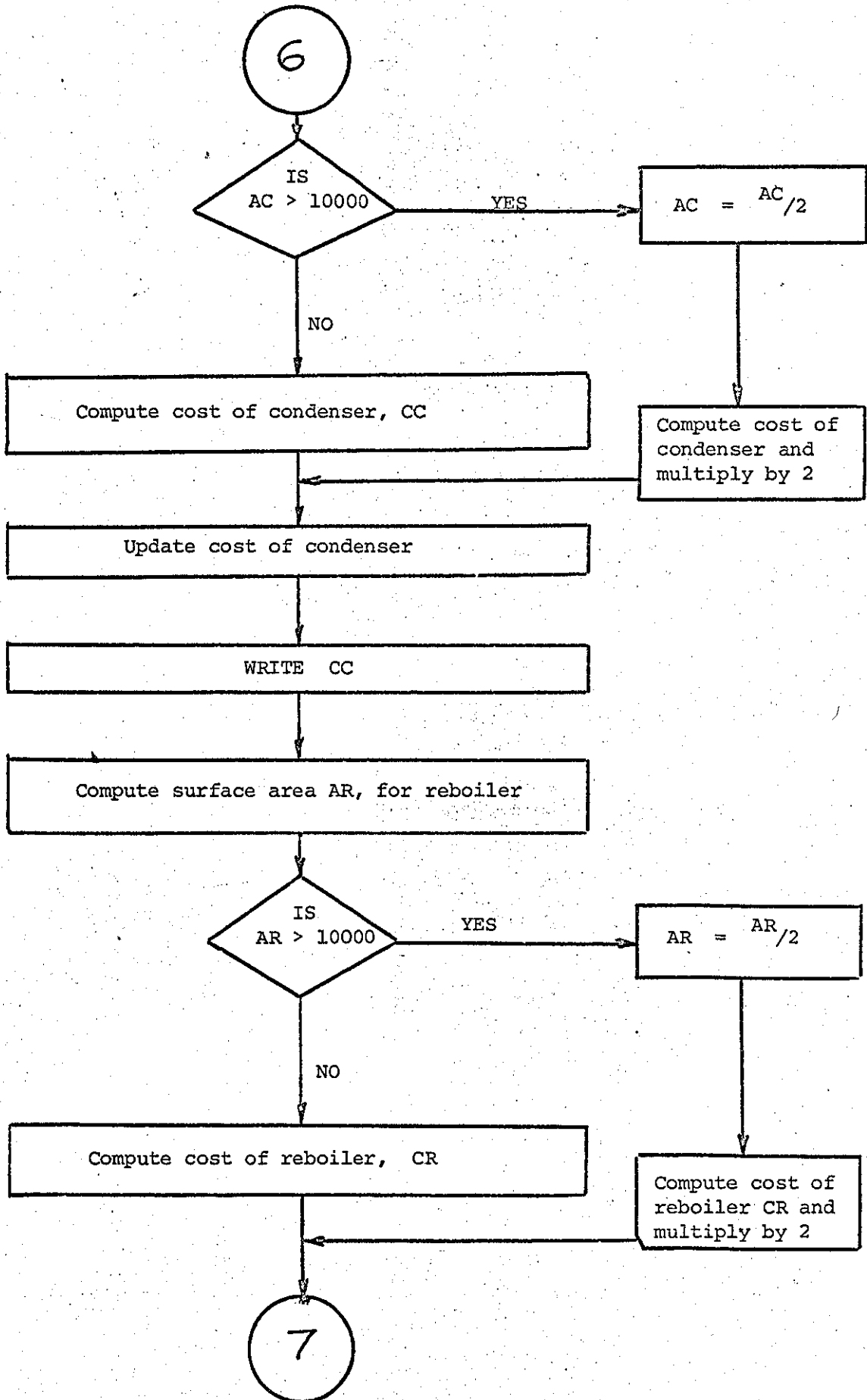
SUBROUTINE DATAR 1

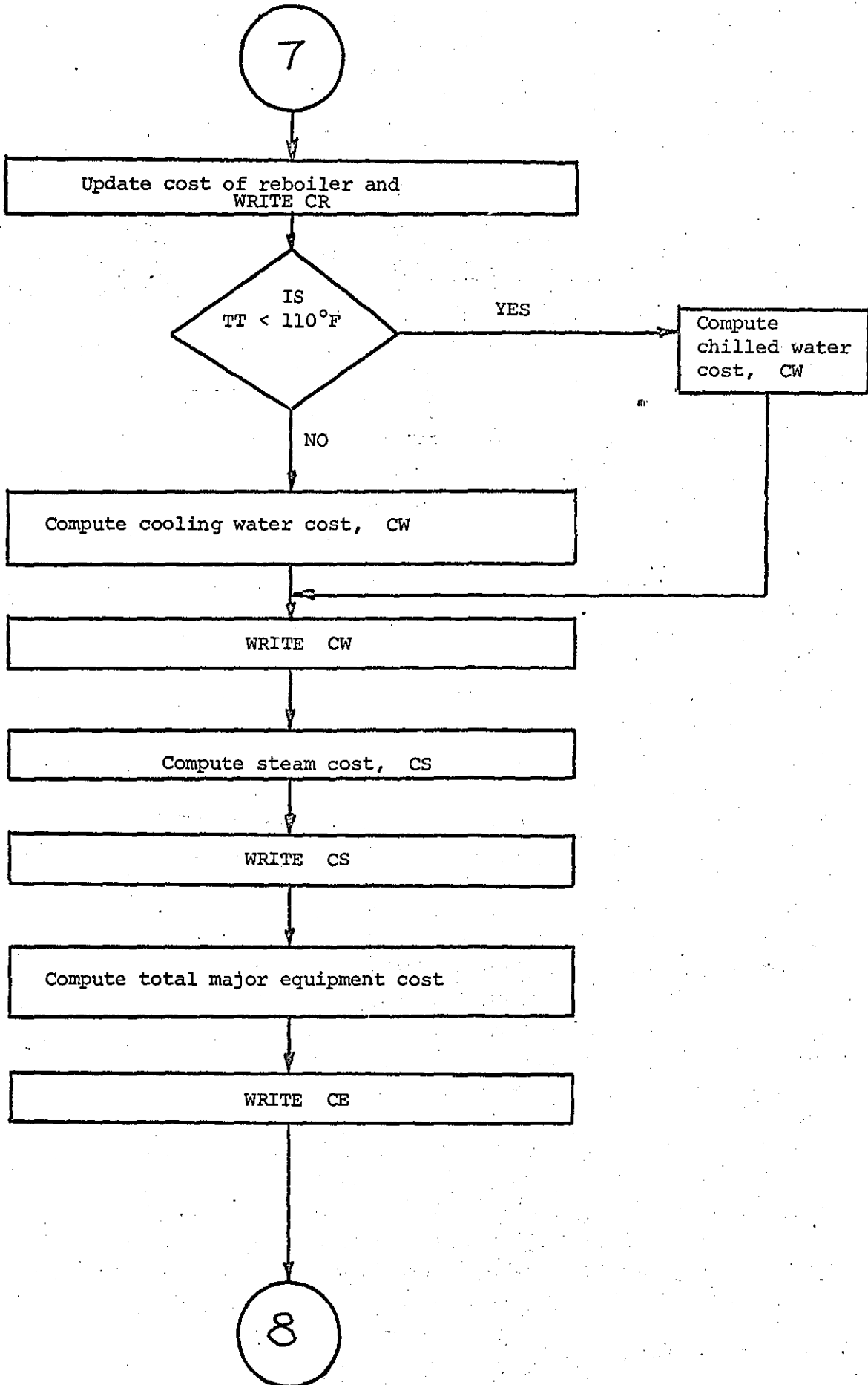
SUBROUTINE COSCA 1

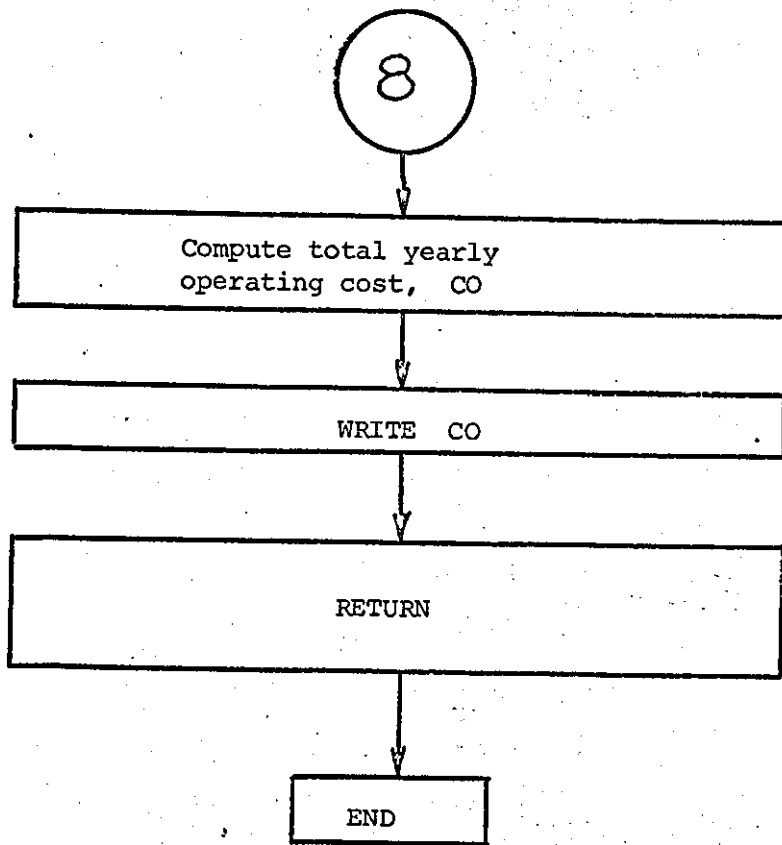




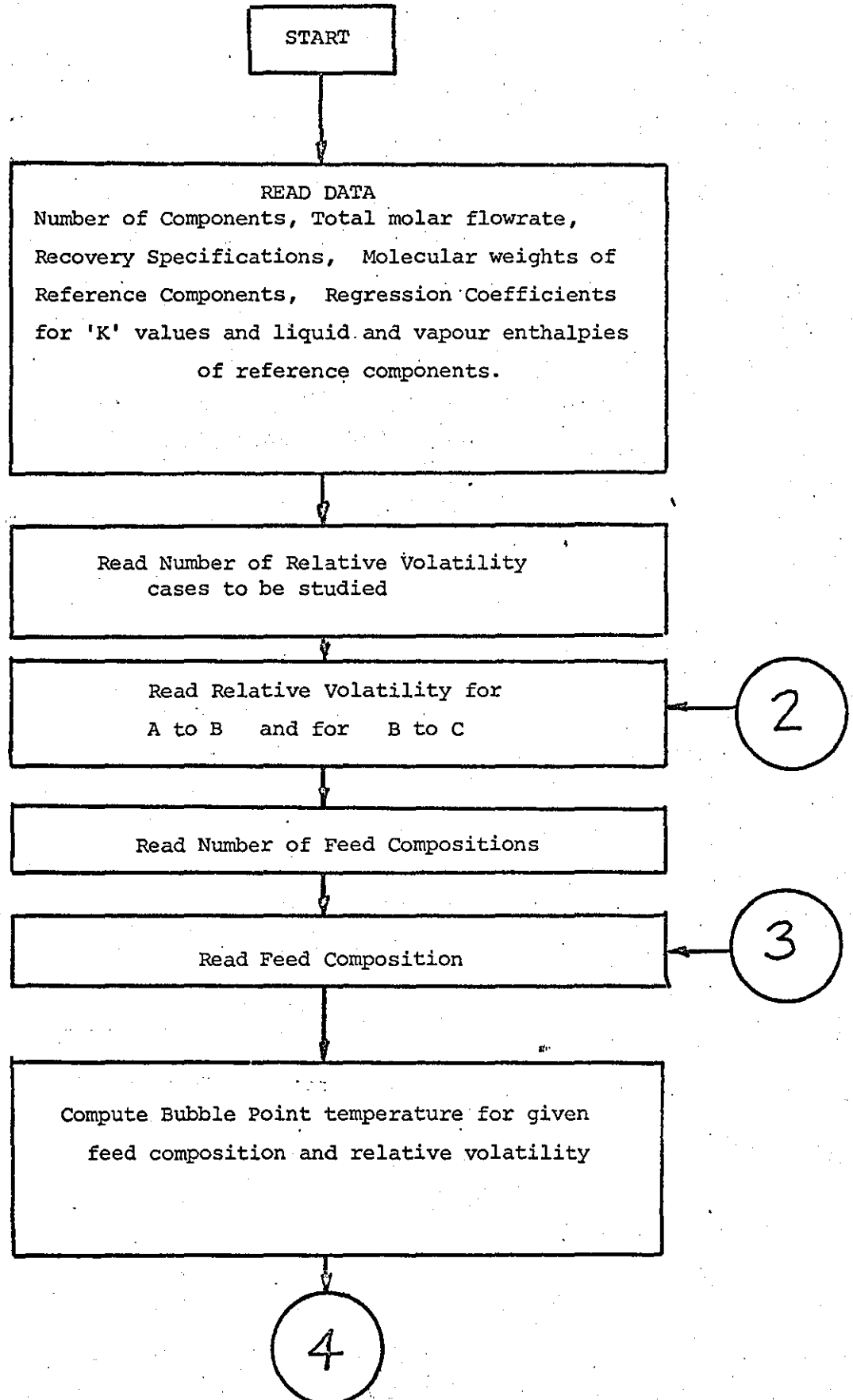








APPENDIX A6.4 - PROGRAMME PSLIDS

Simplified Computer Flowchart

5

Compute for Column one direct amounts of components in both products assuming non-distribution of non-key components

Compute dew point and bubble point temperatures of overhead and bottoms products respectively

10

Compute relative volatilities at these temperatures

Compute geometric mean of these relative volatilities

Compute Total Reflux Ratio using Fenske's Method and Winn's modification

Compute distribution of non-key components at Total Reflux conditions

6

4

230.

Compute K value of components A, B and C
at bubble point temperature

Compute ratio given in Table 5.1 to be
used to generate K values over temperature
range for Components A and B

Call Flow 1 to generate K values
regression coefficients for pseudo
components A and B

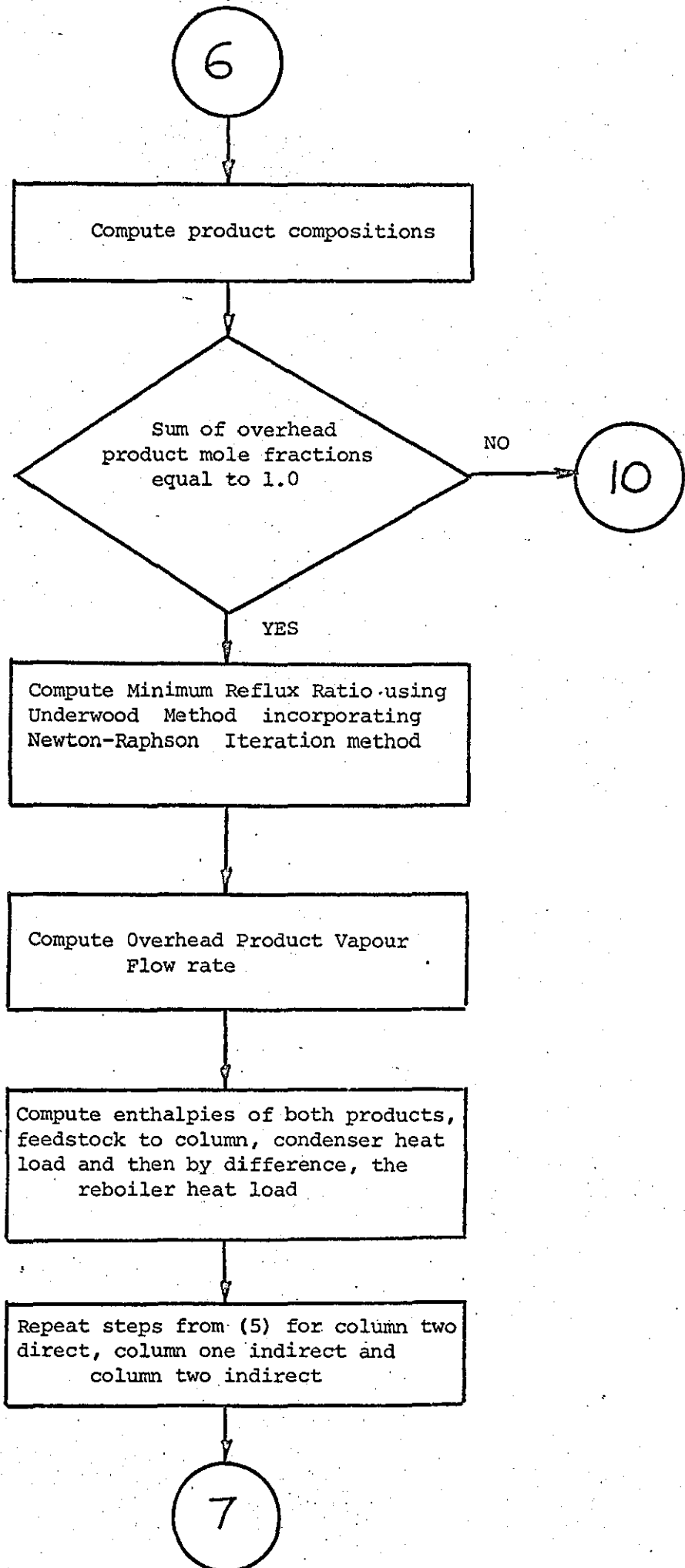
Compute K values for pseudo components
A and B over required temperature range

Compute liquid and vapour enthalpies using
above ratio over required temperature range,
for pseudo-components A and B

Call Flow 1 to generate regression
coefficients for liquid and vapour
enthalpies for pseudo-components A and B

Compute coefficients for Component C

5



7

Compute sum of vapour loads, condenser and reboiler heat loads for two columns in each configuration.

Compute percentage difference relative to configuration one of overhead vapour loads, condenser and reboiler heat loads.

Compute the difference in the reciprocals of the dew point and bubble point temperature of all columns

Compute the product of the overhead vapour flow rate and the difference in reciprocal temperature calculated to give Thermodynamic Net Work Consumption for each column

Compute the percentage difference relative to configuration one between the Thermodynamic Net Work Consumption values.

Compute Indices - Rudd and Tedder's, Heaven's

8

Write following Results:-

" Relative volatilities A to B

B to C

Feed Composition

Feed Bubble Point Temperature

Indices: ESI Heavens

Regression Coefficients K values

Liquid and Vapour enthalpies

Material Balances

Dew point and Bubble point temperature
for all columns

Relative Volatilities for all Columns

Reflux Ratios " " "

Minimum Stages " " "

Theoretical Stages " " "

Underwood Parameter " " "

Vapour Loads " " "

Reboiler Heat Loads " " "

Condenser Heat Loads " " "

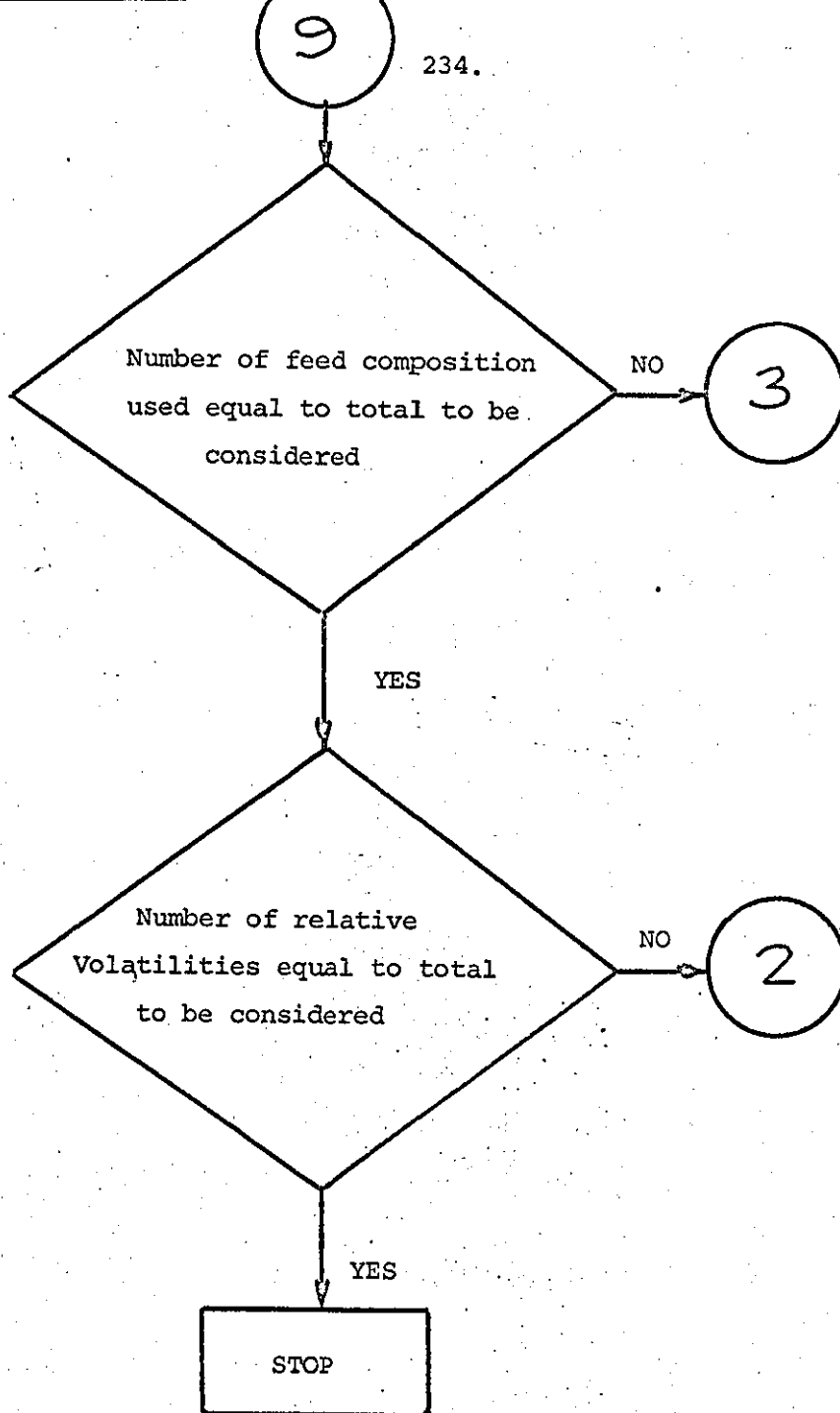
Overhead Vapour Load " " "

Overall Results - Differences in Percent

Condenser and Reboiler Heat Loads, Vapour

Loads and Thermodynamic Net Work

Consumption



A 6.5 Example of 'Flowpack' Printout

FINAL FLOWSHEET RESULTS

UNIT NO. OUTPUT NO.	FEED	1 1	1 2	2 1	2 2	3 1	3 2
TEMPERATURE (°C)	75.600	57.389	119.929	51.440	63.415	105.392	142.884
PRESSURE (MM.HG.)	5170.0000	5170.0000	5170.0000	5170.0000	5170.0000	5170.0000	5170.0000
VAPOUR FRACTION	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

FLOWRATES (KGMOL/HR)

COMPONENT	FEED	1 1	1 2	2 1	2 2	3 1	3 2
1 ISO-BUTANE	100.000	98.918	1.082	89.026	9.892	1.082	0.000
2 NORMAL BUTANE	100.000	95.000	5.000	5.035	89.965	4.999	0.001
3 NORMAL PENTANE	100.000	5.000	95.000	0.000	5.000	89.965	5.035
4 HEXANE	100.000	0.020	99.980	0.000	0.020	9.998	89.982
TOTALS	400.000	198.938	201.062	94.061	104.877	106.044	95.019

MOLE FRACTIONS

COMPONENT	FEED	1 1	1 2	2 1	2 2	3 1	3 2
1 ISO-BUTANE	0.2500	0.4972	0.0054	0.9465	0.0943	0.0102	0.0000
2 NORMAL BUTANE	0.2500	0.4775	0.0249	0.0535	0.8578	0.0471	0.0000
3 NORMAL PENTANE	0.2500	0.0251	0.4725	0.0000	0.0477	0.8484	0.0530
4 HEXANE	0.2500	0.0001	0.4973	0.0000	0.0002	0.0943	0.9470

UNIT NO. 1

NUMBER OF THEORETICAL STAGES ABOVE FEED 10.83651
NUMBER OF THEORETICAL STAGES BELOW FEED 9.83651
REFLUX RATIO 0.78715
CONDENSER SPECIFICATION TEMPERATURE 52.265
PRESSURE 5170.000
HEAT LOAD 2428427.
REBOILER SPECIFICATION TEMPERATURE 122.569
PRESSURE 5170.000
HEAT LOAD 2668864.

UNIT NO. 2

NUMBER OF THEORETICAL STAGES ABOVE FEED 32.85372
NUMBER OF THEORETICAL STAGES BELOW FEED 27.57880
REFLUX RATIO 3.92491
CONDENSER SPECIFICATION TEMPERATURE 50.849
PRESSURE 5170.000
HEAT LOAD 5735707.
REBOILER SPECIFICATION TEMPERATURE 62.628
PRESSURE 5170.000
HEAT LOAD 5738067.

UNIT NO. 3

NUMBER OF THEORETICAL STAGES ABOVE FEED 11.71255
NUMBER OF THEORETICAL STAGES BELOW FEED 12.46456
REFLUX RATIO 1.95815
CONDENSER SPECIFICATION TEMPERATURE 106.839
PRESSURE 5170.000
HEAT LOAD 598010.
REBOILER SPECIFICATION TEMPERATURE 145.491
PRESSURE 5170.000
HEAT LOAD 619632.

UNIT NO.

1

2

3

0

VAPOUR MOLECULAR WEIGHT	79.070880	58.238611	85.635754	0.000000	0.000000
VAPOUR DENSITY (LB./CU.FT.)	1.034825	0.896845	1.063861	0.000000	0.000000
LIQUID DENSITY (LB./CU.FT.)	34.436309	32.894657	36.023278	0.000000	0.000000
VAPOUR LOAD	3.467863	4.889066	2.345409	0.000000	0.000000
NET WORK CONSUMPTION FUNCTION	0.012068	0.005701	0.002312	0.000000	0.000000

COSTS (POUNDS STERLING)

DISTILLATION COLUMN	4955.78	9248.39	3713.50	0.00	0.00
CONDENSER	5483.18	9023.61	2235.82	0.00	0.00
REBOILER	3471.21	2582.53	3847.29	0.00	0.00
TOTAL MAJOR EQUIPMENT COST	13910.18	20854.53	9796.61	0.00	0.00
COOLING OR CHILLED WATER	34631.69	58146.75	26100.00	0.00	0.00
STEAM	38222.70	53874.72	24969.50	0.00	0.00
TOTAL YEARLY OPERATING COST	78413.46	120363.28	54988.14	0.00	0.00

FOR THE CONFIGURATION:-

TOTAL REBOILER LOAD	=	6732395.22
TOTAL YEARLY OPERATING COST	=	253769.89

