ECONOMIC ASPECTS OF THE DESIGN AND IMPROVEMENT OF CHEMICAL ENGINEERING SYSTEMS.

A Thesis submitted to the University of London for the Degree of Ph.D in the Faculty of Engineering

by

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ABSTRACT

A general strategy is presented for deciding on those critical points in a plant complex where improvement can be most profitably effected. The importance of replacement studies in arriving at such a strategy is emphasized, as is the necessity for adopting a realistic economic yardstick.

Certain aspects of the general strategy are employed in a case study on the economics of distillation column design and operation. The influence of the choice of economic criterion on the optimum design conditions is investigated, in conjunction with the reverse approach of studying the effect of variation in the design and operating parameters on the economics of the system. Based on this technique of parameter perturbation a simulation is carried out on the system resulting in the delineation of development alternatives.

A similar case study is carried out on a continuous stirred tank reactor system incorporating a recycle. The feed stream to the system, (which consists of a reactor and separator) contains an inert component which must be purged from the recycle stream to prevent its accumulation within the system. The economics of continuous and intermittent purging, with attendant steady and unsteady state

modes of operation, are examined. Optimal strategies of purging are outlined for alternate profitability criteria. An analytical solution, applicable under certain conditions, is obtained for the time-behaviour of the system.

"The primary function of an engineer in our society is to apply his knowledge and experience to the economic solution of practical problems of a tangible and material nature as opposed to the abstract."

A.I.CH.E. Report 1961. Dynamic Objectives for Chemical Engineering (C.E.P. October 1961).

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CONTENTS.

Introduction

It is commonplace in industry to find that at the higher levels of management, decision-making on, say, major capital investment or research and development programmes is based on some form of profitability criterion. It is equally usual to find that the decisions which are taken lower down the scale, pertaining to the actual expenditures involved in a particular programme, are based on hunch decisions and estimated judgements. In discussing this matter Barrell (1) raises the question of the improvement that would result in a company's overall profitability, if all plant or production modifications were judged in relation to a minimum acceptable rate of return for the additional investment - this minimum acceptable rate of return having been fixed by the company for that particular plant. The implication being that a considerable increase in profitability would be achieved by applying a rigorous economic index to all such individual decisions.

Two main problems arise when attempting to base a decision on an economic criterion, they are:-

(i) the choice of economic criterion and

(ii) the assessment of the degree of accuracy of the result.

The problem of the choice of criterion is discussed at some length in the thesis and it is only necessary to point out here that its importance cannot be underrated, as the choice of criterion may condition the whole structure of the project (or programme) underlying the decision.

The second difficulty, that of assessing the accuracy of the result, reduces to an assessment of the errors present in the forecasted levels of the salient variables. At senior management level this uncertainty might be, for example, in the tax rate or the investment allowances. At the lower decision-making level this may be, for example, the rate of obsolescence of a particular piece of plant. The greater frequency with which decision-making ~~taken~~ at the senior level is based on an economic index may be attributed to two facts:-

(i) the relatively small number of variables (albeit multicomponent ones) all economic in nature on which the decisions are dependent, enables estimates of their probable values to be arrived at more easily.

(ii) the awareness of senior management that continued existence depends on continued profitability.

The engineer, on the other hand, is generally confronted with a large number of heterogeneous variables requiring evaluation, in addition to technical and operational feasibility problems. Faced with such demands, and invariably pressed for time, his solution is to concentrate on solving the technical problems, to the virtual exclusion of all else. Thus expediency (which is frequently difficult to criticize), results in a neglect of the economic implications at this stage. However, since the actual outlay of funds occurs at this point in the structure of any given expenditure programme, it follows that here is where great economies may be most readily effected

The complexity of the problem outlined in the last paragraph is magnified when the development of a process or system is envisaged. A whole new range of variables must be specified and in turn assigned probable values. To date little progress has been made towards the development of methods for handling this problem or towards its solution. No systematic approach appears to have been devised towards selecting those items in a complex plant which should first be replaced by expenditure on research and development.

The work described in this thesis, which has been prompted by the deficiencies in the situation outlined, falls into two parts:

(i) An attempt at devising an approach to the development, measured in economic terms, of a complex plant system.

(ii) A study of the influence of the economic criterion adopted on the optimum design of simple plant systems.

The general strategy presented in Chapter 1 of the thesis is an initial attempt at providing a methodological framework capable of yielding a definitive solution to the problem of improving a complex plant. The strategy involves considering improvement through replacement studies, prior to attempting development of the system. The development theory outlined consists essentially of the execution of a systematic sensitivity analysis of the system. The alternative development possibilities obtained from this analysis are then subjected to selection by means of decision theory.

Application of the strategy presupposes the mathematical formulation of a well-defined model of the whole system. Such a model implies a full knowledge of the physical and economic behaviour of the separate plant units, together with their interactions with the system as a whole. The inability to construct or obtain such a well defined model and the ancillary data, precluded the possibility of undertaking for this thesis a complete development study on the basis outlined. Recourse is therefore made to simpler systems and economic analyses of a design-operating nature are carried out with a view to investigating the effect of the choice of criterion on the optimal design.

The various economic criteria which may be adopted are discussed in Chapter 2. In view of the importance of adopting a realistic profitability criterion, emphasis is laid on the application of an economic criterion which takes into account the time value of money. The two comparative criteria used in the case studies presented are (i) the "unit cost of production" and (ii) the "venture worth" of the project. The "venture worth" criterion is a variant of the better known "net present value" criterion. The problem of applying, in a reasonably workable manner, a criterion of this form to a single item in a complex plant has therefore been encountered.

The systems chosen for study, namely a separation system in the form of a plate distillation column and a reaction system consisting of a reactor, a separator and a recycle to the reactor, are considered as typical chemical engineering systems.

An existing procedure for achieving the economic optimum in the design of plate columns is extended and the mathematical model in question is reconstructed to facilitate development studies using the technique of sensitivity analysis (Chapter 3). The procedure is generalized with the aid of earlier work carried out by Gilliland (52). The effects on the optimal design are considered due to the application of a 'time value of money' criterion as opposed to a conventional criterion. These results, together with an outline of possible developments for the system, may be found in Chapter 4.

The reaction system, which is discussed in Chapter 5, is investigated by a somewhat different approach. Comparative analyses of unsteady state operation as opposed to steady state operation are presented. Since purging is necessary when inert material enters the system, purging strategies are examined and optimized. The influence of the economic criterion selected on the mode of operation of the system is studied in conjunction with the purging policy. The time behaviour of the recycle and other system streams is outlined. Chapter 6 contains the results of the reaction system case study.

CHAPTER 1: A General Strategy for Economic Optimization of Industrial Plant Systems.

1.1 Introduction

1.2 A Methodology of Approach for the Problem.

1.3 Techniques and Aspects of Optimization.

1.4 Replacement Policy.

1.5 Development Theory - Sensitivity Analysis of Systems.

1.6 Decision Theory.

1.1 Introduction:

The presentation of a new strategy of optimization might appear at first sight to require some justification. This may be found in the economic orientation and generalized nature of the strategy. In the first place a broader environment will be considered for the system than is usual in the field of chemical engineering and, secondly, a real attempt will be made to study the economic factors involved. The necessity for considering a chemical plant or process within these terms of reference may seem self-evident - but the complexities which arise when such an analysis is attempted, seem to date, to have been an effective deterrent.

A great deal of work has been carried out in the domain of process optimization. A large part of this work consists of the formulation and solution of mathematical descriptions or models of chemical processes. The optimum design of items of equipment, even whole plants, is another area which has received a great deal of attention. The third area in which a major effort has been made is that of optimum control of plant systems. Two generalizations can be made of the work on process optimization

(i) Exact or semi-exact descriptions of the systems have been required and factors which cannot be represented analytically have tended to be excluded e.g. obsolescence of plant. This requirement has resulted in the work being contained within a close plant or process framework.

(ii) The objective functions being optimized are in the majority of cases a process parameter. In some cases a simple economic criterion may be associated with the parameter or even optimized in its own right, but in general, lip-service has been the order of the day with regard to economics.

In the context of this work an industrial plant system may be ~~equated to~~ considered as any chemical project in which the plant is either in the design or the "in situ" stage. The purpose of the strategy is to provide the optimum solution, as defined by an economic criterion, of the problem of (i) the timing of, (ii) the location of and (iii) the extent of any expenditure on development of, the project.

The timing of the expenditure is important because of the reality of capital rationing. Few companies have unlimited supplies of funds and, in order to avail of future investment opportunities, these funds must necessarily be conserved. At the same time, present advantageous opportunities must not be forgone, in the hope of future ones with an even greater yield.

In a complex project with many interacting components and often with very little knowledge of the overall effect of these interactions, the question of where attempts at development should be carried out is not easily answered. The more complex the project however, the more likelihood there is of development opportunities being present.

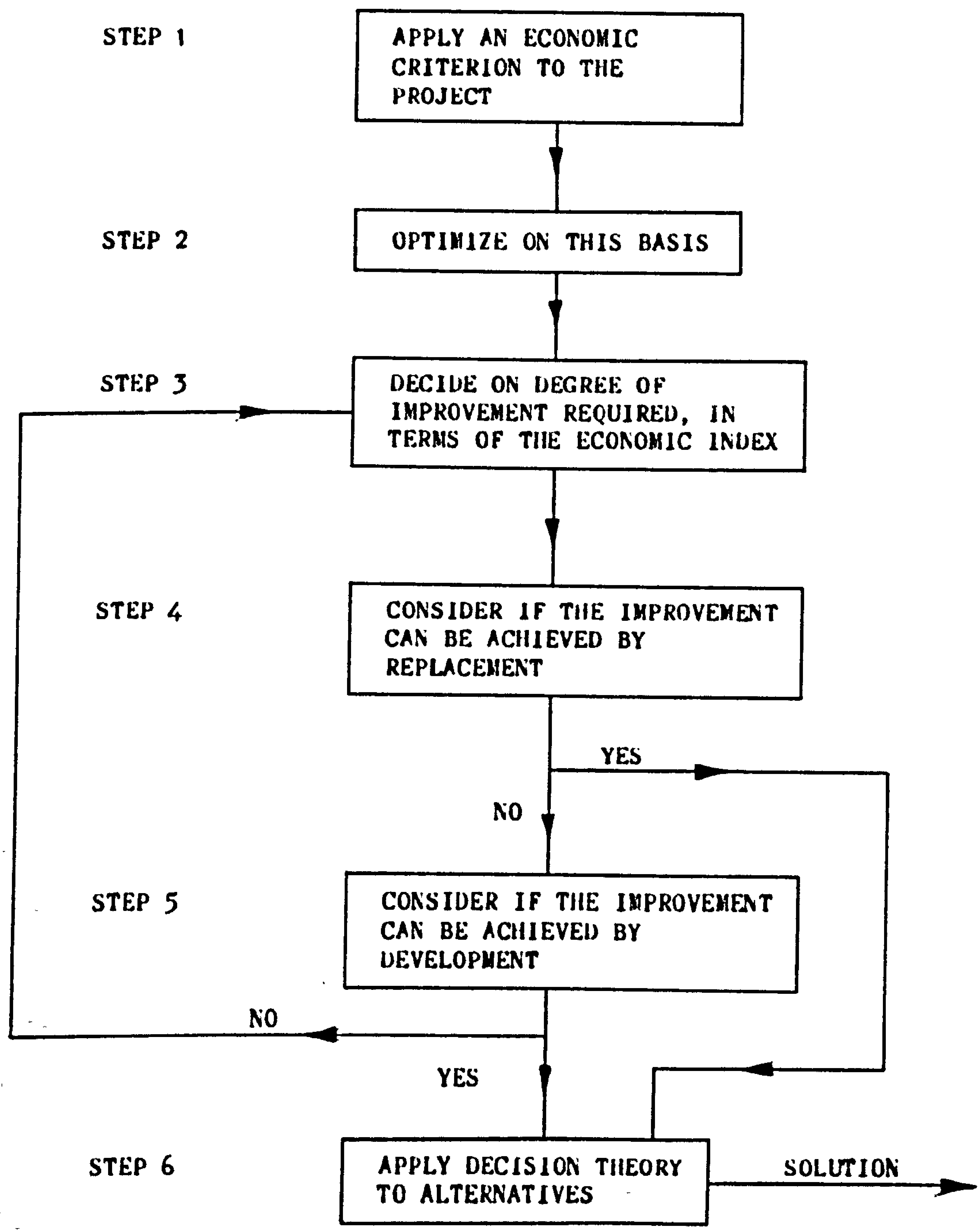
The maximum expenditure which can be allocated to any particular development is equal to the increase, caused by that development or improvement, in the overall return from the project. The two sides of this cash balance must be in consistent terms and allowance must be made for the time required to effect the change or improvement.

Where the project is one which requires a large amount of capital, the desirability of obtaining the optimum solution to the above problems is more acute. The general strategy can be applied to both drawing-board and in situ projects. Where an improvement leads to the replacement of an item of equipment in an operating plant, replacement economics must be introduced. Such a change in a plant during design, avoids this complication.

1.2 A Methodology of Approach for the Problem.

A schematic diagram of the form of the optimization procedure by which the problem can be handled is given in figure 1.1. It will be seen that six major steps are shown and that consideration of improvement by means of replacement precedes that by development. Clearly if the replacement problem can be characterized in an absolute manner, the solution is determined, whereas in the case of development, a probability factor is always present. Other things being equal, an improvement by replacement is preferable to that by development. In order to determine if other things are equal, it is of course necessary to complete the development study. The steps can be detailed in the following manner

SCHEMATIC DIAGRAM OF OPTIMIZATION STRATEGY FIG.1.1



Step 1: Apply an Economic Criterion to the Project.

(i) The measure of profitability, as defined by an economic index, must be specified.

(ii) A simple overall model* of the whole process in terms of the specified criterion must be constructed.

(iii) A more ~~accurate~~ detailed model of the process representing the individual stages and their position in the process must be constructed.

(iv) The economic data required to realize both the models, must be obtained.

As (i) and (ii) are treated in Chapter 2 and (iii) is discussed in Section 1.3, no comments will be made now. The explicit statement of (iv) is important because of the large volume of economic data, mainly costs, which are required if any of the more sophisticated economic criteria are applied. In most projects no provision is made for obtaining such data e.g. the operating costs for unit plant items - (operating costs tend to be bulked) and no critical economic analysis is possible without these cost data.

* The simple model consists, in effect, of the equation expressing the overall economics of the process.

Step 2: Optimize the Project on this Basis.

(i) Optimize the models.

(ii) If the project parameters are non-optimum, alter to optimum.

The complexities behind the statement, optimize the models are dealt with in the next section. Should the values of the parameters specifying the optimum condition of the model be different from the operating values of the corresponding parameters in the project, the slack is taken up, by altering the operating parameters to their optimal values.

Step 3: Decide on Degree of Improvement required in terms of the economic index.

Market conditions and the total economic environment are seldom static and this permanent state of change demands a continuing increase in the profitability of investments. Increases in profitability are effected by improving or developing the plant or process. The degree of improvement required could be dictated by any of a number of factors such as declining product return, rising costs or monetary devaluation. The guideline or yardstick used is a matter of company policy.

Declining product return could be caused ~~either~~ by a falling off, in selling price or in product demand - improvement would then be necessary to maintain the company's position. Similarly, for the other conditions mentioned, ~~under a number of circumstances,~~ improvement is required to maintain the yield on investments. Once the yardstick has been identified, quantitative estimates are necessary in order that the degree of improvement required can be expressed as a percentage increase of the existing index or, possibly, in absolute terms.

Step 4: Consider if the Improvement can be achieved by means of Replacement.

This step is concerned mainly with the plant; how the replacement of certain items in a complex may result in the desired improvement. Product replacement could also be considered, but this type of replacement tends to create a new project, rather than a change in an existing one. Section 1.4 deals with plant replacement analysis.

Step 5: Consider if the Improvement can be achieved by means of Development.

(i) Perturb the models and study how the objective function* responds to variations in the input parameters.

* economic criterion

A systematic approach to a simulation of this nature is presented in section 1.5.

Step 6: Apply Decision Theory.

When alternative solutions are available Decision Theory, which is discussed in section 1.6, enables the optimal decision to be made.

As pointed out in the above steps, certain important aspects will be treated more fully in the succeeding sections. It is evident that there is a continual interchange of information between the simple and the complete models. The simple model indicates the relative importance of the overall parameters, (eg. I, the total capital investment) and is designed in order that their effect is readily observed. If variations in I were indicated as important, then the detailed model would enable the capital cost of each component of the plant to be studied. A very similar approach has been used by Davis (3) in considering bottlenecks in plants.

There is also a major linkage between steps 4 and 5, in that perturbation of the model is required, if an effective replacement analysis is to be carried out.

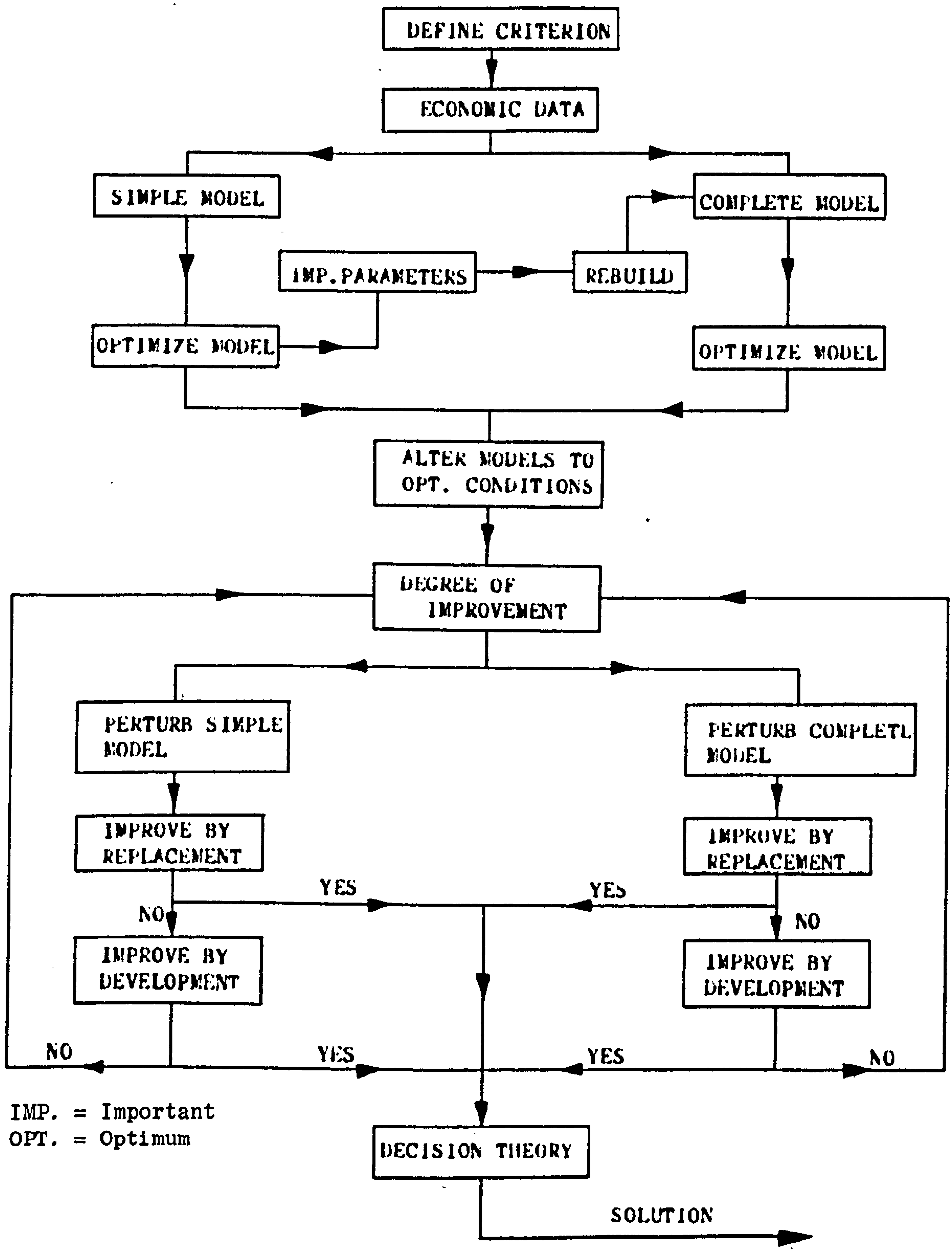
The procedure then encompasses the sequential execution of the outlined series of logical steps. Figure 1.2 presents the procedure in block diagram form.

1.3 Techniques and Aspects of Optimization.

The economic or other performance criterion being investigated is termed, mathematically, the objective function. In order that the effect of changes in the design and operating variables of the plant on the objective function can be studied, it is necessary to have a mathematical model of the plant. The model, which consists of a number of equations derived from the plant design and operating parameters, expresses, in terms of the objective function, the behaviour of the system.

The problem of describing a topologically complex plant by means of an adequate mathematical model is one of some difficulty. Most plants can be thought of, in mathematical terms, as multi-dimensional non linear systems and the models of such systems ~~itself~~ tend to be complex.

In optimization, the optimum value of the specified objective function is sought. A number of

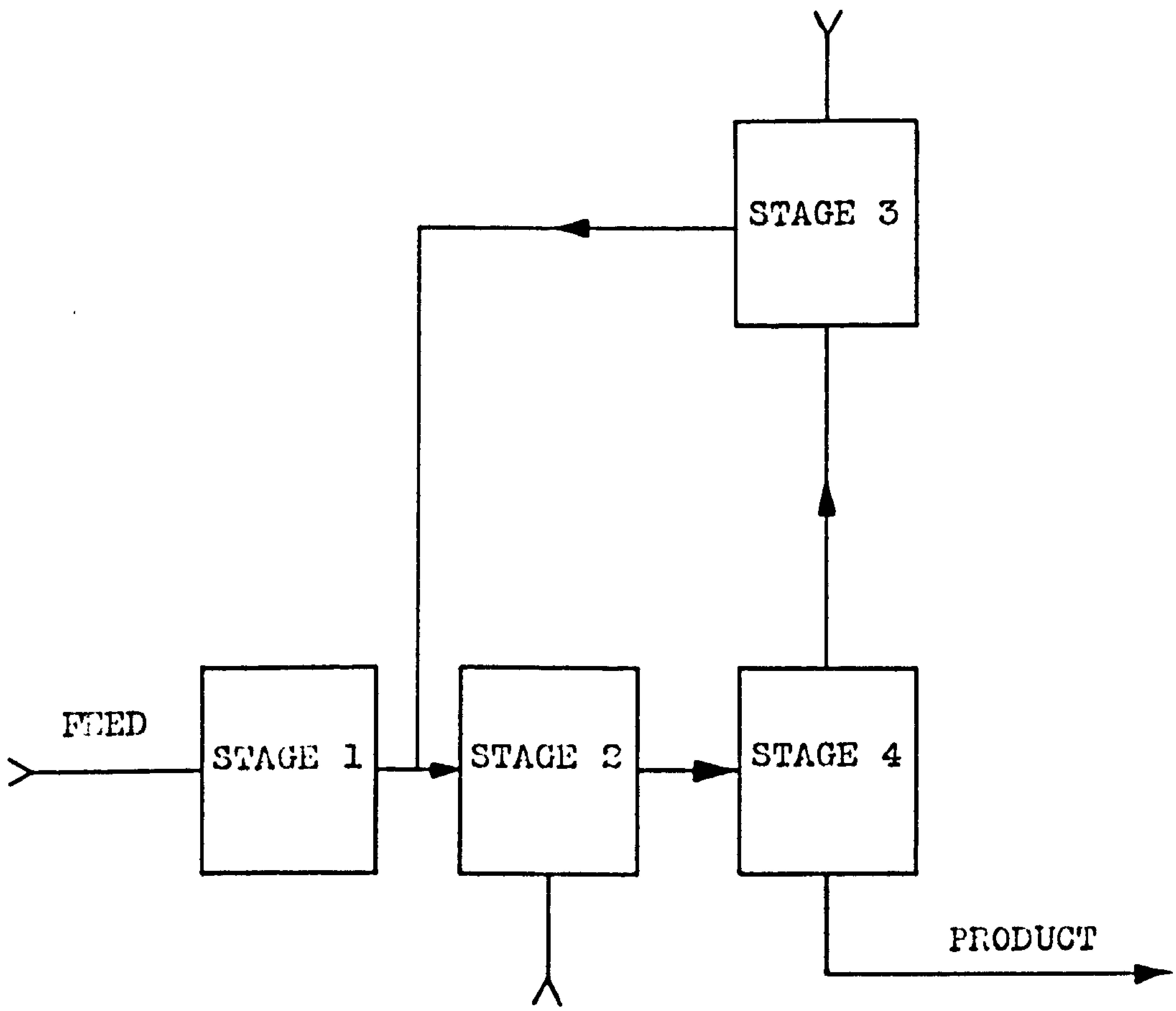


SCHEMATIC DIAGRAM OF OPTIMIZATION STRATEGY FIG. 1.2

techniques have been developed, which enable the difficulties that may arise in carrying out such an optimization, to be overcome. Before considering these techniques, the relationship between the physical structure of the plant and the mathematical model will be examined.

The Mathematical Model.

A chemical plant consists of a number of equipment units or stages in which operations are carried out in a predetermined fashion eg. figure 1.3. The term multi-stage is often applied to plants of this structure. It follows then, that one approach to formulating a model for the process as a whole is, firstly, to obtain models for each of the stages and then attempt to synthesize a complete model for the plant. The stages into which the process is divided are decided arbitrarily, but depend on the degree of optimization required and on the information available on the process. For example, consider a distillation column with 'n' plates and a specified overall column efficiency, 'η_o'. Such a unit may be regarded as one stage in an optimization procedure for an N-stage process. However, if the plate efficiency, ηp, of each plate in the column can be controlled, η_o can be optimized,



TYPICAL BLOCK DIAGRAM FOR A CHEMICAL PLANT

FIG. 1.3

provided the column is considered as an n-stage process.

The mathematical characterization of a unit stage generally results in a set of non-linear equations. The behaviour of the stage is obtained by the simultaneous solution of the set of equations for a given control policy. The whole plant can, in turn, be described by means of a set of such equations, and in theory, the behaviour of the plant can be obtained from the simultaneous solution of these equations. In practice, it may not be possible to solve simultaneously a set of non-linear equations, with the result, that the methods which have evolved in the field of optimization are based on decomposition strategies. This approach endeavours to reduce the dimensionality of the problem, by decomposing it into a series of problems, each of smaller dimensionality.

In the case where the plant consists of only one or two stages, the set of equations which comprise the model may be of small dimensionality and simultaneous solution may be possible. The number of equations which can be solved in this manner cannot be predicted, as it depends on such factors as the nature of the equations eg. differential or algebraic, the degree of non-linearity present and the method of solution being used.

Mathematical Procedures:

The mathematical procedures, by which the decomposed problems are handled, fall into two main categories:-

(i) Variational Calculus and its extensions.

(ii) Dynamic Programming.

Variational Calculus: The classical approach to the solution of this type of optimization problem is through the calculus of variations. Certain disadvantages inherent in the use of this method can be overcome by means of the Maximum Principle of Pontryagin. The Maximum Principle effectively reduces the optimization problem to a maximum or minimum seeking problem, subject to the constraints of a set of linear differential equations and the original constraints. The work of Pontryagin has, for the most part, been applied to continuous problems. Some methods related to the Maximum Principle which enable discrete problems to be handled have been developed mainly by Katz (4), Horn(5) and Jackson (6, 7).

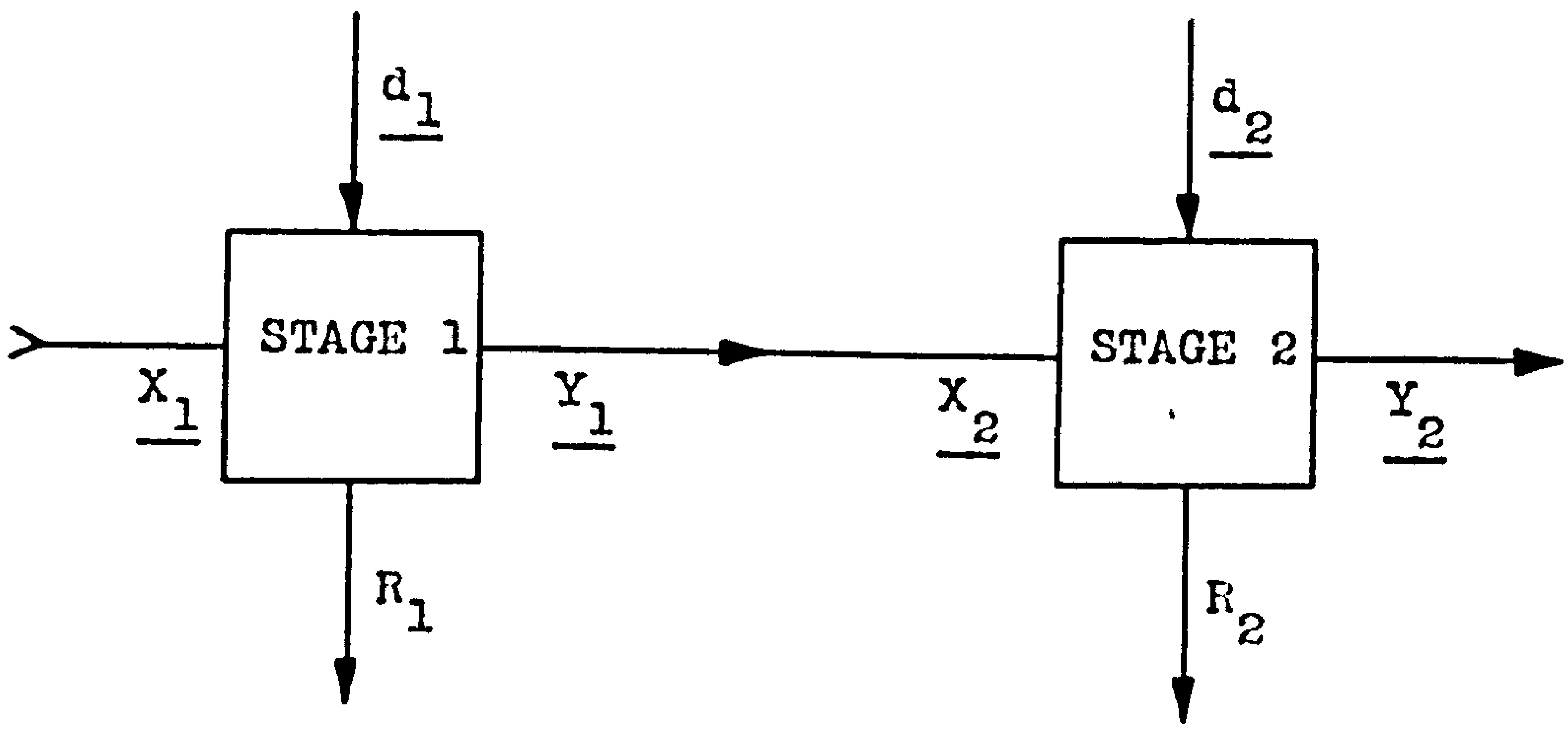
Horn(5) has treated cascade reactor optimization problems by means of what he calls the "forward" and "backward" methods of calculation, as well as by a combination of the two. Jackson (6) has presented a method of decomposing the overall optimization problem into a number of sub-problems with the dimensionalities of the individual units. In all these methods, the maximum is obtained by means of a hill-climbing or other search procedure. The complexity of the procedure required depends on the shape of the function being handled. The many and varied procedures which have been developed in the wake of optimization are enumerated by Wilde (8), who has coined the term "optimum seeking methods" to describe these methods of search.

Dynamic Programming: The term was invented by Bellman to describe those methods which are based on the principle of optimality and which were developed to tackle multi-stage decision problems. It can be thought of as a method for converting an optimization problem into a series of problems each of much reduced dimensionality. The principle of optimality has been defined as follows (9), "an optimal policy has the property that whatever the initial state and initial decision are, the remaining decisions must constitute an optimal policy with regard to the state resulting from the first decision". A diagramatic representation is given in figure 1.4, (see Aris (10)) of the application of dynamic programming to a two-stage process. The procedure is as follows:

(a) The complete system will not be optimized unless stage 2 is operating at its optimum point with respect to its feed. Thus R_2, is calculated for all possible values of the input state vector and the operating policy, that is, the value of $\underline{d_2}$ which maximizes R_2 for each value of $\underline{x_2}$ is obtained.

(b) The two stages are next taken together. To find the maximum return from the two stages, it is only necessary to consider the feed conditions to stage 1, since R_2 max. has already been obtained. All possible values of $\underline{x_1}$ are considered and the operating policy which maximizes the total return from the process is obtained.

The approach involved in applying Dynamic Programming (D.P.), that of starting at the end of the system, is evident from the example. In practice the value of the input vector to the first stage would be specified and, having obtained the optimal control or operating policy, the operating conditions for the whole process



[MAX. RETURN FROM WHOLE PROCESS] = MAX. OF [(RETURN FROM STAGE 1) + (MAX. RETURN FROM STAGE 2, WITH INPUT FROM STAGE 1)]

$\underline{X}_1$	STATE INPUT VECTOR
$\underline{Y}_1$	STATE OUTPUT VECTOR
$\underline{d}_1$	DECISION OR CONTROL VECTOR
R_1	STAGE RETURN

APPLICATION OF DYNAMIC PROGRAMMING TO A TWO-STAGE PROCESS
FIG. 1.4

are known. The above illustration has been given because of the importance of D.P. in optimization work. A more formal statement of the theory can be found in Appendix 1.

Mitten and Nemhauser (11) have applied D.P. successfully to multi-stage optimization in which the process is either a straightforward sequence of steps or a branched separating sequence. Simple combining branch and feed forward systems have also been considered by these authors although the method in these instances requires an increased amount of computation. Aris (10, 12) has used D.P. extensively in reactor optimization work including feed forward sequences. Sargent and Westerberg (13) have presented an algorithm for optimizing the order of computation of unit stages in the design of a complex plant, based on D.P.

The main disadvantage of D.P. is its inability to handle systems where the state vector has more than one or two components. The amount of storage space required for the tabulation of alternatives in systems of more than three dimensions is generally beyond the capacity of existing computers. Lee (14) has reported some work where a three state variable system was optimized. An advantage of the method is that if a general picture of the optimal region is required, then D.P. provides the solution of the complete class of problems. A further advantage, and one which Jackson (6) thinks represents the main virtue of D.P., is that it invariably leads to the maximum or minimum value of the function being optimized. When variational methods are used, problems may arise when non-optimum stationary points are present in the function space.

General:

In cases where the decomposed problem cannot be handled satisfactorily by either variational methods or D.P., combinations of these or other techniques may be used. The strategy is to divide the plant into a number of sections, optimize each of the sections by a suitable optimization procedure and then apply D.P. to optimize the operations of all the sections. This approach has been used by Lee (14) and indications are that a near optimal solution is obtained.

Some studies were carried out on simple two and three stage systems using the D.P. algorithm and effecting the computations by hand. The purpose of this work was to see how different economic criteria could be applied to multi-stage systems and to study how the optimal configuration of the plant varied with the application of the different criteria. The work was mainly qualitative and some aspects are reported briefly in Appendix 1.

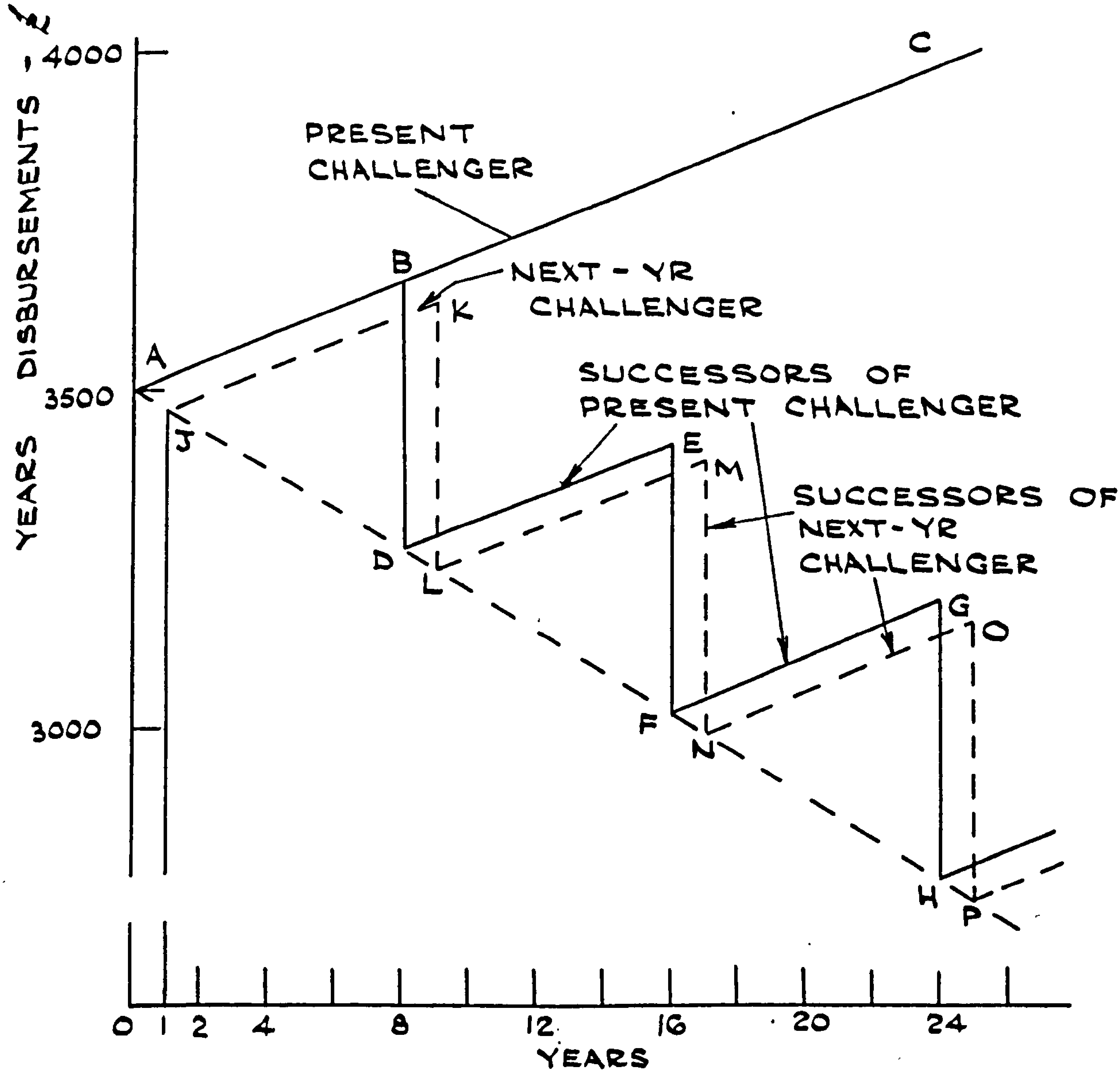
1.4 Replacement Policy.

The problem of replacement has been mentioned in sections 1 and 2 of this chapter. If the word displacement is substituted for replacement, the near equivalence of replacement and development as methods of improving a process is clear. It has been pointed out that improvement by means of replacement can eliminate the probability factor that arises when development per se, is considered. This statement presupposes that the replacement analysis is deterministic, a supposition which, as is discussed later, is incorrect. Nonetheless, the element of uncertainty in most replacement problems is a great deal less than in development studies.

The uncertainty can be attributed mainly to the onset of obsolescence due to technological progress, although other factors involving uncertainty may be involved. Methods have been developed recently which enable an attempt to be made at computing the rate of obsolescence. Modern replacement theory began with the realization by Preinreich (15) that static situation models were inadequate. Such a model assumed that an item of equipment was replaced by another of identical type and operated under the same economic conditions.

Terborgh (16) first formulated a dynamic model in which a quantitative measure was introduced to reflect the technological improvement between an existing plant item, the defender, and its proposed replacement, the challenger. This measure takes the form of an inferiority gradient which describes the operating advantage of future replacements as compared to the present plant item. The gradient from the viewpoint of the defender is a measure of the rate at which it accumulates inferiority relative to future challengers. This concept is illustrated in figure 1.5, which is derived from Alchians work (17), and given by Grant (2). It will be seen from the figure that:-

(i) The total expenses in the first year for the replacement available at present is £3500 and that this figure increases at the rate of £20 p.a.



YEARS DISBURSEMENTS = $\sum$ANN. CAPITAL AND OPERATING COSTS

DIAGRAM OF INFERIORITY GRADIENT.

FOR REPLACEMENT STUDIES (FROM GRANT)

Fig.1.5

(ii) A steady improvement of future replacements is allowed for and that the first year's expenses for next year's replacement is £3,470. It will also be noted that this initial figure decreases by £30 for each succeeding year.

(iii) The assumption is made that the annual increase in yearly expenses for these future replacements is also £20.

It is evident that the present replacement accumulates inferiority at the rate of £50 p.a. with respect to future replacements. This figure represents the inferiority gradient. The adverse minimum, a term used to denote the minimum average annual cost, is then calculated for both the defender and the challenger. In the case of the defender the problem becomes that of finding the period that gives the lowest annual cost if it is not replaced. The adverse minimum of the challenger is obtained by calculating its economic life.

Defenders Adverse Minimum; it will nearly always be reached in the next year from the time of the replacement analysis. It has two components (a) a next-year or minimum annual operating inferiority obtained from the gradient and (b) a next-year or minimum annual cost of capital term.

Challengers Adverse Minimum; this is also comprised of two components (a) the capital recovery cost and (b) a component representing the present worth of the advantage of replacing with the next year challenger and its successors rather than with the present one. It may be obtained by use of the approximate formula

$$\text{C. Adverse Min.} = \sqrt{2Ig} + \frac{iI - g}{2} \qquad (1.1)$$

where I = initial capital cost, i = interest rate and g = gradient.

If the adverse minimum of the challenger is lower then a replacement is made. The difference between the challengers and the defenders adverse minima will be, in nearly all cases, a next-year difference.

Terborgh's theory has been presented at some length because it represents a considerable breakthrough and because its approach is fundamental in considering replacement. Alchian (17) presented a very comprehensive formula but operational difficulties are encountered in its application. Terborgh (18) has continued to develop the ideas presented in this section and considerable advances have been made. A short outline of these developments can be found in Appendix 1. The work of Churchman et al. (19) and others in the operational research field is mainly concerned with optimal replacement policies under simplifying conditions. Problems are generally categorized into (a) equipment items subject to deterioration and (b) equipment items subject to failure. The approach to deteriorating items is similar to that of Terborgh, while sudden failure problems are handled through the use of probability theory.

The concept of an inferiority gradient provides a means of estimating the rate of technological obsolescence and of assessing future replacements. The appraisal and evaluation of these 'ghost' replacements constitutes for Terborgh the heart of replacement analysis. Other major factors which must be evaluated are:-

(i) the design philosophy involved.
(ii) the company policy being followed.
(iii) Government Control measures.
(iv) plant deterioration and changing plant economics.
(v) changing process economics.

Three further points can be made which have specific application to this work. The necessity for considering the replacement analysis and its resultant decisions in the context of time. The importance of time and the time value of money is discussed in the next chapter. The problem of sub-optimization is again present when the replacement of a unit plant item in a plant complex is in question, and any replacement analysis must be imbedded into the overall system. In the field of chemical engineering, the rate of technological progress is high and continued displacement analysis of plants may yield a high dividend in increased profitability.

1.5 Development Theory - Sensitivity Analysis of Systems.

The procedure which is outlined in this section consists of a logical approach to development problems. In essence, a model of the system under investigation is perturbed and the possible development region obtained by simulation. The response of the system to the perturbations is obtained and the critical development parameters identified. The complete solution to the problem is not given but the development alternatives are clearly delineated.

Consider a single stage r of an N-stage process as shown in figure 1.6. The input and output vectors $\underline{x}(r)$ and $\underline{Y}(r)$ are the state vectors of the stage. Two control vectors, one of which $\underline{q}(r)$ is designated a cost vector, are indicated. The following relationships hold

$$\underline{Y}(r) = F_1(\underline{x}(r), \underline{P}(r)) \qquad (1.2)$$

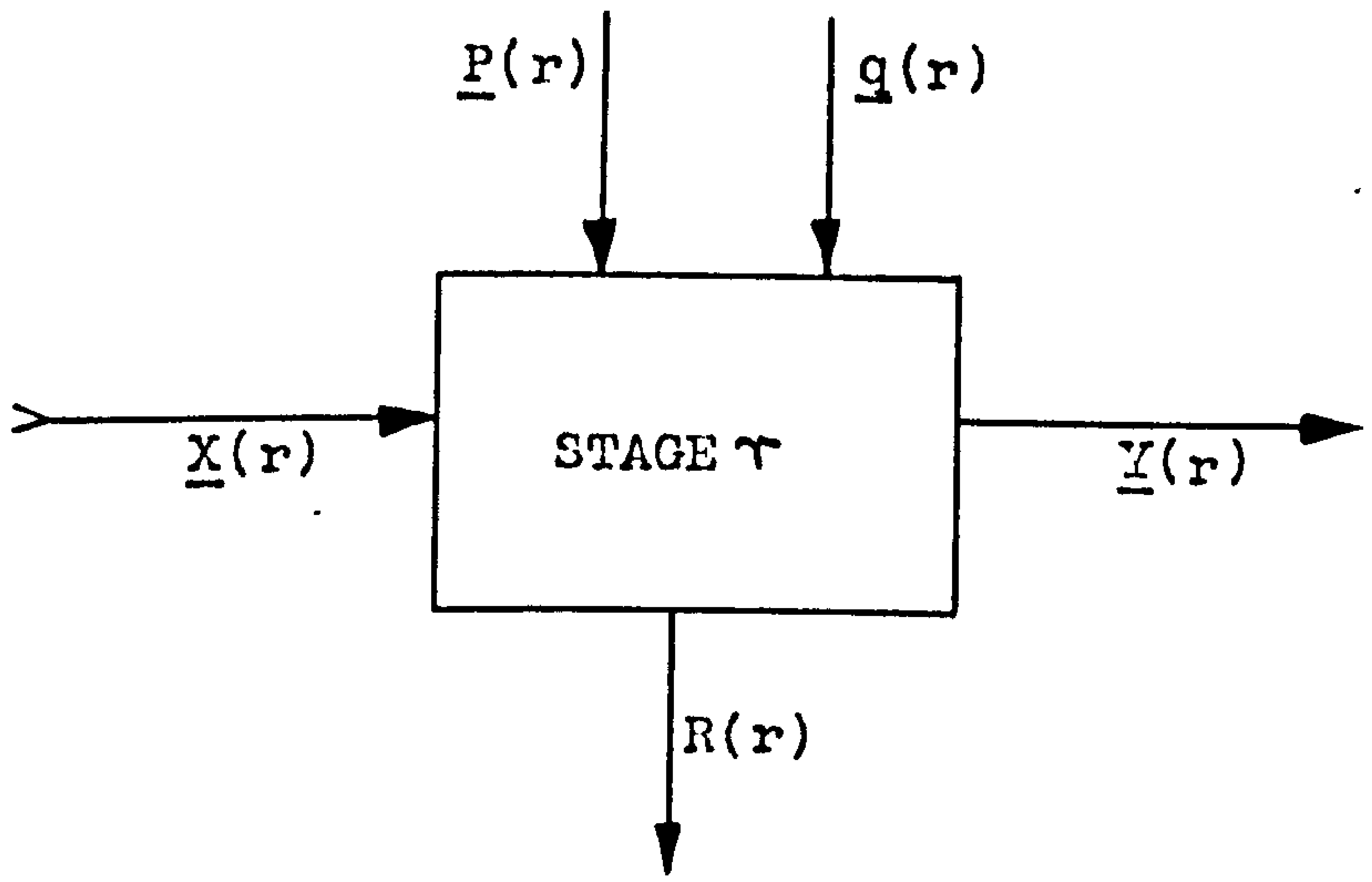
$$R(r) = F_2(\underline{x}(r), \underline{P}(r), \underline{q}(r), \underline{Y}(r)) \qquad (1.3)$$

Since $\underline{Y}(r)$ is a function of $\underline{x}(r)$ and $\underline{P}(r)$ only, the second of these functional expressions can be written

$$R(r) = F_2(\underline{x}(r), \underline{P}(r), \underline{q}(r)) \qquad (1.4)$$

The stage return depends on the input, cost and control vectors of the stage. The resolution of the adjustable variables into the categories, cost and control, assuming that this is possible can result as is shown later in a worthwhile simplification of the problem. $\underline{x}(r)$ will depend on the control policy of the previous stage and/or on fixed external conditions.

From expression (1.2) it will be seen that the process state is independent of the cost vector. The variables included in the cost vector would be, for example, raw material, utility and capital unit costs i.e. £/lb. of raw material, £/lb. of steam used or £/unit



X(r) STATE INPUT VECTOR

Y(r) STATE OUTPUT VECTOR

P(r) CONTROL VECTOR (DESIGN AND OPERATING VARIABLES)

q(r) COST VECTOR (COST VARIABLES)

R(r) STAGE RETURN

UNIT STAGE OF A CHEMICAL PROCESS FIG. 1.6

dimension of plant item. The procedure which is given in a stepwise fashion, is as follows:

Step 1: Obtain the costs for each stage in three categories

(i) Operational Costs

(ii) Capital Costs

(iii) Raw Material Costs i.e. cost of r. matls. to the stage minus value of products from the stage. It is not necessary in the case of the main process stream to allocate an in-process value as the total return may be credited to the final stage.

Step 2: Define the operating and design parameters which are variables for each stage.

Step 3: For any stage r, the vectors $\underline{P}(r)$ and $\underline{q}(r)$ are now specified. The state of the process $\underline{x}(r)$ is defined either by the initial state if $r = 1$, or by the policies of previous stages.

Step 4: $\underline{P}(r)$ and $\underline{q}(r)$ may be written in terms of their components

$$\underline{P}(r) = f(P_i(r))_1, \; i = 1, 2, 3 \ldots \qquad (1.5)$$

$$\underline{q}(r) = f(q_i(r))_1, \; i = 1, 2, 3 \ldots \qquad (1.6)$$

and expression (1.4) can be written

$$R(r) = F_2\{\underline{X}(r),\ P_1(r),\ P_2(r)\ \ldots,\ q_1(r),\ q_2(r)\ldots\} \quad (1.7)$$

<u>Step 5:</u> This relationship i.e. (1.7) can be developed by simulation. The variables $P_1(r)$ and $q_1(r)$ are given a series of values $[P_1(r)j]$ $j=1,2,\ldots$ and $[q_1(r)j]$ $j=1,2,\ldots$ each level of which will give a value of R(r). In this way the effect of variations in the governing variables of a stage on its return can be studied. In practice the number of components of $\underline{P}(r)$ and $\underline{q}(r)$ which have a significant effect would probably be of the order of three or four.

<u>Step 6:</u> The pattern of development for the stage is now available. Unfortunately the stage cannot be considered in isolation from the rest of the process, because of the dependence of the return from the remaining (n-r) stages on $\underline{Y}(r)$.

<u>Step 7:</u> It is necessary therefore to consider the changes in the subsequent stages caused by the variation in $\underline{Y}(r)$. Once $R(r+1)\ldots R(n)$ have been determined, R_t, the total return from the process can be obtained.

$$R_t = f(R(1)\ldots.\ R(r)\ldots.\ R(n)) \quad (1.8)$$

The effect of any given change in a stage variable on R_t, may then be determined. Suppose such a perturbation occurs to stage r, then expression (1.8) becomes

$$R^1_t = f\left(K, R^1(r) \ldots . R^1(n)\right) \qquad (1.9)$$

where R^1_t, $R^1(r) \ldots . R^1(n)$ equal the new values of these quantities.

Variation in $\underline{Y}(r)$ will not affect stages (1)...(r-1) and the return from stages (1) to (r-1) equals a constant, K.

Step 8: In the case where the cost variables alone are being investigated, $\underline{Y}(r)$ will remain constant and the relationship (1.4) can be written

$$R^1_t = f\left(K_1, R^1(r)\right) \qquad (1.10)$$

where $K_1 = \sum R(1) \ldots . R(r-1), \; R(r+1), \ldots R(n)$

Step 9: A considerable simplification is thus introduced in the instance where the state variable is constant. Stage (r) can be considered independently of the rest of the process. The functional relationship of K_1 to $R^1(r)$ is always relatively simple, whereas those which arise in equation (1.9) may be complex. Step 7 requires in effect an optimization for the remaining (n-r) stages. As $r \longrightarrow n$, the magnitude of this problem decreases.

<u>Step 10:</u> Having determined the effect of any given variable eg. $P_i(r)$ on R_t, for a number of different levels of $P_i(r)$, a curve can be plotted. Let such a curve be of the form shown in figure 1.7(a). A change in the value of $P_i(r)$ from $P_i(r)^1$ to $P_i(r)^2$ will increase the total return from the process, R_t, by a sum of money equal to $R^2_t - R^1_t$. This sum represents the maximum amount which can be spent on achieving this change i.e. the maximum permissible development expenditure.

<u>Step 11:</u> If $R^2_t - R^1_t = D$, then figure 1.7(a) can be replotted as shown in figure 1.7(b). A graph of this type would be obtained for each variable studied. The effect of time, which is present in any development study may be introduced at this point. Any delays that may occur in the execution of the development will reduce the maximum permissible level of expenditure for that development i.e. the curve for maximum D, shown in figure 1.7(b) will be closer to the abcissa. Since D is evaluated by considering the increase in revenue that would be obtained if the

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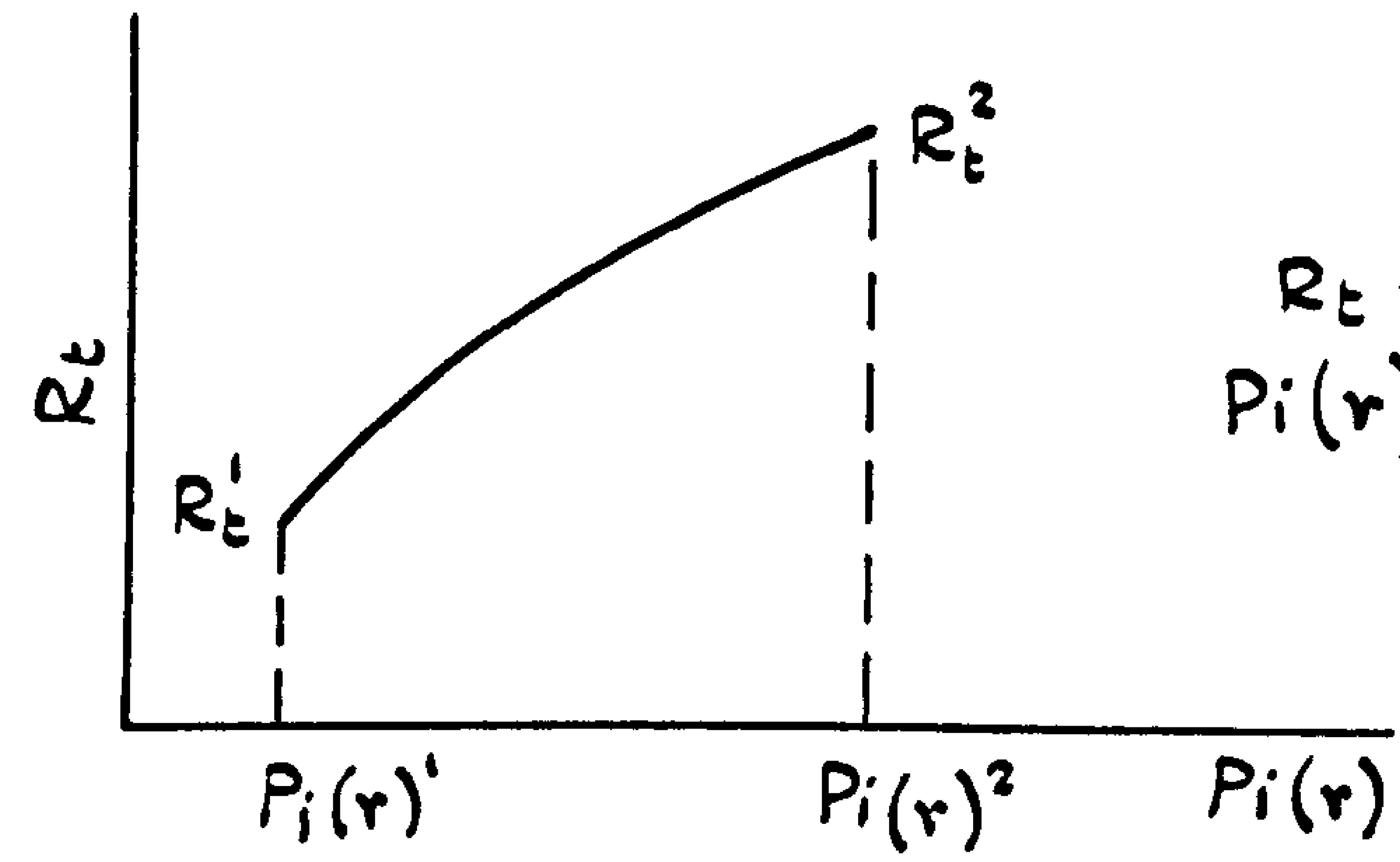
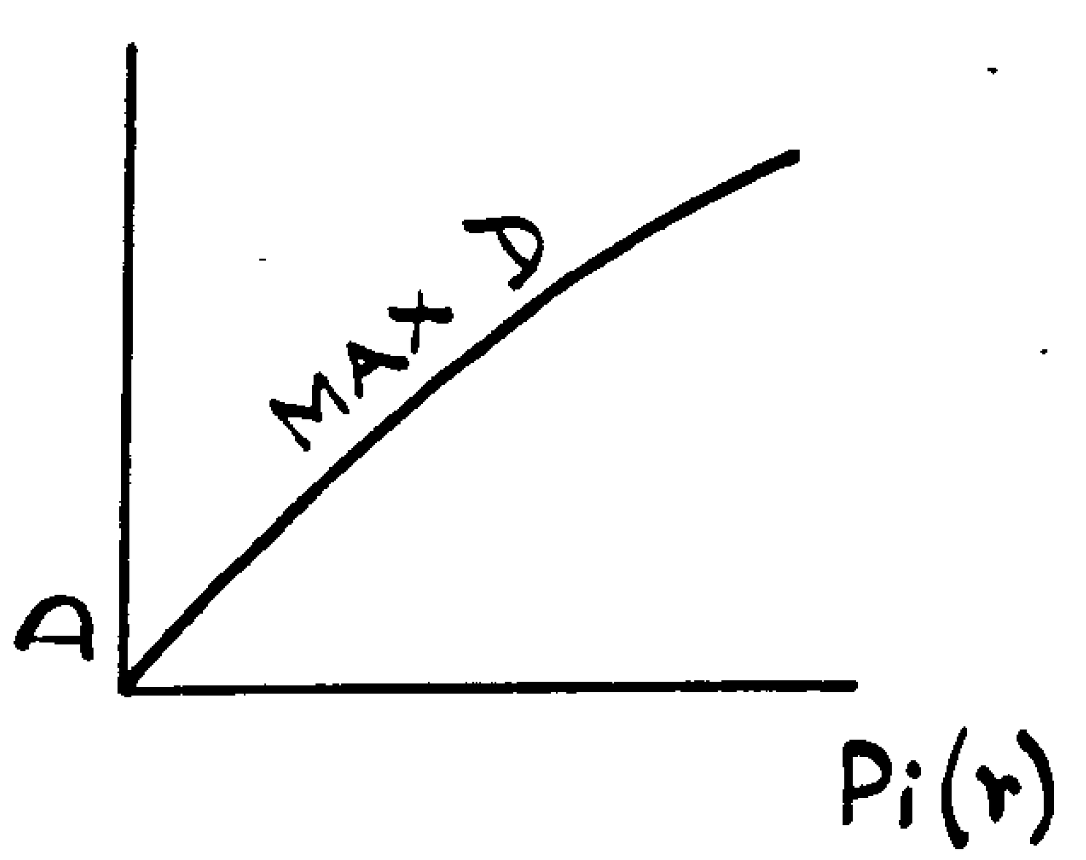


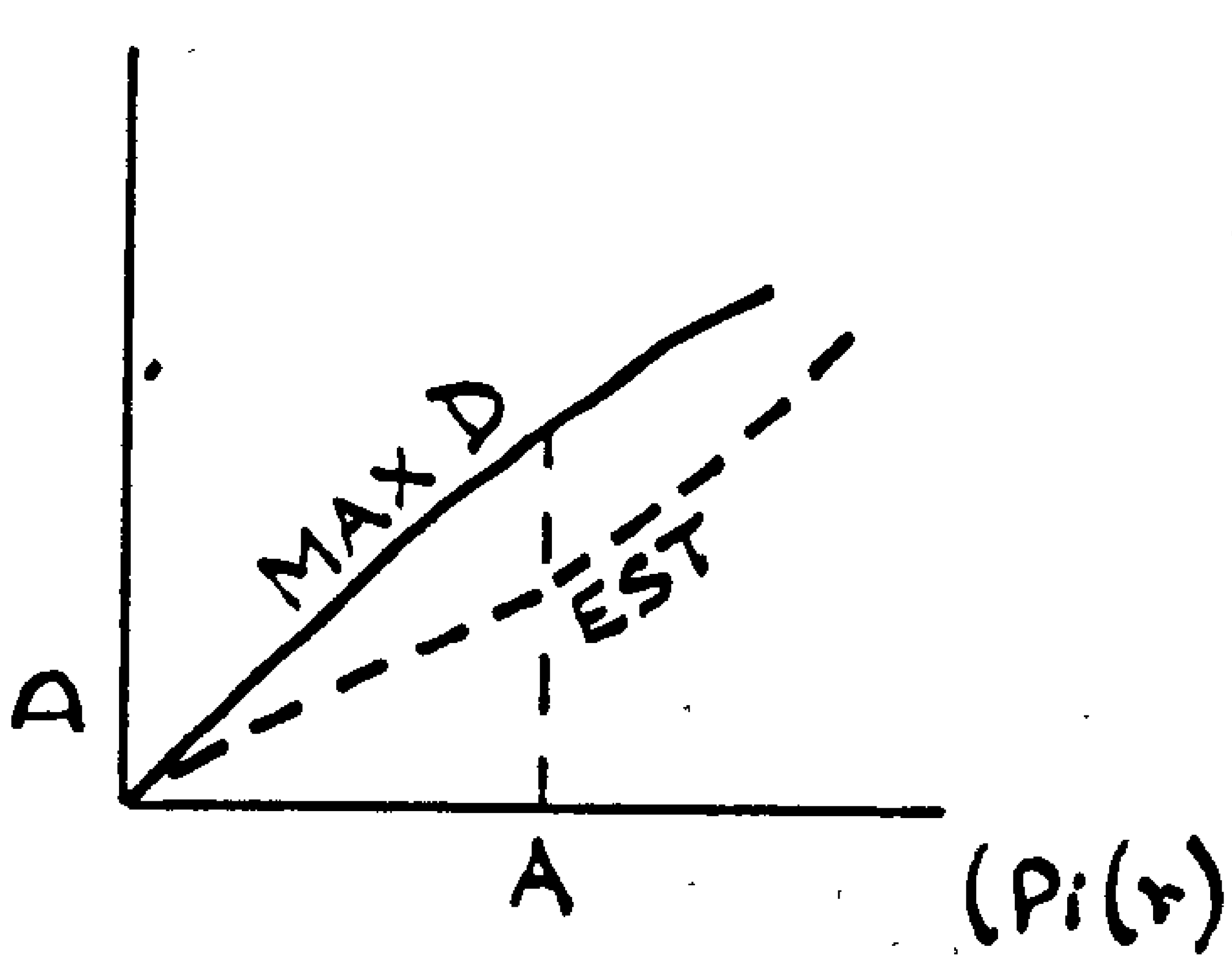
1.7 (a)

R_t = PROCESS RETURN
$P_i(r)$ = VARIABLE P_i
OF STAGE r



1.7 (b)

D = DEV. EXPENDITURE
MAX D = MAX EXPENDITURE
TO ATTAIN A
GIVEN $P_i(r)$



1.7 (c)

EST. = WEIGHTED EST.
EXPENDITURE
TO ATTAIN A
GIVE $P_i(r)$

OUTLINE DEVELOPMENT CURVES

Fig. 1.7

development was carried out, it is clear that a delay in effecting the development will reduce the time available for the increased return to accrue. D will therefore be decreased. In cases where the development expenditure is over a period of time, a more complex analysis is required. When the improvement is measured on an annual basis, then provided there is no change in the conditions, time delays will not affect the curve.

Step 12: The effect of each variable on the whole system and the maximum amount which can be spent to attain a given level of development for each of the variables has now been ascertained. At this point, the problem of uncertainity arises. A factor indicating the probability of attaining success in any given development attempted, must be arrived at - a problem discussed briefly later in this section. An estimated cost of development must also be calculated and subsequently weighted in accordance with the probability of attaining success.* The resultant weighted estimated cost of development curve is plotted on the development graph e.g. figure 1.7(c). Where the weighted estimated cost of development is greater than the maximum permitted, the development would not be

* The word "adjusted" might preferably be used for "weighted" - this initial separation of the cost of development and the probability factor will lead to better estimates.

attempted. The difference between the two curves represents the improvement measured in terms of the overall return from the process brought about by the development.

<u>Step 13:</u> The variable yielding the greatest improvement would be selected for development. The new level for the variable would be that at which the difference between the two curves is greatest e.g. point A in figure 1.7(c).

The method outlined is straightforward and only two points need be mentioned. The recognition of the independence of subsequent stages to perturbations of the cost vector is important. It enables a whole class of problems to be investigated without the repetition of a complex optimization of the system. The quantification of the probability of success is the most difficult step in the procedure. The first step is the move from the abstract to the particular, in this case the variable in question. There may be a great deal of information available about the variable e.g. vapour velocity in a column. A study might have revealed that an increase in vapour velocity will yield a worthwhile increase in profitability. The engineering knowledge and costs may be available to calculate exactly the cost of carrying out the development, giving a probability factor of 1. In other instances there will be more or less knowledge, but seldom will the case occur when nothing is known about the necessary data.

There is, in the literature, a great deal of information on and methods of assessing this probability factor in the context of research and development. The existence of a learning curve "based on experience has been postulated by Hirschmann (20) and comparisons of such curves could help in arriving at the value of the probability of success factor. The successful estimation of this factor is the key to development work.

1.6 Decision Theory.

The quantification of decision making has occurred in the post-war period and mainly within the framework of operations research (19, 21). The difficulty involved in moving from the qualitative to the quantitative in this field can be inferred from the attitude of Keynes.[1]

1. Keynes in 1936 could write on business decisions "most probably, of our decisions to do something positive, the full consequences of which will be drawn out over many days to come, can only be taken as a result of animal spirits - of a spontaneous urge to action rather than inaction and not as the outcome of a weighted average of quantitative benefits multiplied by quantitative probabilities (22).

To make a decision, two prerequisites are necessary:(a) alternatives are required and (b) a measure of the relative importance of the alternatives must be available. The previous two sections have indicated how alternatives can be obtained by means of replacement or development analyses. The problem of the relative importance of the alternatives has been considered in that a criterion for replacement has been given and the necessity for ascertaining a probability factor for the success of a given development has been pointed out. Decision theory is concerned with combining these two factors, such that decisions can be made on a quantitative basis. Anderson (23, 24) has shown how decision theory can be applied to economic problems in chemical engineering.

The main feature of the current approach to decision making is the reduction of the problem to a series of single figures generally arranged in a matrix format. Such a matrix is often termed the pay-off matrix. An example of how a pay-off matrix is obtained is given in Appendix 1. A disadvantage of this approach, which is discussed by Hall (25), is the inherent assumption that a simple number can express the comparative value of a given combination of a decision and a probable result. The number may represent an economic value or any other representation of value, but only one kind of value scale may be used. At the present time the simplifications necessary to make this assumption have not been fully accepted by economists such as Shackle (26) and Carter and Williams (27). Carter and Williams have concluded that the possibility of summing-up a course of action by a single figure is far from obvious.

A typical pay-off matrix might be

PAY-OFF MATRIX
ALTERNATIVE POSSIBLE RESULTS

DECISION	A_1	A_2
D_1	2	$1\frac{1}{2}$
D_2	0	3
D_3	$1\frac{1}{2}$	1

Having obtained a matrix, the next step is to try to simplify the decision problem by reducing the size of the matrix. This can be achieved by the application of dominance relations. In the pay-off matrix shown, no rational person would ever choose the last row, in the language of the theory, row one dominates over row three.

A decision criterion can then be applied, which can be thought of as the quantitative representation of the risk philosophy adopted. Typical decision criteria are,

(i) the maximum expectation criterion,

(ii) the minimax regret criterion.

The Maximum Expectation Criterion, assumes that all alternatives as given in the pay-off matrix are equally likely and that the expected pay-off should be maximized. To apply this criterion to the above example, one merely notes that decision D_2, yields the maximum pay-off i.e. 3.

The Minimax Regret Criterion requires that the maximum regret be minimized. Regret is defined as the difference between the return obtained for a given decision and the return that would have been obtained if the best decision had been made. It can be illustrated by applying the criterion to the matrix of the example, a regret matrix is constructed as follows -

REGRET MATRIX

	A_1	A_2
D_1	0	$1\frac{1}{2}$
D_2	2	0
D_3	$\frac{1}{2}$	2

or alternatively if the last row is eliminated

REGRET MATRIX

	A_1	A_2
D_1	0	$1\frac{1}{2}$
D_2	2	0

If we consider that result A_1 occurs in the pay-off matrix, then the best decision would have been decision D_1, resulting in a pay-off of 2. If however decisions D_2 or D_3 had been made a loss or regret of 2 and $\frac{1}{2}$ respectively would have resulted. The criterion requires that the maximum regret that occurs for any given decision over all the alternative results be minimized. In this case, decision D_1, is the decision that would be taken.

The example shows that the adoption of different decision criteria may lead to different alternatives being specified. It is important therefore that the decision criterion adopted should conform with company risk policy.

CHAPTER 2 ECONOMIC THEORY AND CAPITAL INVESTMENT CRITERIA

2.1 Introduction - The Shape of Engineering Economic Theory

2.2 Conventional Investment Criteria

2.3 Time Value of Money and Discounted Investment Criteria

2.4 Formulation of the Venture Worth Criterion

2.5 Analysis and General Simulation of the Venture Worth Equation

2.6 Application of Venture Worth to Unit Plant Items

2.7 Criteria for Selection of Investment Alternatives

2.1 Introduction - The Shape of Engineering Economic Theory.

Engineers have always been involved with the costs and profitability of the projects and processes under their control. The field of engineering into which these matters fall is designated engineering economics. A considerable number of techniques, formulae and rules-of-thumb have been developed which enable the problems that occur in the area to be handled. Such techniques, formulae and rules-of-thumb constitute what is called the theory of engineering economics. This theory is far removed from pure economic theory and has been developed to meet the specific problems arising in the general industrial and engineering environment.

The scope of engineering economic theory can be both quite broad or quite limited according to the meaning given to the term. In its broadest sense it embraces a great deal of pure economic theory, as can be seen from the content of Grant's (2) classic work. In its narrowed sense it may perhaps be concerned ~~with,~~ only with the production costs of a particular process. This second concept has given rise to the sub-discipline of cost engineering (28, 29) and in many instances what is called engineering economic theory might more accurately be referred to as engineering cost theory.

This contention is borne out by considering the typical works of Tyler (30), Schweyer (31), Aries and Newton (32), Perry (33) and Peters (34) in chemical engineering. The main emphasis is not on economics, that is, in the true sense of the word, but on process, production and particularly plant costs. They are to some extent handbooks for ready use in practice, whereas, that of Grant and Ireson is more in the nature of a theoretical treatise. The concepts of engineering economy expounded by Grant, although closely related to the engineering economic theory contained in the other references, are more generalized and must therefore necessarily be less immediate in application.

Happel's work (35, 36, 37) is intermediate, although it is essentially practical and can be readily applied to real situations. In it, formulae are developed which take account of many of the broader economic factors with which Grant is concerned. Some of Happel's formulae will be examined later in this chapter.

The main features of engineering economic theory are its:

(I) preoccupation with capital costs

(II) general simplicity

(III) applicability.

The preoccupation with capital costs is well justified on a number of counts. In the first place, most engineering projects are capital intensive projects. In the second, the majority of the criteria by which projects are judged involve the capital cost. Again, frequently the capital costs can be calculated in a more exact manner than the other costs involved in the project and are thus rendered capable of a quantitative engineering approach.

The second two features enumerated are complementary. The formulae most generally used are simple, the data required to apply the theory is easily acquired and often readily attainable from existing accounts. The more complex formulae allowing for the time value of money have not yet obtained wide acceptance in industry in this country (38) and need not be considered under this heading.

The primary products of engineering economic theory have been economic criteria. Their main function is to assist decisions on the absolute or relative profitability of projects. The orientation of engineering economic theory is probably due, in addition to the reasons stated, to the fact that industry has always been aware of the importance of measuring its effectiveness in terms of one of its major resources, that is, capital. The investment problem, is one of the most complex and difficult industrial problems and it has been the main concern of engineering economists.

2.2 Conventional Investment Criteria.

The formulae referred to in the previous section are those criteria most commonly in use, some of which will now be examined. The two most frequently used criteria are:

(I) Percentage Return on Investment.

(II) Payout or Payback Time.

A third criterion which is also widely used is:

(III) Cash Position.

(I) Percentage Return on Investment: R

The percentage return on investment can be defined as the annual net profit expressed as a percentage of the total investment

$$R = \frac{Pa}{I + Iw} \times 100 \qquad (2.1)$$

where I = fixed capital investment and I_W = working capital. Pa = net profit p.a., i.e. gross profit minus taxes and depreciation.

(II) Pay-Out Time: T(Yrs)

The pay-out time is the ratio of the fixed capital investment to the annual gross profit

$$T = \frac{I}{R_a} \qquad (2.2)$$

where R_a = gross profit p.a.

(III) Cash Position: P

Cash position is defined as the gross earnings minus taxes and depreciation.

$$P = \left[(1-t)R_a + d\,t\,I\right]n - I \qquad (2.3)$$

where t = tax rate on income, d = depreciation rate for tax purposes and n = no. of years.

The simplicity of these formulae has been pointed out earlier, which is certainly one reason why their current usage is still widespread. The use of more complex criteria, as outlined in Section 2.3 of this chapter, gives rise immediately to considerable difficulties. The recent N.E.D.C. Report (38) presented an analysis of the investment appraisal methods in use in the Machine Tool Industry. 83% of the companies in the survey used either one of the methods mentioned already or no established method of appraisal.

Despite their present wide usage, recent theory and more enlightened practice does not recognise these traditional criteria as acceptable final arbiters in investment decisions - although their value as guides and as complementary standards is considerable. Some points including the disadvantages which occur in the use of these indices of comparison will be considered briefly.

(I) Percentage Return on Investment.

Application of this criterion requires a knowledge of the net profit p.a., the fixed capital investment and the working capital. Normally these data are available. Some disadvantages are:

(a) it makes no allowance for the time value of money

(b) it gives no measure of the magnitude of the project

(c) the original fixed capital investment becomes meaningless in the context of changing time (39).

Where the percentage return is used as a continuing measure of the success of a project, the I term should be updated by the replacement cost of the fixed capital assets. This will inevitably cause the percentage return to decrease.* This modification which is seldom effected

* except when the replacement cost is less than the original cost.

enables a more realistic yield for projects to be evaluated.

(II) Pay-Out Time.

Pay-out time is the most widely used of the criteria under discussion. The formula as given in equation (2.2) can be altered to allow for taxes and depreciation but it is more often used in its simple form. The note in the previous paragraph on updating the I term applies equally to pay-out time, although, since this criterion is more often used for investment decisions than as an operating index, the passage of time may not be relevant. That is, in comparisons between alternative decisions at time $t = o$, the I terms are comparable and their future values need not be considered. The main disadvantages are:

(a) again, no allowance for the time value of money

(b) it gives no measure of the magnitude of the project

(c) no allowance is made for tax or tax credits

(d) the tendency in its application to define an arbitrary pay-out time against which alternative projects are measured

(e) its failure to distinguish between projects which initially have the same returns but subsequently have different ones.

For engineering projects which are capital intensive, the impact of taxation has a large effect on the profitability and no criterion which neglects tax can be satisfactory. The effect of (d) is that when the defined pay-out time is too short, the alternative projects are unable to compete and are rejected. Capital investment is thus restricted, new projects are abandoned and existing plant rather than be replaced is permitted to become more and more unproductive. Furthermore, no indication is given of what occurs to the investment after the end of the pay-out period. The main value of pay-out time lies in its use as a short-term criterion.

(III) Cash Position.

The use of the cash position criterion enables the accumulated cash earnings of a project to be assessed. The fixed capital investment is offset in the first instance against the revenue from the project, which then contributes in total to the net or total earnings. The cash position has an advantage over the previous methods in that the magnitude of the project is ascertained. Its disadvantage is that while it takes account of the revenue over a number of years, it takes no account of the time value of money.

A recent report of the N.E.D.C. (40) on investment criteria outlines in some detail the unsatisfactory aspects of many of the currently used methods of appraisal. It is pointed out that there is much evidence which indicates that these criteria "tend to lead to underinvestment in plant and equipment". The major objection to the three criteria already examined, is that, the time value of money factor is neglected. The importance of the time factor has only recently been recognised and is, as yet, inadequately appreciated.

2.3 Time Value of Money and Discounted Investment Criteria.

Time Value of Money - In its simplest form the time value of money can be explained by saying that one pound to-day is worth more than one pound in five years time, which in turn is worth more than one pound in ten years time. This phenomenon is due to the ability of money, in the form of employed or deposited capital, to earn interest.

It is now accepted that except for certain specific instances, economic criteria which neglect this factor are unsatisfactory for assessing the true economics of a project.[1] Recent years have, therefore, seen the growth of new criteria for evaluating capital projects which take account of the time yield of money. In principle, these criteria result from considering all the cash flows, both positive (in the form of revenue) and negative (in the form of outgoings or disbursements), over the lifetime of the project and assessing their value at some particular point in time. This point in time is nearly always the present time. Hence the term present worth or present value used to describe these or the methods by which they are derived. The description, discounted cash flow techniques is also used. This term comes from the "discounting factor" applied to all cash terms in the future in order that their present value is obtained.

Problems of depreciation, investment allowances and taxation are more easily handled by discounting methods than by conventional ones. The formulae themselves are more complex but their application with reference to these problems is simplified, because these terms and their timing are specifically identified in the formulae developed.

---

1. "There is good reason for supposing that industrial investment in Britain has been more sluggish than it should have been because of a lack of understanding of the true economics of investment and its yield over time", The Economist, Aug. 29, 1964, in A Rationale of Capital Investment (41).

A good outline of the methods and their use in assessing the profitability of projects is given by Steward (42).

DISCOUNTED INVESTMENT CRITERIA - The two main criteria are:

(I) Discounted Cash Flow, D.C.F.

(II) Net Present Value (or Worth), N.P.V.

A criterion related to N.P.V. called Venture Worth has been developed by Happel (35, 36) which is well suited for engineering projects. Hart (43) has recently advocated a new method called the Standard Investor's Rate of Return.

(I) Discounted Cash Flow:

The term internal rate of return is also applied to this criterion. The D.C.F. yield can be defined as the rate of return, p, which will equate the present value of the cash returns to the present value of the investment outlays. p, therefore, represents the maximum "rate of profitability" which the project will yield - the project will pay a rate of interest, p, on the capital invested and recover the initial investment. In application, the rate p, is compared with the interest rate on capital, i, or a risk interest rate, i_m. (The rate, i_m, makes allowance for the risk nature of the project - $i_m \geq i$)

$p > i$ accept project

$p < i$ reject project

A good formulation of the criterion, that given by Amey (44) is, the internal rate of return, is the rate, p, such that

$$-I_o + \sum_{t=1}^{T} \frac{E_t}{(1+p)^t} + \frac{S_t}{(1+p)^t} = 0 \qquad (2.4)$$

For continuous compounding of interest equation (2.4) becomes

$$-I_o + \int_0^T \bar{E}_t e^{-m^* t} dt + \bar{S}_t e^{-m^* t} = 0 \qquad (2.5)$$

where I_o = present value of investment outlays

$\bar{E}_t$ = net cash inflows in the period t, (i.e. benefits - costs)

S_t = disinvestment of working capital and scrap value

T = project lifetime, yrs.

m^* = continuous rate of interest = ln (1 + p)

(II) Net Present Value.

The net present value of a project is obtained by discounting all the cash flows resulting from the project to the present time at a discount rate equal to the cost of capital. If the N.P.V. > o, then the project is worthwhile. The N.P.V. criterion leads to an absolute value or worth of the project in terms of money, whereas the D.C.F. criterion leads to a rate. The following formulation is again taken from Amey:

The net present value is given by V_o, where:-

$$V_o = -I_o + \sum_{t=1}^{T} \frac{E_t}{(1+i)^t} + \frac{S_t}{(1+i)^t} > 0 \qquad (2.6)$$

For continuous compounding of interest equation (2.6) becomes

$$V_o = -I_o + \int_0^T \bar{E}_t e^{-mt} . dt + \bar{S}_t e^{-mt} > 0 \qquad (2.7)$$

where i = cost of capital or other discount rate

m = ln (1+i)

Comparison of D.C.F. and N.P.V.

At present there exists two schools of thought regarding the superiority of one or other of these criteria. In this country the balance at present seems to be swinging in favour of D.C.F. (38, 41, 45), though this may be in part due to the large amount of publicity given to the method. The main argument against N.P.V. is that of the difficulty of determining the cost of capital to the firm, and if so desired, the index i_m. If this cannot be determined accurately, then a range of values for i must be established and since the effect of variations in i are difficult to observe, a series of present worth calculations must be carried out. This difficulty is avoided by the use of the D.C.F. criterion, it is merely necessary to have an estimate of the cost of capital and if the yield is sufficiently greater, a difference immediately obvious, then no further calculation is necessary.

It is true that there are considerable difficulties in arriving at an accurate estimate of i, but it is equally true that the proponents of D.C.F. magnify the difficulty. Grant and Ireson (2) go into this question in some detail from the engineering viewpoint, while Dean (46) in discussing the problem of capital rationing outlines a number of alternative approaches whereby i, can be evaluated. Hart (43) maintains that to avoid the necessity for obtaining, i, is to close one's "eyes to facts". A good discussion is given by Amey (44) who comes out in favour of N.P.V., the statement is made that "the N.P.V. criterion for productive investment is valid and consistent with profit maximization at all points in time".

The arguments in favour of N.P.V. together with its advantage in ranking projects, of giving absolute magnitudes to the alternatives involved, have caused it to be adopted in Happel's form as the discounted criterion in this thesis.

2.4 Formulation of the Venture Worth Criterion.

This Criterion hereafter referred to as the V.W. criterion which has been developed by Happel is an extension of the N.P.V. Criterion. It may be defined as the present worth of all the cash flows from a venture above a minimum risk level, discounted to the present by means of an average rate of earnings. The term, venture, in the context of the criterion is synonymous with project. The risk nature of the project is expressed by means of a minimum acceptable rate of return factor. The criterion is well suited for ranking projects, governed by different risk characteristics. A general mathematical formulation of the criterion is

$$W = \sum_{k=1}^{k=n} \frac{(1-t)R_k}{(1+i)^k} + \sum_{k=1}^{k=r} \frac{d_k t I}{(1+i)^k} - \left[\frac{i}{(1+i)^n - 1} + i_m\right] \sum_{k=1}^{k=n} \frac{I}{(1+i)^k}$$

$$- \sum_{k=1}^{k=n} \frac{i_m I_w}{(1+i)^k} + \left[\frac{i(1-t)}{(1+i)^n - 1}\right] \sum_{k=1}^{k=n} \frac{S_a}{(1+i)^k} \qquad (2.8)$$

where t = tax rate, fraction/yr

R = gross profit p.a.

I = initial or fixed capital investment

I_w = working capital

i = average rate of return on investment, fraction/yr

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i_m = min. acceptable rate of return on investment, fraction/yr

Sa = salvage value

d = depreciation rate for tax purposes, fraction/yr

r = taxable period of plant life, yrs.

n = project lifetime, yrs

k = index, indicating years from start of venture.

R_k and d_k represent the value of these variables in the k^{th} year of the project. It is assumed that I, I_w and Sa do not change from year to year although the criterion can be generalized further if necessary. Since I, I_w and Sa are constants, equation (2.8) can be written

$$W = \underbrace{\sum_{=1}^{k=n} \frac{(1-t)R_k}{(1+i)^k}}_{(1)} + \underbrace{\sum_{=1}^{k=r} \frac{d_k tI}{(1+i)^k}}_{(2)} - \underbrace{\left[\frac{(1+i)^n-1}{i(1+i)^n}\right]}_{(3)} (i_m-i)(I+I_w) \underbrace{-I}_{(4)}$$

$$- \underbrace{\left[\frac{(1+i)^n-1}{(1+i)^n}\right] I_w}_{(5)} + \underbrace{\frac{(1-t)Sa}{(1+i)^n}}_{(6)} \qquad (2.9)$$

The six terms in equation (2.9) represent:

(1) Summation of gross taxed income.

(2) Summation of tax credit on capital investment.

(3) Present worth of incremental return on total investment.

(4) Initial capital investment.

(5) Present worth of cost of working capital.

(6) Present worth of salvage.

The form of the V.W. criterion given in equation (2.9) is much more readily applied in practice than the more general expression. The number of summations have been reduced to two and in nearly all cases it is possible to eliminate the summation for the tax credit. It is possible to obtain an analytical solution for the series, describing the three most common methods of depreciation, namely, straight-line depreciation, double declining balance method and sum-of-the-digits method. Combinations of these three can also be expressed analytically. In the case of the gross return summation, if the fluctuations are regular a formulation may be possible, otherwise tabulation may be necessary.

For continuous compounding, equation (2.9) in the limit becomes

$$W = \int_{=0}^{k=n} (1-t)R_k e^{-mk}.dk + \int_{=0}^{k=r} Itd_k\, e^{-mk}.dk - \frac{1}{m}(1-e^{-mn})(e^{q}-e^{m})(I+I_m)$$

$$-I - (1-e^{-mn})I_w + (1-t)Sa\, e^{-mn} \qquad (2.10)$$

where $m = \ln(1+i)$ and $q = \ln(i_m + i)$

In this equation R_k and d_k represent the values of R and $\bar{d}$ in the whole period k and could be written R and d respectively.

If either R or d, or both, are constant throughout the lifetime of the project, further simplifications of equations (2.9) and (2.10) are possible. When both are constant the first two terms in the equations become respectively

$$\left[\frac{(1+i)^n-1}{i(1+i)^n}\right](1-t)R+\left[\frac{(1+i)^r-1}{i(1+i)^r}\right]dtI$$

These two terms together with the other terms in equation (2.9) will be called equation (2.11) ~~(2.11)~~

and

$$(1-t)\bar{R}\frac{1}{m}(1-e^{-mn})+It\bar{d}\frac{1}{m}(1-e^{-mr})$$

plus other terms in equation (2.10) will be called equation (2.12) The assumption that d is constant is equivalent to assuming straight line depreciation. The combined premise of both R and d constant renders the V.W. equivalent to the summation of the annual venture profits (35), suitably discounted, throughout the lifetime of the project.

2.5 Analysis and General Simulation of V.W. Equation.

Equation (2.8) which is the general formulation of the V.W. Criterion has ten parameters. The following categories may be used to group them

(i) Parameters fixed by the state or country.

(ii) Parameters fixed by the company.

(iii) Variable Parameters.

(i) Parameters fixed by the State:

t = income tax rate. Company policy can on occasion modify the effect of t.

d = depreciation rate for tax purposes.

r = taxable period of plant life. Although there is some flexibility with both d and r, the company's decision will be mainly motivated by state policy.

(ii) Parameters fixed by the Company:

I = initial fixed capital investment.

n = project life as estimated for design. This figure depends on the type of plant, the design philosophy adopted, on the replacement or obsolescence policies being followed and on market forecasts.

i = projected average rate of return on investment. Current economic conditions will influence this decision -

but company policy will in the main decide the value of i (46).

i_m = minimum acceptable rate of return on investment.

(iii) Variable Parameters:

I_w = working capital

R = gross profit

Sa = salvage value

These three parameters can depend largely on the market conditions and although other factors are involved they may be thought of as being subject to the fluctuations of the market.

It is clear that the above categories are very loose but they are helpful when considering the equation and enable the engineering problem to be delineated. Five of the ten parameters have what can be considered as an engineering content and as such are amenable to engineering control. They are I, I_w, n, R and Sa. Of these, three have been categorized as variables and the remaining two placed in the 'parameters fixed by the company' group.

I: this parameter contains the greatest engineering content in the majority of industrial projects.

I_w: the working capital's engineering factor can be thought of as the effect of the plant design on the operating and out-of-pocket expenses.

n: the project lifetime may, depending on the nature of the project, be totally governed by engineering considerations or by market conditions.

R: depends on the labour content, utility consumption and general profitability of the plant.

Sa: the design philosophy can influence the terminal value of the plant.

The above notes on the parameters describing the V.W. criterion have indicated that

(i) five parameters are outside engineering control

(ii) of the other five all have a greater or lesser engineering content.

Simulation of the V.W. Criterion.

A simulation of the project as expressed by its V.W. is a logical step in considering a project. This might correspond to the simple model simulation discussed in the last chapter. The effect on the V.W. of variations in the parameters can be discovered and the critical parameters identified. Such a simulation was carried out to illustrate this approach. It took the form of evaluating the V.W. of a plant of a fixed capital cost for a number of predetermined levels of the other parameters. The parameter variation proceeded in a one variable at a time sequence. Certain simplifications were introduced in assigning values to the parameters R, I_W and Sa. It was assumed that

(i) $R = 0.5I$

(ii) $I_W = QI \qquad Q = 0.2$

(iii) $Sa = PI \qquad 0 < P < 1$

These assumptions were introduced to reduce the dimension of the simulation from ten to seven variables. It will be seen that the three parameters which have been substituted for are the three least controllable ones, and as such cannot be varied at will in reality. The form of the criterion used was that given by equation (2.11).

A programme was written for the University Mercury Computer in which plants with initial capital costs of one, five and ten million pounds were simulated.

Figures 2.1, 2.2 and 2.3 are typical of the results obtained. It will be observed that the responses shown in figure 2.3 are linear, which follows from the linearity of equation (2.11) with respect to t. The information, which can be obtained from curves of this type, is best illustrated if we consider an example:-

A ten percent increase in V.W. is required from a 5 million pound plant, with a project lifetime of 15 yrs., a depreciation period of 5 yrs. and a tax rate of 50%.

From fig. 2.1: V.W. $=$ 6.55x10^6 £

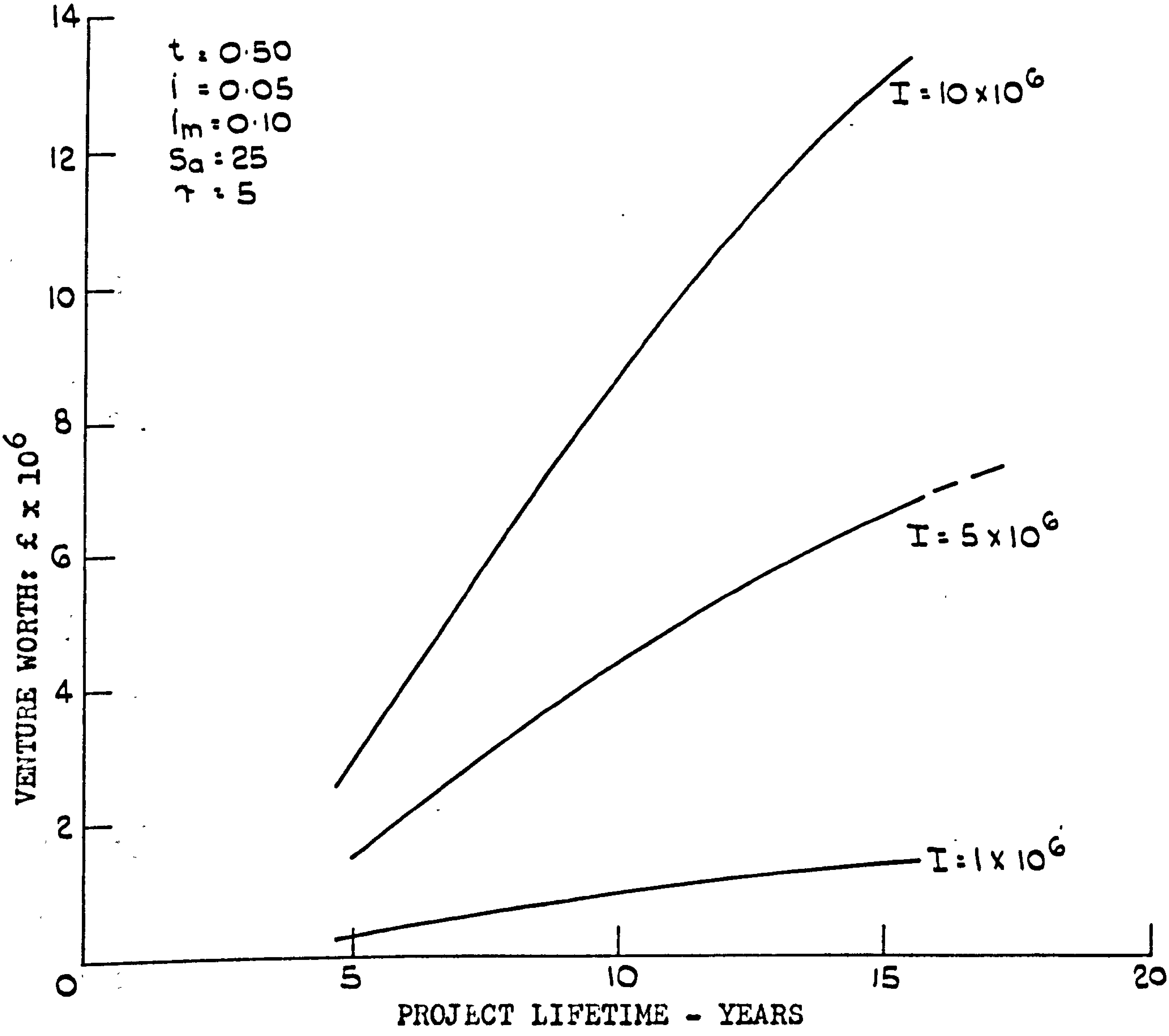
Reqd. V.W. $=$ 7.205x10^6 £

From fig. 2.1 n $=$ 17 yrs.

2.2 can't be achieved

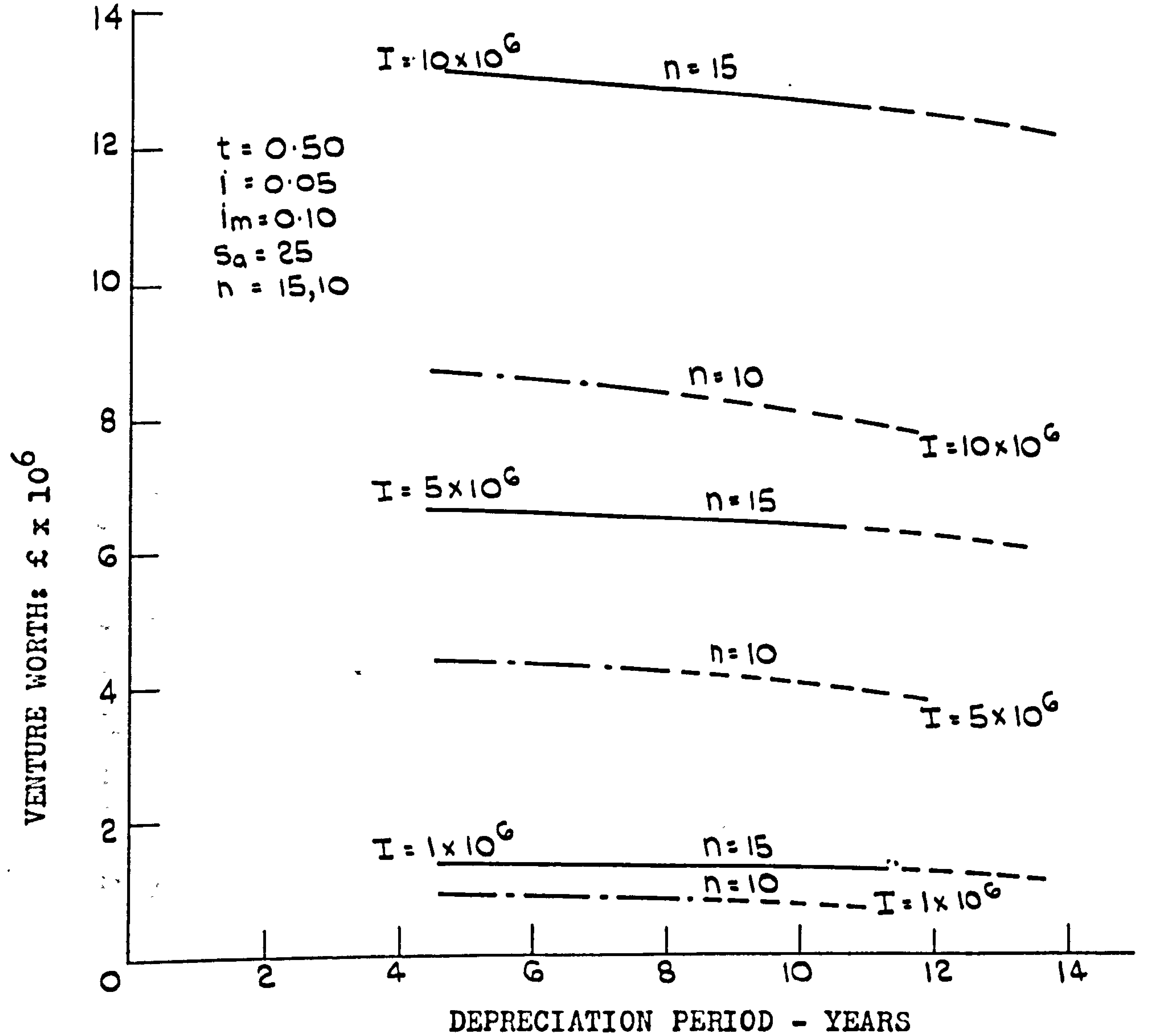
2.3 t $=$ 47%

It will be seen that considering these three variables, a 6% reduction in the tax rate is equivalent to a 13% increase in the project lifetime, either of which could be altered to achieve the desired increase in the V.W. Whereas, no matter what depreciation period is used, resulting in the most favourable tax credit, a ten percent increase



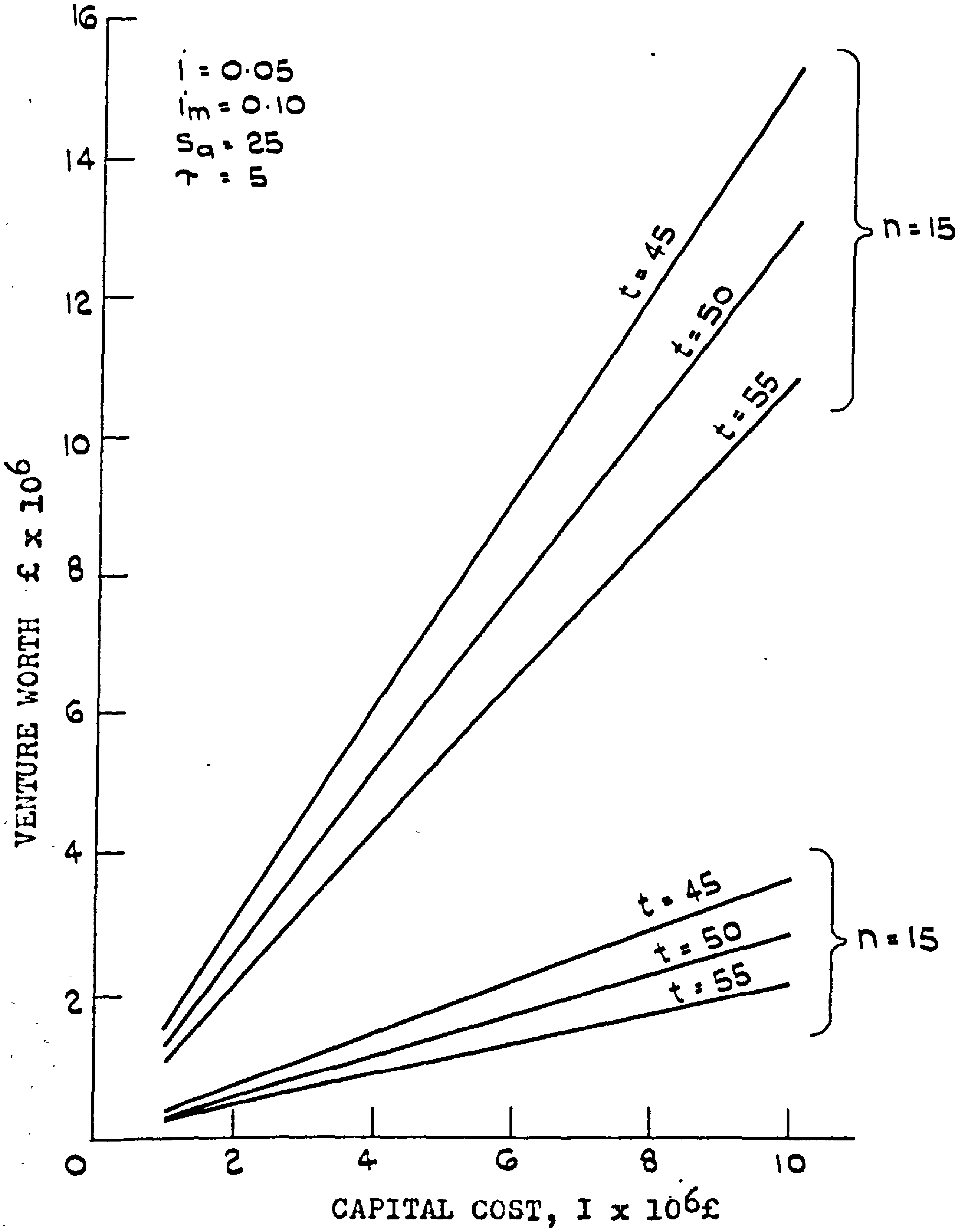
VENTURE WORTH SIMULATION
VARIATION OF n

Fig. 2.1



VENTURE WORTH SIMULATION
VARIATION OF r

Fig. 2.2



VENTURE WORTH SIMULATION
VARIATION OF t

Fig. 2.3

cannot be achieved, the maximum attainable being approximately 2.3%. The decision lies between two alternatives, one of which cannot be controlled by the engineer. If in such circumstances, it should prove that the level of taxation can be more easily reduced by the required 6%, than that the project lifetime be extended by 13%, then further engineering analysis may be of no benefit.

The information which can be obtained from a simulation of this nature is threefold

(i) It will show which parameters are significant and the effect of variations in them on the V.W. of the project. Some order of magnitude figures for the possible variations in the parameter range are given by Bauman (29).

(ii) If the non-engineering parameters are controlling, /arises the necessity for considering the value of continuing engineering studies. ~~arises.~~

(iii) When the engineering parameters are critical, their relative importance is known.

Appendix 2 contains details of the computer programme and some further notes on the simulation.

2.6 Application of V.W. Criterion to Unit Plant Items.

Chemical processes can be represented as inter-linked multi-stage systems. In the previous two sections the application of the V.W. Criterion to complete processes or plants has been outlined. In accordance with the general scheme presented in chapter 1, the application of the criterion to single stages or items in a multistage system must now be considered. If equation (2.11) is written in the form

$$V.W. = J_1R + J_2I - J_3I_w \qquad (2.13)$$

where:

$$J_1 = \left[\frac{(1+i)^n - 1}{i(1+i)^n}\right](1-t)$$

$$J_2 = \left[\frac{(1+i)^r - 1}{i(1+i)^r}\right]dt - (i_m - i)\left[\frac{(1+i)^n - 1}{i(1+i)^n}\right] - 1 - \frac{(1-t)P}{(1+i)^n}$$

$$J_3 = \left[\frac{(1+i)^n - 1}{i(1+i)^n}\right]i_m$$

and $Sa = PI$.

Now: $I_w = Q$ [total annual expense]

$$= Q\left[X + 0\right] \qquad (2.14)$$

The assumption that the working capital, I_w, may be expressed as a constant, Q, times the total annual expense is a fact accepted by Happel (35).

$$R = \left[S - X - O\right] \tag{2.15}$$

where $X =$ raw matl. costs p.a., $O =$ all operating costs p.a., and $S =$ sales revenue p.a.

Substituting (2.14) and (2.15) into equation (2.13)

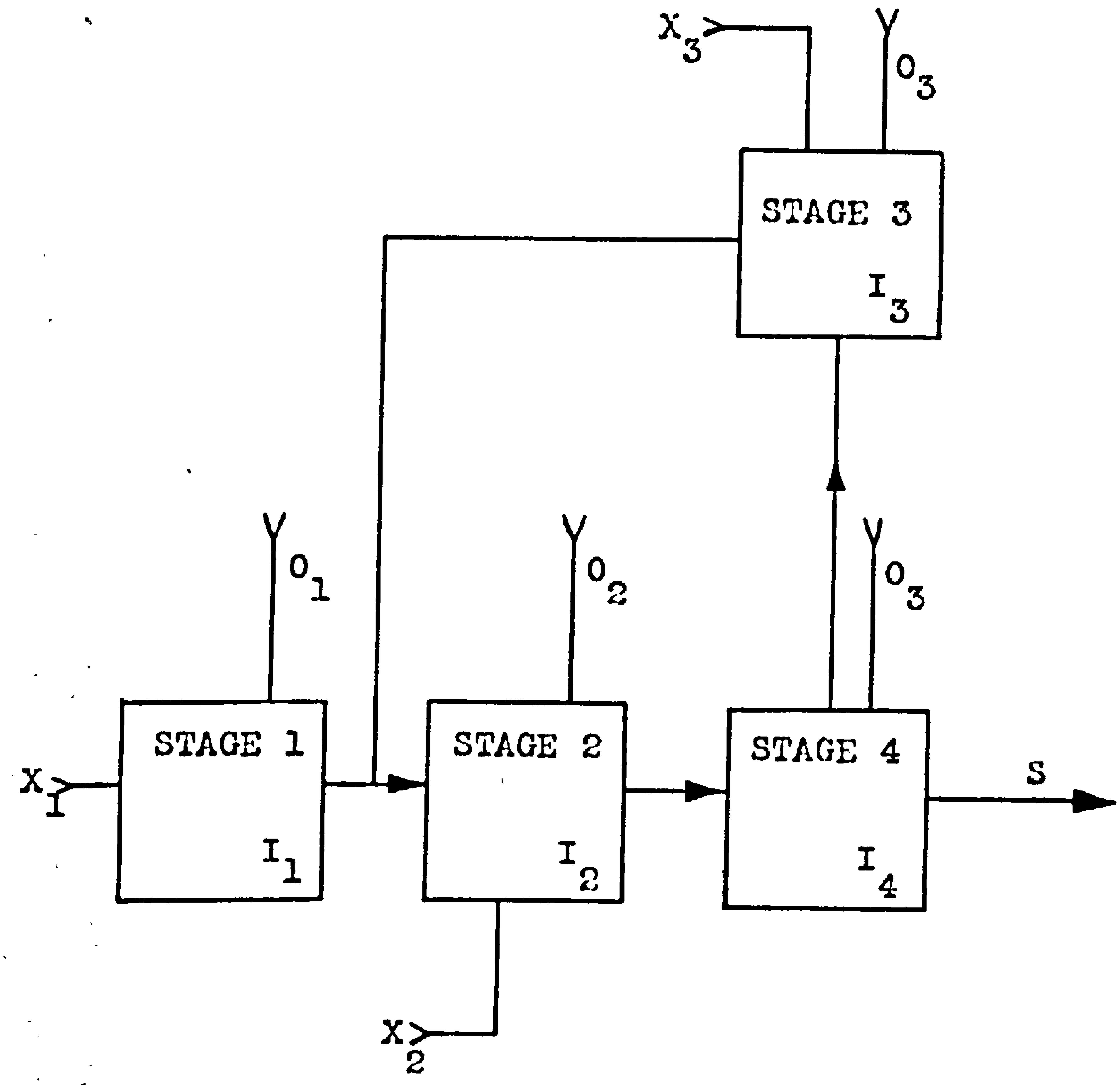
$$V.W. = J_1 S + J_2 I - (J_1 + J_3 Q)\,X - (J_1 + J_3 Q)\,O \tag{2.16}$$

If we assume that the process consists of N stages and that each of the N stages can be described by a capital cost, an annual operating cost and a raw material cost, this equation can be written

$$V.W. = J_1 S + J_2 \sum_{k=1}^{k=N} I_k - (J_1 + J_3 Q) \sum_{k=1}^{k=N} X_k - (J_1 + J_3 Q) \sum_{k=1}^{k=N} O_k \tag{2.17}$$

The V.W. is expressed in equation (2.17) as the sum of a series of costs, each of which represents a single stage of the process, together with the sales from the process as a whole. Since the sales from the whole process only are considered, the necessity for allocating in-system prices to the products of the individual stages is avoided. A typical system is that of figure 2.4 in which a four stage system is depicted.

Should the process yield any other saleable



X_i COST OF RAW MATLS. TO STAGE i p.a.

O_i COST OF OPERN OF STAGE i p.a.

I_i CAPITAL COST OF STAGE i

CONTRIBUTIONS OF VARIOUS COSTS TO VENTURE WORTH OF A TYPICAL PROCESS FIG. 2.4

by-products, $S = \sum S_i$, where S_i = sales revenue p.a. from the i^{th} product. The additive nature of the venture worth of the individual stages is clear from equation (2.17). This characteristic of the criterion reduces the computation, when the effect, on the whole process, of perturbations to single stages must be determined.

2.7 Criteria for Selection of Investment Alternatives.

The effect of allowing for the time value of money as indicated in section 2.3, puts a high premium on cash flows in the present or near present time and minimizes the importance of cash flows in the distant future. Such a financial structure represents the true economic situation, but has certain disadvantages when weighing alternative possibilities at the present time. Where two projects show a small difference when represented by a conventional investment yardstick, the difference may become less evident after discounting for futurity. This possibility occurs because the discounting factor converges to a specific value as $n \longrightarrow \infty$. As i increases, the rate of convergence also increases. A table demonstrating how the discount factor converges can be found in Appendix 2.

For example, consider two processes each with the same output of product, but showing a small but distinct difference in their unit production cost. Over the lifetime of the project, the cumulative total effect of the differential, expressed as say, profit over twenty years might be of some moment and thus a clear-cut decision between the two may be possible. If, however, a discounting criterion is applied the difference may be regarded as insufficient to enable a decision to be made. Thus the application of a more rigorous economic criterion may render the selection between alternatives more difficult.

The recent work of Allen and Edgeworth Johnstone (47) in this field is of interest. It tentatively attempts to rank a number of economic criteria relative to their ability, to distinguish at an early stage between successful and unsuccessful projects. They found that the D.C.F. yield was less satisfactory than shorter term criteria, such as Payout Time from the start of the project. Two new criteria, Equivalent Maximum Investment Period and Interest Recovery Period, which do not involve discounting, were also found to be effective. It is pointed out that the ranking of the D.C.F. Criterion relative to the above criteria improves as the project lifetime decreases.

The corollary of the foregoing is important, which is that small differences in projects as measured by a discounted criterion may be as significant as much larger differences in non-discounted criteria. The necessity for considering the time yield of money, means that discounting must generally be used and it follows that even small differences in N.P.V., D.C.F. yield or V.W. must be examined closely.

CHAPTER 3: CASE I - A SEPARATION SYSTEM DISTILLATION COLUMN

3.1 Introduction

3.2 Mathematical Theory and Development of Equations

3.3 Validity of Efficiency Approximation and Alternatives

3.4 Derivation of an Analytical Expression for Gilliland's Correlation

3.5 Application of the Venture Worth Criterion and General Cost Data for the System

3.6 Mathematics of Solution, Programme Mechanics and Simulation Outline

3.1 Introduction:

A distillation column was selected as a typical unit of equipment and one on which a great deal of process and design data are readily available. The existence of such information is a prerequisite for most economic investigations. The objective of the study was to see how the application of different economic criteria affected the optimum design and operating conditions of the column. It was also wished to study the reverse approach, that is to see how variations in the design and operating parameters affected the economic criteria. The method of perturbing a model of the system outlined in the section on development theory was utilized to this end.

A well known approach to the optimum design of plate columns is to express the optimum condition as a function of the number of plates, N, in the column and the reflux ratio, R (48, 49, 50). These two parameters are chosen because the capital cost of the column can be expressed as a function of N, and the column cost represents in practice virtually the total capital cost of the system. Also, the reflux ratio tends to be the governing factor in the operating costs. It is possible to express all other capital and operating costs as functions of these two variables cf. (51). Underlying all the work which has been carried out in the analysis presented here, is this concept of an optimum design as an economic balance between N and R. Figure 3.1 shows a line diagram of the column and the ancillary items of equipment comprising the system. Two economic criteria, the unit cost of production and the venture worth of the project were considered. The first step in the case study involves the construction of a mathematical model of the system which is described in the next section.

3.2 Mathematical Theory and Development of Equations.

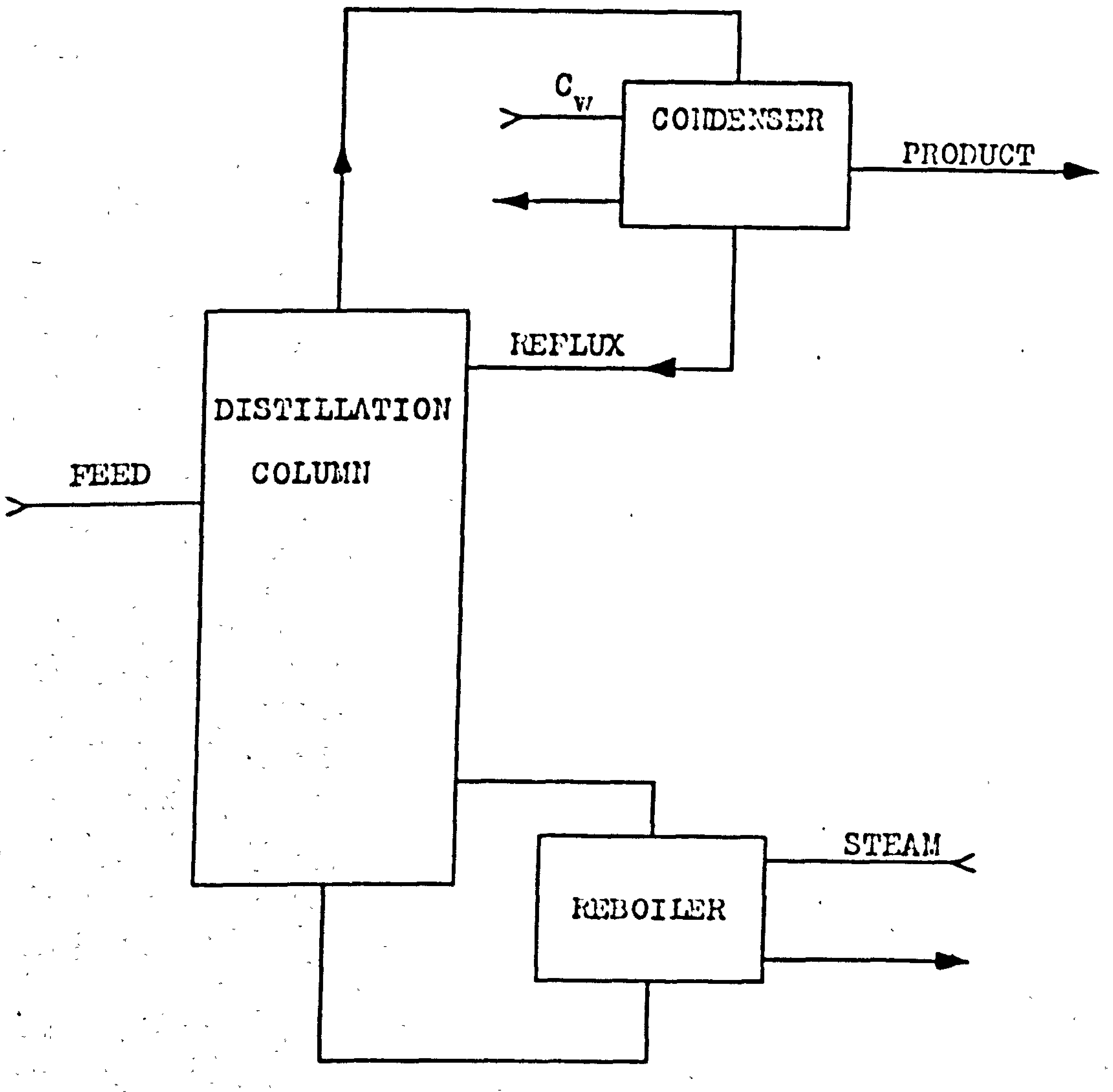
The costs associated with the system shown in figure 3.1 can be represented by the equation given by Happel (35).

$$C = \frac{C_1 N(R+1)}{EhG_a} + \frac{C_2(R+1)}{hG_b} + C_3(R+1) \qquad (3.1)$$

where C = unit cost of production. \$/lb mol product

C_1 = amortized incremental unit investment cost of column. \$/(Ft^2)(plate) (yr).

C_2 = amortized incremental unit investment cost of tubular equipment (T.E.). \$/(Ft^2)(yr.)



LINE DIAGRAM OF SEPARATION SYSTEM FIG. 3.1

C_3 = cost of steam and coolant necessary for 1 lb mol of product. $

h = hrs. operation p.a.

G_a = allowable vap. vel. in column. lb mols/(hr)(FT^2)

G_b = vap. handling cap. of T.E. lb mols/(hr)(FT^2)

E = fractional plate efficiency.

The relationship between N and R mentioned in section 3.1 and on which equation (3.1) is based is dependent on the fact that, for a given separation, as the reflux ratio is increased, the number of plates required decreases. The necessary calculations to produce the N v R curve are usually carried out by the well known McCabe-Thiele method (see, for example, 33, 48, 49). The work of Gilliland (52) which is discussed later, may also be used for this purpose. It is clear that the three terms on the R.H.S. of equation (3.1) represent the column capital costs, the ancillary equipment capital costs and the system operating costs respectively. The make-up of the individual terms is given in Appendix 3. The procedure used by Happel to find the minimum of C was originally devised by Colburn and is as follows. The derivative of equation (3.1) w.r.t. R is equated equal to zero. E, the fractional plate efficiency is assumed independent of R for this purpose. The values of N and R which satisfy the equation

$$\frac{dC}{dR} = 0 \tag{3.1a}$$

are the optimum values for the system.

In this work some extensions have been made to the above procedure. Firstly, E is not assumed independent of R and secondly equation (3.1) is formulated such that the design and operating parameters are readily accessible for the purpose of perturbation. In addition a more generalized treatment is developed through the use of Gillilands work (52) on the relationship between the number of theoretical plates required for a separation and the reflux ratio.

The recent correlation of English and Van Winkle (53) for the efficiency of fractionating columns expresses the plate efficiency as a function of a number of design and operating variables including the reflux ratio. The correlation is for the Murphree vapour plate efficiency and is

$$E_{mv} = 10.84(FA)^{-0.28}\left(\frac{L}{V}\right)^{0.024} h_w^{-0.241} G^{-0.013} \alpha^{-0.028} \left(\frac{\sigma}{\mu_L V_G}\right)^{0.044} \left(\frac{\mu_L}{\rho_L D_L}\right)^{0.137} \tag{3.2}$$

where FA = free area fraction in col. cross section. (C/S).

L/V = reflux ratio

h_w = weir height. ins

G = superfical mass vap. vel. based on col. C/S. lb/(hr)(FT^2)

α = relative volatility.

σ = surface tension of mixture. dynes/cm

μ_L = liq. viscosity of mixture. poise

Vg = vap. vel. based on col. C/S. cm/sec

ρ_L = liq. density of mixture.

D_L = liq. mol-diffusion coeff. cm^2/sec

The two dimensionless groups at the end of the equation represent the liquid Schmidt No. and the surface tension No. respectively.

This correlation was derived from data on, and is applicable to, both bubble cap and perforated plate columns. Although the data analysed were all binary data, the authors consider that the correlation can be used satisfactorily for multi-component systems and illustrate this point with a typical example. When applied to multi-component fractionation μ_L, ρ_L, σ and D_L are the mixture properties of the system.

Equation (3.2) can be written

$$E_{mv} = K\left(\frac{R}{R+1}\right)^{0.024} \qquad (3.3)$$

where $\left(\frac{L}{V}\right) = \frac{R}{R+1}$ and $K =$ other terms in equation (3.2).

The assumption, which is discussed fully in section 3.3, is now made that E_{mv} in equation (3.3) is equal to E in equation (3.1) that is that, the Murphree vapour plate efficiency is equal to the overall column plate efficiency. Equation (3.3) is now substituted in equation (3.1)

$$C = \frac{C_1 N(R+1)}{KhG_a\left(\frac{R}{R+1}\right)^{0.024}} + \frac{C_2(R+1)}{hG_b} + C_3(R+1) \qquad (3.4)$$

In this equation, the unit cost of production is given not only as a function of the two major variables N and R, but also of G_a, G_b, h and K. The constant K contains a number of operating and design variables including $G = MG_a$ where $M =$ mol. wt. These subsidiary variables may be thought of as the development parameters of the system.

Equation (3.4) can be differentiated with respect to R and the condition necessary for the minimum unit cost of production is obtained when this is equated equal to zero.

$$(R+1) = \frac{N - 0.024\ N(\frac{1}{R}) + F^{*}(\frac{R}{R+1})^{0.024}}{-(\frac{dN}{dR})} \qquad (3.5)$$

where $F^{*} = K\frac{G_a}{C_1}(\frac{C_o}{G_b} + hC_3)$ = cost or development constant (3.5a)

The value of R which satisfies (3.5) i.e. L.H.S.=R.H.S. is the optimum value of $R = R_o$. N_θ is defined as the no. of plates corresponding to the value of R_o. In order that equation (3.5) can be solved it is necessary to have curves of N v R and $\frac{dN}{-dR}$ v R for the system, a trial and error solution can then be obtained. The work of Gilliland (52) referred to earlier presents a means by which the N v R curve can be generated for a given system provided that the system is characterized by N_m (the min. no. of plates required for the separation at total reflux) and R_m (the min. reflux ratio required for the separation with an infinite no. of plates). To generalize this work an analytical expression was sought for Gilliland's curve and the following polynomial was obtained.

$$\frac{N-N_m}{N+2} = A\left[\frac{R-R_m}{R+1}\right]^3 + B\left[\frac{R-R_m}{R+1}\right]^2 + C\left[\frac{R-R_m}{R+1}\right] + D \qquad (3.6)$$

where A = -0 359, B = 0.834, C = -1.120 and D = 0.642.

The accuracy of equation (3.6) and the general applicability of Gillilands work is considered in section 3.4, but the above expression was considered capable of generating N v R curves. The values of (dN/dR) necessary for the solution of equation (3.5) are obtained by differentiating equation (3.6),

$$\frac{dN}{dR} = \frac{(N+2)^2}{N_m+2} \cdot \frac{R_m+1}{(R+1)^2}\left[\frac{3A(R-R_m)^2}{(R+1)^2} + \frac{2B(R-R_m)}{R+1} + C\right] \qquad (3.7)$$

Equation (3.5) can now be solved for any given system, i.e. a specified N_m and R_m, for a given value of F^*. Solution for a series of different values of F^* yields the locus of the optimum R and N for the system. The procedure has been carried out for a range of systems enabling the optimum solution to be calculated rapidly and directly. The results, as will be seen later, can be conveniently presented as a family of curves of the form

$$\left(\frac{R_o}{R_m} - 1\right) \text{ v } F^* \quad \text{and} \quad \frac{N_o}{N_m} \text{ v } F^*$$

An equation, differing only in the cost constants and analogous to equation (3.5), is developed in section 3.5 when the venture worth criterion is being evaluated. The subsequent procedure is identical to that described above.

3.3 Validity of Efficiency Approximation and Alternatives.

The Murphree vapour plate efficiency, E_{mv}, is the ratio of the actual change in the average vapour composition accomplished by the plate to the change that would occur, if the mixed vapour stream reached equilibrium with the exit liquid. Thus

$$E_{mv} = \frac{Y_{n avg.} - Y(n-1)avg.}{Y_n^* - Y(n-1)avg.} \qquad (3.8)$$

where $Y_{n\ avg.}$ and $Y(n-1)avg.$ = the average composition of the vapour leaving the n^{th} and $(n-1)^{th}$ plate. Y_n^* = composition of vapour in equilibrium with liquid on n^{th} plate.

The overall plate efficiency, E, is the ratio of the number of theoretical plates required for a given separation to the number of actual physical plates.

Under certain conditions, the two efficiencies are identical

(i) if the plates are 100% efficient or alternatively if E_{mv} is the same for all plates, then $E_{mv} = E$.

(ii) if the equilibrium line and the operating line are straight and parallel, then $E_{mv} = E$.

Where these conditions do not hold the assumption of equality or near equality is frequently made (49, 54), on the grounds that the difference between the two is small. Robinson and Gilliland (49) make the point that where the rectifying section operates from low to high concentrations, E will approximately equal E_{mv}. O'Connell (55) assumes equality in his correlation for plate efficiencies in absorbers. Griswold and Steward (56) found that E_{mv} ranged from 2% to 10% $>$ E, in a study on the effect of operating variables on plate efficiency. English and Van Winkle (53) in assembling the data for their correlation from the literature, used an arithmetic average for E_{mv} where column efficiencies were reported. Furthermore, in the sample calculation outlined, Murphree efficiencies are averaged to give column efficiencies.

The recommended design procedure of English and Van Winkle (53) involves calculating E_{mv} for the top, feed and bottom plates and then averaging to obtain the rectifying and stripping section efficiencies, i.e.

$$\frac{E_{mv}(\text{TOP}) + E_{mv}(\text{FEED})}{2} = E_{\text{RECT. SECTION}}$$

$$\frac{E_{mv}(\text{FEED}) + E_{mv}(\text{BOTTOM})}{2} = E_{\text{STRIPPING SECTION}}$$

Where the two values are similar, the average value is taken and the number of plates required for the column is calculated on this average. If the two values are widely different they recommend that the number of plates for each section be calculated independently. The decision to substitute E_{mv} as given by the correlation (3.2) for E was arrived at mainly on the basis of the author's own practice.

In some cases where the substitution $E_{mv} = E$ may be unacceptable, expressions are available giving E as a function of E_{mv}.

(i) where the equilibrium line and the operating line are straight but not parallel, the following expression has been derived by Lewis (59) :-

$$E = \frac{\ln\left[1 + E_{mv}(J-1)\right]}{\ln J} \qquad (3.9)$$

where J = ratio of the slopes of the equilibrium and operating lines. Equation (3.9) was developed from consideration of binary mixtures but as with equation (3.2) can be applied to multicomponent systems provided E_{mv} is correctly calculated.

(ii) where efficiencies are very small equation (3.9) can be written:-

$$E = E_{mv}\left(\frac{J-1}{\ln J}\right) \qquad (3.10)$$

(iii) it may be possible to approximate the equilibrium diagram in a piecewise linear fashion cf. (58) and if so two or more expressions similar to equation (3.9) will enable E to be expressed as a function of E_{mv}. An averaging procedure similar to that of English and Van Winkle could then be adopted.

(iv) where no relationship holds between E and E_{mv}, a plate to plate calculation must be carried out to obtain E.

In section 3.2, equation (3.3) i.e.

$$E = E_{mv} = K \left(\frac{R}{R+I}\right)^{0.024} \tag{3.3}$$

was given as the substitution for equation (3.1) when $E = E_{mv}$. When $E \neq E_{mv}$ but can be expressed by either equation (3.9) or (3.10), the following substitutions can be readily made in respect of these equations for E in equation (3.1)

$$E = \lambda_1 \ln\left[1+\lambda_2 K \left(\frac{R}{R+I}\right)^{0.024}\right] \tag{3.11}$$

$$E = \lambda_3 K \left(\frac{R}{R+I}\right)^{0.024} \tag{3.12}$$

where $\lambda_1 = 1/\ln J$, $\lambda_2 = (J-1)$, $\lambda_3 = (J-1)/\ln J$

It is clear that no additional computational difficulties will arise from the use of either equation (3.11) or (3.12) instead of (3.3) in the procedure described in the previous section.

3.4 Derivation of an Analytical Expression for Gillilands Correlation.

Gilliland in his work on multicomponent rectification (51) produced a correlation relating the number of theoretical plates required for a given separation to the reflux ratio. The correlation was based on systems containing from two to eleven components and with widely varying physical properties. The minimum reflux ratios, R_m, varied from 0.53 ⟶ 7 and the minimum no. of theoretical plates, N_m, from 1.4 ⟶ 42. It is widely used in the design of multicomponent distillation systems (33, 48, 50) and it has the advantage from the economic viewpoint, that it is most accurate near the limiting conditions of R_m and N_m, that is, the region of the economic optimum. Figure 3.2 shows the form in which the correlation is generally presented. The points on the graph are the actual data of Gilliland.

For use in the procedure outlined in section 3.2, it was necessary to express this curve in a form suitable for computer work. Accordingly an analytical expression was sought for the curve. A least squares curve fit (59) was carried out on Atlas using all Gillilands data and the following third order polynomial was obtained.

$$Y = -0.359\,X^3 + 0.834\,X^2 - 1.120\,X + 0.642 \qquad (3.13)$$

[Gillilands: $S_m = N_m + 1$]

where $Y = \frac{N-N_m}{N+2}$, $\quad X = \frac{R - R_m}{R+1}$

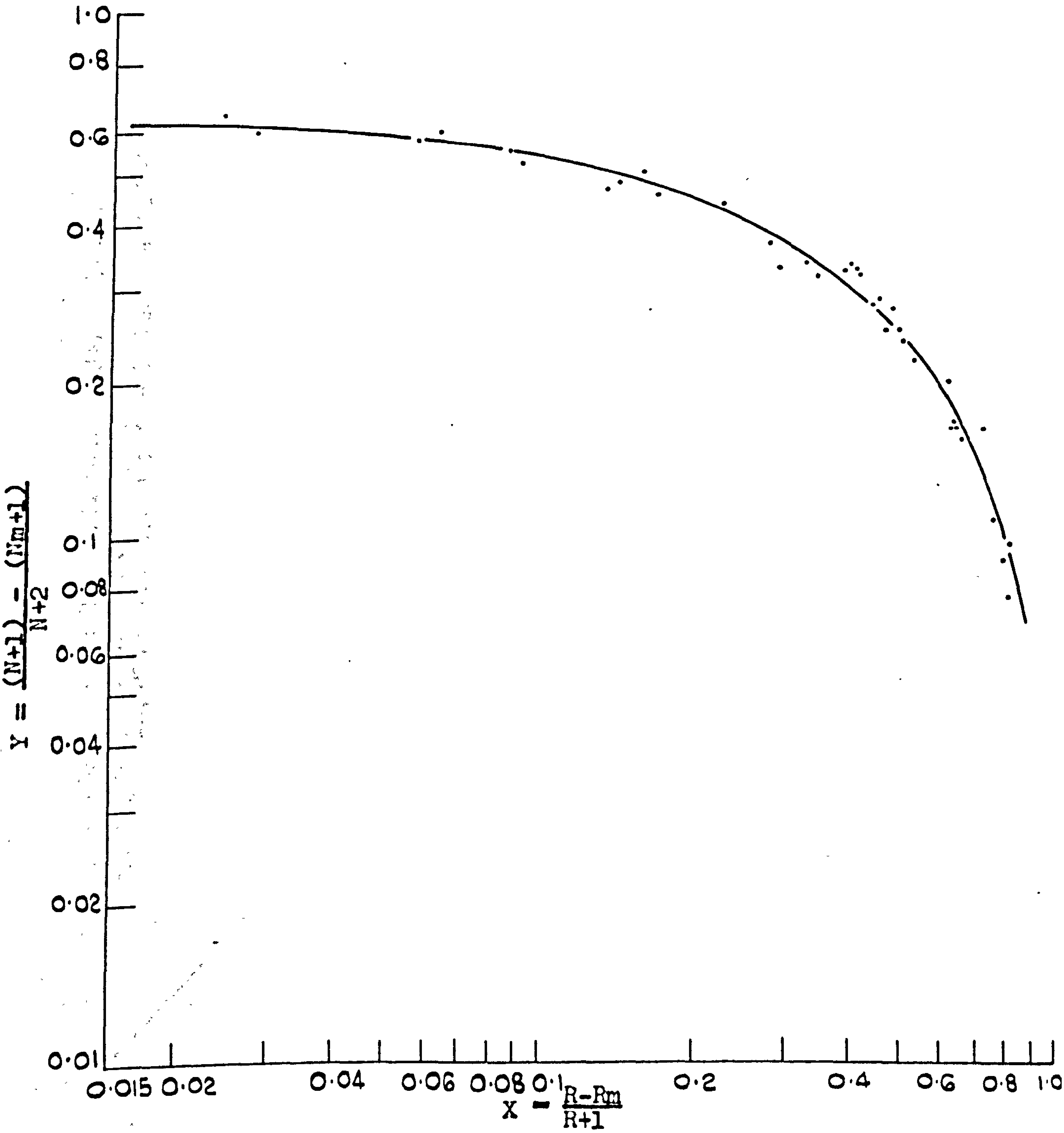
The curve plotted in figure 3.2 is given by this equation. In figure 3.3 the normal, as opposed to the log-log, form of the curve has been plotted and again the points are those of Gilliland. The error criteria for equation (3.13) are

(i) max residual $= 0.0457$

(ii) residual sum of sqs $= 0.0146$

The fit was considered to be satisfactory and the expression capable of generating N v R curves.

Programme 1000, a standard library programme was used for these computations. The data used, as has been indicated, was that of Gilliland. All the data for the seventeen systems correlated by Gilliland were utilized with the exception of the end points for each system, that is the values of $Y = 1.0$, $X = 0$ and $Y = 0$, $X = 1.0$. It will be observed that these values correspond to $N = \infty$, $R = R_m$ and $N = N_m$, $R = \infty$ respectively and that the omission



GILLILAND'S CURVE: PTS. ARE ACTUAL DATA
CURVE GIVEN BY EQN.
$Y = -0.359\,x^{3} + 0.834\,x^{2} - 1.120\,x + 0.642$

Fig. 3.2

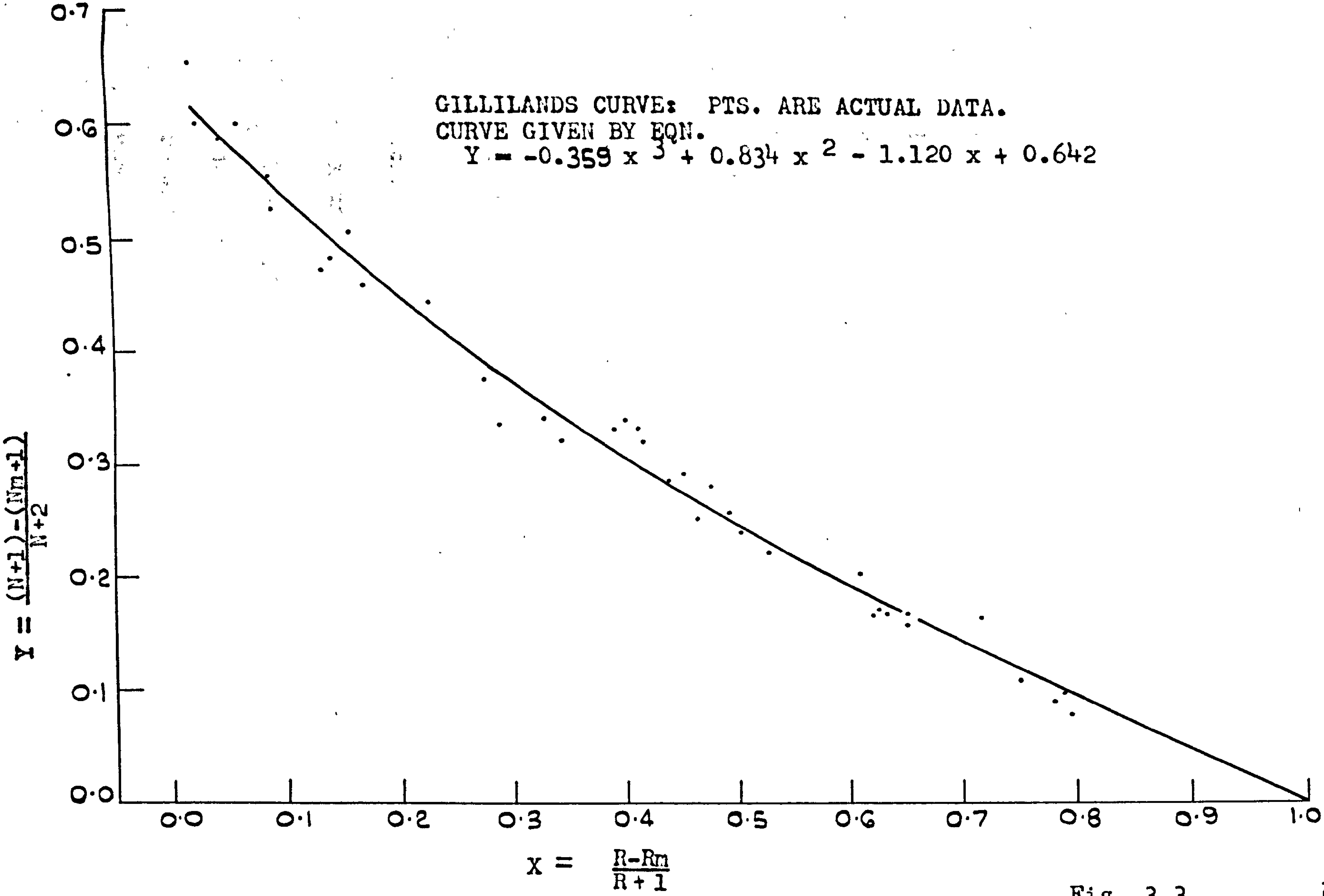

GILLILANDS CURVE: PTS. ARE ACTUAL DATA.
CURVE GIVEN BY EQN.
Y = -0.359 x 3 + 0.834 x 2 - 1.120 x + 0.642
0·7
0·6
0·5
0·4
0·3
0·2
0·1
0·0
Y = (N+1)-(Nm+1) / N+2
0·0
0·1
0·2
0·3
0·4
0·5
0·6
0·7
0·8
0·9
1·0
X = R-Rm / R+1

Fig. 3.3

of these points effectively neglects the two fixed boundary points of the curve.

A number of curve fits were obtained incorporating the end points in a variety of ways (i) including the points as data of equal weight (ii) including the points with a greater weighting than the remaining data and (iii) including ghost points between the end of the other data and the end points. It was found, however, that the most accurate fit to the data as a whole, by means of a polynomial expression, was obtained by omitting the end points.

A further point in connection with the applicability of the analytical relationship needs to be made, as it has a bearing on the computational procedure presented in section 3.2 which will become evident in section 3.6.

It will be observed from figure 3.2 that the workable ranges for the groups plotted are approximately

$$X = \frac{R-R_m}{R+1} \qquad 0.02 \longrightarrow 0.85 \qquad (3.14)$$

$$Y = \frac{N-N_m}{N+2} \qquad 0.07 \longrightarrow 0.60 \qquad (3.15)$$

The systems with which Gilliland was concerned had R_m ranging from $0.53 \longrightarrow 7.0$ and N_m from $1.4 \longrightarrow 42.1$. They may be assumed to include a wide variety of typical systems and therefore the following ranges for R_m and N_m may be considered as embracing the majority of normal systems.

$$R_m \quad 0.50 \longrightarrow 10.0$$

$$N_m \quad 1.0 \longrightarrow 50$$

It will be noted from the ranges (3.14) and (3.15) that the values of R and N may therefore vary in the following manner

$$\begin{array}{ll} R & 0.53 \longrightarrow 72 \\ N & 1.23 \longrightarrow 128 \end{array} \qquad (3.16)$$

The ranges given in (3.16) effectively define the limits of the system characteristics which can be handled by this expression i.e. equation (3.13). If we consider the systems which Gilliland correlated from the same view-point, the range of values apart from the infinite cases was

$$R \quad 2.0 \longrightarrow 35$$

$$N \quad 8.0 \longrightarrow 57$$

Thus it will be seen that the ranges defined in (3.16) are sufficiently extensive to cover all the typical systems investigated by Gilliland. Equation (3.13) is therefore capable of generating satisfactory N v R curves for most normal separation systems.

Due to the neglect of the end point conditions the expression does not satisfactorily describe the behaviour of the curve outside the limits given in (3.14) and (3.15). This limitation is not severe, in practice, but imposes a restraint on the computational procedure outlined later.

3.5 Application of the Venture Worth Criterion and General Cost Data for the System.

The venture worth of a project can be represented under certain simplifying conditions by the equation (2.13) developed in the last chapter i.e.

$$V.W = J_1 S + J_2 I - (J_1 + J_3 Q)X - (J_1 + J_3 Q)O \qquad (2.13)$$

To apply this equation, it is necessary to express the variables in the equation in terms of the system variables and to develop an expression similar to equation (3.5).

Capital Costs: The capital costs are

$$I_{COL.} = \frac{C_4 ND(R+1)}{EG_a}$$

$$I_{T.E.} = \frac{C_5 D(R+1)}{G_b}$$

$$I = I_{COL.} + I_{T.E.} = D(R+1)\left[\frac{C_4 N}{EG_a} + \frac{C_5}{G_b}\right] \qquad (3.17)$$

The derivation of these and subsequent costs is given in Appendix 3. The nomenclature is the same as that in section 3.2, additionally C_4 = incremental unit investment cost of column. \$/(FT^2)(Plate)

C_5 = incremental unit investment cost of T.E. \$/FT^2

D = distillate or product rate lb mols/hr

Material Costs: If D lb. moles/hr. of product are obtained from F lb. moles/hr. of feed and if y = yield, then

$$D = yF$$

Raw Material requirement p.a. = Fh lb. moles

$$= \frac{D}{y} h \text{ lb. moles}$$

Let p = cost of 1 lb. mole of raw material, then the raw material costs, X, can be expressed

$$X = \frac{D}{y} \cdot p\, h \qquad \$ \text{ p.a.} \qquad (3.18)$$

Annual Operating Costs:

Operating Cost of equipment p.a. $= C_3hD(R+1)$ \$

Maintenance Cost p.a. $= mI$ \$

where m = fraction p.a.

The total annual operating cost is given by

$$O = C_3hD(R+1) + mD(R+1)\left[\frac{C_4N}{EG_a} + \frac{C_5}{G_b}\right] \qquad \$ \quad (3.19)$$

Annual Sales: $S = shD$ (3.20)

where s = selling price of product $ / lb mol

Equations (3.17), (3.18), (3.19) and (3.20) can be substituted into equation (2.13) to give

$$V.W. = k_1 \frac{(R+1)DN}{E} + k_2RD + k_3D \qquad (3.21)$$

where $k_1 = J_1sh - (J_1+J_3Q)\frac{hp}{y}$

$$k_2 = J_2\frac{C_5}{G_b} - (J_1+J_3Q)(C_3h - m\frac{C_5}{G_b})$$

$$k_3 = J_1sh + J_2\frac{C_5}{G_b} - (J_1+J_3Q)(C_3h - m\frac{C_5}{G_b} - \frac{hP}{y})$$

E is now eliminated from equation (3.21) by means of equation (3.3) and we obtain for the V.W. the expression

$$V.W. = \frac{k_1DN(R+1)^{1.024}}{KR^{0.024}} + k_2RD + k_3D \qquad (3.22)$$

Maximization of V.W.: For the V.W. to be a maximum the condition $\frac{d(V.W.)}{dR} = 0$

must hold. If the output from the system is fixed, then D is a constant and on differentiating and equating = 0, we obtain

$$(R+1) = \frac{N - 0.024\,N(\frac{1}{R}) + v^*\left(\frac{R}{(R+1)}\right)^{0.024}}{-\left(\frac{dN}{dR}\right)} \qquad (3.23)$$

$$\text{where } V^{*} = \frac{K\left(\left[J_2 - m(J_1 + J_3Q)\right]\frac{C_5}{G_b} - C_3h(J_1 + J_3Q)\right)}{\left[J_2 - m(J_1 + J_3Q)\right]\frac{C_4}{G_a}} \qquad (3.24)$$

It will be seen that equations (3.23) and (3.5) differ only in the constants V^{*} and F^{*}, and accordingly both are solved by the same procedure.

Cost and Design Data:

It has been shown that the indices F^{*} and V^{*} include all the cost and design parameters in equations (3.5) and (3.23) with the exception of N and R. Typical values of F^{*} and V^{*} are 50 and 85 respectively - the various cost and design assumptions for the parameters in question can be found in Appendix 3. Many of the assumptions are those of Happel. The assumptions made for the economic variables in the venture worth instance were (see section 2.4)

$i = 0.10$, $i_m = 0.125$, $t = 0.50$, $n = 10$ yrs, $r = 5$ yrs, $S_a = 0.10I$, straight line depreciation and $Q = 0.25$(35).

3.6 Mathematics of Solution, Programme Mechanics and Simulation Outline.

A number of numerical methods have been developed and can be found in Scarborough (59), to solve algebraic equations of the form of equation (3.5). A combination of the Method of False Position and the Newton-Raphson Method was used to effect the solution in this instance. The procedure followed required writing equation (3.5) in the form

$$e = (R+1) - \left[\frac{N - 0.024N(\frac{1}{R}) + F^{*} \left(\frac{R}{R+1}\right)^{0.024}}{-\left(\frac{dN}{dR}\right)} \right] \qquad (3.25)$$

and the computing sequence is as follows: Select R, calculate N and $\frac{dN}{dR}$ from equations (3.6) and (3.7) and hence evaluate e. Correct R by predetermined increment and repeat process with new value of R. The iteration is continued with $e \longrightarrow 0$, until the error is sufficiently small to satisfy the accuracy required. The variables in equation (3.25) and their ranges are

R	$R_m \longrightarrow \infty$	(infinity)
N	$\infty \longrightarrow N_m$	
$\frac{dN}{dR}$	$-\infty \longrightarrow 0$	

The following points should be noted about equation (3.25)

(i) It will be seen that as $R \longrightarrow R_m$, $\frac{dN}{dR} \longrightarrow -\infty$ and $N \longrightarrow \infty$. Consideration of any N v R curve will show that $\frac{dN}{dR} \longrightarrow -\infty$ more rapidly than $N \longrightarrow \infty$.

Under this condition then, i.e. $R \longrightarrow R_m$, the term within the brackets $\longrightarrow 0$ and

$$\therefore \quad e \longrightarrow (R+1)$$

(ii) As $R \longrightarrow \infty$, $\frac{dN}{dR} \longrightarrow 0$ from the negative direction and does so more rapidly than $R \longrightarrow \infty$, thus the term within the brackets $\longrightarrow \infty^-$.

$$\therefore \quad e \longrightarrow \text{a negative value.}$$

It is clear that the function e has its maximum value at $R = R_m$ and goes from positive to negative as R increases. Due to the behaviour of the function in this manner, the first guess is $R = R_m$. R is then incremented in large steps until e becomes negative at which stage the method of False Position begins computation. Under some conditions the final steps may be carried out by the Newton-Raphson Method. The Method of False Position gives the incremental correction to R and is based on the assumption that the curve is linear between the two points which yield the sign change in the function. The result is tested for error and, if satisfactory, the computation finishes. If not, the programme moves on to the Newton-Raphson method, and continues to use this method until a solution of the required accuracy is found.

In this method the graph of the function is replaced by the tangent at each successive step. This combination procedure was used because the Method of False Position operates satisfactorily in cases where the curve of f(x) is nearly horizontal where it crosses the x-axis. The Newton-Raphson Method is, on the other hand, superior when the curve is nearly vertical where it crosses the x-axis.

For certain systems, defined in terms of N_m and R_m and having a specific value of F^*, the function e may be negative when $R = R_m$ is selected initially. This phenomenon is due to the limitations of equation (3.13) mentioned in the preceding section. It arises when the optimum value of R is extremely close to R_m, the condition is given by

$$\frac{R - R_m}{R + 1} > 0.02$$

Under this condition, which does not occur in practice very often, this method will not yield a solution.

A schematic diagram of the programme mechanics is given in Appendix 3.

The above work was verified independently by means of a programme which effected solution by means of the method of repeated plotting. This programme was much less economical from the point of view of computer time usage.

Simulation Outline: The range of systems considered was

$$N_m = 1, 5, 10, 15, 20, 25, 50$$

$$R_m = 0.5, 1, 2, 4, 6, 8, 10$$

$$F^*, V^* = 10(+10)\ 100, 150, 200, 250, 300$$

In the second section of this work to study the effect of changes in the cost and design variables on the optimum conditions, equations (3.5a) and (3.24) were programmed and the variation in F^* and V^* respectively noted. The previous work enables the change in F^* and V^* to be related directly to the optimum economic design. A number of typical parameters which were independently varied were chosen for perturbation, they were:-

Design Parameters:			Range		
(i)	h_w	= weir height	1.0	5.0	ins
(ii)	FA	= fractional free area	0.01	0.21	
(iii)	G	= mass vapour velocity	50	2000	lbs/(FT^2)(HR)
(iv)	$F(\geq E)$	= plate efficiency factor	0.3	1.0	

Cost Parameters:		Range		
(i)	C_p = incremental plate cost	20	50	\$/FT^2
(ii)	C_s = steam cost	0.2	0.80	\$/1000 lbs
(iii)	h = hrs. operation	6115 (0.70)	8736(1.0)	HRS/YR

In addition to varying these parameters two pay-out times 2 yrs. and 5 yrs. were considered in the unit production cost case.

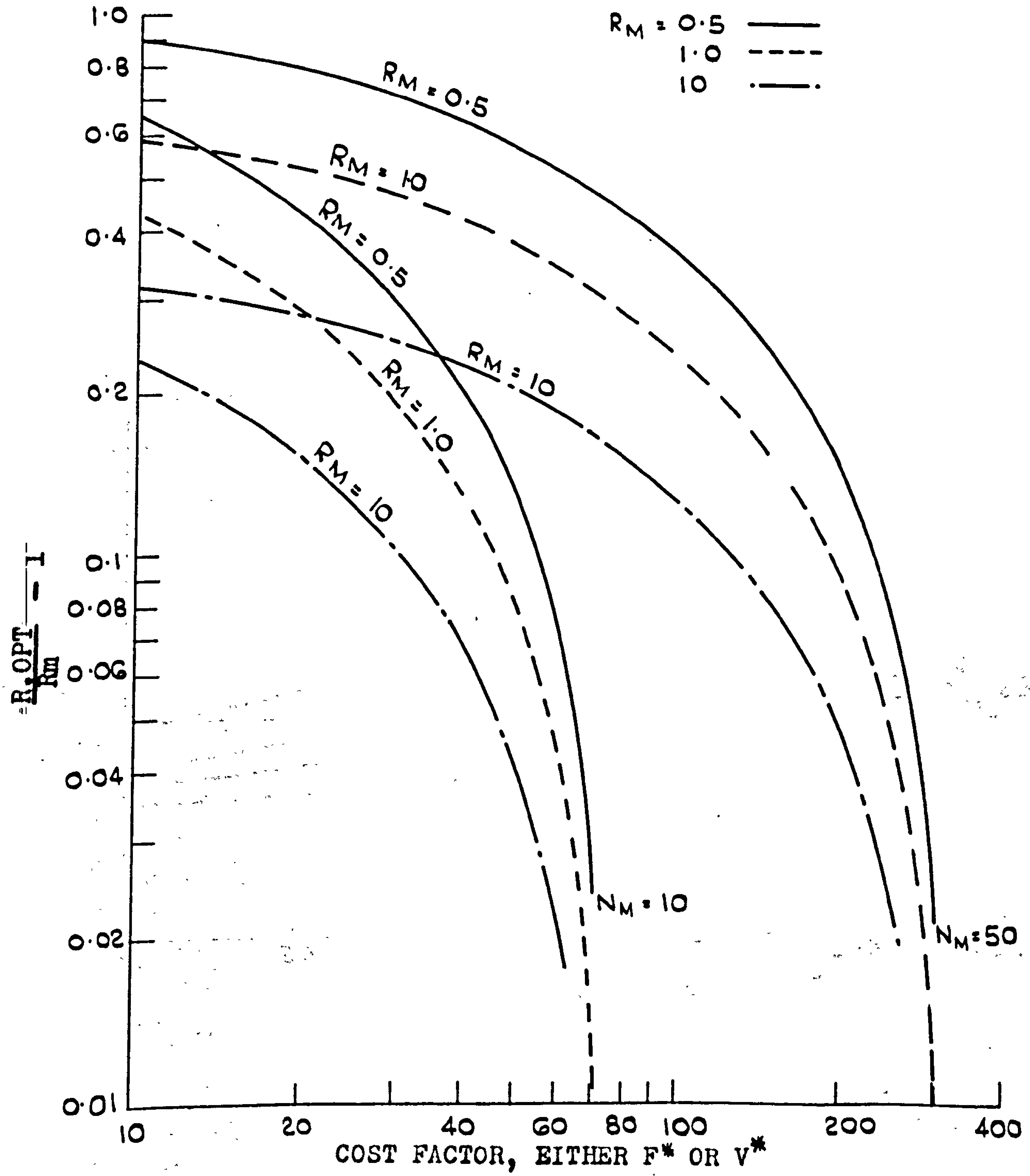
CHAPTER 4. DISCUSSION AND RESULTS OF STUDY ON THE DISTILLATION SYSTEM.

4.1 Comparison with Previous Analysis

The results obtained on solution of equations (3.5) and (3.23) are shown in figures 4.1 and 4.2. In figure 4.1, the spread is shown of the optimum curves for various minimum reflux ratios for systems in which N_m may vary from 50 to 10. It will be observed in figure 4.2 that for reflux ratios in the range considered ($R_m = 0.5$ to 10), a single curve only is shown for each value of N_m. A specific curve is obtained for each value of R_m, but for any given N_m, these fall so closely together that they can be represented by one curve. A number of similar curves obtained by Happel from the analysis discussed in the last chapter are shown in figure 4.3. The points used to plot these curves, which represent the situation when E is assumed independent of R, were obtained from figure 7.3 ref. (35). The equation used in this previous analysis was

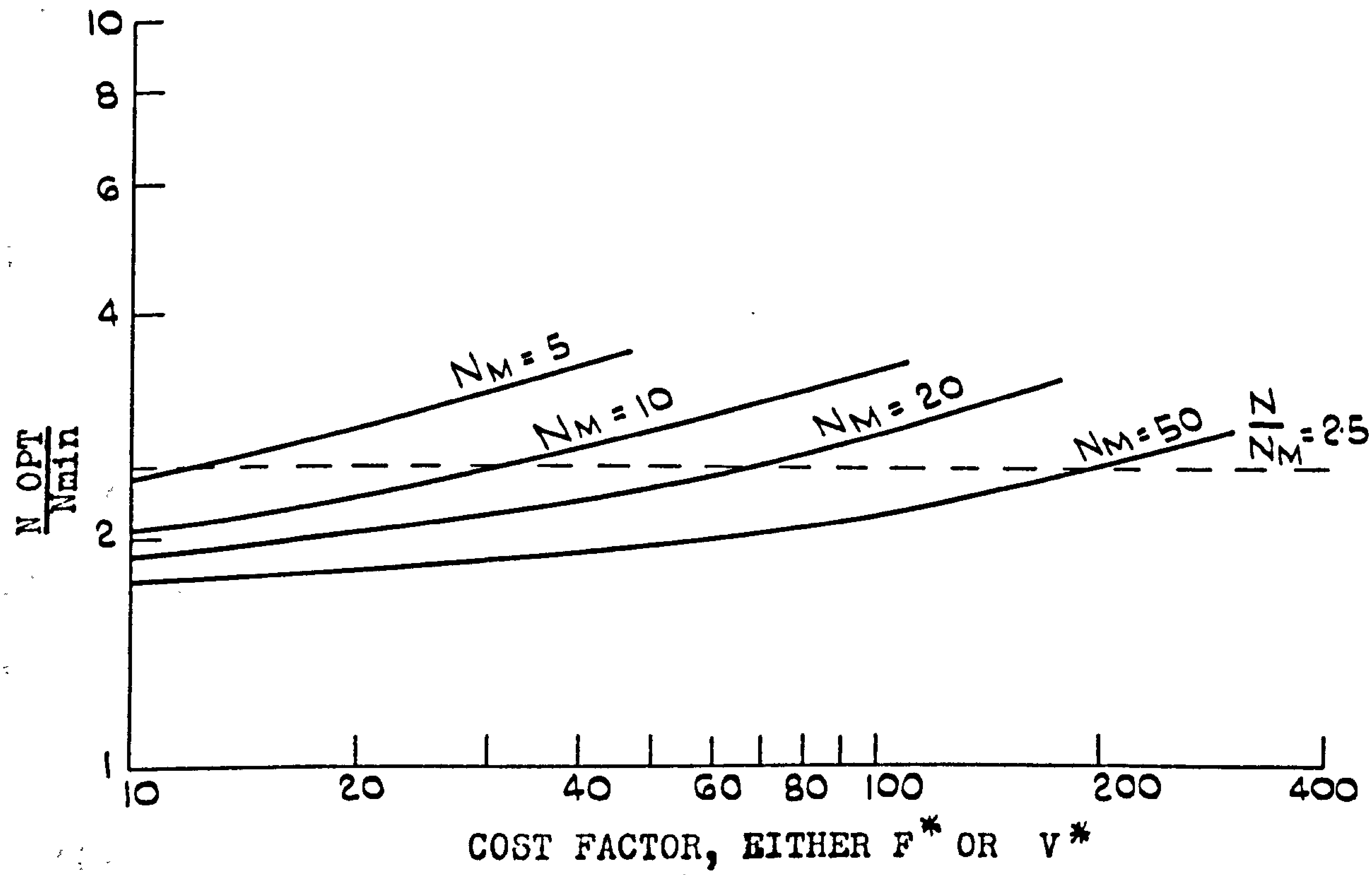
$$(R + 1) = \frac{N + F}{-(\frac{dN}{dR})} \qquad (4.1)$$

where $F = \left[\frac{C_2 G_a}{C_1 G_b} + C_3 \frac{hGa}{C_1}\right] E$



OPTIMUM REFLUX RATIO

Fig. 4.1



OPTIMUM NUMBER OF PLATES
CURVES VALID FOR Rm = 0.5 ⟶ 10

Fig. 4.2

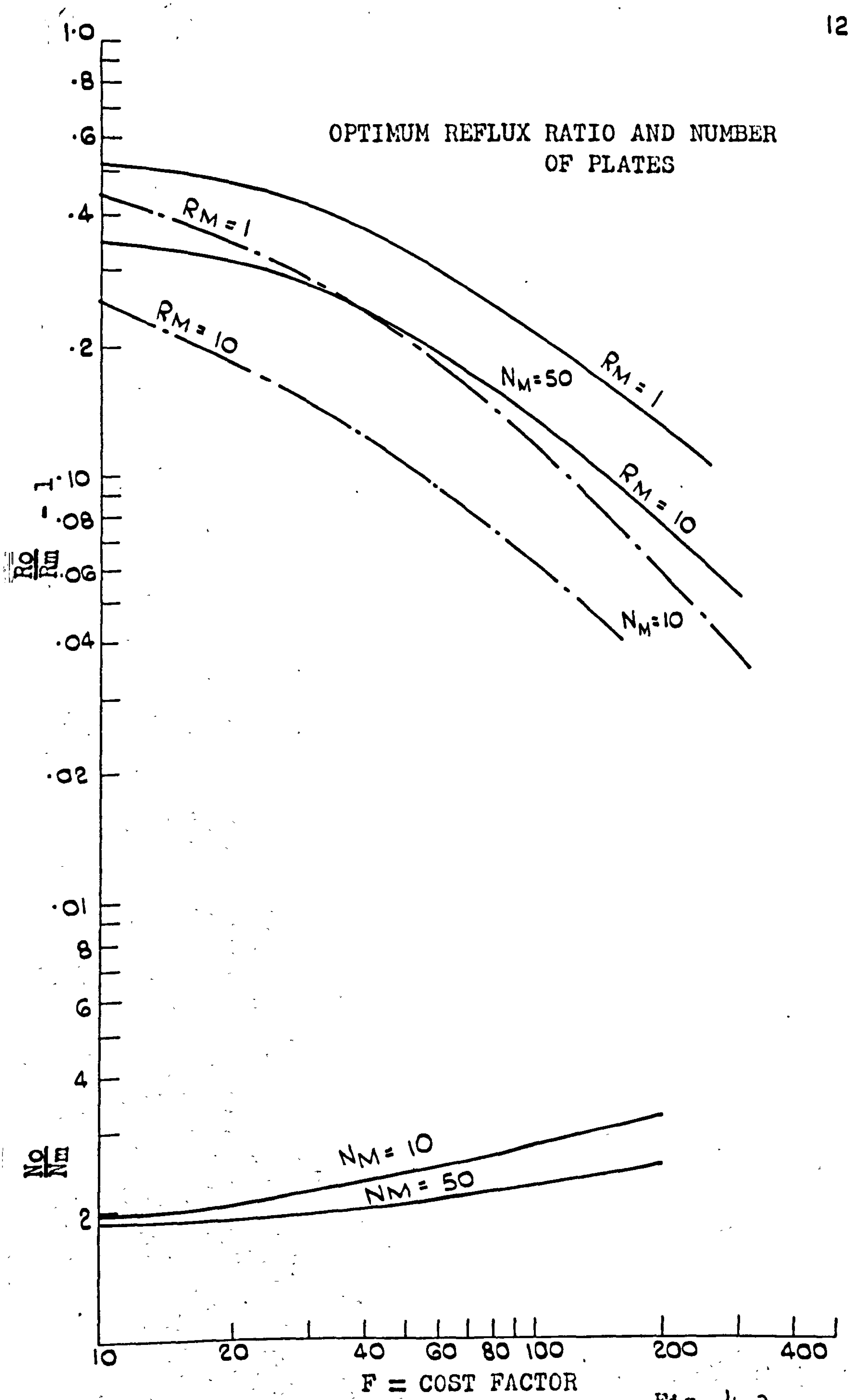

OPTIMUM REFLUX RATIO AND NUMBER OF PLATES
$R_M = 1$
$R_M = 10$
$N_M = 50$
$R_M = 1$
$R_M = 10$
$N_M = 10$
$N_M = 10$
$N_M = 50$
$\frac{R_o}{R_m} - 1$
$\frac{N_o}{N_m}$
1·0
·8
·6
·4
·2
·10
·08
·06
·04
·02
·01
8
6
4
2
10
20
40
60
80
100
200
400
F = COST FACTOR

Fig. 4.3

as opposed to equation (3.5) used in this work

$$(R+1) = \frac{N - 0.024N(\frac{1}{R}) + F^{*}\left(\frac{R}{R+1}\right)^{0.024}}{-(\frac{dN}{dR})} \qquad (3.5)$$

where $F^{*} = \left[\frac{C_2G_a}{C_1G_b} + C_3\frac{hGa}{C_1}\right] K$

The relationship between the cost factors F and F^{*} occurring in these equations is therefore

$$\frac{F^{*}}{K} = \frac{F}{E} \qquad (4.2)$$

Equation (3.3) can be rewritten to incorporate the assumption that $E_{mv} \neq E$ as

$$E = K\left(\frac{R}{R+1}\right)^{0.024} \qquad (4.3)$$

From equation (4.3) it is clear that K will always be greater than E and that its value will approach that of E, as R increases. The extent of the differences in value between K and E, can be outlined by considering possible values of the parameters in equation (4.3).

R	$\left(\frac{R}{1+R}\right)^{0.024}$	K	E(HIGH) = 1,K =	E(LOW)=0.4,K=
0.5	0.974	1.026 E	1.026	0.410
10	0.997	1.002 E	1.002	0.401

The maximum difference in this table is 2.6%, a figure which will not be exceeded unless reflux ratios < 0.5 are being used. Thus in many cases as $K \longrightarrow E$ it is possible to equate $F^{*} = F$ in equation (4.2).

A comparison between the two sets of results, shows that the curves in figure 4.1 fall more rapidly than the equivalent curves in figure 4.3. In the case of the N/N_m curves in figure 4.2, they will be observed to rise more rapidly than the corresponding curves in figure 4.3, although as N_m increases the differences between the curves decrease and, at $N_m = 50$, both curves nearly coincide. The effect of these differences is that for any given value of the cost constant the optimum column design, as derived from the curves calculated in this work, is one operating at a lower reflux ratio and having a greater number of plates compared with the optimum column design obtained using curves from Happel's analysis.

For example, consider the system $R_m = 10$, $N_m = 10$ and let $F^{*} = 50$. From figures 4.1 and 4.2, $R_o = 10.4$ and $N_o = 28$ is obtained. If this value of R (i.e. 10.4) is substituted into equation (4.3), E can be expressed in terms of K

$$E = 0.9975\ K$$

From equation (4.2)

$$F \simeq 0.9975\ F^{*} \simeq 49.9$$

Thus the equivalent cost constant in equation (4.1) $\simeq$ 49.9. From figure 4.3 for this value of F and the same system, the optimum design is given by $R_o \simeq 11.03$ and $N_o \simeq 23.9$. The two designs are therefore

	This Work	Happel
R_o	10.4	11.03
N_o	28	23.9

The assumption of $F \simeq F^{*}$ would make a negligible difference to this result.

4.2 Verification of Optimum Solutions and Comparison of Economic Criteria.

In order to verify the optimum solutions plotted in figures 4.1 and 4.2 the unit cost of production (U.C.) and the venture worth (V.W.) were calculated independently for a number of particular systems. The systems chosen were $R_m = 0.5$ and $N_m = 25$, 20 and 15. The cost constants F^{*} and V^{*}, when evaluated using the data given in Appendix 4, had values in this instance of 99.9 and 84.6 respectively.

The U.C. was calculated for a series of values of R by means of equation (3.4) and a like procedure using equation (3.22) was carried out for the V.W. The results obtained are shown in figures 4.4 and 4.5. A minimum U.C. and a maximum V.W. is obtained for each system. The optima indicated on these figures can be compared with those previously obtained and the necessary curves for the comparison are plotted in figure 4.6. Table 4.1 shows that the agreement, as would be expected, is very good.

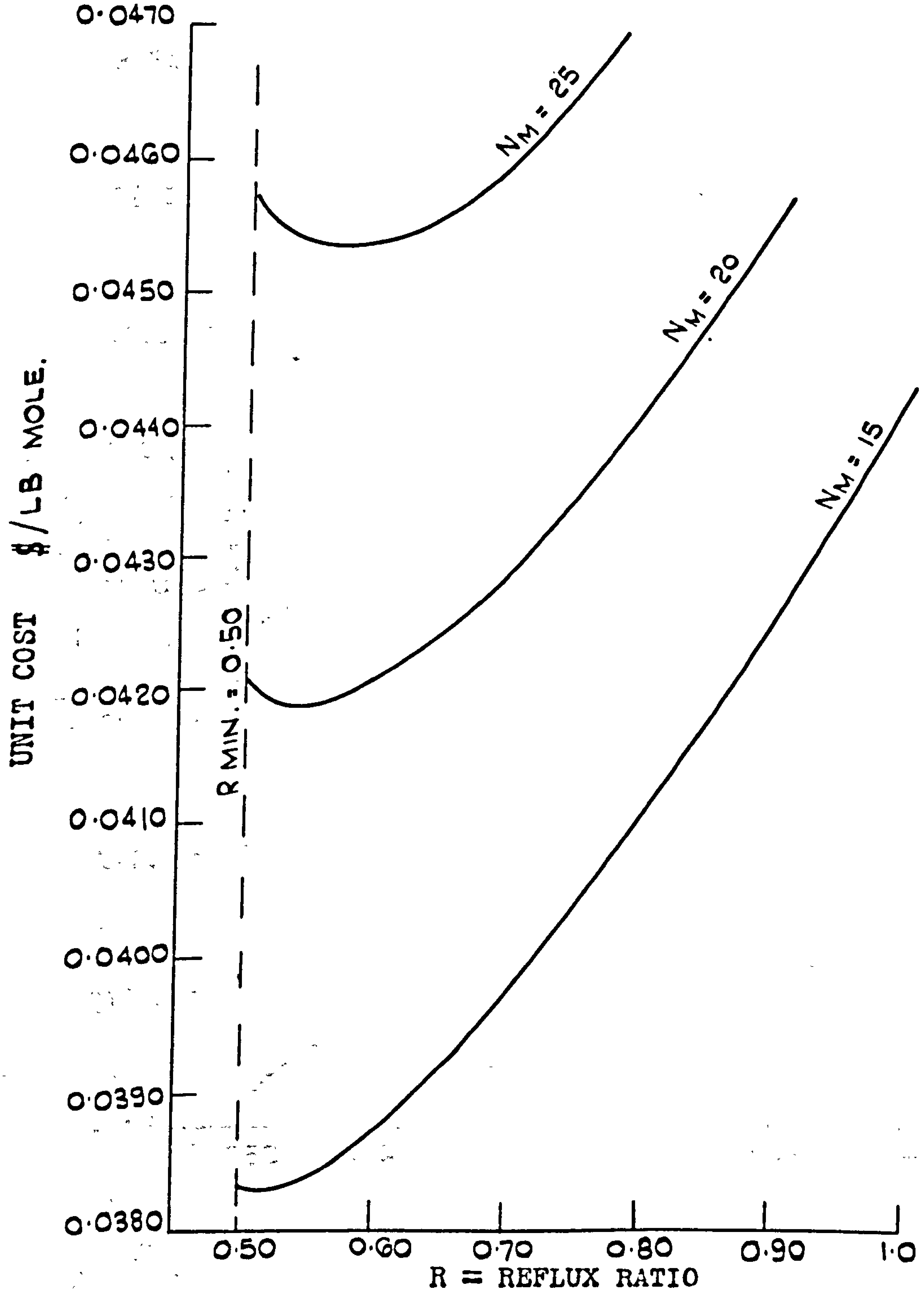
When we come to consider the two criteria in question, it is obvious that different optimum designs will be obtained since two different cost factors are being

TABLE 4.1

VERIFICATION OF OPTIMUM COLUMN SOLUTIONS

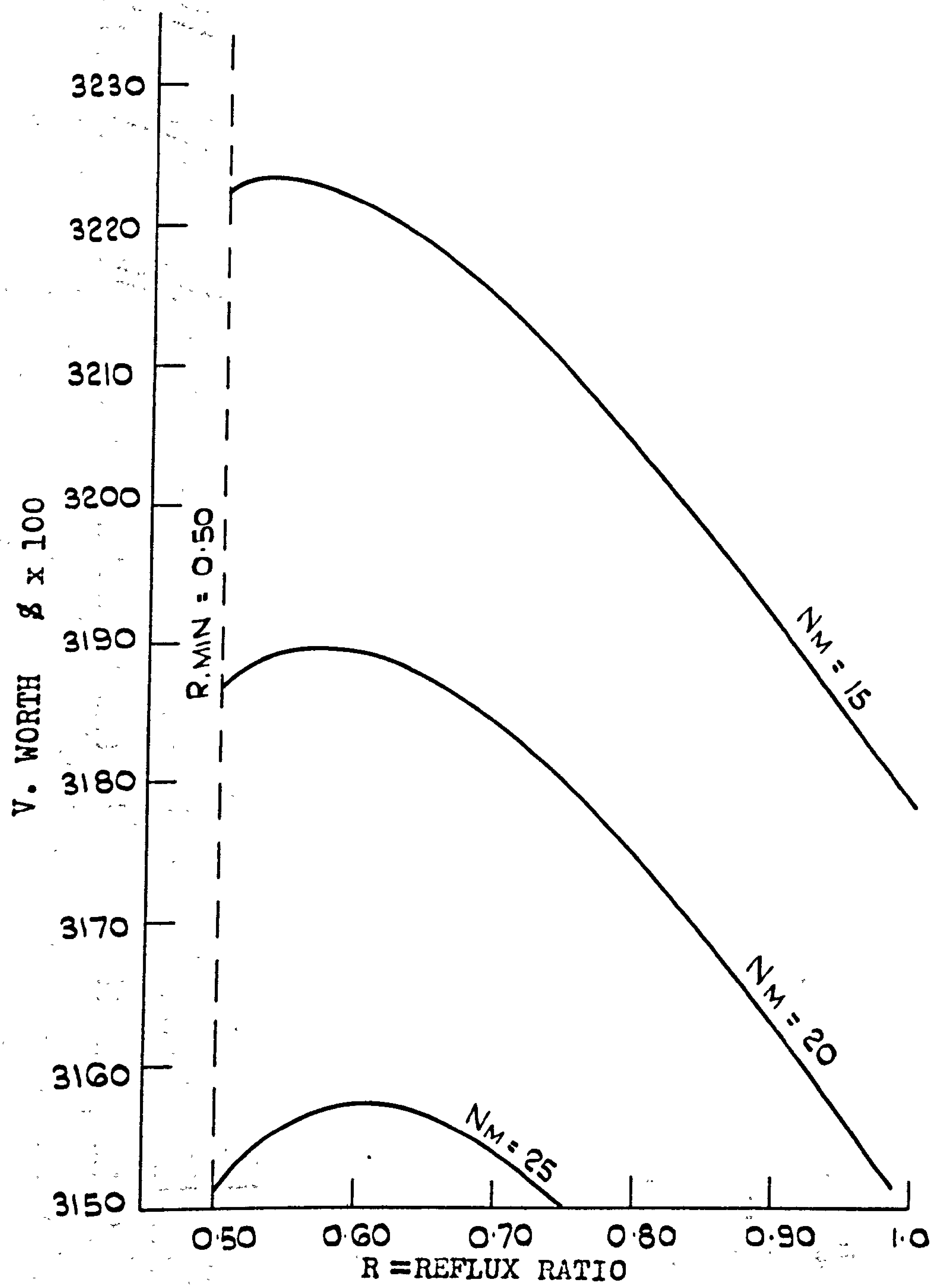
	SYSTEM			
F*	R_m	N_m	R_o (Fig. 4.6)	R_o (Fig. 4.4)
99.9	0.5	20	0.546	0.543
		25	0.576	0.575
V*	R_m	N_m		R_o (Fig. 4.5)
84.6	0.5	20	0.570	0.570
		25	0.602	0.603

used in conjunction with any particular curve. It can be seen from figures 4.1 and 4.2 that as the cost factor



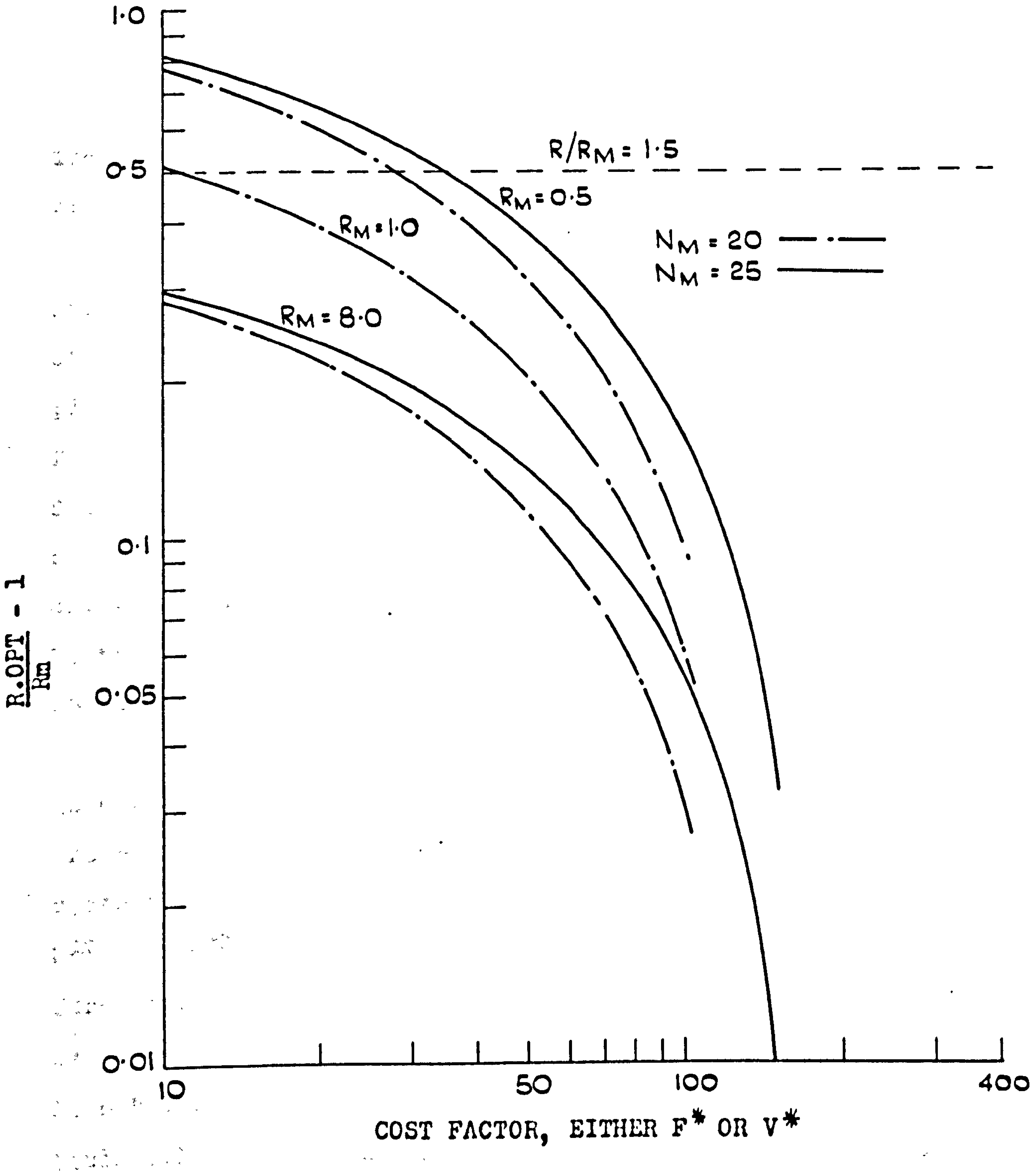
OPTIMUM UNIT COST OF PRODUCTION CURVES
UNIT COST V REFLUX RATIO F ÷ 100

Fig. 4.4.



OPTIMUM VENTURE WORTH CURVES.
V. WORTH V REFLUX RATIO $V^* \doteq 85$.

Fig. 4.5



OPTIMUM REFLUX RATIO.

Fig. 4.6

increases the optimum reflux ratio will decrease and the optimum number of plates will increase for any given system.

Thus if the V.W. criterion is applied to a system already optimized to satisfy the U.C. criterion, the direction in which changes in the optimum design will take place is dependent on the relative magnitudes of the cost factors V^* and F^*. If $V^* > F^*$ then the optimum design using the V.W. criterion will have a lower reflux ratio and a greater number of plates compared with that using the U.C. criterion. If $V^* < F^*$, the reverse will be true. The parameters involved are given in equations (3.5a) and (3.24).

In Appendix 3, it can be seen that when the assumptions outlined are made, the cost factors F^* and V^* are equivalent when they have values of 47.3 and 84.6 respectively. Equivalent in this context means that both F^* and V^* are evaluated using the same data and therefore apply equally to the system. In the case of F^* however, certain of the data such as tax rate or interest rate is not utilized. In the case of the systems considered in table 4.1, the optimum values of the reflux ratios for these equivalent cost factors are:-

SYSTEM		UNIT COST	V. WORTH	
N_m	R_m	R_o (MIN.U.C.)	R_o MAX(V.W.)	%R_o(U.C.) > R_o (V.W.)
20	0.5	0.664	0.570	16.5
25	0.5	0.697	0.603	15.6

Some additional results, showing the same behaviour for a number of other systems are given in Table 4.2. The values of F^* and V^* are, as before, equal to 47.3 and 84.6.

TABLE 4.2.

OPTIMUM REFLUX RATIOS FOR ECONOMIC CRITERIA

SYSTEM				
N_m	R_m	R_o (U.C.)	R_o (V.W.)	% R_o (U.C.) > R_o (V.W.)
15	0.5	0.624	0.533	17.1
	1.0	1.160	1.042	11.4
	10	10.850	10.200	6.4
N_m	R_m			
25	0.5	0.697	0.603	15.6
	1.0	1.254	1.130	11.0
	10	11.360	10.695	6.2
N_m	R_m			
50	0.5	0.789	0.703	12.2
	1.0	1.381	1.264	9.3
	10	12.060	11.430	5.5

The optimum operating reflux ratio is lower when the criterion used is V.W. which follows from $V^{*} > F^{*}$ in the example. R_o (U.C.) has values up to 17% greater than R_o (V.W.).

4.3. Note on Preliminary Design Methods for Columns.

The suggestion is frequently made (35,49) that a suitable design value for the reflux ratio is 1.5 R_m and it is maintained that the effect of this approximation on the economics of the process is small. Likewise a similar rule of thumb, that of $N = 2.5\ N_m$ is used to calculate the number of plates required. The validity of these assumptions can now be investigated.

If the system $R_m = 0.5$, $N_m = 20$ is considered and the value of $F^{*} = 100$ used earlier in the verification programme assumed, then for the U.C. criterion, the following situation occurs:-

The minimum U.C. = 0.04187 ($/lb. mole) occurs at a reflux ratio (deemed the optimum in this case) $R_o = 0.54$. If the approximation $R = 1.5\ R_m$ is used, a value of 0.75 is obtained for R, the operating reflux ratio, which gives a unit cost of production = 0.04350 ($/lb. mole). The approximation in this instance increases the unit cost of production by a factor of 1.039 or 3.9%. This result, together with some further comparisons, is shown in Table 4.3. The basic data for this table can be found in Appendix 4 (table A4/1). In connection with Table 4.3, the unit cost ($/lb. mole) and venture worth ($) results cannot be compared as $F^{*} = 99.9$ is not equivalent to $V^{*} = 84.6$.

TABLE 4.3.

ECONOMIC OPTIMA FOR OPTIMAL AND APPROXIMATE DESIGN METHODS

SYSTEM			OPT. DESIGN		APPROX. DESIGN			
F^{*}	R_m	N_m	R_o	MIN.U.C.	$R = 1.5R_m$	U.C.	%$R > R_o$	%U.C. > MIN.U.C.
99.9	0.5	20	0.54	0.0419	0.75	0.0435	38.9	3.9
		30	0.60	0.0488	0.75	0.0497	25	1.8
	8.0	20	8.24	0.2494	12.0	0.3004	48	20.4
		30	8.60	0.2900	12.0	0.3360	39.5	15.8
V^{*}	R_m	N_m	R_o	MAX.V.W.	$R = 1.5R_m$	V.W.	%$R > R_o$	%V.W. < MAX.V.W.
84.6	0.5	20	0.57	318,980	0.75	317,950	31.6	0.3
		30	0.63	312,580	0.75	312,050	19	0.2
	8.0	20	8.4	140,500	12.0	101,200	42.8	28.0
		30	8.7	102,700	12.0	67,000	38	34.7

It will be seen that when the approximate method is used the differences, as measured in terms of the economic indices, are small for systems which have a low minimum reflux ratio. In cases where R_m is large, this is not so and the use of the short-cut method leads to large errors. Such behaviour is to be expected since the operating costs increase with increasing R and, as R_m increases, the absolute value of the increase in costs (caused by operating at $R = 1.5\ R_m$ as opposed to R_o) will become larger. The increased operating costs will be offset in some instances by a decrease in the capital costs, due to the number of plates N, corresponding to R, being less than N_o.

If $R = 1.5\ R_m$ is written as $R/R_m - 1 = 0.5$, then the L.H.S. of this expression is in the form of the ordinate in figures 4.1, 4.3 and 4.6. Thus the assumption that, $R = 1.5\ R_m$, is equivalent to assuming that the straight-line curve $R/R_m - 1 = 0.5$, plotted on figure 4.6 gives a satisfactory solution for all systems with their differing cost factors. Accordingly, the error involved for any given system will be proportionate to the divergence of the optimum curve for the system from the curve $R/R_m - 1 = 0.5$.

Figure 4.1 could equally well be used to illustrate this point. The extent of the divergence which may occur is exemplified in Table 4.4. This table has been constructed from the curves given in figure 4.1 and from similar additional data not plotted. The cost factor (C.F.) may be either that for U.C. or V.W.

TABLE 4.4.

DIVERGENCE FROM OPTIMUM REFLUX RATIO THROUGH USE OF APPROXIMATE DESIGN METHOD

		R_o C.F. = 20		R_o C.F. = 100	
R_m	$R = 1.5\ R_m$	$N_m = 50$	$N_m = 15$	$N_m = 50$	$N_m = 15$
0.5	0.75	0.894	0.764	0.627	0.510
1.0	1.5	1.517	1.346	1.231	1.010
4.0	6.0	5.276	4.850	4.565	4.017
8.0	12.0	10.290	9.524	9.013	8.028
10.0	15.0	12.797	11.861	11.236	10.033

From this table it will be noted that for the low values of R_m and low cost factor, the value of R given by the approximate method is lower than R_o. A study of figure 4.6 will show that the condition of $R < R_o$, occurs for those curves or parts of curves which have higher values than $R/R_m - 1 \approx 0.5$.

If the parameter N is examined a similar pattern emerges. The curve $N/N_m \approx 2.5$ is shown in figure 4.2 and the degree of divergence of any specific curve from this straight-line curve is a measure of the accuracy of the approximate method. If the optimum point for any particular system lies on a curve above the $N/N_m \approx 2.5$ curve, then the value of N obtained through usage of the approximate rule is $< N_o$, if below, then N will be $> N_o$. It will be noticed in figure 4.2, when those curves above the approximation line are considered that

(i) for a fixed cost factor, as N_m decreases, $N \ll N_o$ and
(ii) for any given system, as the cost factor increases $N \ll N_o$.

In the area below this line (i.e. $N/N_m \approx 2.5$), the inverse of these two observations holds, that is, for a fixed cost factor N_m increasing results in $N \gg N_o$ and for a given system a decreasing cost factor will make $N \gg N_o$. These trends can be seen in Table 4.5.

TABLE 4.5.

DIVERGENCE FROM OPTIMUM NUMBER OF PLATES THROUGH USE OF APPROXIMATE DESIGN METHOD

SYSTEM			OPTIMUM	APPROXIMATE	
F*	R_m	N_m	N_o	$N = 2.5\ N_m$	% N >/< N_o
99.9	0.5(8.0)	20	55	50	< 9.1
		50	110	125	> 13.6
V*	R_m	N_m			
84.6	015(8.0)	20	53	50	< 5.6
		50	106	125	> 18.0

Table 4.6 presents a summary of the results from the optimum and approximate methods and has been constructed with the aid of figure 3.2 (Gillilands Curve).

TABLE 4.6.

COMPARISON OF COLUMN PRELIMINARY DESIGN METHODS

SYSTEM			OPTIMUM		3		4		5	
F^*	R_m	N_m	R_o	N_o	$R = 1.5R_m$	N	R	$N=2.5N_m$	$R=1.5R_m$	$N=2.5N_m$
99.9	0.5	20	0.54	55	0.75	41	0.60	50	0.75	50
		30	0.60	74	0.75	60	0.64	70	0.75	70
	8.0	20	8.24	55	12.0	33	8.58	50	12.0	50
		30	8.60	74	12.0	49	8.86	70	12.0	70
V^*	R_m	N_m								
84.6	0.5	20	0.57	53	,,	,,	0.60	50	,,	,,
		30	0.63	70	,,	,,	0.64	70	,,	,,
	8.0	20	8.40	53	,,	,,	8.58	50	,,	,,
		30	8.70	70	,,	,,	8.86	70	,,	,,

Three non-optimum methods are compared in the table.

(i) Column 3, the rule $R = 1.5\ R_m$ and use of Fig. 3.2 to obtain N.

(ii) Column 4, the rule $N = 2.5\ N_m$ and use of Fig. 3.2 to obtain R.

(iii) Column 5, the rules $R = 1.5\ R_m$ and $N = 2.5\ N_m$.

Of the three methods that of Column 5 yields the least satisfactory results and a very considerable improvement is made by using either of the other methods. Within the scope of this study, the approximate rule $N = 2.5\ N_m$ applied in conjunction with the use of Gillilands Correlation results in the design approximating the optimum design most closely. This observation is true for both the economic criteria examined. In line 6 of the table it will be noted that the optimum design and that given in Column 4 are virtually identical. This good result is obtained due to the cost factor in question, giving an optimum point on the $N_m = 30$ curve in figure 4.2 in close proximity to the value $N/N_m = 2.5$.

4.4. Sensitivity of the Cost Factor to Perturbations of the Cost and Design Parameters.

The effect on the optimum column design, for a given system, of variations in the cost and design parameters will now be investigated. The design method outlined in the previous pages can deal very rapidly with changes in the cost factor of any system. In order that the effect of changes in the basic cost and design parameters on the overall design of the system may be determined it is necessary only to know their effect on the cost factor.

A number of these parameters have been plotted as a function of F^* and V^* in order that these effects may be studied. Equations (3.5a) and (3.24) express the cost factors in question in terms of the cost and design parameters and if:-

(i) for G_a, the allowable vapour velocity (lb. moles/HR.FT^2), $G/_M$ is substituted, where $G =$ mass vapour velocity (lbs/HR.FT^2) and $M =$ average molecular weight of the vapour stream and

(ii) the following additional substitutions are made :-

(a) $\left[J_2 - m\,(J_1 + J_3Q)\right] = \Omega$

(b) $-(J_1 - J_3Q) = \Pi$

the equations may be written

$$F^* = \left[\frac{C_2}{G_b} + hC_3\right]\frac{GK}{MC_1} \qquad (4.4)$$

$$V^* = \left[\frac{C_5}{G_b} + hC_3\frac{\Pi}{\Omega}\right]\frac{GK}{MC_4} \qquad (4.5)$$

where $K = 0.1084\,(FA)^{-0.28}h_w^{0.241}G^{-0.013}\alpha^{-0.028}\left(\frac{\sigma}{\mu_L V_g}\right)^{0.044}$

$$\left(\frac{\mu_L}{\rho_L D_L}\right)^{0.137} \qquad (4.6)$$

The parameters which were chosen for perturbation and their range of variation have been outlined in section (3.6). Any of the other cost and design variables contained in these three equations could equally well have been chosen. In equation (4.4), C_p, the incremental plate cost is contained in C_1, the amortized incremental plate cost and C_s, the steam cost in C_3, the cost of steam and coolant required to produce 1 lb. mole of product. In equation (4.5) $C_p = C_4$ and C_s is included in C_3 as before.

It has been pointed out that K is approximately equal to E and in order that a representative area should be covered, the simulation procedure was carried out for values of K in the high, medium and low ranges e.g. K = 0.90, 0.60, 0.30. The importance or otherwise of the relative magnitude of K in the equations (4.4) and (4.5) can also be investigated for this reason.

For the simulation, suitable values of the variables were chosen such that K was approximately equal to the values quoted (i.e. 0.90, 0.60, 0.30). The values chosen together with any other necessary data are given in Appendix 4.

The computational procedure followed was :-

(i) K was computed accurately by means of equation (4.6).

(ii) The specific value of the cost parameter being investigated was inserted into equation (4.4) or equation (4.5).

(iii) Fixed values were given to the other parameters in the equation i.e. either equation (4.4) or equation (4.5).

(iv) F^* or alternatively V^* was computed.

(v) A new value was given to the variable being studied in (ii) and the cycle was repeated.

When the design parameters were being examined a slightly different procedure was necessary due to the parameters in question being variables in equation (4.6).

(i) K was computed accurately by means of equation (4.6).

(ii) K was multiplied by the specific value of the design parameter being investigated and divided by the initial value used in the computation of K. This new value of K was then used subsequently in either equation (4.4) or equation (4.5).

e.g. $$K_{NEW} = \frac{K(FA)^{-0.28}}{(FA)_i^{-0.28}}$$

(iii) Fixed values were given to the other parameters in the cost factor equation. (When G was being studied its value in equations (4.4) or (4.5) was equal to its particular value for the cycle).

(iv) F^* or alternatively V^* was computed.

(v) A new value was given to the variable being studied in (ii) and the cycle was repeated.

The effect of variations in the cost parameters, steam cost and hours of operation per annum on F^* can be seen in figure 4.7. The steam cost C_s may be expressed by the equation

$$C_s = \frac{C_3 - \lambda}{\theta} \tag{4.7}$$

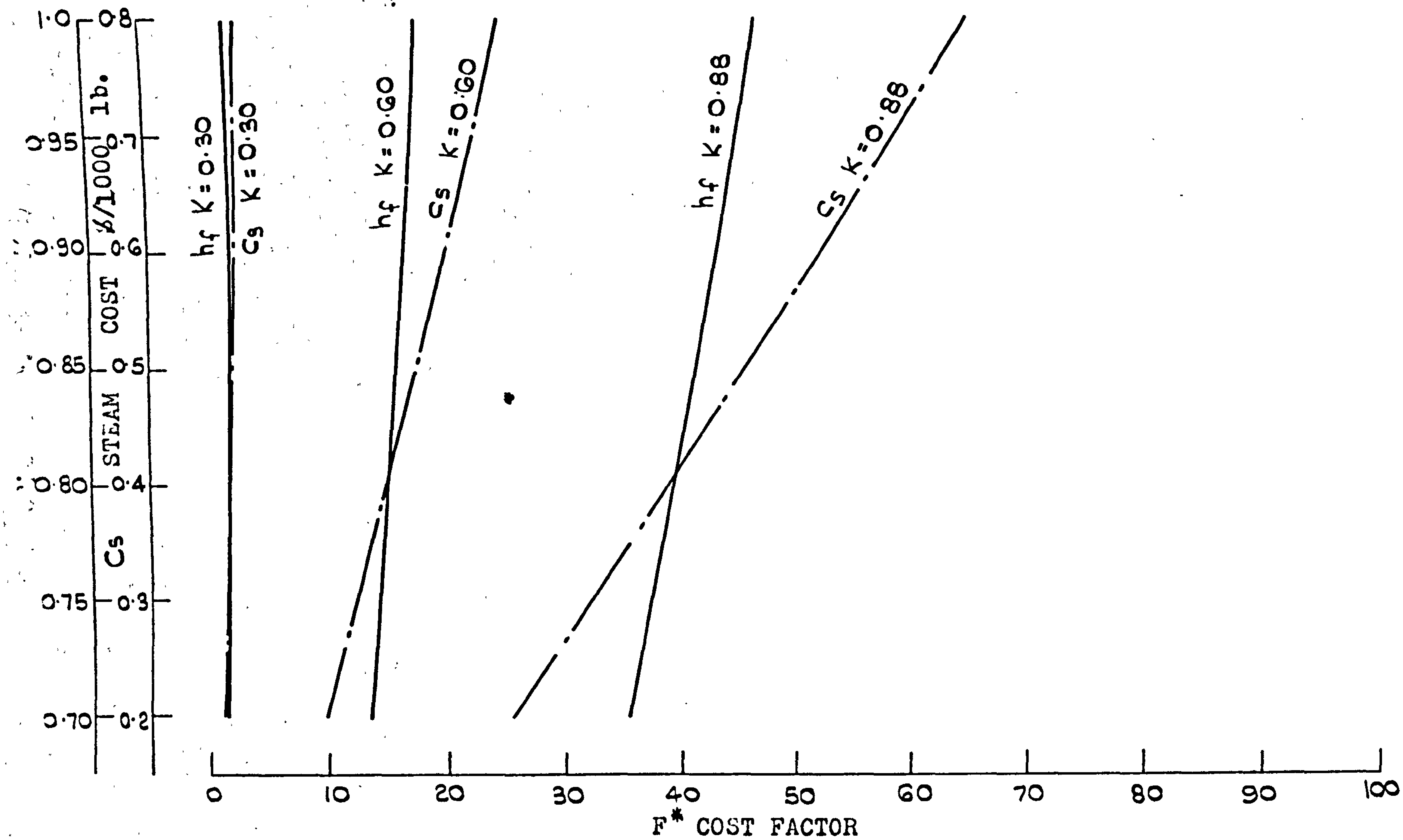
where λ and θ are evaluated in Appendix 4. The "hours of operation per annum" is expressed as the fraction hf, of the total hours (H) in a year i.e. hf.H = h. In figure 4.7 the curves representing the variation in these two parameters are expressed by the equations

$$C_s = -\left[\frac{C_2}{\theta hG_b} + \frac{\lambda}{\theta}\right] + \left[\frac{MC_1}{hGK}\right] F^* \tag{4.8}$$

and

$$hf = -\left[\frac{C_2}{HC_3G_b}\right] + \left[\frac{MC_1}{HC_3GK}\right] F^* \tag{4.9}$$

Since K in both equations is contained within the term giving the slope of the curve, it follows that variation in K will lead to different slopes being obtained. It can



VARIATION OF F* WITH COST PARAMETERS

Fig. 4.7

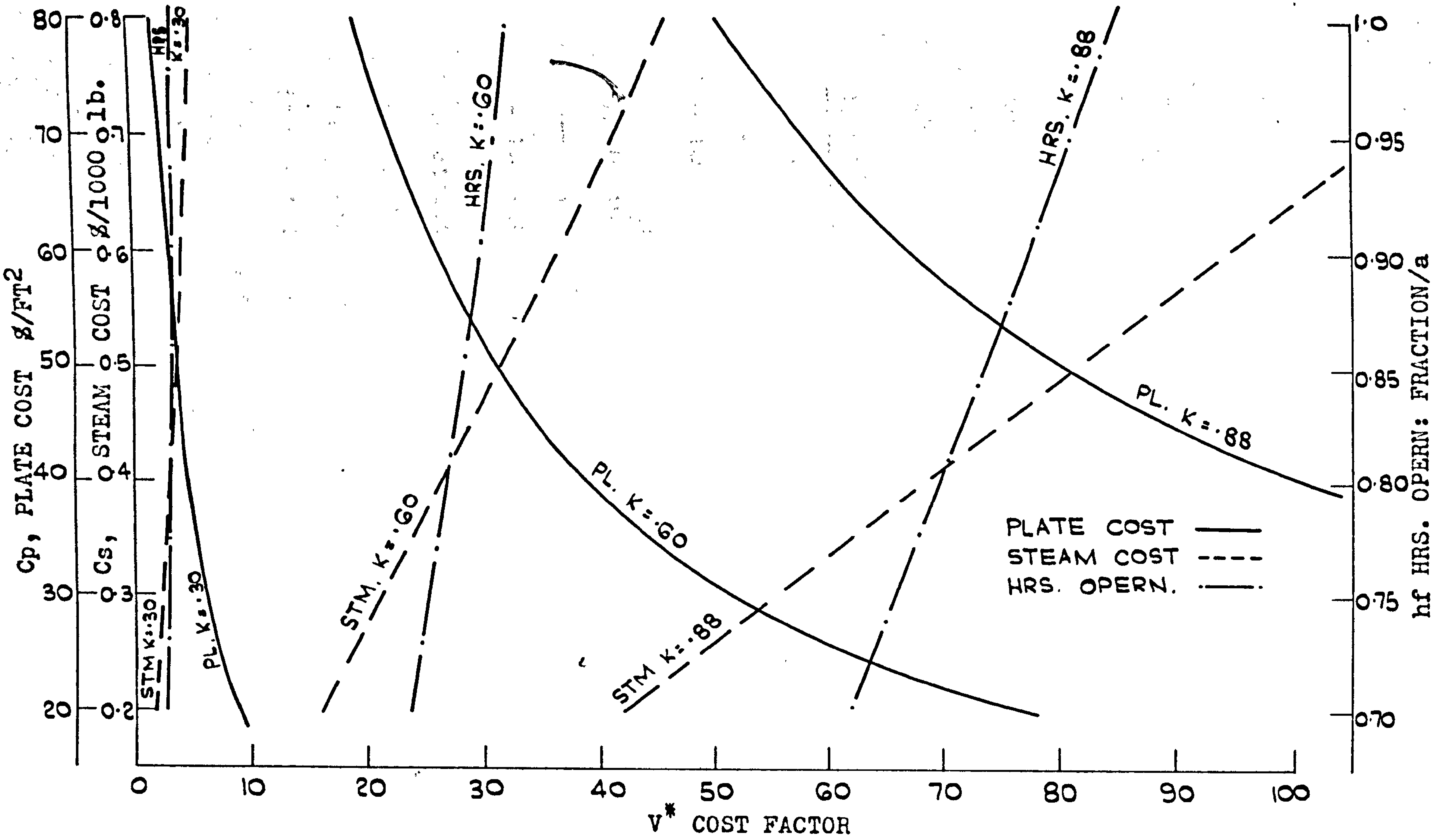
be observed that the slope of the hf v F^* curve is always greater than that of the C_s v F^* curve for any given value of K and further that the slopes of both curves decrease as K increases.

As might be expected from the similarity of equations (4.4) and (4.5) an identical pattern arises in figure 4.8, in which C_s and hf are plotted against V^*.
The respective equations in this instance are

$$C_s = \left[\frac{C_5}{\theta^{hG_b}} \cdot \frac{\Omega}{\Pi} + \frac{\lambda}{\theta}\right] + \left[\frac{MC_4}{\theta^{GK}} \cdot \frac{\Omega}{\Pi}\right] V^* \qquad (4.10)$$

$$hf = \left[\frac{C_5}{HC_3G_b} \cdot \frac{\Omega}{\Pi}\right] + \left[\frac{MC_4}{HC_3GK} \cdot \frac{\Omega}{\Pi}\right] V^* \qquad (4.11)$$

The slopes of the curves in figures 4.7 and 4.8 are given in Table 4.7 as are some figures showing the effect on the cost factor of a 10% change in C_s and hf.



VARIATION OF V* WITH COST PARAMETERS.

Fig. 4.8

TABLE 4.7.

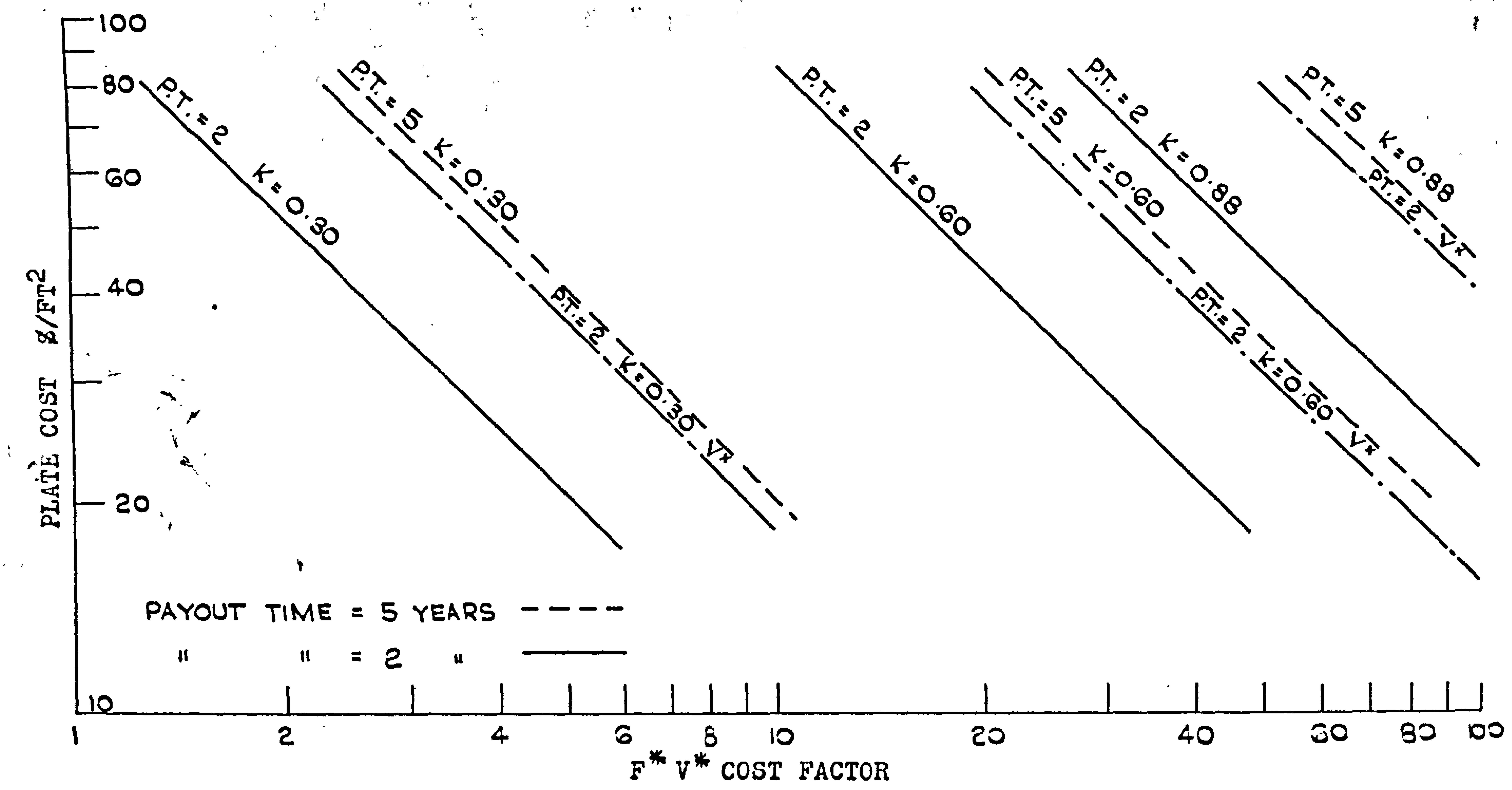
CURVE GRADIENTS AND EFFECT ON COST FACTOR OF 10% VARIATION IN STEAM COST AND HOURS OPERATION PER ANNUM

	C_s V C.F. GRADIENT			hf V C.F. GRADIENT		
C.F.	K = 0.30	K = 0.60	K = 0.88	K = 0.30	K = 0.60	K = 0.88
F*	0.3296	0.0391	0.0150	0.5555	0.0662	0.0254
V*	0.1686	0.0200	0.0077	0.2865	0.0339	0.0130

%PERT^{BN}	C_s	F*			V*		
+10	0.55	2.21	18.71	48.79	3.99	33.65	87.83
—	0.50	2.06	17.43	45.45	3.69	31.15	81.34
- 10	0.45	1.91	16.15	42.12	3.39	28.65	74.84
	hf						
+10	0.99	1.99	17.98	45.26	3.82	32.24	84.16
—	0.90	1.97	16.62	43.39	3.50	29.58	77.23
- 10	0.81	1.95	15.26	41.42	3.19	26.92	70.30

The effect of the gradient on the variation in the cost factor for the specified changes in C_s and hf can be seen. The greater the gradient, the smaller is the unit change in the cost factor.

F* and V* are shown as a function of the incremental unit plate cost, C_p, in figure 4.9. It will



VARIATION OF COST FACTOR WITH PLATE COST

Fig. 4.9

be seen that the slope is independent of K and constant for both cost factors. Equations (4.12) and (4.13) which describe the C_p v F^* and C_p v V^* curves, show why this is so

$$\log C_1 = \log \left[\left(\frac{C_2}{G_b} + hC_3\right) \frac{GK}{M} \right] - \log F^* \qquad (4.12)$$

$$\log C_4 = \log \left[\left(\frac{C_5}{G_b} + hC_3 \frac{\Pi}{\Omega}\right) \frac{GK}{M} \right] - \log V^* \qquad (4.13)$$

The effect of a change in the payout time on the U.C. may also be seen from this figure. If the case of $K = 0.60$ and $C_p = 50$ (¢/FT^2) is taken, then if P.T. = payout time, in years, we have

C_p	P.T.	F^*
50	2	17.4
50	5	34.7

$F^* = 34.7$ for a P.T. = 2 yrs, means that $C_p = 25$, ¢/FT^2, whereas $F^* = 17.4$ for a P.T. = 5 yrs is equivalent to a plate cost equal to 100 ¢/FT^2. Pursuing this example somewhat further it will be seen in Table 4.8, that the optimum design conditions are different depending on the payout time used.

TABLE 4.8.

EFFECT OF PAY-OUT TIME ON OPTIMUM SYSTEM DESIGN

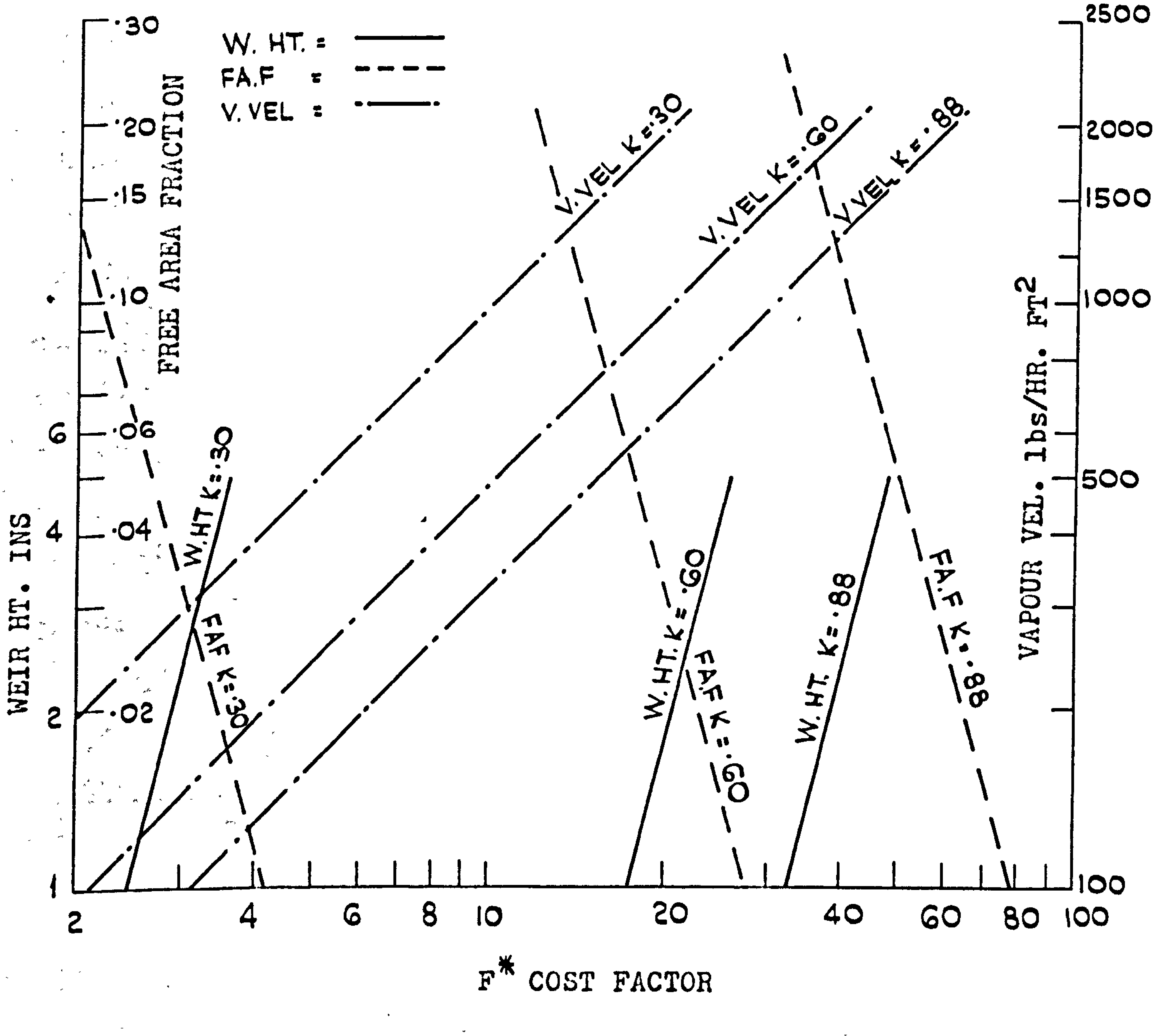
SYSTEM				OPT. DESIGN	
F^*	R_m	N_m	P.T	R_o	N_o
17.4	0.5	10	2	0.75	22.1
34.7			5	0.C2	25.5
17.4	10	50	2	12.89	90.3
34.7			5	12.37	95

The effect of increasing the payout time is to increase the number of plates in the optimum design and to reduce the reflux ratio. This is of course to be expected, because increasing the payout time reduces the fixed capital costs per annum and the optimum will therefore shift in the direction of increased capital cost.

Figures 4.10 and 4.11 show how F^* and V^* vary with changes in the design parameters studied. As in the case of the plate cost curves, the slopes of the curves are independent of K and are the same for both F^* and V^*. The equations for these curves all take the same form, a typical example is that for G v F^*

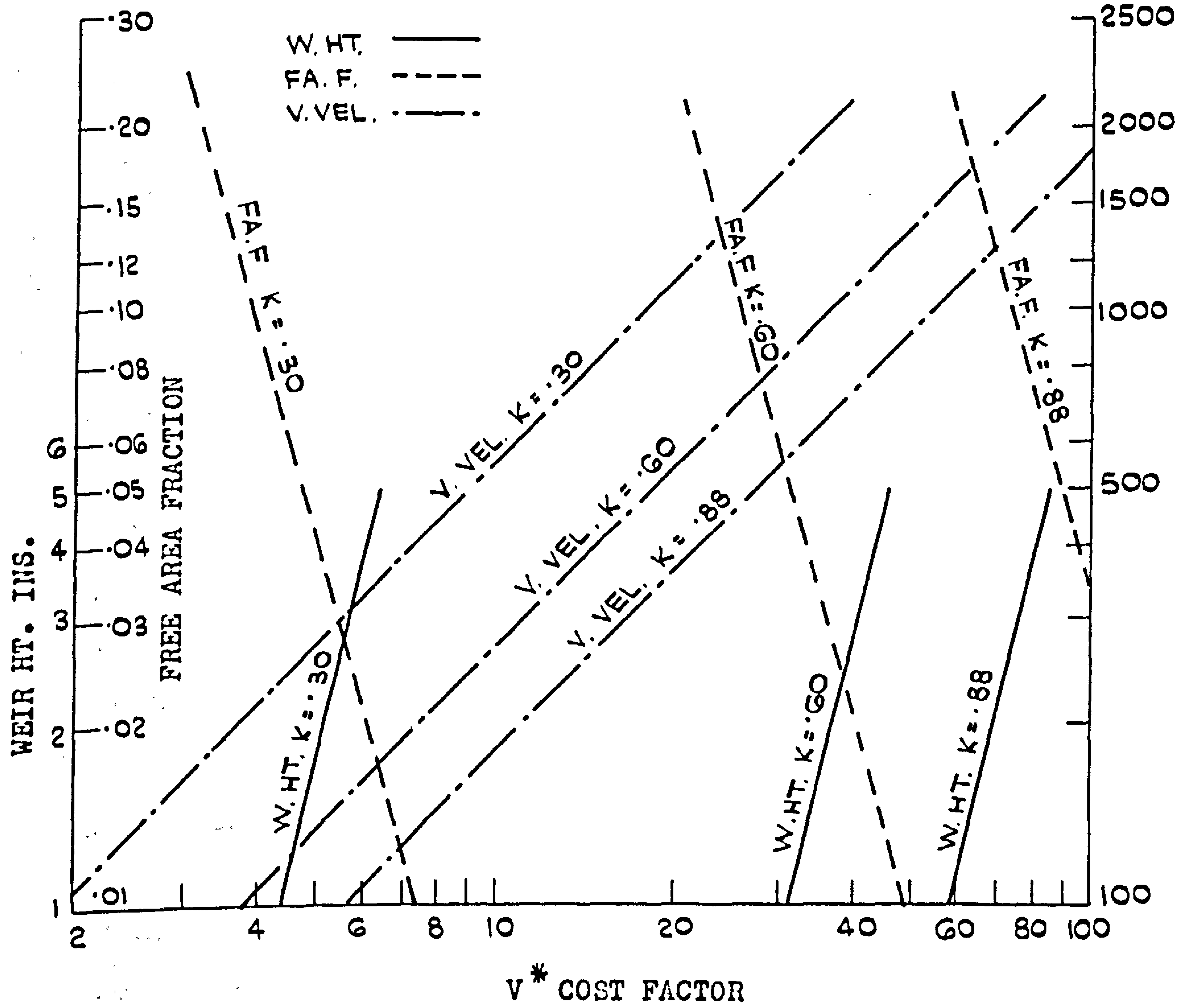
$$\log G = -1.0143 \log \epsilon + 1.0143 \log F^* \qquad (4.14)$$

where $\epsilon = \left(\frac{C_2}{G_b} + hC_3\right)\left[\frac{1}{MC_1} \cdot \frac{K}{G_1 - 0.013}\right]$



VARIATION OF F* WITH DESIGN PARAMLTERS

Fig. 4.10



VARIATION OF V* WITH DESIGN PARAMETERS

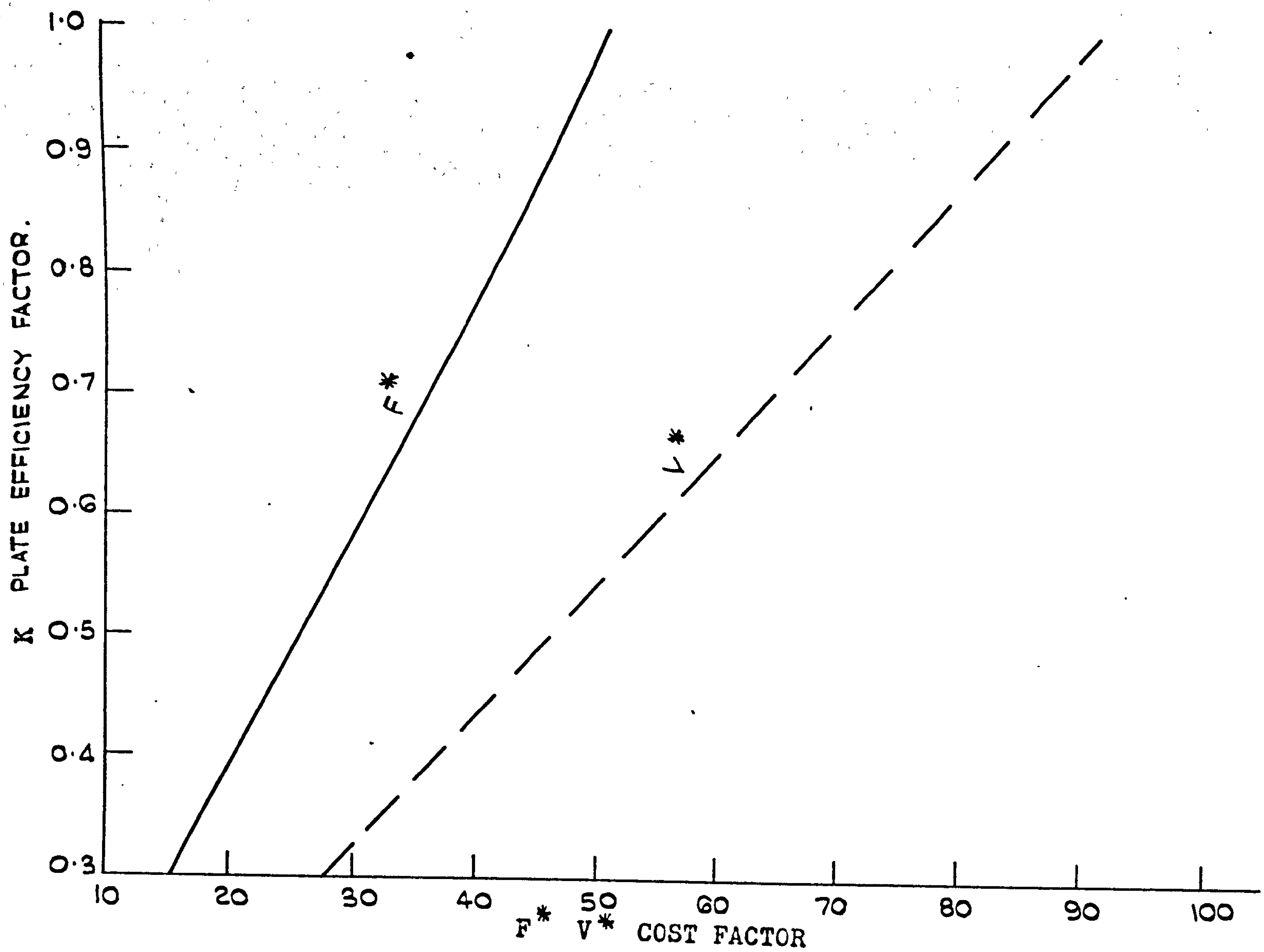
Fig. 4.11

The equations expressing the remaining curves in figures 4.10 and 4.11 can be found in Appendix 4. Tables similar to Table 4.5 can be drawn up which show how a given percentage or absolute perturbation of any of these design variables will change the value of the cost factor. Again it is clear that the change in F^* or V^* will be proportional to the slopes of the curves.

In figure 4.12, the parameter K is plotted against both F^* and V^*, should the effect of changes in the group factor K be required. These curves can be expressed by rewriting equations (4.1) and (4.2), which are given in Appendix 4.

4.5. Equivalent Development Alternatives for the System.

It is now possible to examine the effect on the optimum design for a given system of a change in any of these parameters. For example consider the system $R_m = 1.0$, $N_m = 20$ and let the previous assumptions hold for the cost and design parameters, resulting in cost factors of 47.3 and 84.6 for the U.C. and V.W. criteria. The optimum design for the U.C. criterion is $R = 1.212$, $N = 46.4$ and for the V.W. criterion $R = 1.091$, $N = 52.6$. Table 4.9



VARIATION OF COST FACTOR WITH K.

Fig. 4.12

TABLE 4.9.

EQUIVALENT DEVELOPMENT ALTERNATIVES FOR THE SEPARATION SYSTEM

PARAMETER	%PERT[BN]	F*	OPT. DESIGN R	OPT. DESIGN N	V*	OPT. DESIGN R	OPT. DESIGN N
C_s	+10	50.8	1.198	47.0	91.4	1.076	53.8
= 0.50	—	47.3	1.212	46.4	84.6	1.091	52.6
	-10	43.8	1.229	45.8	77.8	1.109	51.8
hf	+ 5	49.3	1.203	46.6	88.4	1.082	53.4
= 0.95	—	47.3	1.212	46.4	84.6	1.091	52.6
	- 5	45.3	1.221	46.0	80.8	1.100	52.0
C_p	+10	43.0	1.233	45.6	76.9	1.112	51.6
=50	—	47.3	1.212	46.4	84.6	1.091	52.6
	-10	52.7	1.190	47.4	94.0	1.070	54.2
K	+ 5	49.7	1.201	46.8	88.8	1.081	53.4
= 0.92	—	47.3	1.212	46.4	84.6	1.091	52.6
	- 5	44.9	1.223	46.0	80.2	1.101	52.2
hw	+10	48.4	1.207	46.6	86.6	1.087	52.8
= 4.0	—	47.3	1.212	46.4	84.6	1.091	52.6
	-10	46.1	1.217	46.2	82.5	1.096	52.2

TABLE 4.9 Continued:

PARAMETER	%PERT[BN]	F^*	OPT. DESIGN R	OPT. DESIGN N	V^*	OPT. DESIGN R	OPT. DESIGN N
FA	+10	46.1	1.217	46.2	82.4	1.097	52.2
= 0.07	—	47.3	1.212	46.4	84.6	1.091	52.6
	-10	48.7	1.206	46.6	87.1	1.086	53.0
G	+10	52.0	1.193	47.2	92.9	1.073	54.0
=1500	—	47.3	1.212	46.4	84.6	1.091	52.6
	-10	42.6	1.234	45.4	76.3	1.113	51.4

shows the effect on F^* and V^* of perturbing the parameters chosen from their base levels to plus or minus 10% of these levels except in the case of hf and K, where the table shows a 5% variation. The optimum designs for the system at the perturbed levels of the parameters are also given. It will be noticed that the effect of a change in one parameter, is in some cases, approximately equal to that caused by a change in another parameter. Some equivalent or nearly equivalent perturbations given in Table 4.9, which apply to both F^* and V^* are :-

(i) +10% FA $\doteqdot$ -10% hw $\doteqdot$ -5% K $\doteqdot$ -5% hf

(ii) +10% C_s $\doteqdot$ +5% K $\doteqdot$ +10% G

Thus a 10% increase in FA, the plate free area, for example, will result in the same cost factor being obtained as would result from a 10% reduction in the weir height, h_w. In order to obtain the absolute value of the U.C. or the V.W. for any particular perturbation it is merely necessary to evaluate equation (3.4) or equation (3.22) using the values of R and N given in the table. Since these values of R and N are optimum design values for the cost factors specified, it follows that the U.C. and V.W. obtained from the equations will be the minimum and maximum values respectively. A new optimum design for the system is thus arrived at, subsequent to a determined perturbation of the system. Should an improvement occur in the economic index as a result of a change in the cost factor, the parameter or parameters which are capable of effecting this change, together with the degree of variation necessary in the parameter are identified.

Equivalent alternative possibilities for developing the system are therefore delineated and subject to the qualifications outlined in section 1.5 on the probability of success factor, the strategy for developing the system will be known.

4.6. Summary and Conclusions:

Certain modifications have been made to the method of Happel for the economic design of distillation systems. The incorporation of the correlation for Murphree vapour plate efficiency derived by English and Van Winkle has enabled E, the fractional plate efficiency to be expressed as a function of R, the reflux ratio. A satisfactory analytical expression has been obtained for Gilliland's Curve, enabling the design method to be generalized.

A set of design curves has been calculated based on the developed analysis which yields the optimum design for a given cost factor. It has been shown that the design curves can be utilized to handle more complex economic criteria provided the form of the cost factor remains unchanged. A comparison with Happel's analysis indicates that designs based on the newly calculated curves tend to have a lower reflux ratio and a larger number of plates. The differences between the optimum designs produced by the two analyses, are such as to suggest that the use of the analysis given in this work is to be prefered.

The effect on the design of having the Unit Cost, U.C., as opposed to the Venture Worth, V.W., as the objective function to be optimized, depends on the relative magnitude of the respective cost factors F^* and V^*. In a typical case examined in this study, V^* was greater than F^*, with the result that the optimum design had a lower reflux ratio and a greater number of plates when V.W. was the objective function. This behaviour is true for all systems defined in terms of R_m and N_m.

An examination of some common rule-of-thumb design methods results in the conclusion that a considerable departure from the optimum design is occasioned by their use. The nearest approach to the optimum is achieved by the approximation $N \simeq 2.5\ N_m$, together with the use of Gilliland's Curve to calculate R. In terms of the economic yardsticks, wide divergences from the optimum values are experienced when the approximate design methods outlined are used for systems where R_m is large.

The advantage of formulating the cost factors in the manner described is reflected in the ease with which sensitivity analyses can be carried out using them. The effect of perturbing the various parameters contained in the cost factors has been demonstrated. The variation in optimum design for any particular system, where an optimal condition is expressed in terms of a given economic criterion, may be obtained from the curves given for any perturbation of the cost and design parameters studied. The absolute value of the criterion can easily be obtained by use of the equations derived for the Unit Cost, U.C., and Venture Worth, V.W.

Consequent on this capability for ready analysis by perturbation, a method of delineating equivalent possibilities for development and improvement of the system has been indicated.

CHAPTER 5: CASE 2 - A REACTOR SYSTEM, C.S.T.R. WITH RECYCLE

5.1 Introduction

5.2 Related Work on Similar Systems

5.3 Description of and Assumptions involved in the Physical Models.

5.4 Formulation of the Mathematical Model

5.5 Cost, Design and Process Data and Development of Economic Criteria Equations

5.6 Simulation Outline, Mathematics of Solution and Programme Mechanics

5.1 Introduction.

As in the previous case study, the primary purpose of this work was to consider how the optimum design of a unit chemical plant stage was affected by the choice of economic criterian. A chemical reactor is not only a typical unit stage but is, in one form or another, one of the most frequently encountered units in a chemical plant. In view of the fact that a generalized treatment of unsteady state recycling systems has not yet been satisfactorily devised, it was also thought that a specific study on a simple system of this nature was worth carrying out. Finally, very little work has been done on purging strategies for this form of system and some insight into this aspect should prove valuable.

The general approach and the methods used in carrying out the investigations on the reactor system were similar to those employed in the distillation work. A mathematical model of the system was devised and certain key parameters were perturbed in order that their effect on the system could be studied. In addition, as has been indicated, a number of interesting economic problems arising from the nature of the system were investigated.

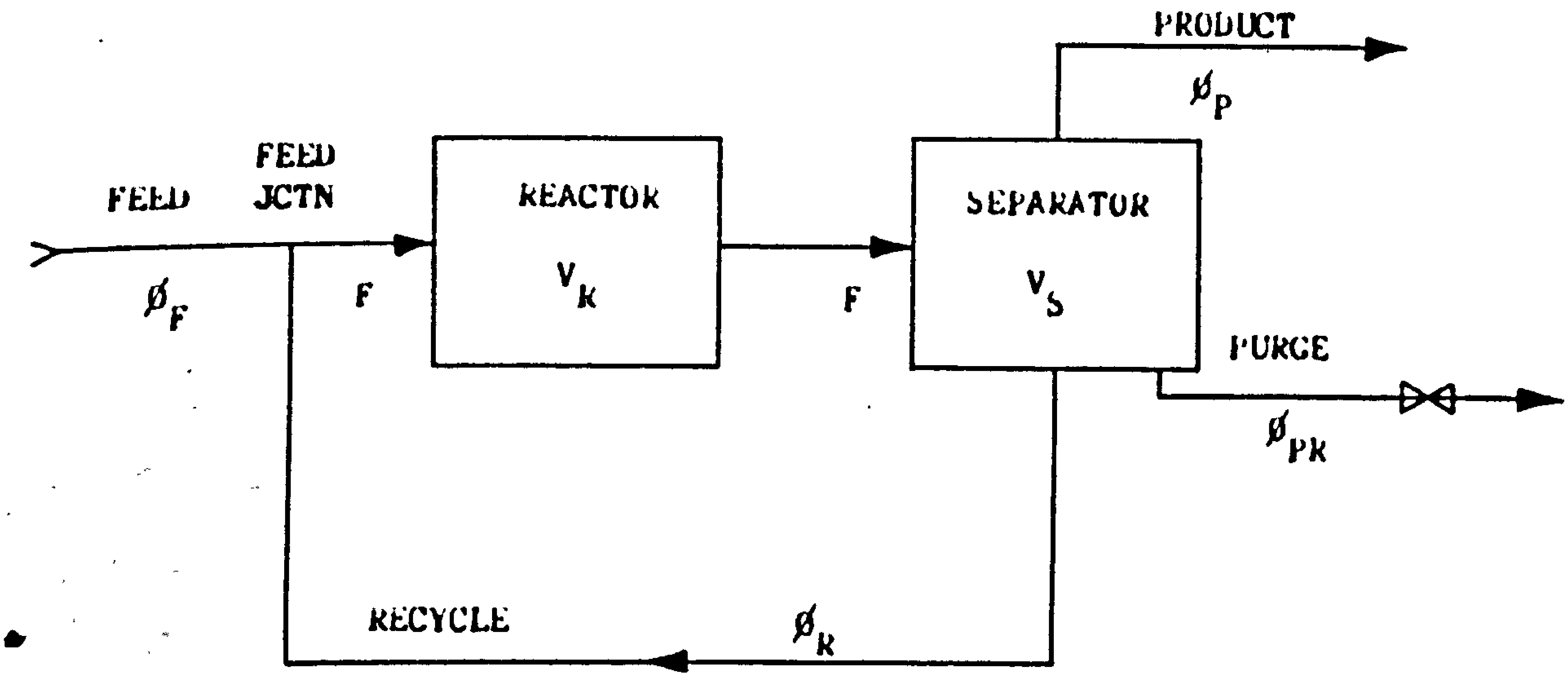
The reactor system studied consisted basically of a continuous stirred tank reactor and a separator in which the desired reaction product was separated from any unconverted feed material in the reactor outlet. This unconverted feed material together with any by-products, was recycled to the feed stream. Furthermore, the feed contained an inert material which must be purged to prevent its accumulation within the system. Depending on whether purging is carried out in a continuous or intermittent manner, the system will operate as a steady state system or as an unsteady state system. A line diagram of the system is given in figure 5.1.

The economics of continuous and intermittent purging were examined and, as before, two economic criteria, the unit cost of production and the V.W. were considered. Both first and second order chemical reactions of the type

$$A \rightleftharpoons B \qquad (5.1)$$

$$A + C \rightleftharpoons B + D \qquad (5.2)$$

were studied as alternatives in the reactor. Two models were postulated to describe the behaviour of the separator and a general model of the system incorporating the separator was derived for each of these two variants. Before describing the models used and their mathematical aspects, some related work will be considered.



FLOW RATES

ϕ_F = FRESH FEED STREAM FT^3/HR

F = REACTOR INLET STREAM "

ϕ_P = PRODUCT STREAM "

ϕ_{PR} = PURGE STREAM "

ϕ_R = RECYCLE STREAM "

V_R, V_S = REACTOR AND SEPARATOR VOLS. FT^3

GENERAL SCHEME OF REACTOR SYSTEM FIG. 5.1

5.2 Related Work on Similar Systems.

The term similar systems in this instance covers a wide field and the relevant work can be conveniently divided into a number of loose categories.

(i) Continuous Stirred Tank Reactors (C.S.T.R.).

(ii) Unsteady State Operation of a C.S.T.R.

(iii) Recycling Reactor Systems.

(iv) General Recycling Theory.

(i) Continuous Stirred Tank Reactors.

The general characteristics of the C.S.T.R. are well known and have been described both in the literature of chemical engineering kinetics and in that of reactor design (60, 61, 62). A very clear presentation of the nature of the C.S.T.R. is given in the recent work of Denbigh (63) on reactor theory. When a C.S.T.R. is operating at a steady state, the process may be described as a continuous one. However, when the reactor is operated on an intermittent basis the process is a semi-continuous or semi-batch process, despite the application of the word continuous to the reactor. This distinction has been drawn by Klinkenberg (64) and is noted here, since the modes of operation of the systems studied in this work, place them in these two categories. Thus the economic arguments presented in continuous v batch considerations cf. Kramers and Westertorp (62), correspond to some extent to the steady and unsteady state categories, described later. A graphical design method for certain complex reactions and reflux conditions in C.S.T.R.'s has been developed by Bilous and Piret (65) by means of analogy with batch reactors.

Westbrook and Aris (66) in their work on the optimum design of a C.S.T.R. operating at steady state show how a response surface for an economic objective function can be constructed in terms of the reactor temperature and throughput. The objective function studied was the percentage return on investment, Unfortunately, the effect of changes in this criterion on the optimum design was not investigated.

(ii) Unsteady State Operation of a C.S.T.R.:

The dynamic behaviour of a C.S.T.R. can be described easily in mathematical form and the references given earlier (60, 61, 62, 63), all consider the subject to a greater or lesser extent. Broadly speaking the transient behaviour has been of interest, primarily, as a state through which a process must pass before reaching the steady state condition. Starting-up or shutting down a reactor are examples of such conditions. Piret and Mason (67, 68) have with the aid of some simplifying assumptions, developed a number of equations describing such behaviour for both single C.S.T.R.'s and C.S.T.R. sequences. Among the assumptions are, that the reaction rate can be expressed in a first order form and that the reaction takes place isothermally (in any given reactor). Furthermore, only constant density first order reactions are considered.

It is possible to represent a system of this type by a linear differential equation and an analytical solution is therefore possible. Acton and Lapidus (69) present some design equations for 2nd order reactions in cascade systems. The equations are analytic approximations based on numerical solutions. This work has been extended by Standart (70). It should be pointed out that frequently a non-linear equation will be obtained for C.S.T.R. systems and analytical solutions are not possible. Solutions can, however, in many cases be obtained by means of numerical analysis.

The control problem which is concerned with the transient behaviour of the system has been studied by Bilous et alii (71), and has also been the subject of a series of papers by Aris and Amundson (72).

(iii) Recycling Reactor Systems:

The term recycling as applied to a chemical plant system implies that a material component (or components) is recirculated from an exit point in the system to an entry point. Recycling can also occur between units of a plant complex. In the instance of a reactor, the recirculated component may be unconverted feed material which has been separated from the reactor outlet stream or a by-product stream. The conditions governing the degree and type of recycling used are dependent on either the kinetics of the reaction or the economics of the system.

Hornibrook's (73) paper on the manufacture of styrene provides a description of an industrial recycling process. In a discussion on extractive reaction, Piret et al. (74, 75), show how recycling of the reactive phase may result in better utilization of the reactants. Kramers and Westerterp (62) considered the recirculation of unconverted reactant in a tubular reactor and showed that an economic optimum exists for such a system. The optimum is presented in terms of conversion as a function of the reactor volume and the recycle ratio. Shahbenderian (76) has demonstrated for a similar system how different economic criteria alter the optimum design conditions. The above work has all been concerned with steady state operation of the reactor systems in question.

Bilous and Amundson (77) while investigating reactor stability have considered fluctuations from the steady state for a recycle system. Horn (78) discusses unsteady state operation of a reactor in an optimization analysis of a complete process. The concept of the attainable region is used to illustrate the differences between open loop and recycle optimization problems.

Two recent papers of interest are those by Beveridge and Schechter (79) and Fan et al. (80). The first of these is concerned with the determination of the optimal operating policy for a tubular reactor system with recycle. That of Fan et al. considers the optimal design for carrying out a single reaction in a sequence of C.S.T.R.'s with product recycle.

(iv) General Recycling Theory:

There are two main approaches to the solution of unsteady state recycle problems, the Dynamic Programming (D.P.) approach and the calculus of variations approach. The D.P. approach has been used among others by Mitten and Nemhauser (11), Rudd and Blum (81) and Sargent and Westerberg (13), that of variational calculus by Jackson (7, 82) and Brosilow and Lasdon (83).

In the first two of the above references, solutions are obtained under simplifying conditions to unsteady state problems although Jackson (82) has given counter-examples which indicate that an optimum is not always obtained. Sargent and Westerberg present an algorithm in which the recycle stream is broken and its value estimated. An iterative procedure is then used to match the two broken ends of the recycle stream. A similar method of breaking the stream is used by Brosilow and Lasdon (83), although the overall optimization is based on a gradient technique. These authors present an economic interpretation, in terms of the inter-stage cash values of the process streams, as a method of estimating the values of the two ends of the broken recycle stream.

Underlying all this work is the necessity for decomposing the system. Jackson (84) currently maintains that recycle problems cannot be satisfactorily treated in a decomposed manner, because the recycle constitutes one of the most influential variables in the system. Some evidence in support of this view can be found in ref. (77) in which it is pointed out that instabilities may be expected in recycle systems. It will be seen that a great deal of further work is necessary, before a satisfactory theory of unsteady state recycling applicable to complex systems is available.

5.3 Description of and Assumptions involved in the Physical Model.

The general scheme for the system has been outlined in figure 5.1 and if it is described as a constant density, isothermal system, the two major assumptions involved become explicit.

The constant density assumption implies that no volume changes due either to mixing or reaction occur. This assumption enables an analytical solution to be obtained under certain circumstances for the equations of the system. Furthermore, the changes in volume occurring in liquid systems are generally fairly small and, as a first approximation, may be neglected. The isothermal condition is imposed in order that the effect of temperature, a parameter which is not being investigated, can be neglected. Perfect mixing in the reactor is also assumed, (for a discussion on this assumption see Denbigh (63)). In practice, this assumption is justified when the mixing time is much smaller than the mean residence time. From figure 5.2, it will be noted that (where concentrations are in lb. moles/cu.ft.) :-

C_{io} = concentration of the i^{th} component in the feed stream.

C_{ir} = concentration of the i^{th} component in the recycle stream.

$C_{i(i)}$ = concentration of the i^{th} component in the reactor inlet stream.

C_i = concentration of the i^{th} component in the reactor.

C_{ip} = concentration of the i^{th} component in the product stream.

It will be seen that the concentrations of the components in the reactor outlet stream (and therefore in the separator inlet stream) are the same as the concentrations in the reactor. This condition arises from the

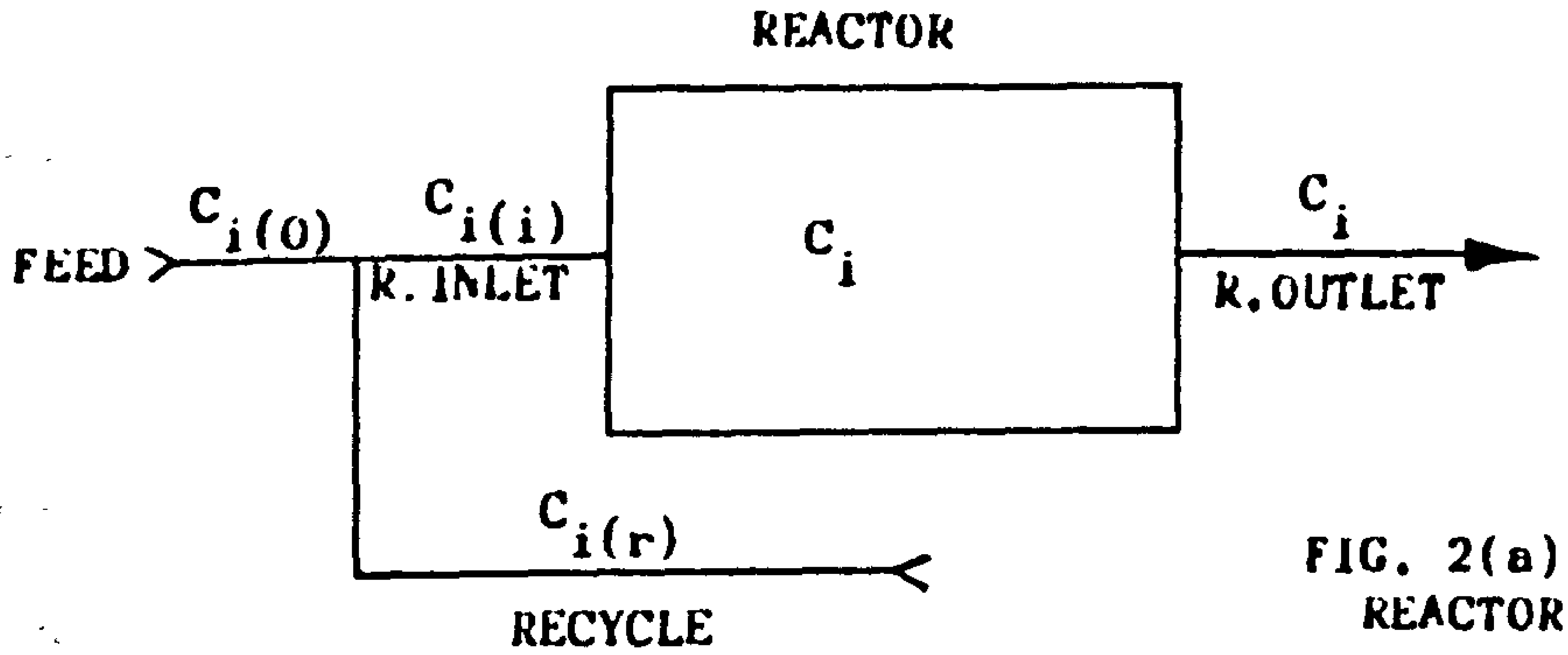


FIG. 2(a)
REACTOR

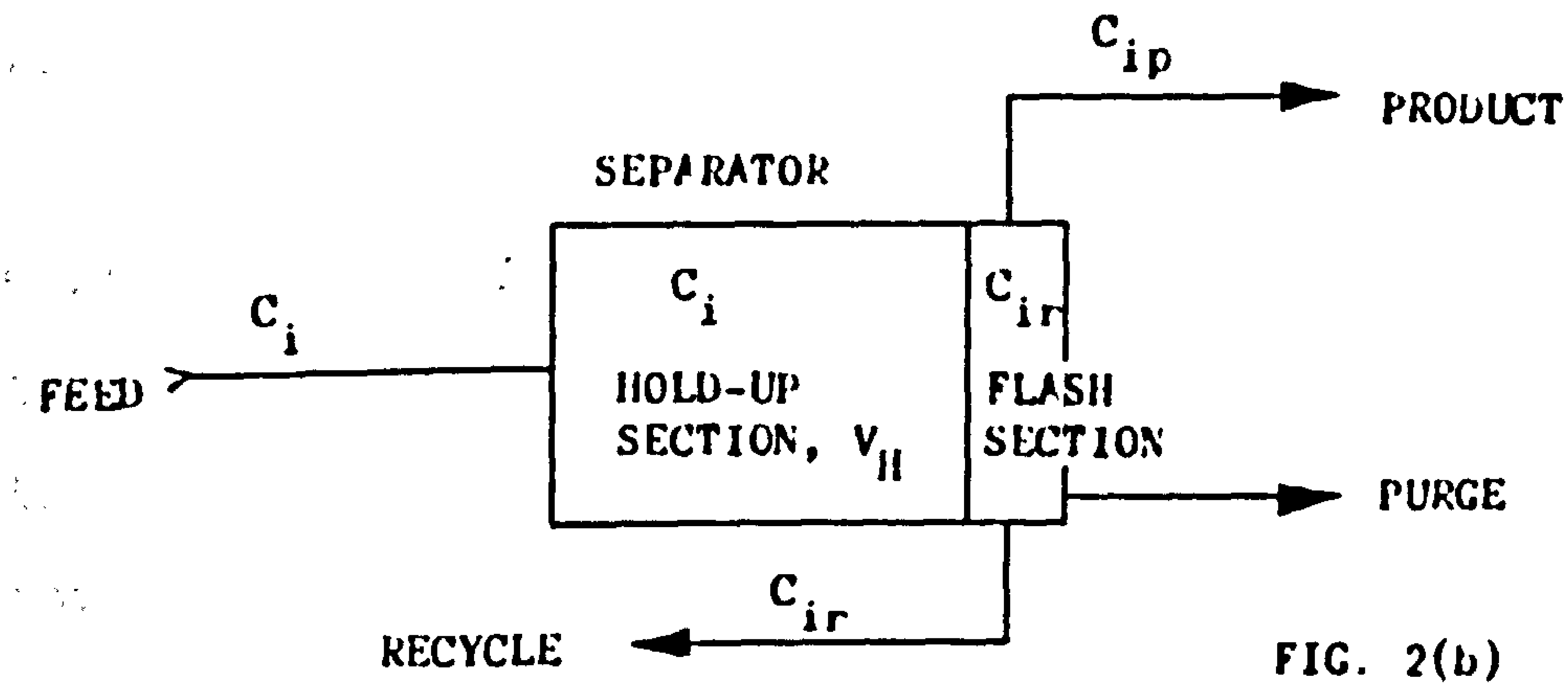


FIG. 2(b)
MODEL 1

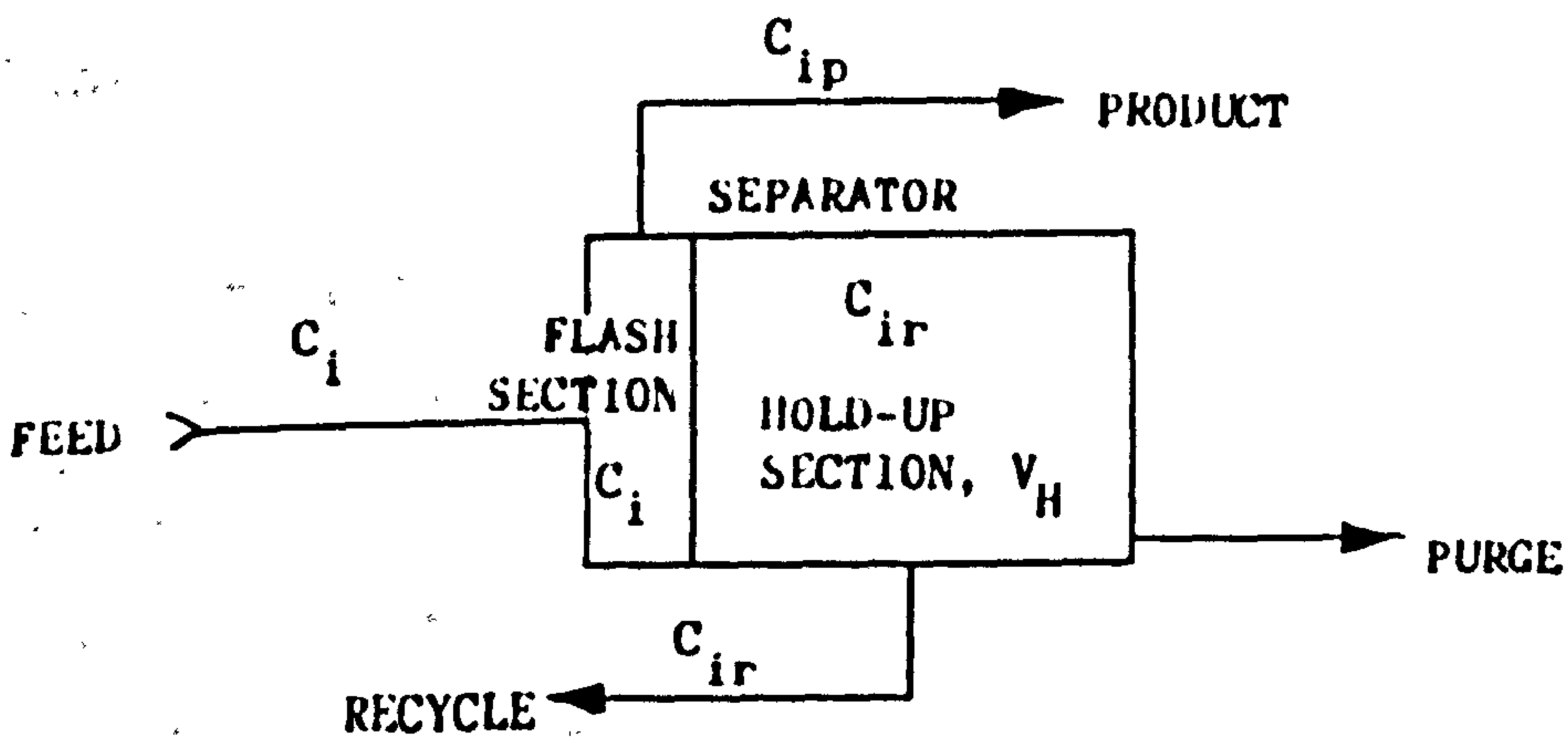


FIG. 2(c)
MODEL 2

PHYSICAL MODELS FOR REACTOR SYSTEM FIG. 5.2

assumption of perfect mixing in the reactor. Figures 5.2(b) and 5.2(c) show the two separation models studied.

Figure 5.2(b) represents the case where a buffer tank is inserted in the process stream between the reactor and the separating unit. The concentrations of the components in this section, that is the hold-up section, will be identical to those in the reactor. The liquid hold-up in the separating section is considered negligible. Figure 5.2(c) illustrates the case where the liquid hold-up in the post-separating section is considerable. This model is, in fact, the well known single-stage distillation model. The liquid hold-up prior to separation is neglected in this case. The effect of changing the volume of liquid in the hold-up section (i.e. V_H), in both these models was investigated and is discussed in the following chapter.

The purge stream from the system can be drawn off either from the separator or from the recycle stream itself. It is shown in the diagram as coming from the separator because when unsteady state operation is considered, the intermittent purging of the system consists, in effect, of emptying the reactor and the separator of their respective contents. In this connection another assumption, that of negligible volume of the flow lines in comparison with the volumes of the reactor and the separator, should be stated.

The mode of operation of the system was based on a constant volumetric flow rate (F) to, and a constant volume of material (V_R) in the reactor - resulting in a constant mean residence time (τ) for the reactor. It can be envisaged more clearly with the aid of an example, and unsteady state operation will first be described.

Unsteady State Operation.

The reaction $A \rightleftharpoons B$ is in question. The inert material in the feed stream is designated component X. At time t minus, the system is assumed to be full of feed material of composition C_{Ao} and C_{Xo}, all of which is being recycled. Since the system is full, the feed stream (ϕ_F), the product stream (ϕ_P) and the purge stream (ϕ_{PR}) all equal zero.

At time t plus, the reaction is started, say by an instantaneous increase in temperature and product B is produced in the reactor. B is then withdrawn from the system through the separator and any unconverted A, all X and if the separation of B is not complete, the remaining B are recycled. In order that the condition F = constant is maintained, once product is withdrawn from the separator some feed enters the system. The feed stream ϕ_F is controlled such that

$$\phi_F + \phi_R = F = \text{constant}$$

This behaviour can be expressed in outline as

$$\phi_p > 0 \longrightarrow \phi_R < F \longrightarrow \phi_F > 0$$

With increasing t, the concentration of X in the system will build-up and hence the conditions most favourable to the production of B, obtain at t plus. ϕ_p and therefore ϕ_F, reach their maximum values at this time and decrease with increasing t. The volumetric behaviour of the various streams may be shown

Stream/Time	Vol. Magnitude of Stream (FT^3/HR)		
	$t < 0$	$t > 0$	$t \longrightarrow \infty$
ϕ_F	0	MAX	$\longrightarrow 0$
ϕ_P	0	MAX	$\longrightarrow 0$
ϕ_R	F	MIN	$\longrightarrow F$

The time is reached when the rate of conversion to B, due to the reduced concentration of A, becomes unsatisfactory.

The system is then purged and the cycle repeated. In practice the maximum permissible concentration of X would be determined by process and/or economic factors. The term unsteady state operation as used subsequently, applies to cyclic operations of this nature.

Steady State Operation.

As in the unsteady state case, constant F and V_R are taken as preconditions. In steady state operation, the concentrations in both reactor and separator and the magnitudes of the various streams in the system are invariant with time. By having a continuous purge from the system, it is possible to control the level of X in the system and, for any given reactor conditions, it is possible to arrive at the steady state condition by control of the inlet stream. The resultant input and output streams from the system can then be calculated.

The main purpose of considering steady state operation was to obtain comparisons between the two types of operation. The steady state operating conditions were calculated from the unsteady state information as follows:- The values of the concentrations C_1 in the reactor at a series of times were obtained by unsteady state analysis.

Each of these sets of values represent a feasible reactor condition and the values can be inserted into the steady state equations for the system, which on solution, yield the required steady state levels for the various streams ϕ_F, ϕ_P, ϕ_{PR} and ϕ_R. It is thus possible to obtain the steady state operating conditions at a series of points over the whole range of concentrations of the reactants which occur in unsteady state operation. This procedure is discussed more fully in section 5.6.

Separator Efficiency.

Since incomplete separation of the product from the system was investigated, the following simple criterion for efficiency of separation was adcpted.

$$\eta = \frac{\text{no. of moles of product in system product stream}}{\text{no. of moles of product in reactor outlet stream}}$$

It was assumed throughout that the product stream contains only pure product.

5.4 Formulation of the Mathematical Model

A reactor coupled with a model 1 type separator (see figure 5.2(b)), in which a first order reversible reaction occurs will first be examined. An analytical solution can be obtained for this system. The kinetics of the reaction can be written

$$A + (X) \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B + (X)$$

where k_1 and k_2 are the forward and backward velocity constants. All flows in the system are expressed in ft^3/hr. All concentrations are expressed as lb mols/ft^3 and all volumes in ft^3. Since the product is pure B, if the mol. wt of $B = M_B$ and if the density of the product stream $= \rho_B$ (lbs/ft^3), then

$$C_{BP} = \frac{\rho_B}{M_B}$$

Unsteady State Analysis:

1. The material balances for the system can be written

(i) Reactor

Component A $\quad FC_{Ai} - FC_A = (k_1C_A - k_2C_B)\, V_R + V_R\frac{dC_A}{dt} \qquad (5.1)$

Component B $\quad FC_{Bi} - FC_B = (k_1C_A - k_2C_B)\, V_R + V_R\frac{dC_B}{dt} \qquad (5.2)$

Component X $\quad FC_{Xi} - FC_X = V_R\frac{dC_X}{dt} \qquad (5.3)$

(ii) Separator

Component A $$FC_A - \phi_R C_{Ar} = V_H \frac{dC_A}{dt} \qquad (5.4)$$

Component B $$FC_B - \phi_P C_{BP} - \phi_R C_{Br} = V_H \frac{dC_B}{dt} \qquad (5.5)$$

Component X $$FC_X - \phi_R C_{Xr} = V_H \frac{dC_X}{dt} \qquad (5.6)$$

(iii) Feed Junction

Component A $$FC_{Ai} = \phi_F C_{Ao} + \phi_R C_{Ar} \qquad (5.7)$$

Component B $$FC_{Bi} = \phi_R C_{Br} \qquad (5.8)$$

Component X $$FC_{Xi} = \phi_F C_{Xo} + \phi_R C_{Xr} \qquad (5.9)$$

(iv) Overall Balances

Feed Junction $$F = \phi_F + \phi_R \qquad (5.10)$$

Separator $$F = \phi_P + \phi_R \qquad (5.11)$$

(v) By Definition

$$\phi_P C_{BP} = \eta F C_B \qquad (5.12)$$

2. Equations (5.10), (5.11) and (5.12) together with the fact that $C_{BP} = \rho_B / M_B$ gives

$$\phi_F = \phi_P = F\left(\frac{\eta M_B}{\rho_B}\right) C_B \qquad (5.13)$$

3. Equations (5.1), (5.4), (5.7) and (5.13) give

$$\frac{dC_A}{dt} = \left[\frac{F(\eta\frac{M_B}{\rho_B})C_{A0} + k_2V_R}{V_R + V_H}\right]C_B - \left[\frac{k_1V_R}{V_R + V_H}\right]C_A \tag{5.14}$$

Equations (5.2), (5.5), (5.8) and (5.12) give

$$\frac{dC_B}{dt} = \left[\frac{k_1V_R}{V_R + V_H}\right]C_A - \left[\frac{k_2V_R + \eta F}{V_R + V_H}\right]C_B \tag{5.15}$$

Equations (5.3), (5.6), (5.9) and (5.13) give

$$\frac{dC_X}{dt} = \left[\frac{F(\eta\frac{M_B}{\rho_B})C_{X0}}{V_R + V_H}\right]C_B \tag{5.16}$$

4. The terms within the square brackets in equations (5.14), (5.15) and (5.16) are all constants and may be written

$$\frac{dC_A}{dt} = \lambda_1 C_B - \lambda_2 C_A \tag{5.17}$$

$$\frac{dC_B}{dt} = \lambda_2 C_A - \lambda_3 C_B \tag{5.18}$$

$$\frac{dC_X}{dt} = \lambda_4 C_B \tag{5.19}$$

5. These equations can be solved readily as follows, C_B is substituted for in (5.18) using (5.17). Equation (5.18) is then solved for C_A. C_B can then be expressed in

terms of C_A and C_X obtained from (5.19). Substitution of C_B in (5.18) results in a linear 2nd order differential equation with constant coefficients.

$$\frac{d^2C_A}{dt^2} + (\lambda_2 + \lambda_3)\frac{dC_A}{dt} + \lambda_2(\lambda_3 - \lambda_1)C_A = 0 \qquad (5.20)$$

The solution of (5.20) is given by the complementary function

$$C_A = Ae^{m_1t} + Be^{m_2t}$$

Boundary conditions are (i) $t = 0$ $\quad C_A = C_{A0}$

(ii) $t = 0$ $\quad C_B = 0$, hence

$$\frac{dC_A}{dt} = -\lambda_2 C_{A0}$$

(i) gives $C_{A0} = A + B$

(ii) gives $m_1A + m_2B = -\lambda_2 C_{A0}$

and hence

$$A = \left(\frac{m_2 + \lambda_2}{m_2 - m_1}\right) C_{A0} \qquad B = \left(\frac{m_1 + \lambda_2}{m_1 - m_2}\right) C_{A0}$$

The solution of (5.20) is then

$$C_A = C_{A0}\left(\frac{m_2 + \lambda_2}{m_2 - m_1}\right) e^{m_1t} + C_{A0}\left(\frac{m_1 + \lambda_2}{m_1 - m_2}\right) e^{m_2t} \qquad (5.21)$$

where m_1 and m_2 are the roots of the auxiliary equation and are given by

$$m_1 = -\tfrac{1}{2}(\lambda_2+\lambda_3) + \tfrac{1}{2}\sqrt{(\lambda_2+\lambda_3)^2 - 4\lambda_2(\lambda_3-\lambda_1)}$$

$$m_2 = -\tfrac{1}{2}(\lambda_2+\lambda_3) - \tfrac{1}{2}\sqrt{(\lambda_2+\lambda_3)^2 - 4\lambda_2(\lambda_3-\lambda_1)}$$

6. The value of C_B can now be obtained from (5.17)

$$C_B = \frac{(m_1+\lambda_2)(m_2+\lambda_2)}{m_2 - m_1}\frac{C_{A0}}{\lambda_1}\left(e^{m_1t}-e^{m_2t}\right) \qquad (5.22)$$

7. Substitution for C_B in equation (5.19) gives $\frac{dC_X}{dt}$, and C_X on integration, with the aid of the boundary condition $t = 0$, $C_X = C_{X0}$ is

$$C_X = \frac{(m_1+\lambda_2)(m_2+\lambda_2)}{m_2 - m_1} \cdot \frac{\lambda_4}{\lambda_1}C_{A0}\left[\frac{e^{m_1t}-1}{m_1} - \frac{e^{m_2t}-1}{m_2}\right] + C_{X0} \qquad (5.23)$$

8. By means of equation (5.13) we have

$$\phi_F = \phi_P = \frac{(m_1+\lambda_2)(m_2+\lambda_2)}{m_2 - m_1}\;\frac{F}{\lambda_1}\left(\eta\frac{\bar{M}_B}{\bar{\rho}_B}\right)C_{A0}\left(e^{m_1t}-e^{m_2t}\right) \qquad (5.24)$$

and since $\phi_R = F - \phi_F$, all the stream volumes are known.

9. The ranges which can be obtained for the variables C_A, C_B, C_X, ϕ_F and ϕ_R from these solutions are

	$t = 0$	$t = \infty$
C_A	C_{A0}	0
C_B	0	0
C_X	C_{X0}	$C_{X0} - \frac{\lambda_4}{\lambda_1} C_{A0}\frac{(m_1+\lambda_2)(m_2+\lambda_2)}{m_1 m_2}$
ϕ_F	0	0
ϕ_R	F	F

It will be observed that $C_X \longrightarrow$ a constant as $t \longrightarrow \infty$. For this condition to hold $\lambda_2(\lambda_3 - \lambda_1)$ must be positive. This occurs when $\frac{M_B C_{A0}}{\rho_B} < 1$.

10. Output from the system. Equation (5.24) which gives the instantaneous value of the output stream can be written

$$\phi_P = \frac{dP}{dt} = K(e^{m_1 t} - e^{m_2 t})$$

where P = product output in ft^3 (1) and K = constants in equation (5.24). Integrating from t = 0 to t = t and using the boundary condition P = 0, t = 0 we obtain

$$P = \frac{(m_1 + \lambda_2)(m_2 + \lambda_2)}{m_2 - m_1} \cdot \frac{F}{\lambda_1} \left(\eta \frac{M_B}{\rho_B}\right) \left[\frac{e^{m_1 t} - 1}{m_1} - \frac{e^{m_2 t} - 1}{m_2} \right] \quad (5.25)$$

A complete mathematical description of the system is given by equations (5.21), (5.22), (5.23) and (5.24) together with the relationship $\phi_R = F - \phi_P$. The concentrations and flow rates at any time can be obtained. Equation (5.25) enables the cumulative output (and therefore input) to be calculated. The total cumulative value R, of the recycle stream is obtained by noting that

$$R = Ft - P$$

The total volume purged as mentioned in section 5.3 equals $(V_R + V_H)$.

(1) P AND R IN THIS SECTION ARE SYNONYMOUS WITH ϕ_P^* AND ϕ_R^* USED LATER.

(iv) Overall Balances

Feed Junction $$F = \phi_F + \phi_R \tag{5.10}$$

Separator $$F = \phi_P + (\phi_R + \phi_{PR}) \tag{5.30}$$

2. From equations (5.10), (5.12) and (5.30) we obtain

$$\phi_R + \phi_{PR} = F\left[1 - \left(\frac{\eta M_B}{\rho_B}\right)C_B\right] \tag{5.31}$$

3. Equations (5.9), (5.10), (5.26), (5.29) and (5.31) enable ϕ_F to be expressed in terms of C_X and C_B

$$\phi_F = \frac{\left(\eta\frac{M_B}{\rho_B}\right)C_B.C_X}{\left[1-\left(\eta\frac{M_B}{\rho_B}\right)C_B\right]} \Bigg/ \frac{C_X}{F\left[1-\left(\eta\frac{M_B}{\rho_B}\right)C_B\right]} - \frac{C_{XO}}{F} \tag{5.32}$$

4. The values of C_X and C_B (also C_A) are known in terms of t and the system constants from the unsteady state analysis. It is therefore possible to take any particular set of values, C_i (corresponding to a particular t) and obtain the corresponding steady state level of ϕ_F by means of equation (5.32). ϕ_R and ϕ_{PR} may then be obtained from equations (5.10) and (5.31). By carrying out a series of such calculations, the equivalent steady state operating conditions can be obtained for the reactor conditions which

exist throughout any given unsteady state cycle.

If the composition of the recycle stream is required equations (5.27), (5.28) and (5.29) will give values to C_{Ar}, C_{Br} and C_{Xr}.

5. If information on values of C_A, C_B and C_X is not available from an earlier analysis, it is possible by manipulation of these equations for a constant τ, to get relationships of the form

$$C_A = f(\phi_F, C_B)$$

$$C_B = f(C_A)$$

$$C_X = f(\phi_F, C_B)$$

whence if C_A or C_B is specified with fixed ϕ_F, the system may be determined.

Model 2 Type Separator System:

To complete the mathematical outline of the systems, the equations for the system incorporating the single-stage model will be developed. The steady state analysis is exactly the same as for the model 1 type system and unsteady state operation need only be reviewed. Non-linear differential equations are obtained and no analytical solution is given.

1. A similar procedure is used and the material balances are first set up

(i) Reactor

Equations for components A, B and X are the same as (5.1), (5.2) and (5.3)

(ii) Separator

Component A $$FC_A - \phi_R C_{Ar} = V_H \frac{dC_{Ar}}{dt} \qquad (5.33)$$

Component B $$FC_B - \phi_P C_{BP} - \phi_R C_{Br} = V_H \frac{dC_{Br}}{dt} \qquad (5.34)$$

Component X $$FC_X - \phi_R C_{Xr} = V_H \frac{dC_{Xr}}{dt} \qquad (5.35)$$

(iii) Feed Junction

Balances are again expressed by equations (5.7), (5.8) and (5.9)

(iv) Overall Balances

Balances are given by equations (5.10) and (5.11)

2. By combining these equations in a similar manner as before, the following set of equations is obtained

$$\frac{dC_A}{dt} = \left(\frac{F}{V_R}\right)C_{Ar} - \left[\frac{\eta M_B}{\rho_B}\left(\frac{F}{V_R}\right)\right]C_B C_{Ar} - \left[\frac{F}{V_R} + k_1\right]C_A + \left[\frac{\eta M_B}{\rho_B}\left(\frac{F}{V_R}\right)C_{A0} + k_2\right]C_B \tag{5.36}$$

$$\frac{dC_B}{dt} = \left(\frac{F}{V_R}\right)C_{Br} - \left[\frac{\eta M_B}{\rho_B}\left(\frac{F}{V_R}\right)\right]C_B C_{Br} - \left[\frac{F}{V_R} + k_2\right]C_B + k_1 C_A \tag{5.37}$$

$$\frac{dC_X}{dt} = \left(\frac{F}{V_R}\right)C_{Xr} - \left[\frac{\eta M_B}{\rho_B}\left(\frac{F}{V_R}\right)\right]C_B C_{Xr} - \left(\frac{F}{V_R}\right)C_X + \left[\left(\frac{\eta M_B}{\rho_B}\right)\frac{F}{V_R}\, C_{X0}\right]C_B \tag{5.38}$$

$$\frac{dC_{Ar}}{dt} = \left(\frac{F}{V_H}\right)C_A - \left(\frac{F}{V_H}\right)C_{Ar} + \left[\frac{\eta M_B}{\rho_B}\left(\frac{F}{V_H}\right)\right] C_B C_{Ar} \tag{5.39}$$

$$\frac{dC_{Br}}{dt} = \left[\left(\frac{F}{V_H}\right)(1-\eta)\right]C_B - \left(\frac{F}{V_H}\right)C_{Br} + \left[\frac{\eta M_B}{\rho_B}\left(\frac{F}{V_H}\right)\right]C_B C_{Br} \tag{5.40}$$

$$\frac{dC_{Xr}}{dt} = \left(\frac{F}{V_H}\right)C_X - \left(\frac{F}{V_H}\right)C_{Xr} + \left[\frac{\eta M_B}{\rho_B}\left(\frac{F}{V_H}\right)\right]C_B C_{Xr} \tag{5.41}$$

$$\frac{dP}{dt} = \left(\frac{\eta M_B}{\rho_B}\right)F.C_B \tag{5.42}$$

$$\frac{dR}{dt} = F\left(1 - \frac{\eta M_B}{\rho_B}\right).C_B \tag{5.43}$$

Equations (5.36) through to (5.41) describe the behaviour of the system and a simultaneous solution is therefore required of these six non-linear equations. An analytical solution cannot be obtained and a numerical technique will be used. It will be observed that the $\left(\frac{F}{V_H}\right)$ term in the equations describing the concentration changes in the separator is analogous to the $(\frac{F}{V_R})$ term in the reactor equations. It can be considered as representing the inverse of an "average residence time" in the separator.

Second Order Reactions:

The reaction considered was

$$A + C \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B + D$$

An exactly similar procedure to that outlined for the first order reaction systems was followed. For the system incorporating a model 1 separator, five non linear equations are obtained. The model 2 separator system is described by ten such equations. In both cases an analytical solution is not feasible, but again a numerical solution is possible. The two sets of equations obtained for the 2nd order reactions are given in Appendix 5.

The steady state analysis for the 2nd order reaction systems can be carried out with the equations developed for the first order systems.

The complete mathematical description of the reaction kinetics and the reactor systems studied has been given in this section, the next section deals with the objective functions chosen to measure the changes in the system.

Steady State Analysis:

In the steady state model the purge stream flow rate, ϕ_{PR}, is introduced as a separate variable. The material balances incorporating ϕ_{PR} are set up as in the unsteady state analysis.

1. Material balances for the system.

(i) Reactor

The balances are the same as those for the unsteady state except, that since there is no accumulation in the system, the differential term in each of the equations equals zero eg.

Component X: $$FC_{Xi} - FC_X = 0 \qquad (5.26)$$

(ii) Separator

Component A $$FC_A = (\phi_R + \phi_{PR})C_{Ar} \qquad (5.27)$$

Component B $$FC_B = \phi_P C_{BP} + (\phi_R + \phi_{PR})C_{Br} \qquad (5.28)$$

Component X $$FC_X = (\phi_R + \phi_{PR})C_{Xr} \qquad (5.29)$$

(iii) Feed Junction

Steady state equations are identical to equations (5.7), (5.8) and (5.9).

5.5 Cost, Design and Process Data and Development of Economic Criteria.

The same two economic criteria were employed in the reactor study as in the distillation study, namely, the unit cost of production (U.C.) and the Venture Worth (V.W.) of the project. The unit cost was defined as

$$\text{Unit Cost} = \frac{\text{total annual cost}}{\text{annual production}}$$

The annual cost is given by the summation :-

$$\text{Cost} = \sum(\text{depreciation, maintenance, labour and overhead, utilities and raw material costs})$$

The V.W. is given by equation (2.8) and is used in the form of equation (2.11).

In order to apply the criteria it was necessary to obtain the system costs in the categories required. The following cost data have been assumed, but the figures are thought to be fairly realistic cf. Shahbonderian (76). As before all cash figures are dollars:

Capital Costs: It was assumed that the total system costs could be expressed as a function of the reactor and separator costs.

Reactor: $I_R = 2500\ V_R^{0.7}$ \$. (V_R and $V_S = FT^3$)

Separator: $I_S = 500\ V_S^{0.7}$ \$

Total Capital Cost $I = 100\ (25\ V_R^{0.7} + 5\ V_S^{0.7})$ \$ (5.44)

Depreciation and Maintenance:

Depreciation $= 0.10\ I$ \$ p.a. (straight line assumed)

Maintenance $= 0.05\ I$ \$ p.a.

Labour and Overhead: Assumed independent of any changes in the system $= 10{,}000$ \$ p.a.

Utilities: Pumping is assumed to be the dominant component of the utility figure and the costs for each of the streams are considered to be the same $= 0.10$ \$/FT^3

Total Utilities Cost $= 0.10\ N\ (\phi_F^* + \phi_P^* + \phi_{PR}^* + \phi_R^*)$ \$ p.a. (5.45)

where ϕ_F^*, ϕ_P^*, ϕ_{PR}^* and ϕ_R^* represent the total volume per cycle of each stream. N = number of cycles p.a. and is calculated as follows: If t = any given cycle time (hrs), then $t^* = 1.05\ t$, where t^* = effective cycle time and N is then given by

$$N = \frac{h}{t^*} \tag{5.46}$$

$h =$ total hrs. operation p.a. A five per cent turn around time is thus included in arriving at the cycles per year figure. $h = 8320$ hrs., a 95% online factor has been assumed.

For steady state operation N can be considered equal to 1 and the flow quantities the total volumes p.a.

Raw Material Costs: The raw material costs are based on the quantity of A in the feed stream. Cost of A is assumed equal to 0.08 \$/lb. If the mol. wt. of A is taken equal to 30, the raw material cost, $M_c = 2.4$ \$/lb mol A

Raw Material
Total Cost $= 2.4\, C_{A0} N \phi_F^*$ \$ p.a.

Purging Costs (Raw Materials): With unsteady state operation the system $(V_R + V_H)$ is entirely purged of its contents at the end of each cycle and refilled with feed material before operation is recommenced. The annual raw material cost for refilling the system is $2.4\, C_{A0}\, N\, (V_R + V_H)$ \$ p.a.

Selling Price of Product: A selling price of 0.20 \$/lb for B is assumed.

Total Sales Return $= 0.2 \rho_B\, N\, \phi_P^*$ \$ p.a.

Unit Cost Criterion:

The total cost p.a. is given by

$$\text{Total Cost} = 0.15\text{x}100(25V_R^{0.7} + 5V_s^{0.7}) + 10,000 + 0.10N (\phi_F^* + \phi_P^* + \phi_{PR}^* + \phi_R^*) + 2.4\, C_{A0}N\phi_F^* + 2.4\, C_{A0}N(V_R + V_H) \ \$ \text{ p.a.} \quad (5.47)$$

The unit cost production is obtained by dividing the total cost by the annual production.

Venture Worth Criterion:

In order that this can be applied the following additional assumptions are made (see section 2.4).

$i = 0.10$, $i_m = 0.125$, $n = 10$ yrs., $r = 5$ yrs., $t = 0.5$, $S_a = 0.10$

Straight line depreciation and working capital $I_w = 0.25$ x annual operating expense (35) are assumed. The annual operating expense, E, is given by

$$E = 0.10N(\phi_F^* + \phi_P^* + \phi_{PR}^* + \phi_R^*) + 0.05\, I + 10,000 + 2.4\, C_{A0}N\phi_F^* + 2.4\, C_{A0}N(V_R + V_H) \quad (5.48)$$

The gross return per a. is

$$R = 0.2\, \rho_B N\phi_P^* - E \quad \$ \text{ p.a.}$$

The V.W. is given by equation (2.11)

$$V.W. = J_1R + J_2I - J_3I_w$$

where J_1, J_2 and J_3 are defined in section (2.6).

Design Data and Assumptions:

F: the volumetric flow rate into the reactor was fixed $= 60$ FT^3/HR

V_R: the reactor volume was taken $= 60$ FT^3. The mean residence time τ, is thus $= 1$ hr.

V_S: the separator volume $= 100$ FT^3. This figure was used to calculate the cost of the separator, which was approximately the right order of magnitude relative to the reactor cost.

V_H: the hold-up volume in the separator $= 10$ FT^3

η: the separator efficiency $= 0.9$

Process Data:

C_{A0}: concentration of A in feed $= 1.0$ lb mol/FT^3

C_{X0}: concentration of X in feed $= 0.10$ lb mol/FT^3

C_{C0}: concentration of C in feed $= 1.0$ lb mol/FT^3 (for 2nd order reactions)

k_1: forward velocity constant $= 1.0$ f(conc)/HR

k_2: backward velocity constant $= 0.1$ f(conc)/HR

ρ_B: density of product B $= 60$ lbs/FT^3

M_B: mol. weight of B $= 30$

5.6 Simulation Outline, Mathematics of Solution and Programme Mechanics.

The method of operation of the system was described in section 5.3 and the mathematical model has been derived. The necessary process and design data to determine the system and the associated cost data has been assumed in the last section. The simulation remains to be considered.

Scheme for Simulation.

Two Models: (i) Reactor with Model 1 Separator (hold-up type).

(ii) Reactor with Model 2 Separator (single-stage type).

Two Criteria:

(i) Unit Cost of Production

(ii) V.W. of project.

Two Reactions: (i) $A + (X) \rightleftharpoons B + (X)$

(ii) $A + C + (X) \rightleftharpoons B + D + (X)$

The first model will be called a type 1, the second a type 2 system.

Variables which will be perturbed.

Design Variables (i) $\eta = (0.9), 0.6, 0.8, 1.0$

(ii) $V_H = (10), 1, 20$

(iii) $V_R = (60), 10$

Cost Variables (i) $R_C = (25), 5, 15$

(ii) $M_C = (2.4), 0.6, 1.2$

(iii) $V_S = (100), 1, 20$

When $V_R = 10$, τ will change. R_C = reactor cost factor and M_C = raw material cost. V_S is in fact a design variable, but it operates as a cost variable in the circumstances of this analysis. In addition the initial condition, C_{XO}, given in the last section was examined at a second level of 0.05 lb mol/ft^3. The behaviour of the system was studied for cycle lengths up to 20 hours throughout the simulation.

Mathematics of Solution:

The system equations were in all cases solved simultaneously by means of the INTSTEP Routine (85) on the Atlas Computer. The method employed in the routine is the Rünge-Kutta fourth order approximation, in which the truncation error is proportional to the (step-length)^5. The Runge-Kutta method for the solution of differential equations can be found in Mickley, Sherwood and Reed (86) and the fourth order approximation is described in Levy and Baggot (87).

Since it was decided to adopt this method of solution in all cases, the analytical solutions derived for the first order type I system were not used. Instead equations (5.14), (5.15) and (5.16) were programmed together with the two ancillary equations (5.42) and (5.43). This set of equations was solved simultaneously and the values of the variables in question C_A, C_B, C_Y, P and R were obtained at half-hour intervals. This provides us with all the information necessary to evaluate the unit cost of production with the aid of equation (5.44) and the venture worth with equations (5.45) and (2.11). The values of C_B and C_X were then inserted into equation (5.32) and the steady state value of ϕ_F calculated. ϕ_R, ϕ_P, and ϕ_{PR} are obtained from equations (5.10), (5.12) and (5.30) respectively, thus defining the steady state operating conditions for this particular set of C_i. The unit cost of production and the venture worth can be evaluated using the same equations as before.

A similar procedure was carried out for the first order type 2 system equations (5.36) to (5.43) and for the second order systems given in Appendix 5.

Programme Mechanics.

The stop length adopted was $t = 0.01$. This step length was adopted because further reduction made no change in the solutions of the equations within the stipulated accuracy of the results i.e. rounded to the third decimal place. It has been pointed out that the error is approximately equal to $(\Delta t)^5$, for $\Delta t = 0.01$, the error $= 1.10^{-10}$.

The computational work was broken down into eight programmes. The various combinations of the two types of system, the two criteria and the two orders of reaction comprised the eight. A typical flow diagram is shown and a list of the programmes given in Appendix 5.

CHAPTER 6: RESULTS AND DISCUSSION OF STUDY ON THE RECYCLING REACTOR SYSTEM (CASE 2).

6.1 Comparison of Separator Models and Significance of Hold-up Volume.

In order to facilitate the presentation of the results obtained from the simulation described in section 5.6, the following convention will be adopted.

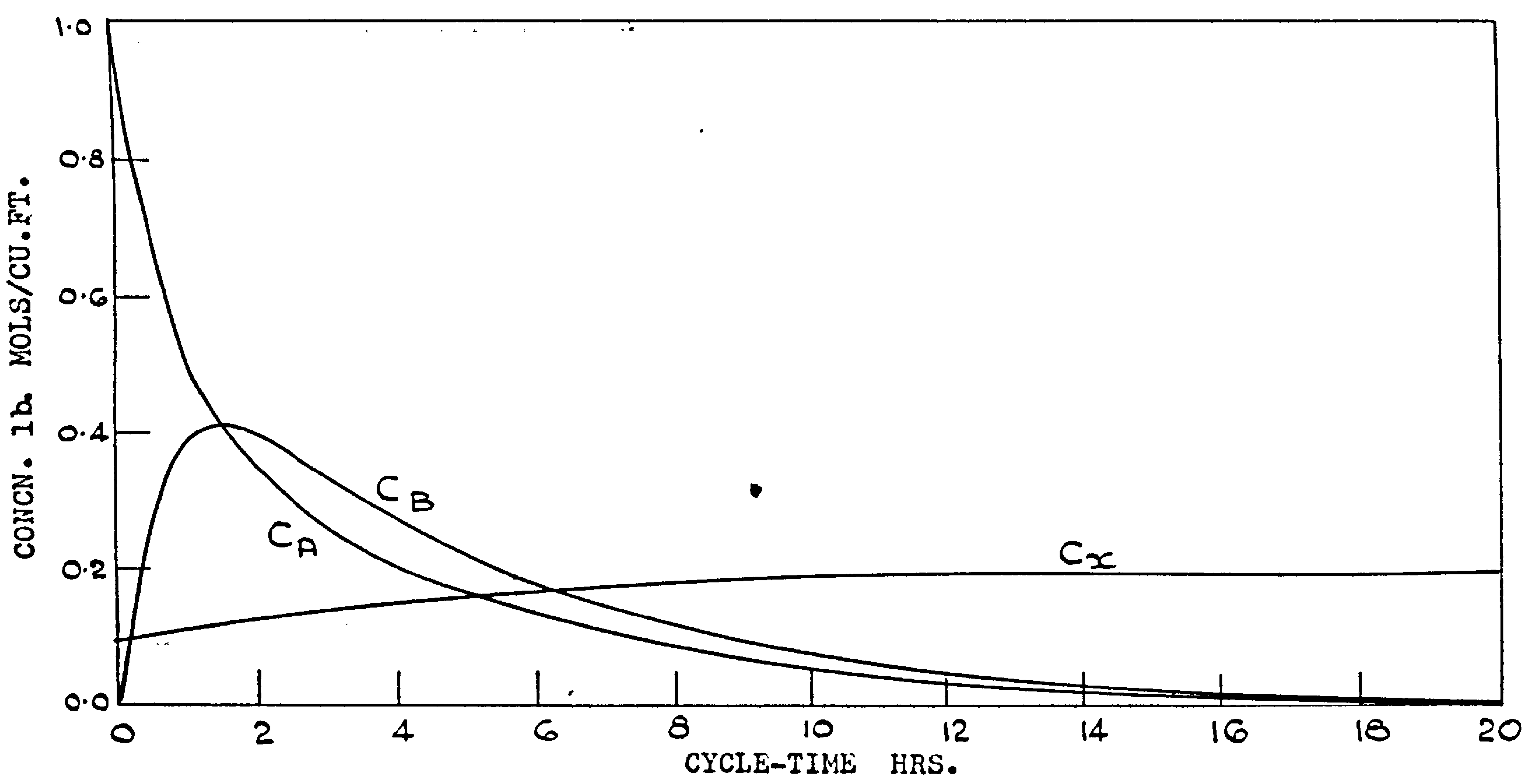
(i) When the reactor is coupled with a model 1 type separator the system will be designated, system 1.

(ii) When the reactor is coupled with a model 2 type separator the system will be designated, system 2.

(iii) When a second order reaction is taking place in the reactor, the designation will be system 1 (2nd ORD.) and system 2 (2nd ORD.), for systems 1 and 2 respectively.

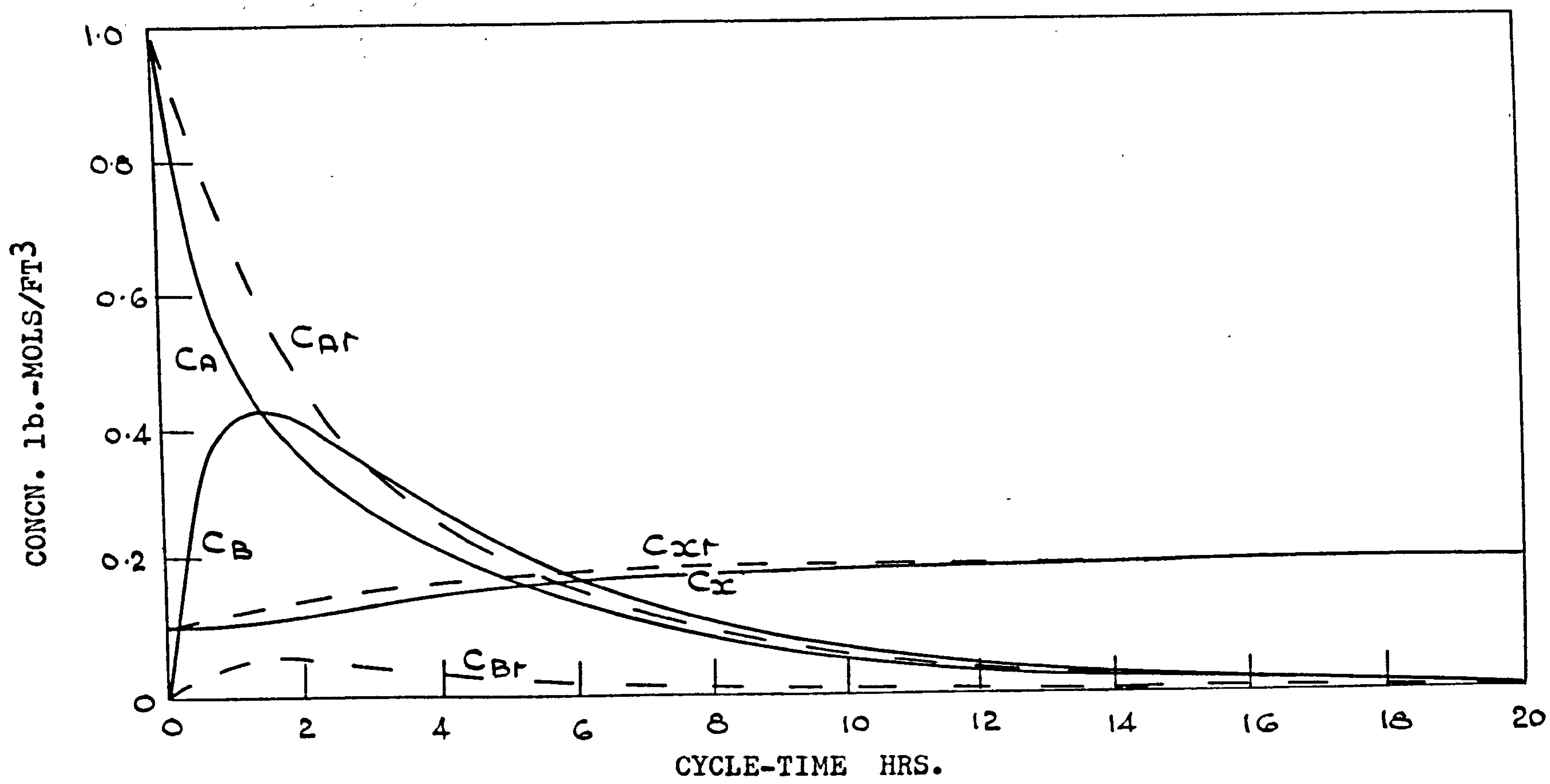
It is recognised that in general Model 2 approximates more closely to the normal separation system than Model 1. However, as has been pointed out, Model 1 has the advantage that an analytical solution can be obtained for the behaviour of the system. The typical time behaviour of the two systems is shown in figures 6.1 and 6.2 over a cycle length of 20 hours.

The behaviour is as expected. In figure 6.2 for example, it will be seen that at any particular time



TYPICAL TIME-BEHAVIOUR OF SYSTEM 1

Fig. 6.1



TYPICAL TIME-BEHAVIOUR OF SYSTEM 2.

Fig. 6.2

the concentration, C_{Ar}, of A in the separator hold-up section is somewhat higher than the concentration, C_A, in the reactor - for two reasons :-

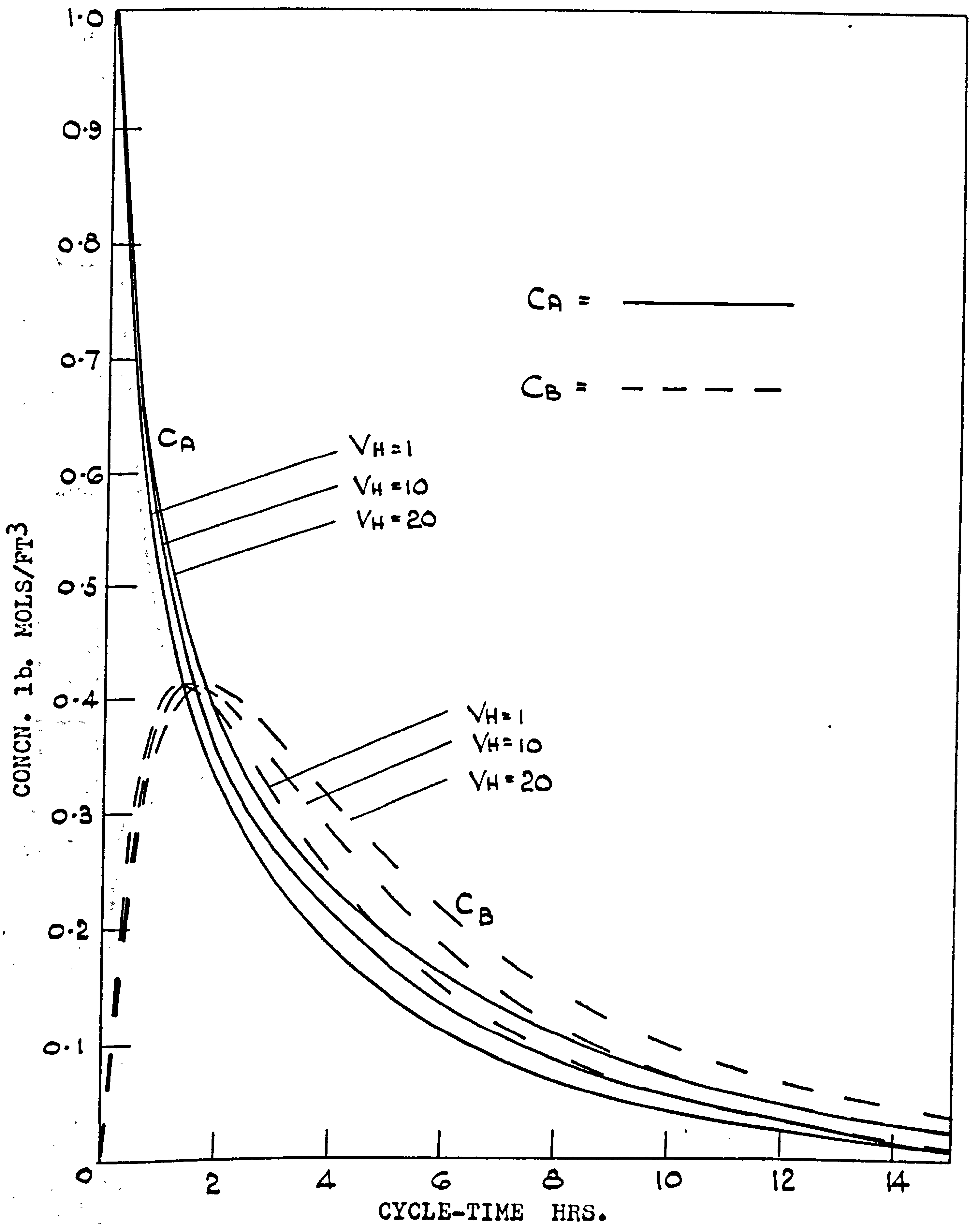
(i) Initially the concentration of A is the same, C_{AO}, throughout the system, but at time $t > 0$, a reduction in the concentration of A first takes place in the reactor and

(ii) the withdrawal of B from the separator results in an increase in the concentration of A and also X. This latter point is also the explanation why $C_{Xr} \geq C_X$. The C_{Br} value is low, as it represents the concentration of B in the separator hold-up section after the product has been withdrawn.

The differences arising in the two systems can be seen from figures 6.1 and 6.2. One difference which can be seen readily on inspecting the concentration curve for B, is that it reaches a maximum value of 0.412 in the case of system 1 and 0.428 in the case of system 2. The process and design data for these curves may be found in Appendix 5 and the values given for the various parameters may be assumed as applying in all instances, except when otherwise specified. In conjunction with this difference in the C_B v t curves, it can be seen that over the first six hours of the cycle time the concentration of A falls off more rapidly in system 1 than in system 2. It is also found that the values of Φ_P^* , the product output per cycle, are somewhat higher (particularly over the shorter cycle lengths) for system 2 than those for system 1, a fact indicating the buffer tank action of system 1.

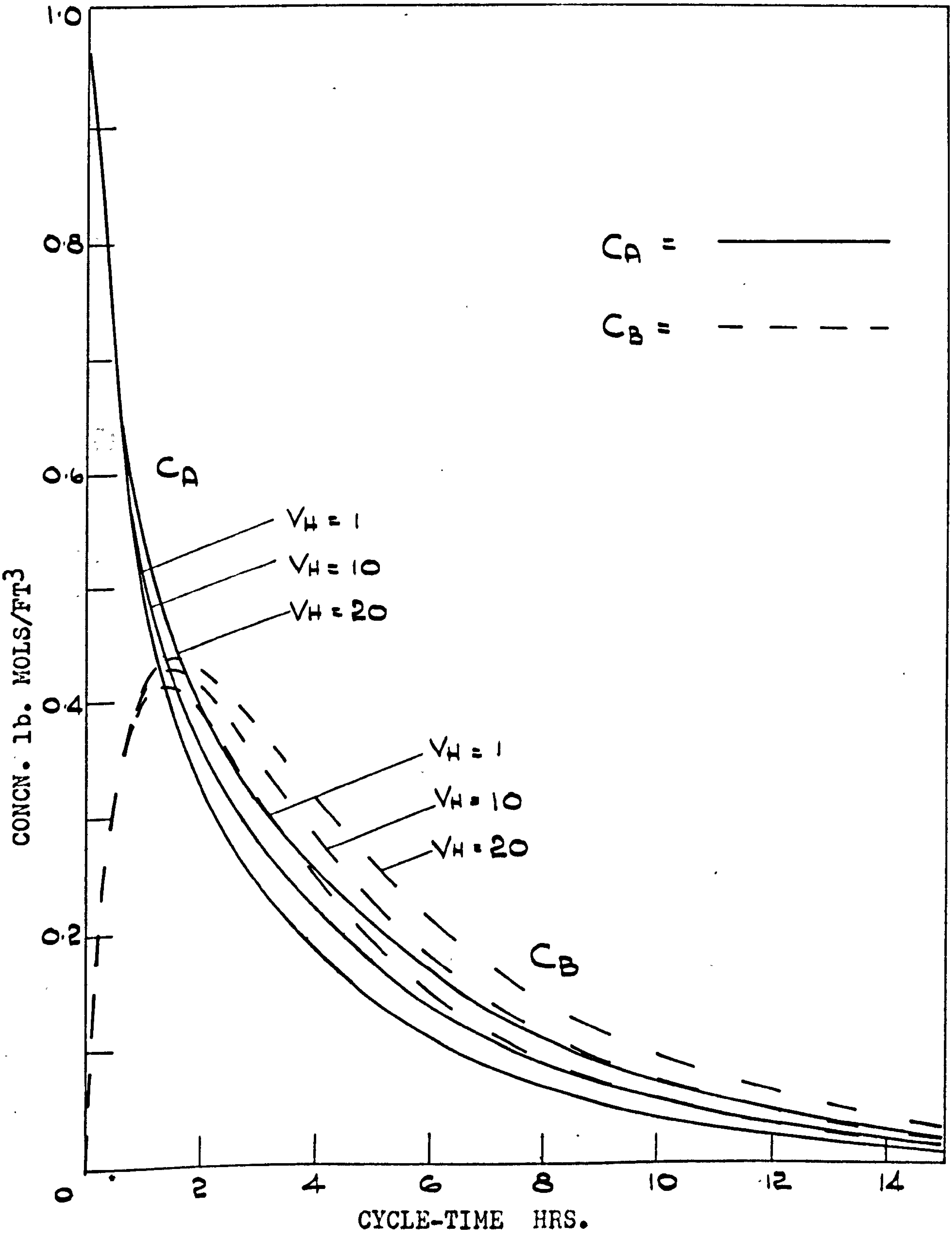
The main parameter in question in comparing the two systems is the separator hold-up volume, V_H. As expected when $V_H \longrightarrow 0$, the behaviour of the two systems becomes nearly identical. Some studies on this aspect, show that C_A falls off and C_X builds up more rapidly as $V_H \longrightarrow 0$. Thus is accompanied by C_B reaching its maximum value within a shorter time. Evidence to this effect is shown in figures 6.3 and 6.4.

It will be seen in figure 6.3 that the maximum point of the C_B v t curve is reached earlier in the cycle as V_H decreases, although the maximum value itself does not change. Whereas in figure 6.4, as V_H decreases the maximum value of C_B attained is reduced and again the point occurs at a shorter cycle length. The curves for $V_H = 10$ in figures 6.3 and 6.4 correspond to those in figures 6.1 and 6.2. Since the production for any given cycle is



EFFLCT OF VARIATION IN VH, SYSTEM 1.

Fig. 6.3.



EFFECT OF VARIATION IN VH. SYSTEM 2.

Fig. 6.4

proportional to the area under the C_B curve, these changes in the C_B v t curve with varying V_H will be reflected in the output from the system.

Some production figures are given in Table 6.1:-

TABLE 6.1.

EFFECT OF VARIATION IN SEPARATOR HOLD-UP VOLUME ON PRODUCTION RATES FOR SYSTEMS 1 AND 2.

SYSTEM NO.	CYCLE LENGTH	PRODUCTION - LB.MOLS/ANN.		
		$V_H = 20$	$V_H = 10$	$V_H = 1$
1	0.5 (HRS)	63,115	69,813	77,120
	1.0	101,214	108,953	116,705
	2.0	136,825	141,323	144,694
	2.5			147,086*
	3.0		147,082*	
	3.5	147,025*		
	10.0	105,342	96,711	87,731
	15.0	79,097	70,822	62,775
	20.0	61,847	54,690	47,983

TABLE 6.1 continued:

SYSTEM NO.	CYCLE LENGTH	$V_H = 20$	$V_H = 10$	$V_H = 1$
2	0.5	77,772	77,861	78,015
	1.0	118,624	118,482	117,791
	2.0	151,757	149,630	145,655
	2.5			147,944*
	3.0	158,392 *	153,719 *	
	10.0	108,496	98,244	87,874
	15.0	80,336	71,345	62,816
	20.0	62,317	54,864	47,995

Points which can be noted from the Table, in which the maximum outputs are marked with an asterisk, are;

(i) In system 1, changing V_H does not decrease the maximum output that can be attained, but as V_H decreases, the maximum output is obtained through the use of a shorter cycle length. This behaviour is in accordance with C_B (Max.) constant and t for C_B (Max.) decreasing as V_H decreases, i.e. figure 6.3.

(ii) In system 2, the maximum output is decreased as V_H decreases and, as before, shorter cycle lengths are required. In figure 6.4, it will be seen that this is in agreement with the fact that C_B (Max.) decreases as V_H increases and C_B (Max.) occurs earlier in the cycle.

(iii) The production rate increases for a given cycle time as V_H decreases. This behaviour which is more marked for system 1, is true for both systems.

(iv) The approach to similarity of the two systems as $V_H \longrightarrow 0$, is evident from the figures for $V_H \neq 1$ in the table.

(v) An important point is the corollary of (ii) above which is that as V_H increases, the output of system 2 relative to system 1 increases.

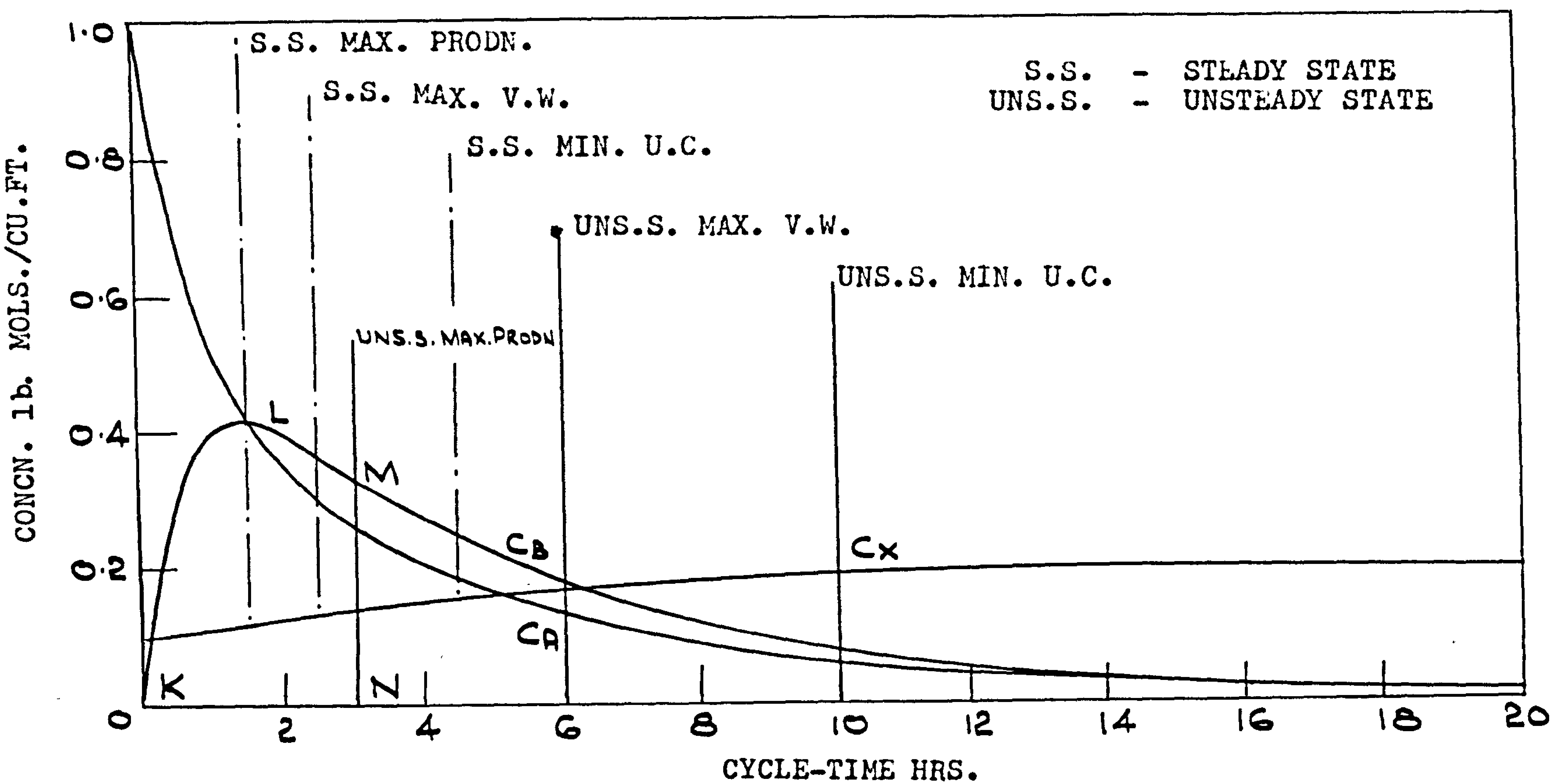
Two important results which emerge in part from the discussion above and which are substantiated by the calculated results are :-

1. For system 1, changes in V_H make very little difference to the absolute magnitude of the optima, although the associated optimum cycles shorten as V_H decreases. This has been demonstrated for the maximum production criterion in Table 6.1 and it is also true for the U.C. and V.W. criteria.

2. For system 2, as V_H decreases both the maximum production and the maximum V.W. decrease and the minimum U.C. increases. Shorter optimum cycles accompany these changes.

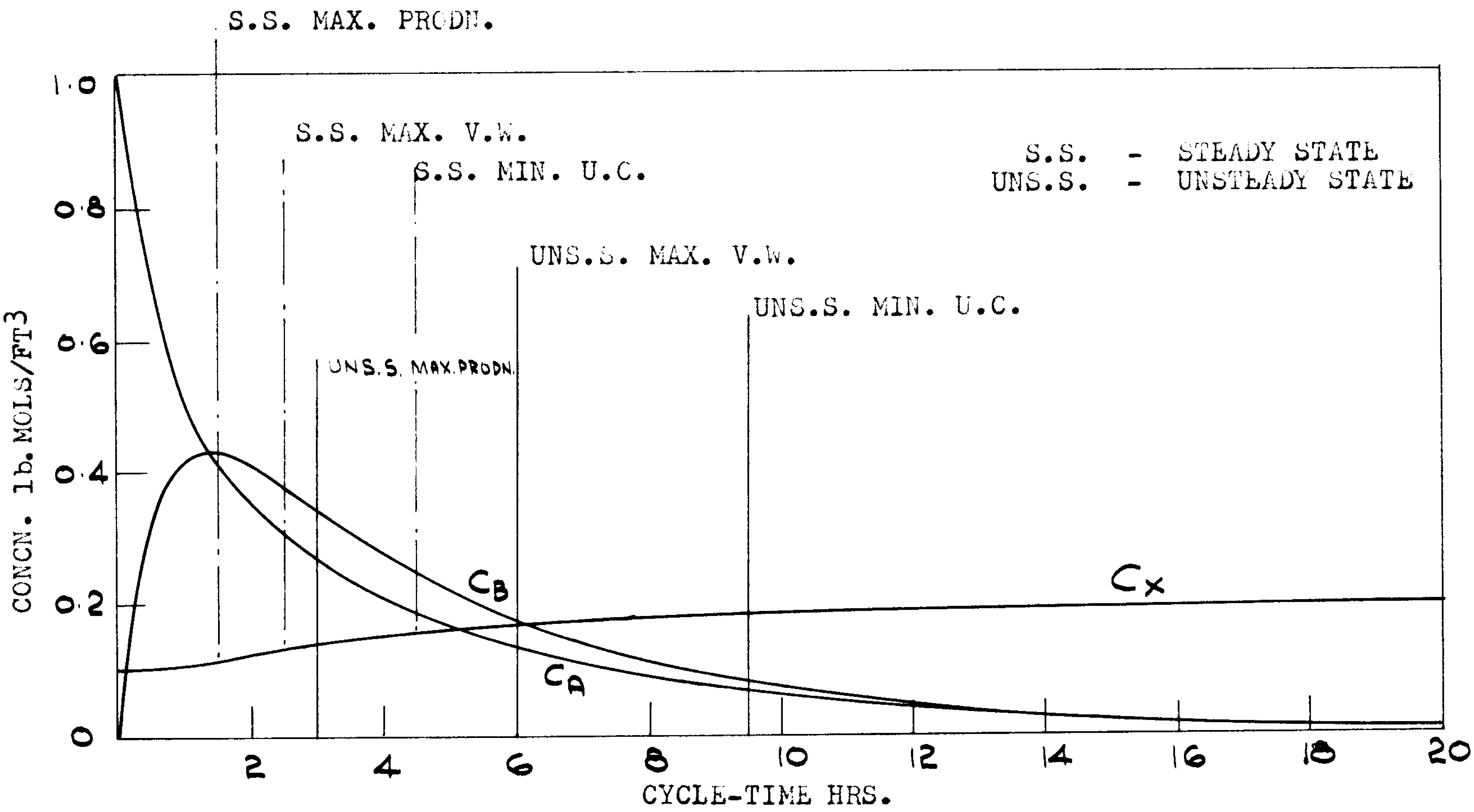
6.2 Comparison of Economic Criteria.

Figures 6.5 and 6.6 show typical optimum points of operation for the systems. It must be borne in mind that where a steady state (S.S.) point or curve is shown on a graph which has cycle time as the abcissa, the S.S. refers to operation at the reactor conditions i.e. the component concentrations, as shown for example in figure 6.1, existing at that time in the cycle. It should also be mentioned that the optimum points presented represent the optimum values taken from a table of results at half-hourly intervals. The true optimum values may lie on one side or other of the value indicated. They can be obtained by plotting curves of the V.W. and U.C. against time. From figures 6.5 and 6.6 it will be seen that each of the two economic criteria and each of the two modes of operation have different optimum points of operation, although to the nearest half hour these points coincide in all but one instance (UNS. S., MIN. U.C.) for both systems. For UNS. S. operation (system 1), a 10 hour cycle represents the optimum cycle length for the U.C. criterion and a 6 hour cycle for the V.W. criterion. The reactor conditions for the corresponding S.S. optima can also be noted e.g. U.C.



TYPICAL OPTIMUM POINTS OF OPERATION FOR SYSTEM 1.

Fig. 6.5



TYPICAL OPTIMUM POINTS OF OPERATION FOR SYSTEM 2.

Fig. 6.6

criterion, $C_A = 0.185$, $C_B = 0.248$, $C_X = 0.157$ lb.moles/FT^3.

The points of operation for maximum production are also indicated and again different optima are obtained for this further criterion. The maximum output in both systems occurs for S.S. operation at the maximum value of the concentration term, C_B, - a fact to be expected. For UNS. S. operation, the area under the C_B v t curve up to the specified cycle length i.e. the area KLMN in figure 6.5, multiplied by the number of cycles per year, (in this case 8320/3.0 x 1.05), is greater than any other area multiplied by its equivalent number of cycles per year.

It will be seen in the figures that a very considerable divergence in operating conditions exists for the optima of the various criteria. This divergence may also be observed in figures A6.2 and A6.3 (in Appendix 6) for the 2nd order reaction studies. The significance of the situation portrayed in figure 6.5 is shown in Table 6.2. Considering UNS. S. operation first, it will be seen that maximization of the output results in a U.C. equal to 1.44 times the minimum U.C. and a V.W., 56% less than the maximum possible. On the other hand, minimization of the U.C. will reduce the production to 66% of its maximum level and the

V.W. rating to 84% of the maximum attainable. A third alternative exists for the optimization of the V.W. and a similar series of possibilities is present for S.S. operation.

TABLE 6.2.

VARIATION OF OPTIMUM OPERATING CONDITIONS (SYSTEM 1) WITH CHOICE OF CRITERION.

MODE OF OPERATION	CRITERION: PRODN. lb mols/a.	CRITERION: U.COST $/lb mol	CRITERION: V.WORTH $	CYCLE LENGTH (HRS)	COMPONENT CONCNS AT TERMINATION OF CYCLE: C_A	C_B	C_X
UNS. S.	147,082 *	4.8414	362,577	3.0	0.263	0.339	0.140
	127,408	3.5821	834,597 *	6.0	0.132	0.178	0.169
	96,711	3.3664 *	695,761	10.0	0.055	0.074	0.187
				(CYCLE LENGTH)	OPERATING COMPONENT CONCNS.: C_A	C_B	C_X
S.S.	185,014 *	4.4362	707,086	1.5	.412	.412	.118
	166,867	3.7574	1,005,091 *	2.5	.299	.371	.133
	111,445	3.5006 *	756,647	4.5	.185	.248	.157

CRITERIA VALUES EXPRESSED AS A % OF THE OPTIMUM

MODE OF OPERN.	PRODN	U.COST	V.WORTH
UNS. S.	100	143.6	43.5
	86.6	106.5	100
	65.7	100	83.5
S.S.	100	126.7	70.4
	90.1	107.2	100
	60.2	100	75.3

Note: the optimum value for the particular criterion is marked with an asterisk.

It is clear that the decision to adopt a particular criterion is important, insofar as the adoption of one criterion will lead to, in most instances, highly non-optimal solutions for the others. In the case of the V.W. criterion, it will be seen from table 6.2 that for both UNS. S. and S.S. operation, optimization subject to this index, yields the next most optimal solution for the other two criteria i.e. for the three solutions given. For UNS. S. operation a 13% reduction in output and a 7% increase in the U.C., and for S.S. operation a 10% reduction in output and a 7% increase in U.C. result from maximizing the V.W.

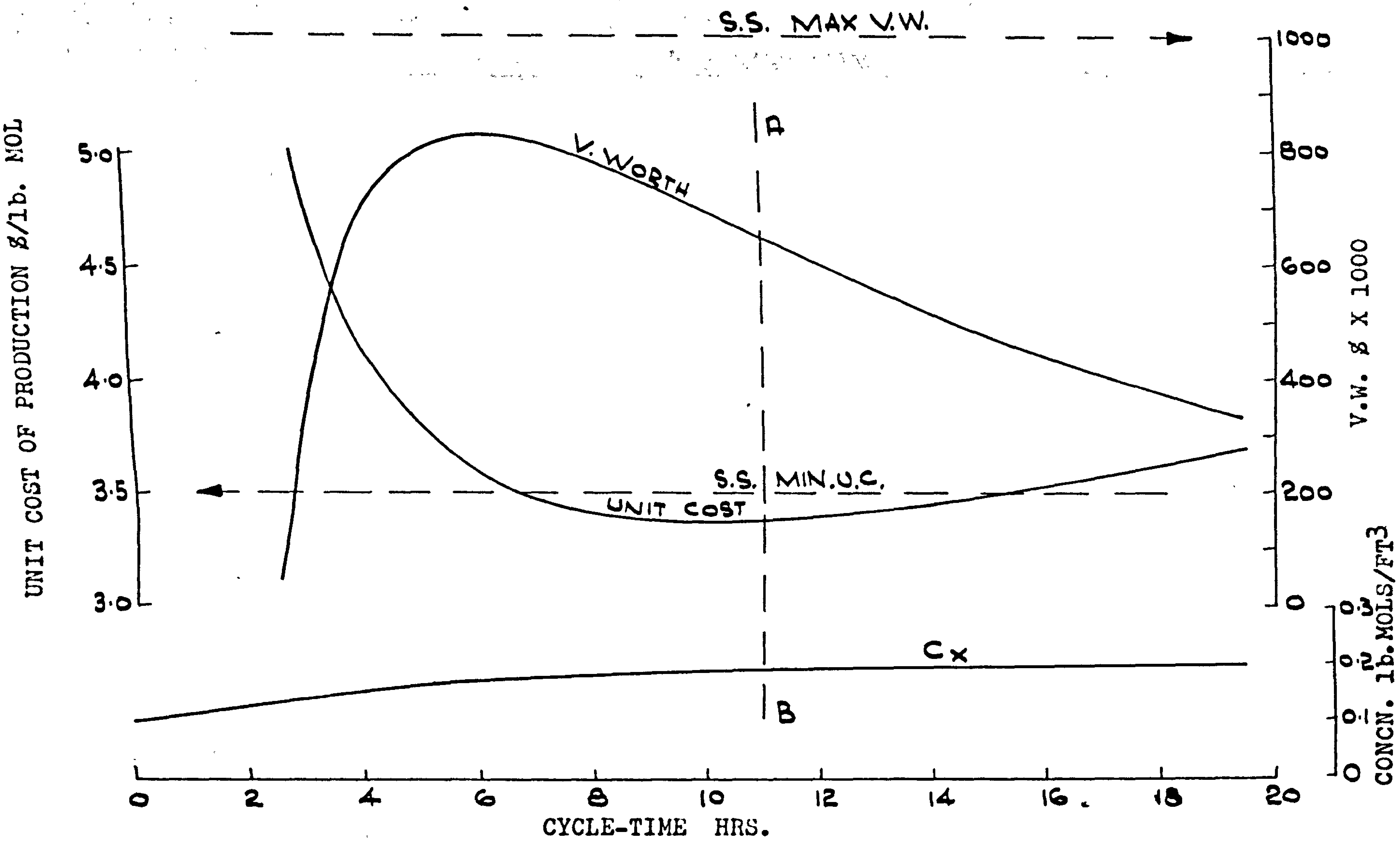
The adoption of a particular criterion will also lead to a decision concerning the mode of operation for the system. In table 6.2 it is obvious that minimization of the U.C. will result in UNS. S. operation being chosen while maximization of the production per annum or the V.W. is attained through S.S. operation.

The conditions under which UNS. S. operation is preferable to S.S. are discussed in the next section.

6.3 Strategy of Purging. Steady State and Unsteady State Operation.

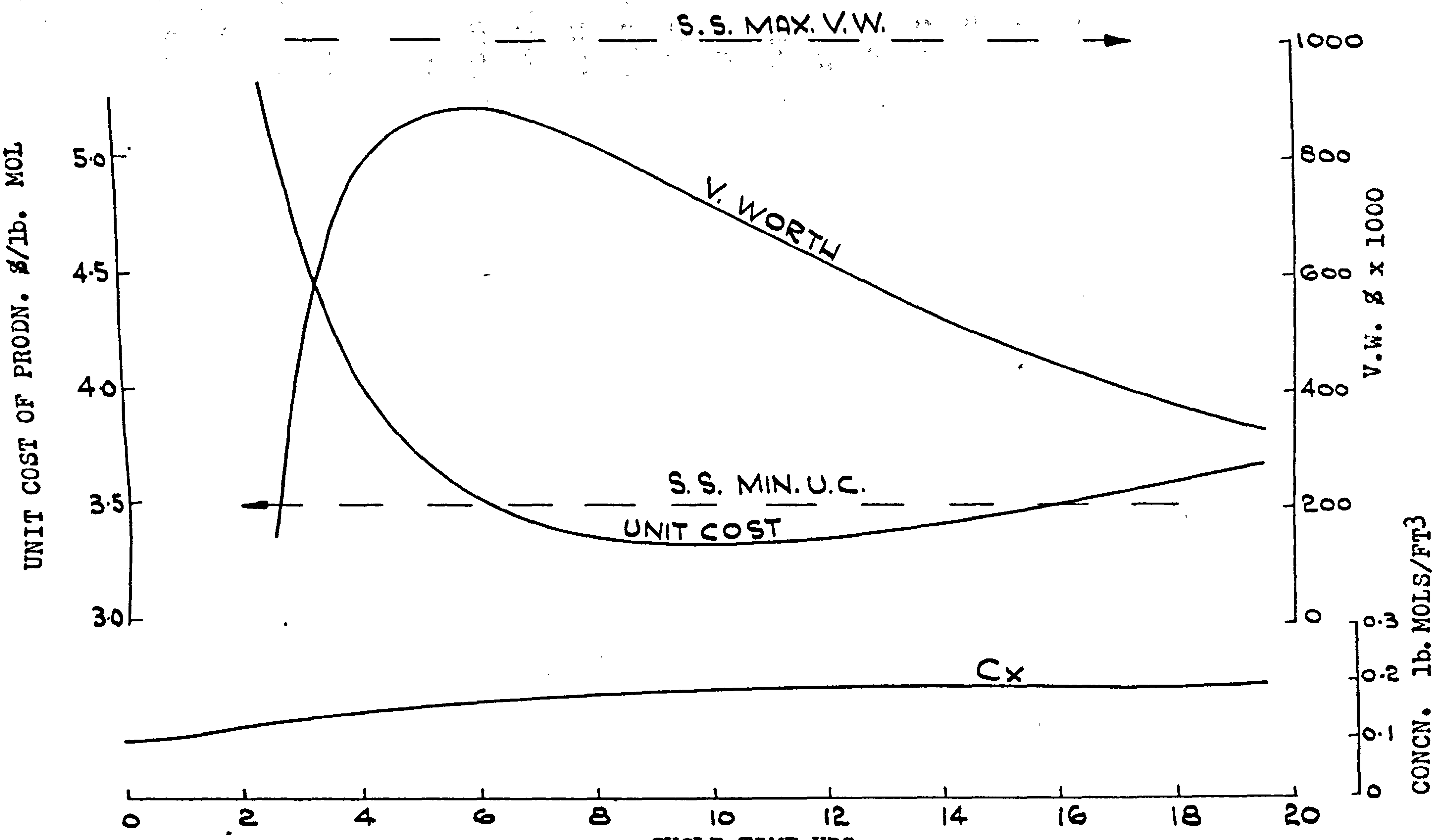
The U.C. and V.W. obtained by means of cyclic operations are plotted against the cycle length in figures 6.7 and 6.8 for systems 1 and 2 respectively. In figure 6.7, the minimum U.C. occurs at a cycle length of approximately 10 hours and the maximum value of the V.W. is given by a 6 hour cycle. The minimum U.C. and the maximum V.W. which can be obtained by S.S. operation are also shown on the graph, as is the C_X curve indicating the rate of build-up of inert material in the system. If, for the moment, no restriction is placed on the concentration of inert material permissible in the system, then the following purging strategy may be outlined: It is clear that within the range studied, provided a cycle length of up to 15 hours is feasible UNS. S. operation with intermittent purging is preferable over cycle lengths of 7 to 15 hours when the index of profitability adopted is U.C. For the V.W. criterion, S.S. operation is uniformly more favourable.

A similar situation is present in figure 6.8, except that the range of cycle lengths favourable to UNS. S. operation in U.C. considerations is slightly greater, that



PURGING STRATEGY FOR SYSTEM I.

Fig. 6.7



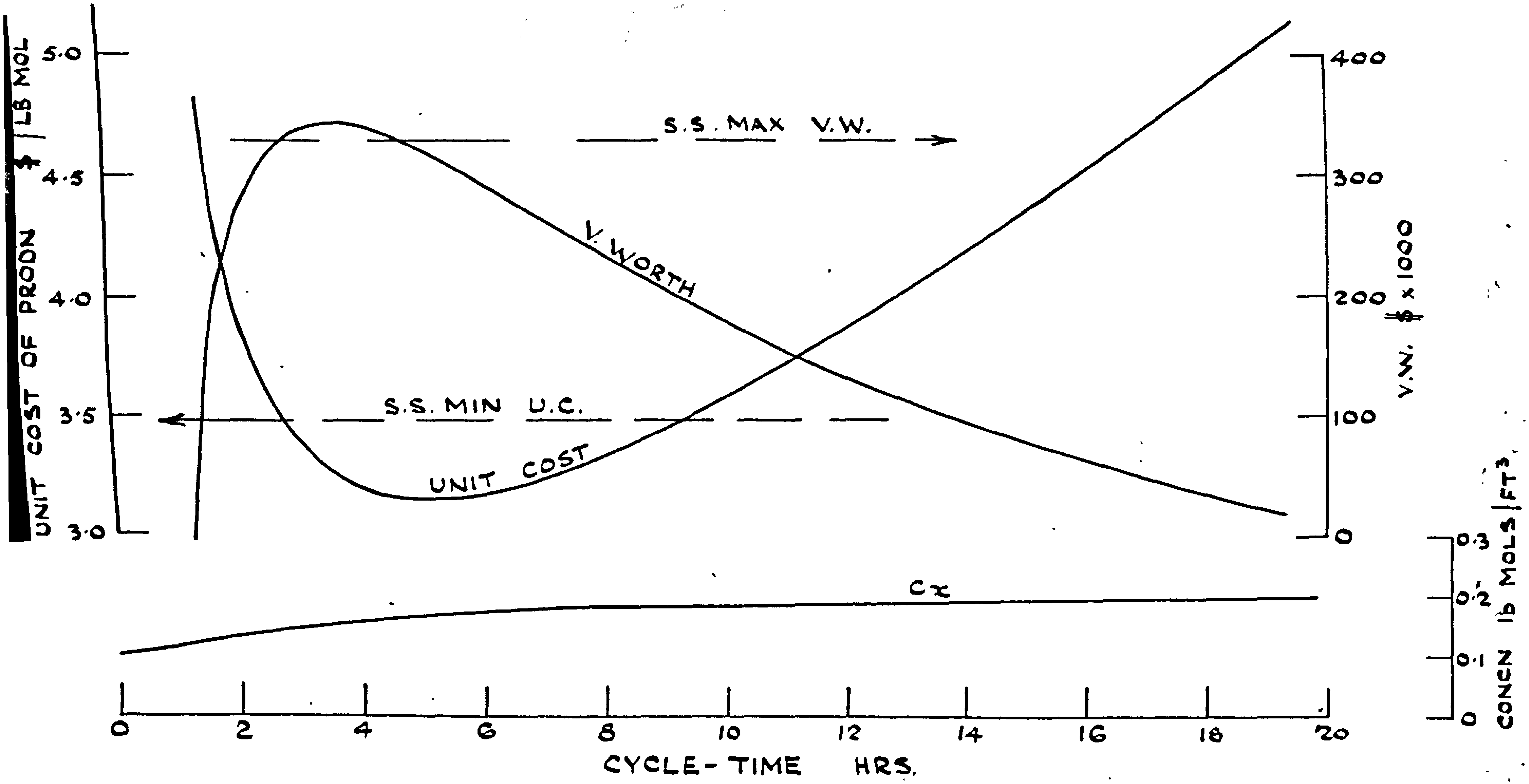
PURGING STRATEGY FOR SYSTEM 2.

Fig. 6.8

is, cycle lengths $>$ 6 hours and $<$ 16 hours.

Should a restriction be placed on the level of inert material permissible in the system, a limit may be imposed on the length of cycle which can be used. Such a limit might be the line AB in figure 6.7, equivalent to a maximum concentration of X of 0.190 lb moles/ft^3. In an instance such as this, the upper limit of the feasible cycles would be 11 hours, rather than 15 hours for the U.C. example discussed. It should also be noted that associated with the S.S. optima shown in figure 6.7, there are operating C_X concentrations. These concentrations are shown in figure 6.5. An important point is that the concentration of X present at the optimum S.S. condition for a given criterion is less, in all instances, than the level of X present at termination of the optimum cycle length for UNS. S. operation (see for example, Table 6.2). This observation holds for all the results obtained in the study.

A case in which the use of V.W. as the economic criterion could lead to UNS. S. operation being preferred to S.S. is indicated in figure 6.9. In this example the reactor volume is smaller and the raw material costs are less than in the case of figure 6.7.



PURGING STRATEGY FOR SYSTEM 1.
$V_R = 10, \quad M_C = 1.2$

Fig. 6.9

Comparison of figures 6.7 and 6.8 enables the effect of the increased production obtained from system 2, to be measured in terms of the greater V.W. and the lower U.C. of the system relative to system 1 in the case of UNS. S. operation. If the S.S. optima shown on these figures are compared, it will be noted that those for system 1 are slightly more favourable than the system 2 equivalents i.e.

	SYSTEM 1	SYSTEM 2
U.C.	3.5006	3.5145
V.W.	1,005,091	1,000,083

a feature opposed to the situation present in UNS. S. operation. Table 6.3 shows the trend in this direction for S.S. operation. Increasing the raw material costs (M_C) will improve the standing of system 1 relative to system 2 for both the U.C. and V.W. criteria. A few results obtained for V_R, reactor volume, indicate that reduction of V_R causes a like result, as is shown in the same table.

TABLE 6.3.

EFFECT ON ECONOMIC CRITERIA OF VARIATION IN RAW MATERIAL COSTS FOR SYSTEMS 1 AND 2.

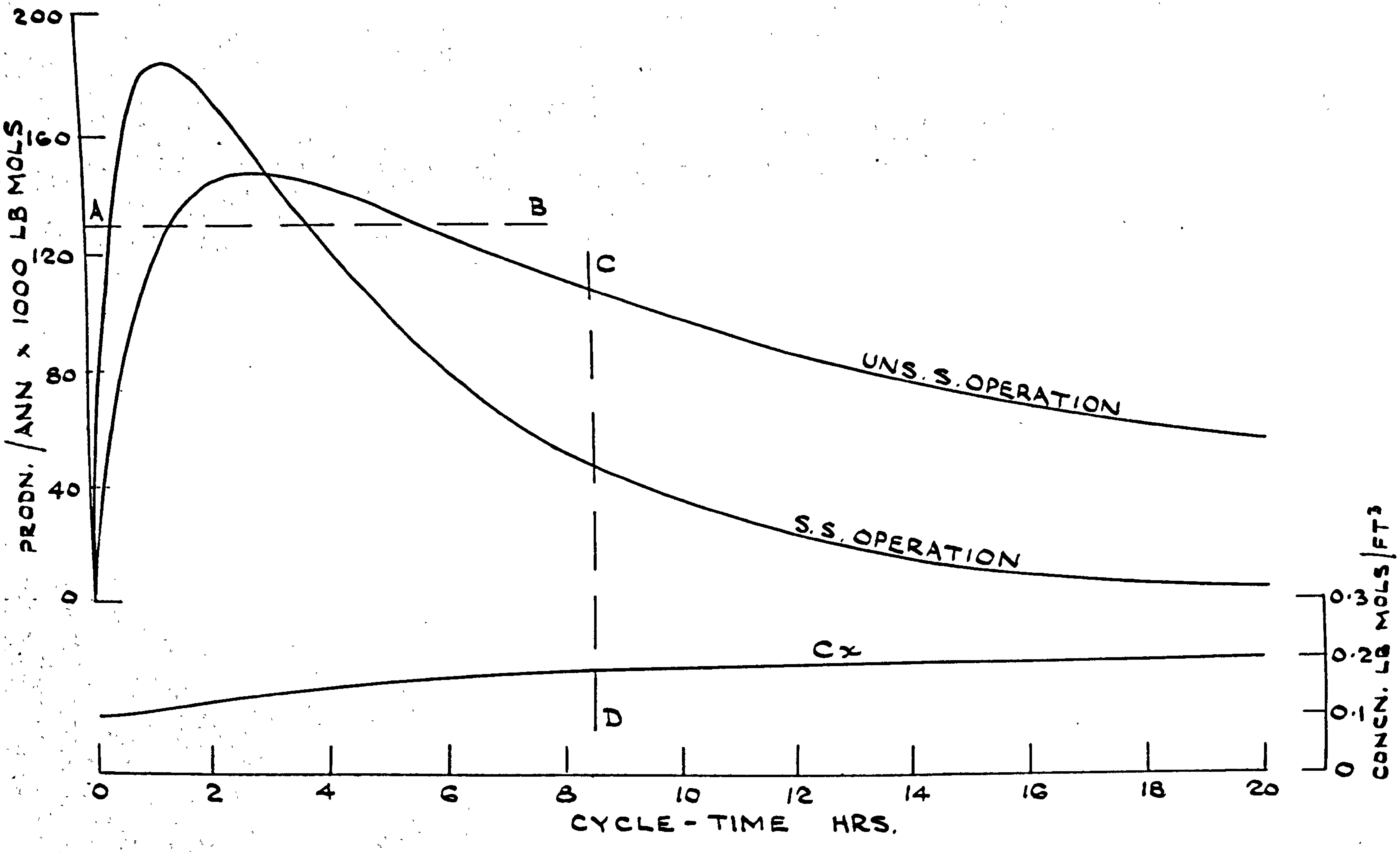
UNIT COST (\$/lb mol)

M_C (\$/lb mol)	SYSTEM 1	SYSTEM 2	DIFF. [SYS.1 < SYS. 2]
0.6	1.3375	1.3423	0.0048
1.2	2.0825	2.0930	0.0105
2.4	3.5006	3.5145	0.0139
V_R (FT^3)			
60	2.0825	2.0930	0.0105
10	3.4791	3.5345	0.0554

VENTURE WORTH (\$)

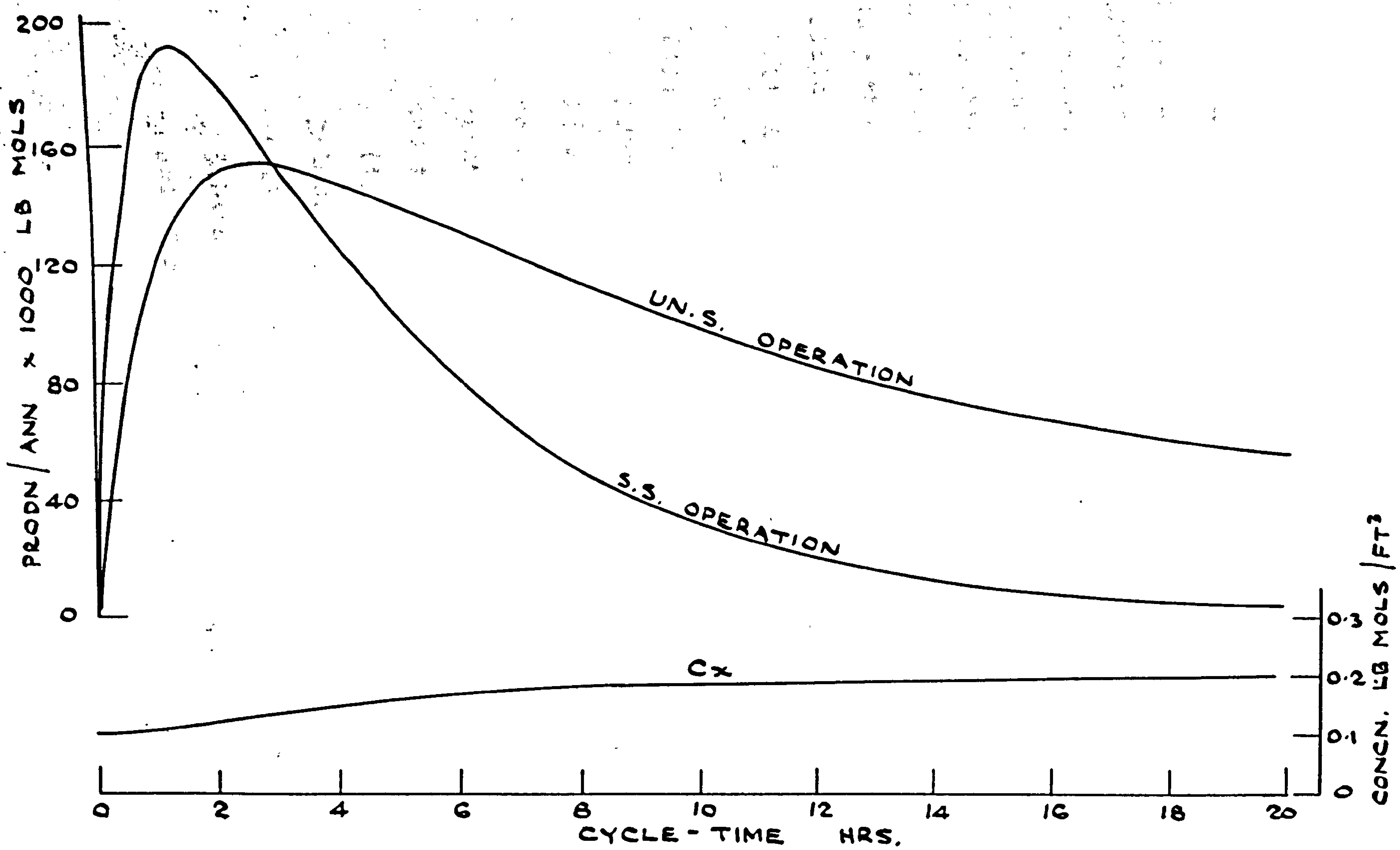
M_C	SYSTEM 1	SYSTEM 2	DIFF. [SYS. 2>SYS. 1]
0.6	2,475,364	2,568,289	92,925
1.2	1,957,386	1,996,544	39,158
2.4	1,005,091	1,000,083	- 5008
V_R			
60	1,957,386	1,996,544	39,158
10	329,346	311,535	- 17,811

In figures 6.10 and 6.11, it may be seen that S.S. operation is more favourable to high production rates,



PURGING STRATEGY FOR MAX. PRODN. FROM SYSTEM 1

Fig. 6.10



PURGING STRATEGY FOR MAX. PRODN. FOR SYSTEM 2

Fig. 6.11

a fact true for both systems. Thus, for situations in which a maximum production criterion is being adhered to, a different strategy (as has already been indicated) will be necessary. It is also evident from figure 6.10, that any given production rate below the maximum of the curves may be attained by two or more methods of production. Consider an annual production requirement of 130,000 lb mols - the line AB on figure 6.10, four alternatives are possible

(i) S.S. operation at the reactor conditions present at t = 0.50 hours or 3.80 hours or

(ii) UNS. S. operation with cycle lengths of 1.50 or 5.70 hours. Depending on which economic criterion is used to judge the production, one method will be the optimum. Table 6.4 demonstrates a typical situation. Points which may be noted in the table are :

(i) S.S. operation is necessary for production > 150,000 lb mols/ann.

(ii) In no case is operation at the conditions present at the shorter cycle lengths more desirable for S.S. operation.

(iii) In no case is the shorter of the two cycle lengths preferable for UNS. S. operation.

(iv) The table ignores the effect of the build-up of X in the system whereas a limitation on the amount of X permissible may change the position. Let the line CD on figure 6.10 represent such a limiting concentration of X = 0.180 lb mols/ft^3.

TABLE 6.4.

OPTIMAL PRODUCTION STRATEGIES FOR SYSTEM 1.

	S. STATE		UNS. S. STATE	
	POINTS OF OPERN(CYCLE)		CYCLE LENGTHS(HRS)	
PRODN (lb.mol/a.x1000)	FIRST	SECOND	FIRST	SECOND
180	1.10	1.90	-	-
160	0.80	2.75	-	-
140	0.60	3.40	1.90	4.50
120	0.45	4.20	1.25	6.90
100	0.35	5.00	0.85	9.50

Table 6.4 Continued:

	STEADY STATE				UNSTEADY STATE			
	UNIT COST ($/lb mol)		V.W. ($ x 1000)		UNIT COST ($/lb mol)		V.W. ($ x 1000)	
PRODN	FIRST	SECOND	FIRST	SECOND	FIRST	SECOND	FIRST	SECOND
180	4.98	4.07*	≑200	975*	-	-	-	-
160	>15	3.67*	< 50	995*	-	-	-	-
140	>25	3.56*	< 0	930*	≑6.3	3.93	<-500	770
120	>40	3.50	<-1000	805	>10	3.46*	<-2000	820*
100	>50	3.51	<-1500	671	>15	3.37*	<-4000	700*

Note: optimal decisions for each criterion, marked with asterisk.

	OPTIMAL MODE OF OPERN.	
PRODN	U.C.	V.W.
180	S.S.	S.S.
160	S.S.	S.S.
140	S.S.	S.S.
120	UNS.S.	UNS.S.
100	UNS.S.	UNS.S.

Production at the rate of 100,000 lb. moles per annum is not now possible by UNS.S. operation at the longer and preferable cycle length. The choice is restricted to S.S. operation or UNS.S. operation at the shorter cycle length - a choice favouring S.S. operation.

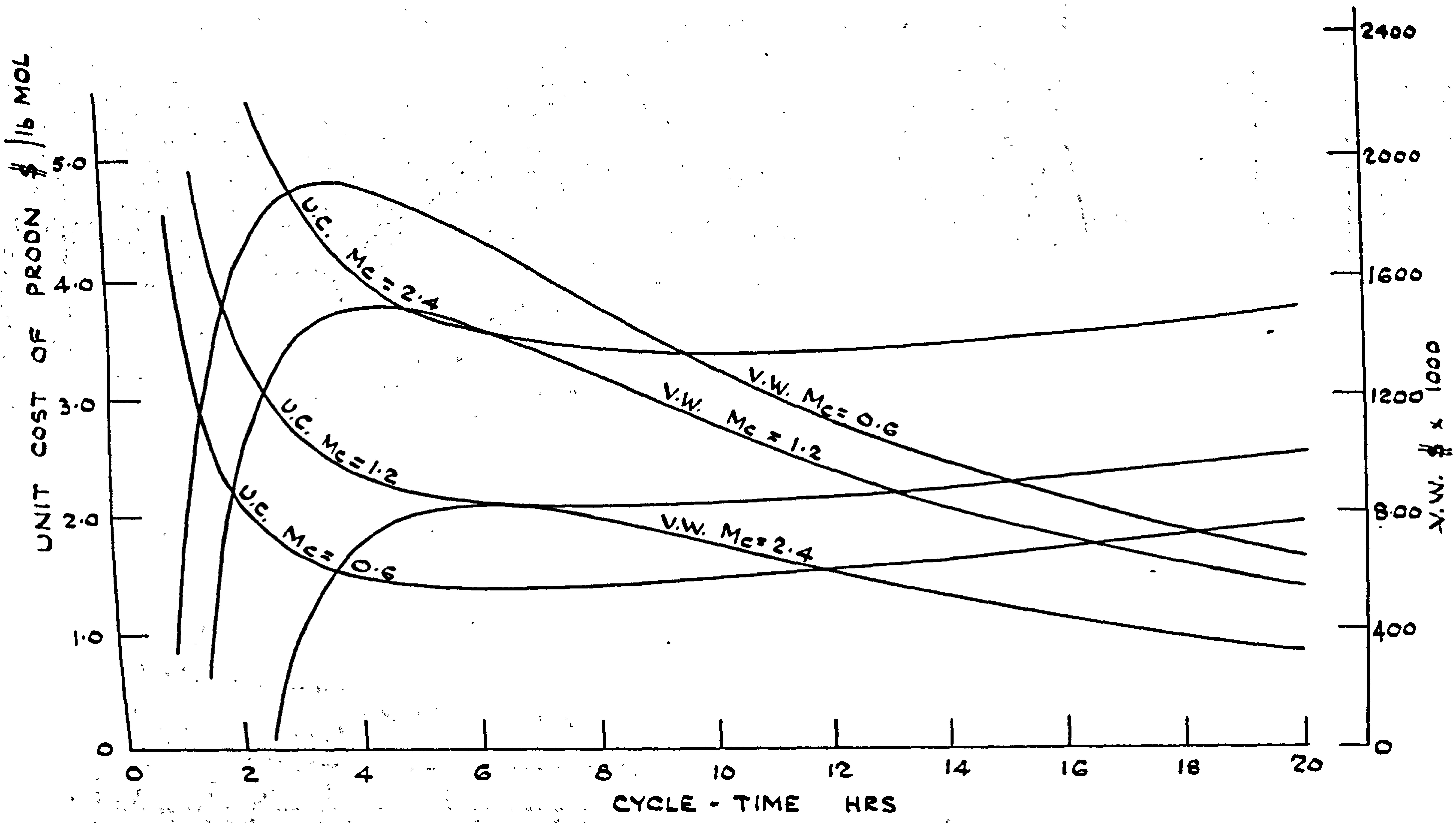
6.4 Effect of Variation in Parameters on the Optimal Points of Operation.

The effects caused by changes in the parameter M_C (Raw Material Cost) are shown in figures 6.12, 6.13 and 6.14. In figure 6.12, the changes that occur in the U.C. and the V.W. can be observed as a function of the cycle length. As M_C decreases the minimum U.C. and the maximum V.W. occur at shorter cycle lengths. For example, for $M_C = 2.4$ ¢/lb mole, maximum V.W. occurs when a cycle length of 6.3 hours is operated, but at $M_C = 0.6$, a cycle length of 3.8 hours will result in the maximum V.W. For S.S. operation, reduction in M_C produces the same result, although to a somewhat lesser degree, as shown for example in Table 6.5.

TABLE 6.5.

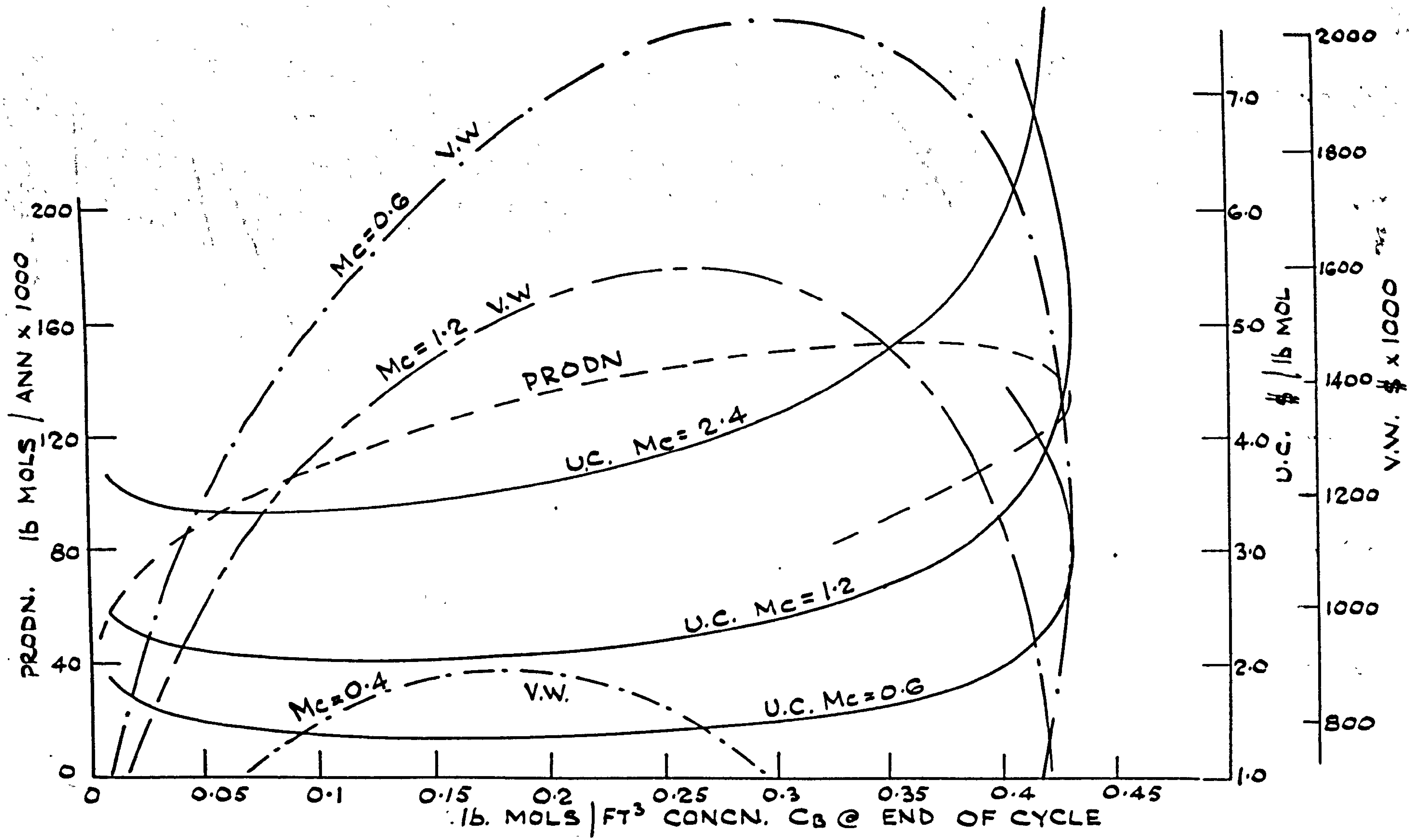
VARIATION IN OPTIMUM OPERATING CONDITIONS FOR SYSTEM 1 WITH RAW MATERIAL COST.

	UNS.S. OPERN CYCLE (HRS)		S.S.OPERN AT CONCNS AT CYCLES (HRS)	
M_C(¢/lb mol)	MIN. U.C.	MAX. V.W.	MIN. U.C.	MAX. V.W.
2.4	10.1	6.3	4.50	2.5
1.2	8.2	4.5	3.50	2.0
0.6	6.6	3.8	3.0	1.5



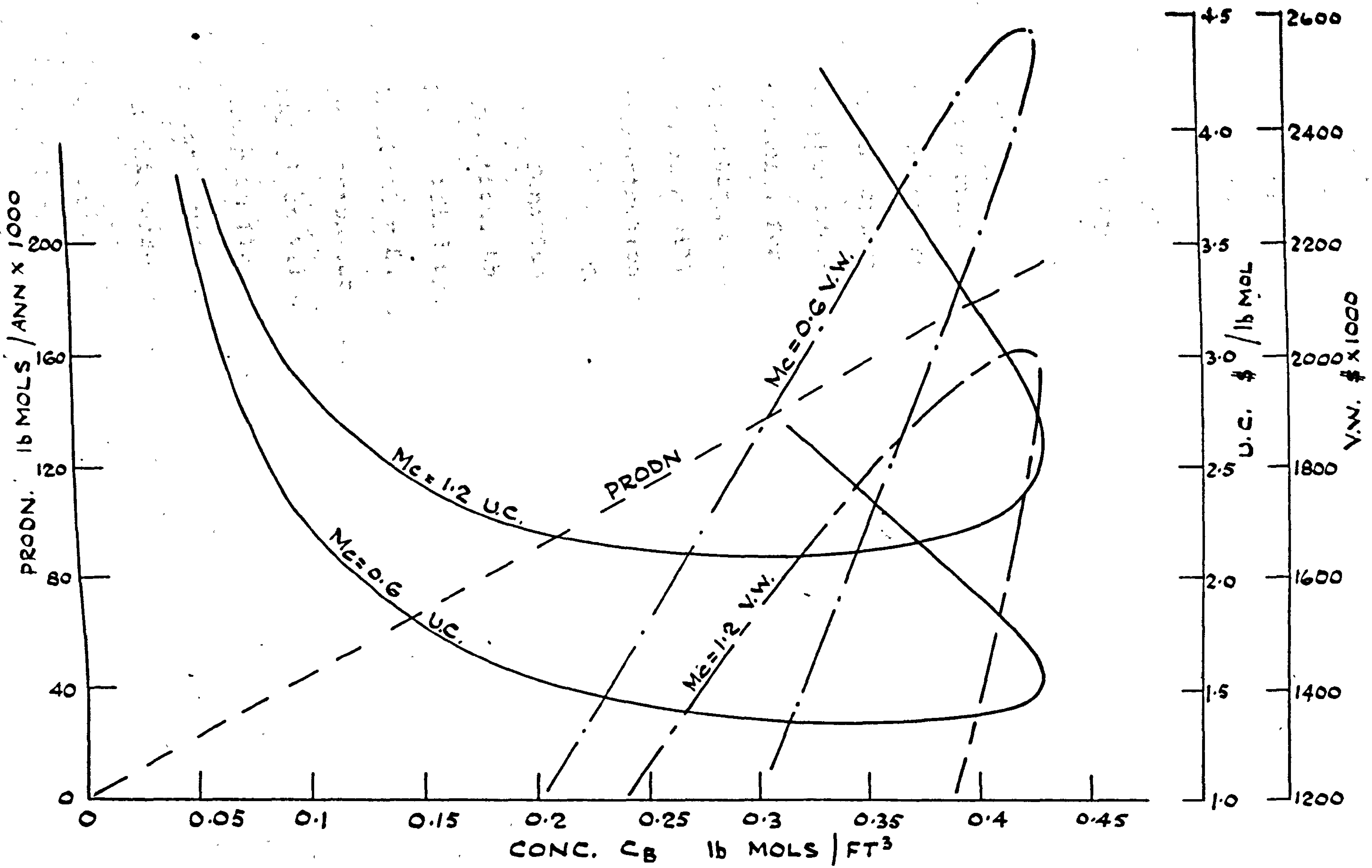
EFFECT OF VARIATION IN RAW MATERIAL COST ON ECONOMIC CRITERIA FOR SYSTEM 1. (UNS.S. OPERATION).

Fig. 6.12



EFFECT OF VARIATION IN RAW MATERIAL COST ON ECONOMIC CRITERIA FOR SYSTEM 2. (UNS.S. OPERATION).

Fig. 6.13



EFFECT OF VARIATION IN RAW MATERIAL COST ON ECONOMIC CRITERIA FOR SYSTEM 2. (S.S. OPERATION).

Fig. 6.14

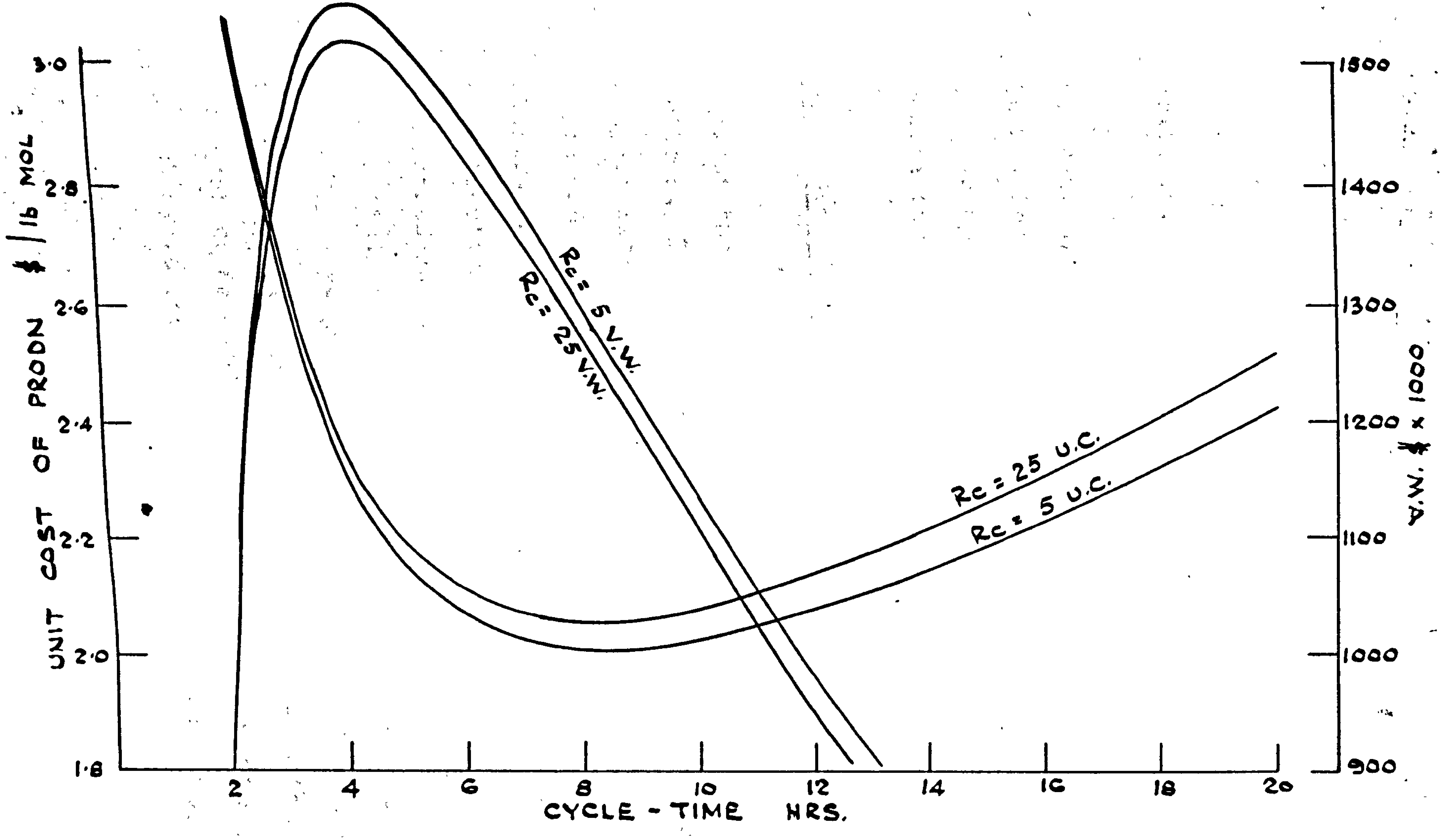
The operating conditions for the S.S. equivalent to the cycle lengths shown may be obtained from figure 6.1.

Figures 6.13 and 6.14 give the position for system 2 and a like effect occurs. In these two figures the curves for the economic criteria are plotted against the concentration of C_B, as opposed to cycle time. For UNS.S. operation i.e. figure 6.13, the concentration of C_B is that present at the termination of the cycle. For example, for $M_C = 1.2$, the maximum V.W. will be obtained by operating a cycle, at the termination of which the concentration of B will be 0.263 lb mols/ft^3. In figure 6.14, the concentration of B is the actual S.S. operating concentration.

The production per annum has also been plotted as a function of C_B in the two figures. In the case of S.S. operation, the output is a linear function of C_B. This may be verified by consideration of the steady state equations in Chapter 5. It will be noticed that the shape of the production curve in figure 6.13 permits two solutions for any given value of C_B. The same is true for S.S. operation shown in figure 6.14, in which the production curve returns exactly upon itself. The existence of the two solutions in this case may be observed from the U.C. and V.W. curves.

This phenomenon is analogous to that of obtaining the same output for different cycle lengths, as discussed in section 6.3. The steepness of the V.W. curves, and the U.C. curves to a lesser extent, in figure 6.14 are indicative of the critical nature of the optima for these criteria when operating at S.S. Somewhat flatter curves are obtained for UNS.S. operation, a feature probably due to the fact that the output is the result of an integration over the range of the concentration of B present during the cycle. This 'average' is opposed to a single fixed value of C_B governing the output in the S.S. case.

The effect of changing the capital cost of the reactor is shown in figure 6.15. The U.C. and V.W. curves are altered, although the cycle lengths at which the optimum points occur are practically constant. Within the assumed economics of this study the effect of changes in the raw material costs are more pronounced than the effect of variation in the reactor costs. For example, for assumed values of $M_C \approx 1.2$ and $R_C \approx 25$, a reduction in M_C by a factor of 2 reduces the minimum U.C. by 33% and increases the maximum V.W. by 27%. On the other hand, a reduction in the costs of the reactor by a factor of 5, produces changes



EFFECT OF VARIATION IN REACTOR COST ON ECONOMIC CRITERIA FOR SYSTEM 1. (UNS.S. OPERATION)

$M_C = 1.2$

Fig. 6.15

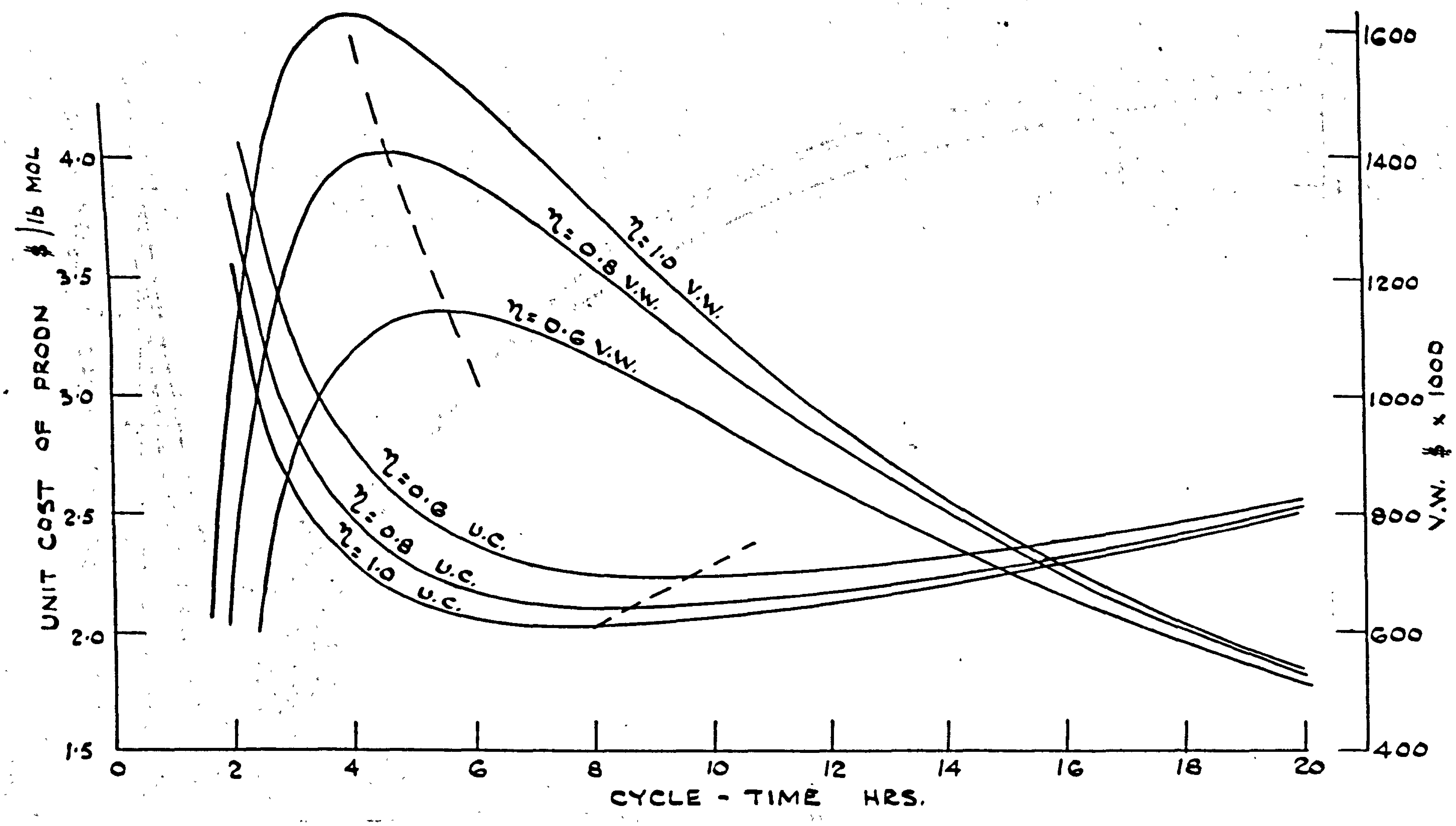
of the order of only 2.3% and 2.2% respectively, for the criteria.

The effect of variation in the efficiency of separation, η, is shown in figure 6.16. The result of increasing efficiency is to cause the optima to occur at shorter cycle lengths, an effect similar to that caused by decreasing raw material costs.

6.5 Some Observations on the Recycle Stream.

The 'average' recycle rate, which is plotted against the cycle time in figure 6.17, has been deduced as follows. In the course of computation, the integrated recycle flow per half hour was calculated on a cumulative basis and obtained as an output from the programme. To obtain, the recycle flow in any particular half-hour period, a subtraction was merely required. The figure obtained was considered as an average recycle rate for the period and was plotted at the mid-point of the two times in question.

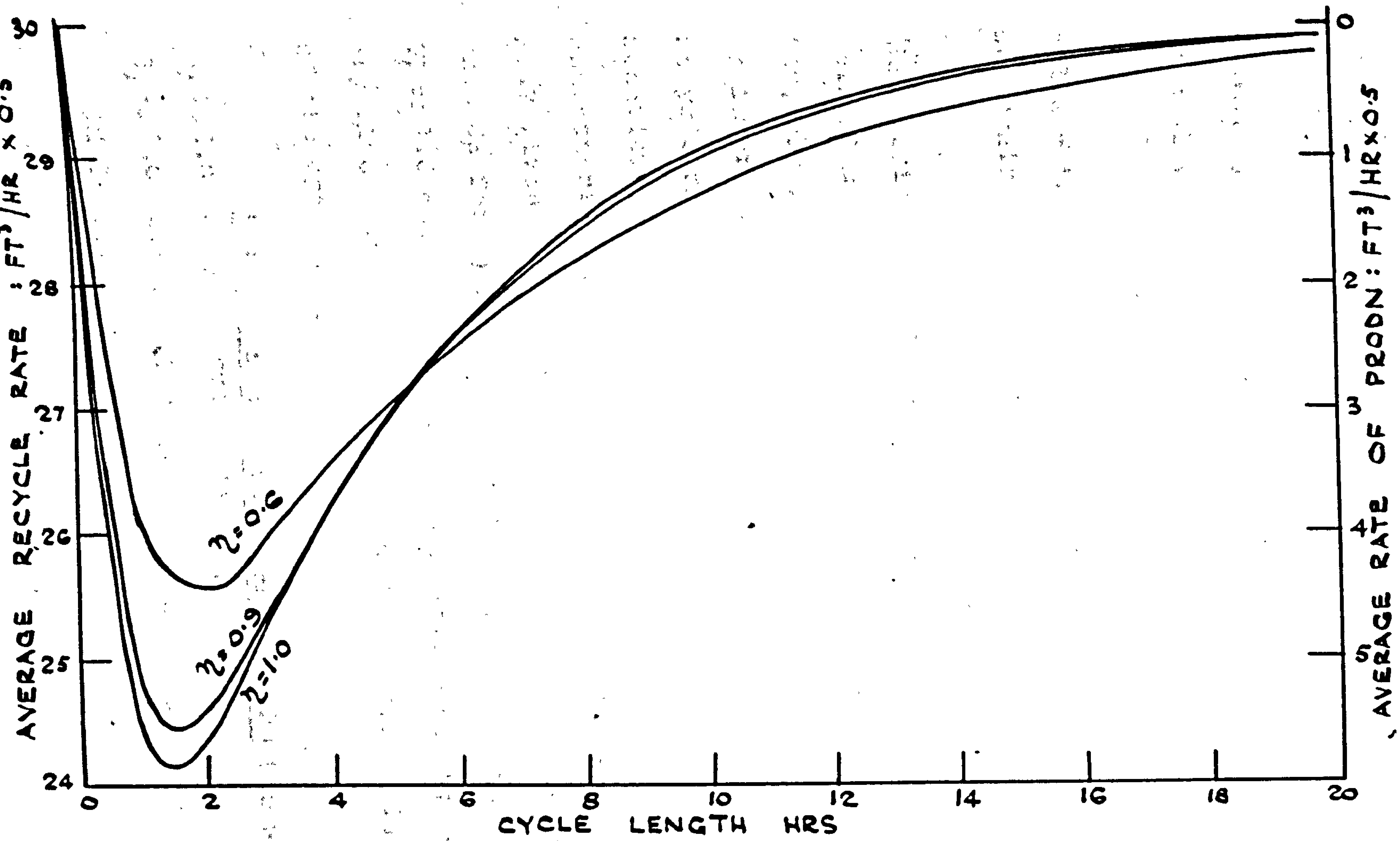
It will be seen that at time $t=0$, the recycle rate, ϕ_R, is equal to F, the flow rate into the reactor, an equation dependent on the assumed start-up conditions. As the cycle starts, it drops rapidly, goes through a



EFFECT OF EFFICIENCY OF SEPARATION ON ECONOMIC CRITERIA FOR SYSTEM 1. (UNS.S. OPERATION)

$M_C = 1.2$

Fig. 6.16



VARIATION OF RECYCLE RATE WITH η

UNS.S. OPERATION SYSTEM 1

Fig. 6.17

minimum value and then increases more gradually back to its initial value. Since the equation

$$F = \phi_R + \phi_P \tag{5.11}$$

holds - the average (instantaneous) rate of production may be obtained directly from this graph.

The changes in the recycle occasioned by changes in the efficiency of separation are plotted in this figure. Initially the lower the efficiency of separation, the greater the recycle rate but as the cycle progresses an inversion takes place, and as the η decreases the recycle rate becomes less. An explanation for this behaviour, due to a combination of dynamic and kinetic characteristics, may be postulated with the aid of figure A6.7 given in Appendix 6. In figure A6.7, it will be seen that C_B for $\eta = 0.6$ is at all times greater than C_B for $\eta = 1.0$ and that the difference between the two values at any given time is significant over a considerable period of the cycle i.e.

	$\bar{t} = 2$	$\bar{t} = 6$	$\bar{t} = 10$	$\bar{t} = 14$	$\bar{t} = 20$ (hours)
$\eta = 0.6$	0.487	0.275	0.139	0.070	0.025
$\eta = 1.0$	0.375	0.158	0.062	0.024	0.006
DIFF	0.112	0.117	0.077	0.046	0.019

Considering the curve for $\eta = 0.6$ in figure 6.17, only 60% of the B being produced is being separated off and the remaining 40% is contributing to the volume of the recycle stream. As the reaction gets under way, the concentration of B in the stream entering the separator increases, the rate of output of product, ϕ_P, increases and ϕ_R decreases. The concentration of B falls in the reactor as the cycle progresses, after going through a maximum, with a resulting fall in the output of B from the separator and an increase in ϕ_R. For $\eta = 1.0$, the same behaviour occurs although in this case the initial decrease in ϕ_R is aided by the total absence of B in the recycle. The curves cross as the cycle proceeds because due to the more rapid fall-off in C_B when $\eta = 1.0$, there is relatively less product with increasing t and hence in agreement with equation (5.11), $\phi_R \longrightarrow F$. When $\eta = 0.6$, with C_B falling off more slowly, a relatively greater amount of product is produced at the longer cycles. From figure 6.17, we have values for, ϕ_P average, e.g.

	$t = 10$	$t = 15$	$t = 19$ (hours)
$\eta = 0.6$	1.25	0.54	0.28
$\eta = 1.0$	0.93	0.29	0.11

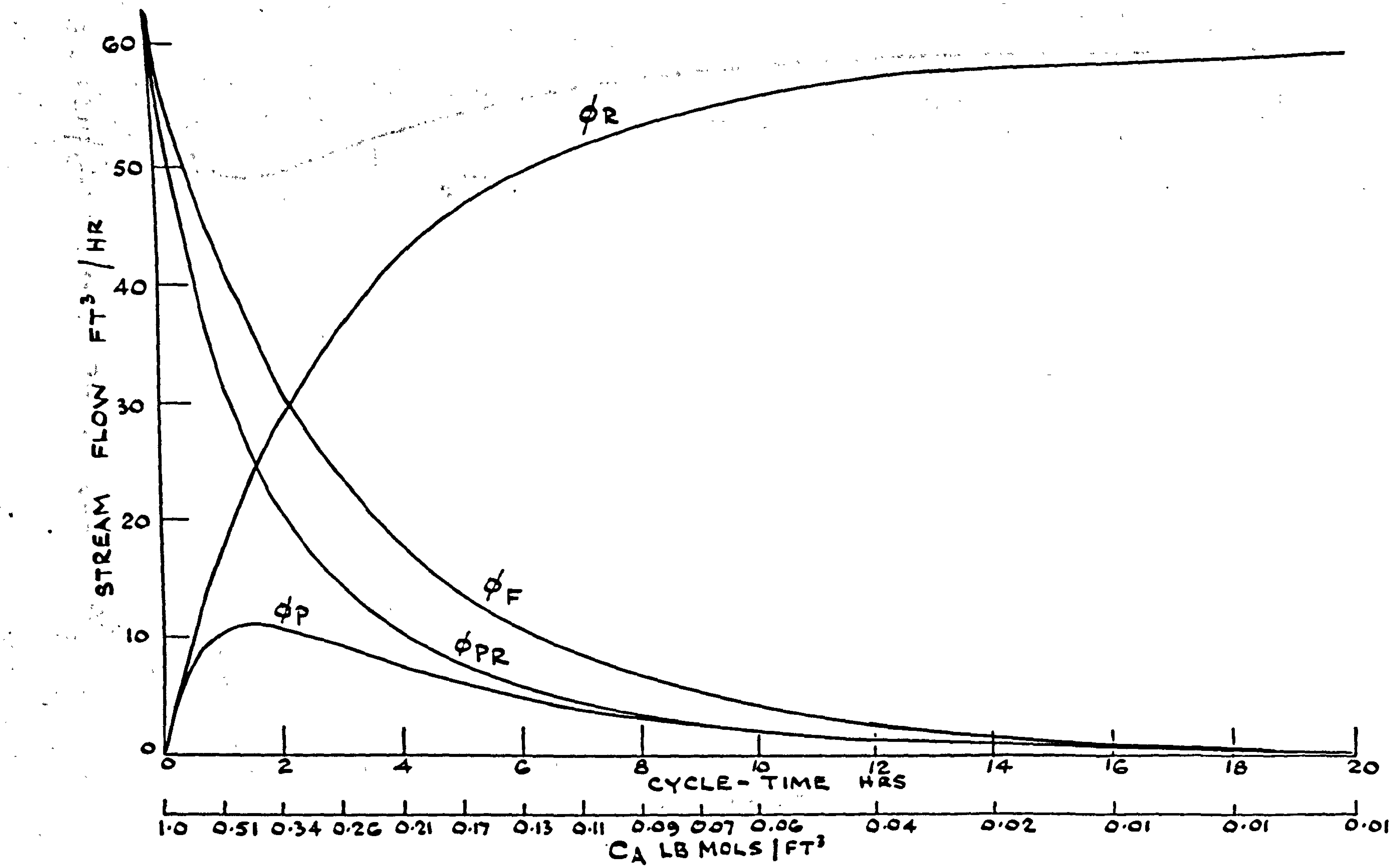
The pattern of stream flows for steady state operation is shown in figure 6.18 and in figure 6.19 a comparison is made of the recycle streams for the two modes of operation. The equations in question for figure 6.18 are:

$$\text{(i)} \quad \phi_F + \phi_R = F \quad (= 60) \qquad (5.10)$$

$$\text{(ii)} \quad \phi_F = \phi_P + \phi_{PR}$$

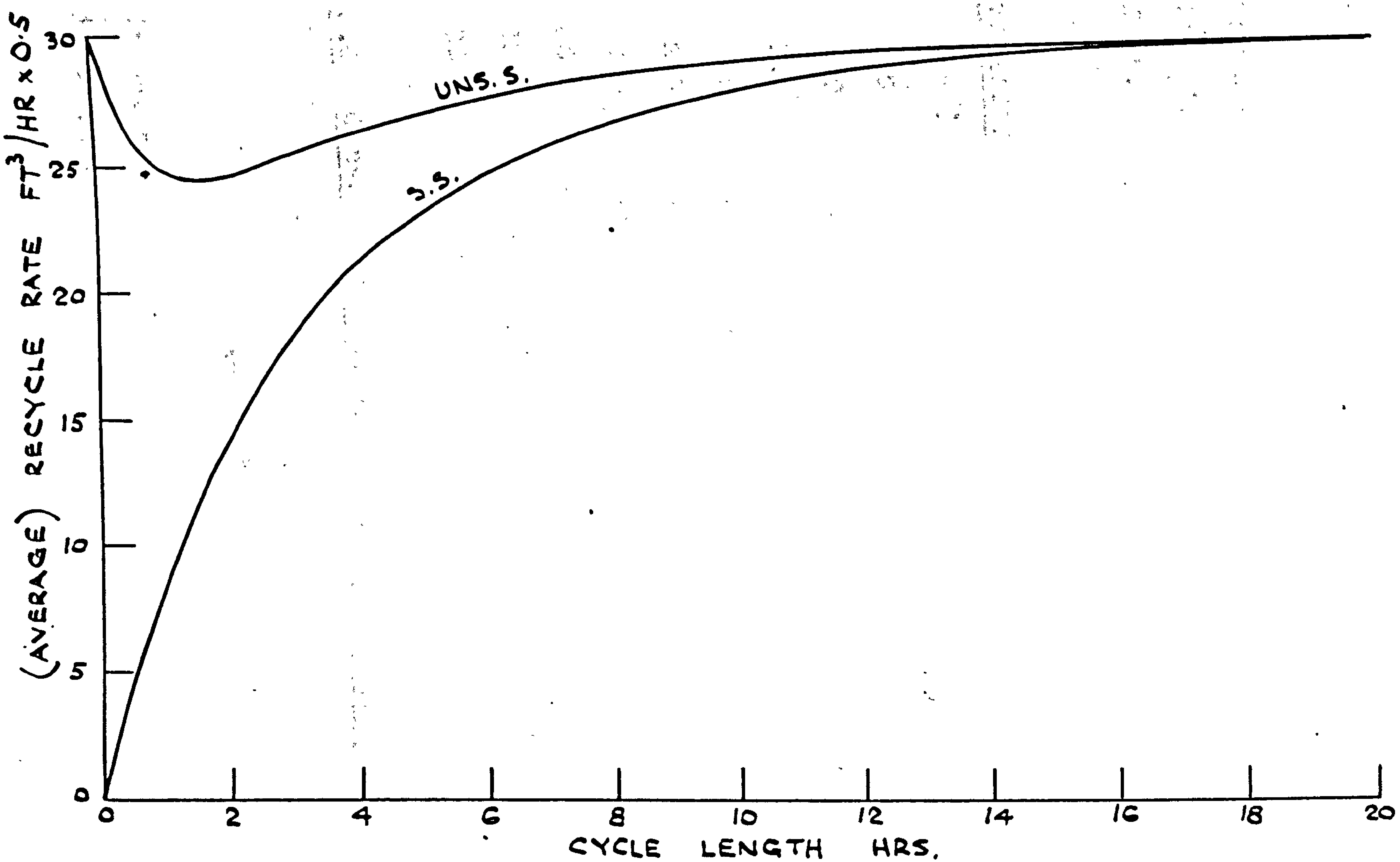
It can be seen that at the maximum production rate of $\phi_P = 11.1$ ft^3/HR, the purge stream has a value of 25.1 ft^3/hr and $\phi_F = 36.2$ ft^3/hr. At this point of operation C_A has a value of 0.412 lb moles/ft^3 and it may be shown that the loss of A in the purge stream is equal to 38.6% of the total A entering the system. The cycle length for maximum production, UNS.S. operation, is 3.0 hours giving an effective cycle time of 3.15 hours. The equivalent loss of A through purging at this cycle frequency is 66.1% of the entering A. The corresponding loss of A through purging at the minimum U.C. optima are 13.5% for S.S. operation and 6.3% for UNS.S. operation.

The position of the recycle stream as an influential variable in the system is evident from figure 6.17 in which a relatively small change in the recycle rate



TYPICAL PATTERN FOR SYSTEM FLOWS
S.S. OPERATION, SYSTEM 1.

Fig. 6.18



BEHAVIOUR OF RECYCLE STREAMS, SYSTEM 1.

Fig. 6.19

may correspond to large changes in the component concentrations in the reactor. Table 6.6 helps to demonstrate this fact.

TABLE 6.6.

VARIATION IN SYSTEM OPERATING CONDITIONS WITH RECYCLE RATE.

t (HRS)	C_A	C_B	C_X	ϕ_R(UNS.S.)	ϕ_R(S.S.)
0.5	0.685	0.284	0.103	27.80	10.34
1.0	0.513	0.389	0.110	25.32	17.80
1.5	0.412	0.412	0.118	24.54	23.83
2.0	0.346	0.399	0.125	24.50	28.88
2.5	0.299	0.371	0.133	24.80	33.14
3.0	0.263	0.339	0.140	25.20	36.74
10	0.055	0.074	0.187	29.06	55.89
15	0.018	0.024	0.196	29.68	58.67
20	0.006	0.008	0.199	29.89	59.56

6.6 Consideration of Second Order Reactions.

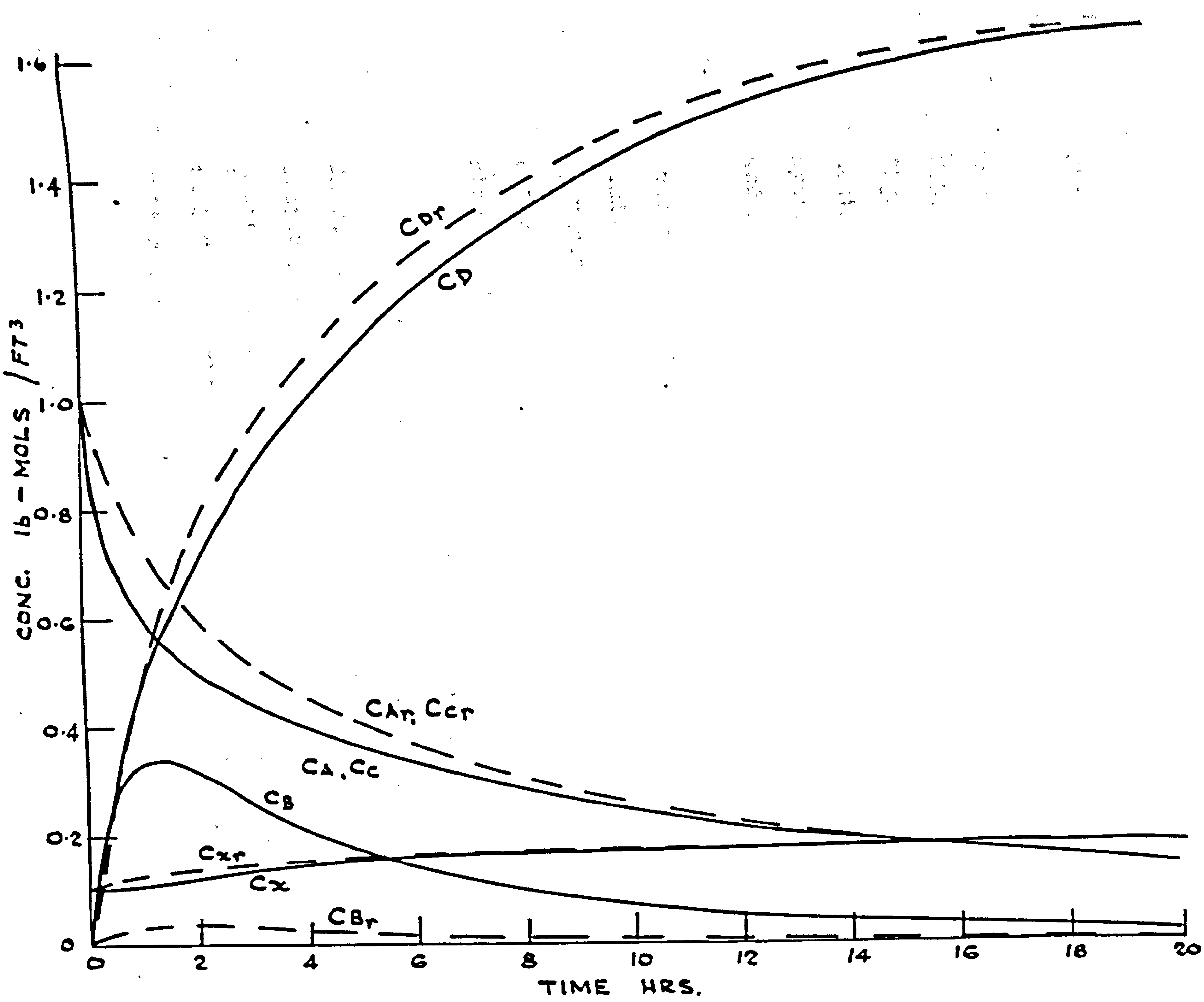
The reaction taking place is

$$A + C \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B + D$$

It was assumed that A and C were present in the feed stream in equal concentrations and thus the C_C v t curve is identical to the C_A v t curve. The second point that follows from this reaction is that since the output is pure B only, a considerable build-up of D will occur in the system. These two points will be observed in Figure 6.20 in which the time behaviour of system 2 (2^{ND} ORD.) is given and in figure A6.1 for system 1 (2^{ND} ORD.). The form of the curves are similar to those presented earlier for first order systems and need little comment. In fact, the introduction of a second order reaction fails to alter in character the behaviour pattern of the system.

The C_{Dr} v t curve may be noted in figure 6.20. At time $t = 0$, no D is present in the system. At time $t > 0$, the production of D starts in the system and the concentration of D, C_D, in the reactor will be greater than the concentration of D, C_{Dr}, in the separator due to time lags in the system. This situation remains until the increase in the concentration of D, due to the withdrawal of B from the separator, causes C_{Dr} to become greater than C_D.

Figures A6.2 and A6.3 given in Appendix 6, show typical optimum points of operation for the two second order systems. The optima shown are, as before, U.C., V.W., and maximum production and these figures are equivalent to



TYPICAL TIME-BEHAVIOUR OF SYSTEM 2 (2nd ORD).

Fig. 6.20

figures 6.5 and 6.6.

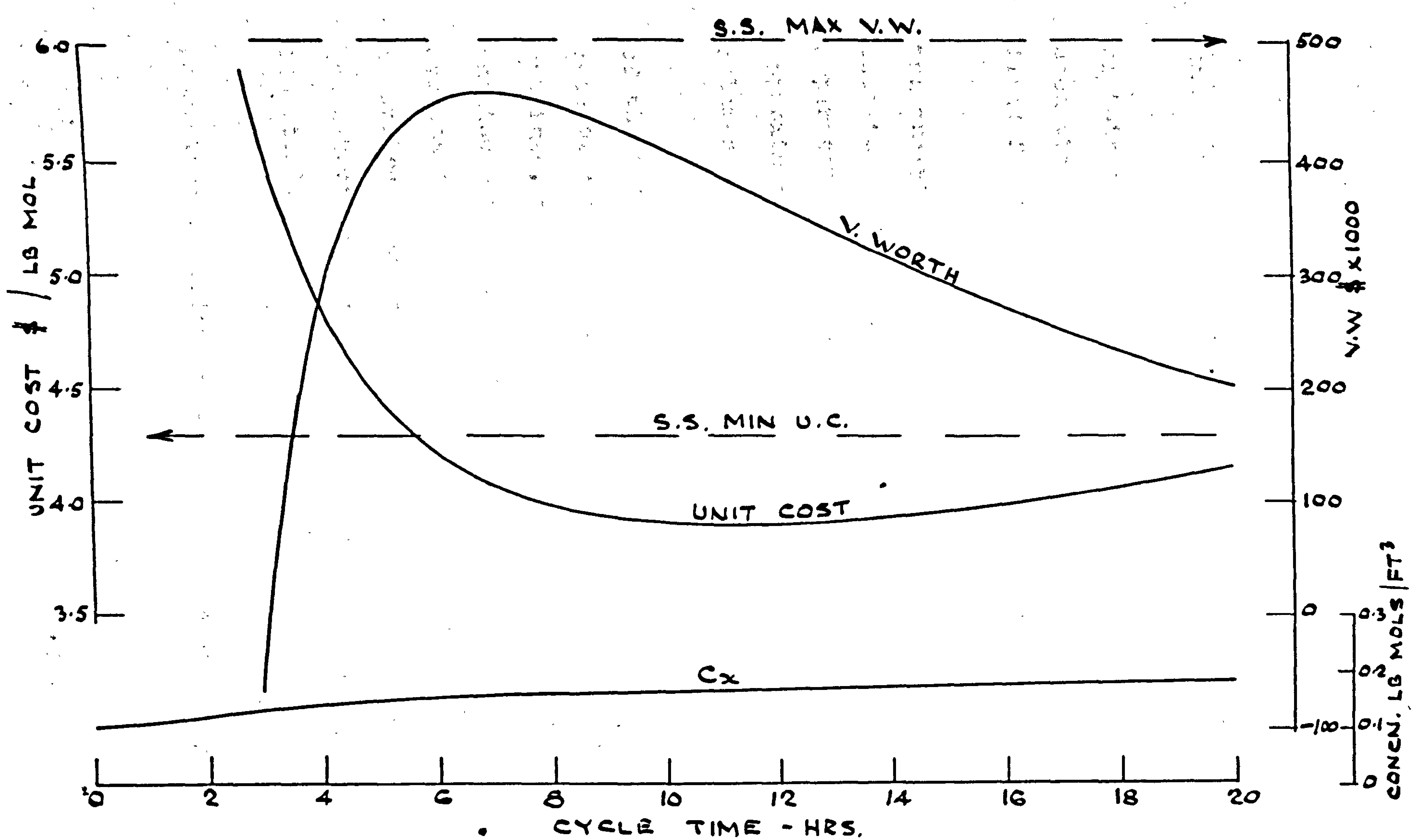
The purging strategy for system 2 (2^{ND} ORD.) may be obtained from figure 6.21 and that for system 1 (2^{ND} ORD.) from figure A6.4 in Appendix 6. Graphs analogous to figures 6.10 and 6.11, enabling the purging strategy for maximum production to be outlined for the second order systems, are also shown in this Appendix (i.e. figures A6.5 and A6.6).

The favourable position of UNS.S. operation when the accepted criterion is U.C. may be seen from figure 6.21. A U.C. less than the S.S. minimum U.C. can be achieved by UNS.S. operation for cycles of $>$ 5.5 and $<$ 23 hours (approx.). Also the difference between the minima is sizeable i.e.

S.S. MIN. U.C. $\simeq$ 4.295 $/lb mol.

UNS.S. MIN. U.C. $\simeq$ 3.900 " " "

There is very little change in the purging strategies as compared with those indicated earlier. In general the position of UNS.S. operation is improved slightly, relative to S.S. operation and this improvement holds for all the criteria studied.



PURGING STRATEGY FOR SYSTEM 2 (2nd ORD.).

Fig. 6.21

6.7 Summary and Conclusions:

The results presented in the foregoing sections of this chapter are mainly comparative in nature, having been obtained from investigations on the two variants outlined for the recycling reactor system.

For the two systems studied it was found that the analytical expression derived from system 1 can be used to describe the behaviour of system 2, when the separator hold-up volume is small. In this study, the approximation was satisfactory for cases where the relative volumes of the separator and reactor were $V_H \leqslant 0.05\ V_R$.

The effect of varying V_H on the optimum values of the three criteria studied is not significant in the case of system 1. In system 2 more marked variation is obtained, the maximum output and maximum V.W. increasing and the minimum U.C. decreasing as V_H increases. In both systems reducing the value of V_H results in the optima occurring at shorter cycle lengths. Furthermore as $V_H \longrightarrow 0$, the behaviour of the two systems will become nearly identical.

It has been demonstrated that under certain conditions intermittent purging, involving operations of an unsteady state, is more profitable than steady state operation with continuous purging. The level of inert material present in the system was less in all cases studied, at the S.S. optima than that present at the comparable UNS.S. optima.

The purging strategy will vary depending on the criterion, economic or otherwise adopted. The optimum cycle length will also vary when different economic criteria are chosen as yardsticks. The considerable divergencies which are present between optima, emphasize the necessity for making the correct choice of criterion.

Variation in either the cost or design parameters will affect both the magnitude and location of economic optima. The magnitude of a production optimum is unaffected by changes in the cost parameters, nor will the operating conditions, e.g. cycle length to effect the maximum output, change.

The importance of the recycle stream as an operating variable in the system has been indicated, together with the relative importance of the raw material cost, reactor capital cost and efficiency of separation.

The analysis presented represents an initial study in an area in which apparently little investigation has hitherto been carried out.

NOTATION

It will be found in certain instances that symbols have been used with different meanings in the various sections of the thesis. The symbols are defined in the text, usually adjacent to the expressions in which they appear. Equations, Section and Appendix locations are shown for example as (3.12), (s.16) and (A3(i)) respectively.

A.	Numerical constant (3.6). Reactant, Chapters 5 and 6.
A_i.	Alternative possible result i (s.1.6).
B.	Numerical constant (3.6). Reaction product, Chapters 5 and 6.
C.	Numerical constant (3.6). Unit cost of production, \$/ /lb.mole (3.1). Reactant, Chapters 5 and 6.
C_1.	Amortized incremental unit investment cost of column, \$ /ft^2 plate. yr.
C_2.	Amortized incremental unit invbstment cost of tubular equipment, \$ /ft^2 yr.
C_3.	Cost of steam and coolant necessary for 1 lb. mole of product, \$.

C_4, C_F.	Incremental unit investment cost of column, \$ /ft.^{2} plate.
C_5, C_T.	Incremental unit investment cost of tubular equipment, \$ /ft.^{2}
C_i.	Concentration of ith component, lb.moles/ft^3.
C_{io}, C_{ir}, C_{ip}, $C_{i(i)}$	Concentration of ith component in the feed, recycle, product and reactor inlet streams respectively, lb.moles/ft.^{3}
C_M.	Challengers adverse minimum (A1 (iii)).
C_S.	Cost of steam, \$ /1000 lbs.
C_W.	Cost of cooling water, \$ /1000 U.S. gals.
D.	Numerical constant (3.6). Reaction by-product, Chapters 5 and 6. Development expenditure, £ or \$ (s.1.5). Distillate or product rate, lb.moles/hr.
D_i, d_i.	Decision i (s.1.6)
D_L.	Liquid mol.diffusion coefficient, cm^2/sec.
D.C.F.	Discounted Cash Flow.
D.P.	Dynamic Programming.
d.	Depreciation rate for tax purposes, fraction /yr.
E.	Fractional or overall plate efficiency. Annual operating expense (5.48), Chapters 5 and 6.

E_{MV}.	Murphree vapour plate efficiency.
E_t	Net cash inflows in period t (s.2.3).
e.	Function (3.25).
F.	Column feed rate, lb.moles/hr. Reactor Inlet rate, ft^3/hr., Chapters 5 and 6. Cost factor (s.4.1).
F^*	Cost factor, defined (3.5a).
FA	Free area fraction in column cross section.
G.	Superficial mass vapour velocity based on column cross section, lbs./hr.ft.^{2}
G_a.	Allowable vapour velocity in column, lb.moles/hr.ft.^{2}
G_b.	Vapour handling capacity of tubular equipment, lb.moles/hr.ft.^{2}
g.	Inferiority gradient.
H.	Total hours in year, hrs. Total area of tubular equipment, ft.^{2} (A3(i)). Constant, defined (A5 (ii)).
h.	Hours operation, hrs/yr.
h_f.	Hours operation, fraction/yr.
h_w.	Weir height, ins.
I.	Initial or fixed capital investment, £ or \$. I_R, I_S, reactor and separator capital cost, respectively, \$.

I_c	Present value of investment outlays, £ or \$ (s.2.3).
I_w.	Working capital, £ or \$.
i.	Average interest rate on capital, fraction/yr.
i_m.	Minimum acceptable rate of return on capital, fraction/yr.
J.	Ratio of the slopes of the equilibrium and operating lines (s.3.3).
J_1, J_2, J_3.	Constants, defined (s.2.6).
K.	Plate efficiency factor. Constant, defined (s.1.5).
K_1.	Constant, defined (s.1.5).
k.	Index, indicating years from start of venture, (s.2.4-s.2.6)
k_1, k_2, k_3.	Constants, defined (s.3.5).
k_1, k_2.	Forward and backward reaction velocity constants, f(conc)/hr.
L.	Column liquid flow.
L.H.	Latent heat, btus/lb (A3 (ii)).
LH_s.	Available heat in steam, btu's/lb (A3(ii))
M.	Average molecular weight of the vapour stream.
M_i.	Molecular weight of component i.
M_c.	Raw material cost, \$/lb.mole A, Chapters 5 and 6.

m.	Maintenance, fraction/yr. Continuous rate of interest (2.6 and 2.7).
m*	Continuous rate of interest (2.4).
m_1, m_2.	Constants, defined (s.5.4).
N.	Number of stages in proces, Chapters 1 and 2. Number of theoretical plates in column, Chapters 3 and 4. Number of cycles/yr. Chapters 5 and 6.
N_m, N_M.	Minimum number of plates required for a separation at total reflex.
N_o, N_{oPT}.	Optimum number of plates.
N.P.V.	Net Present Value, £ or \$.
n.	Project lifetime, yrs.
O.	All operating costs, £ or \$ / yr.
O_1, O_2.	Alternative possible objectives (Al(iv)).
P.	Cash position, £ or \$ (2.3). Numerical factor relating S_a to I, fraction. Product output, ft^3 (5.25), Chapters 5 and 6.
P_a.	Net profit, £ or \$ (2.1).
$\underline{P}$ (r).	Control vector of stage r.
p.	Raw material cost, \$ /lb. mole. D.C.F. yield, fraction/yr. Chapter 2.

P.T.	Payout time, yrs.
Q.	Numerical factor relating I_w to I, fraction.
q.	Constant, defined (2.10).
$\underline{q}$ (r).	Cost vector of stage r.
R.	Percentage return on investment (2.1).
	Gross profit per annum (V.W. equations).
	Reflux ratio, Chapters 3 and 4.
	Recycle flow, ft^3, Chapters 5 and 6.
R_1, R_2.	Return from stage 1 or 2 (s.1.3).
R_a.	Gross profit, £ or $/ yr (2.2.)
R_c.	Reactor cost factor $.I_R=100R_c(5V_R+V_S)$, Chapters 5 and 6.
R_m; R_M.	Minimum reflux ratio for a separation with an infinite number of plates.
R_o. R_{OPT}.	Optimum reflux ratio.
R(r).	Return from stage r.
R_t.	Return from total N stage process.
r.	Taxable period of plant life, yrs.
S.	Sales revenue, $ /yr. Cross sectional area in column, ft^2 (A3.1).
S_a.	Salvage value of plant, £ or $.
S_t.	Disinvestment of working capital and scrap value (s.2.3).
S.S.	Steady state.

T.	Payout time, yrs. Project lifetime, yrs (s.2.3).
t.	Tax rate, fraction/yr.
t*.	Effective cycle time, hrs., defined (s.5.5).
U.C.	Unit cost of production, $ /lb.mole.
UNS.S.	Unsteady state.
V.	Vapour throughput rate in column.
Vg.	Vapour velocity based on column cross section, cm/sec.
Vo.	Net present value, £ or $ (s.2.3)
V_R, V_H, V_S.	Volume of reactor, hold-up section and separator, respectively, ft^3, Chapters 5 and 6.
V*.	Cost factor defined (3.24).
V.P.	Venture profit, £ or $.
V.W.	Venture worth, £ or $.
W.	Venture worth, £ or $.
X.	Raw material costs, $ /yr. Inert component, Chapters 5 and 6.
X_r.	State vector for stage r (Ai(i)).
$\underline{x}_i$, $\underline{x}(i)$	Input state vector (s.1.3).
Y.	Constant, defined (Ai(ii)).
$\underline{Y}(r)$.	Output state vector from stage r.
y.	Reaction yield, faction.

y_n avg., $y_{(n-1)}$avg: Average composition of the vapour leaving the n^{th} and $(n-1)^{th}$ plate.

y_n^*. Composition of vapour in equilibrium with liquid on the n^{th} plate.

Z. Constant, defined (Ai(ii)).

α Relative volatility. Constant, defined (A4(iv)).

β Constant, defined (A4 (iv)).

γ Constant, defined (A4(iv)).

δ Constant, defined (A4(iv)).

ϵ Constant, defined (s.4.4).

ζ Constant, defined (A4(iv)).

η Separator efficiency (s.5.3).

η_o Overall column efficiency (s.1.3)

η_p Plate efficiency (s.1.3)

θ Constant, defined (A3(ii)).

λ Constant, defined (A3(ii)).

$\lambda_1, \lambda_2, \lambda_3$. Constants, defined (s.3.3).

$\lambda_1, \lambda_2, \lambda_3 \lambda_4$. Constants, defined (s.5.4), Chapters 5 and 6.

μ_L Liquid viscosity of mixture, poise.

π Constant, defined (s.4.4).

ρ_i Density component i.

ρ_L.	Liquid density of mixture.
σ	Surface tension of mixture, dynes/cm.
τ	Mean residence time, hrs.
ϕ	Flow rate, ft^3/hr.
ϕ^*	Total flow/cycle, ft^3.
Ω	Constant, defined (s.4.4).

Subscripts:

i.	i^{th} component of vector, system or stage in question.
k.	k^{th} year of project.
r.	Stage r.
P,R,F,PR.	Product, recycle, feed and purge streams, Chapters 5 and 6.

Superscripts:

1, 2.	Perturbed level of variable (s.1.7).
j.	Specific level of variable.

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APPENDICES

No. 1 Appendix to Chapter 1.

No. 2 Appendix to Chapter 2.

No. 3 Appendix to Chapter 3.

No. 4 Appendix to Chapter 4.

No. 5 Appendix to Chapter 5.

No. 6 Appendix to Chapter 6.

APPENDIX 1

(i) Formal Statement of Dynamic Programming Technique.

(ii) Note on Application of Dynamic Programming to Simple Systems.

(iii) Recent Developments in Replacement Models.

(iv) Construction of a Pay-Off Decision Matrix.

(i) Formal Statement of Dynamic Programming Technique.

The following outline is nearly identical to that given by Mitten and Nemhauser (11). The simple multi-stage process illustrated in figure A1.1 may be subjected to an optimization analysis by the technique of dynamic programming in the following manner: Consider a single stage, r, of the N stage process.

Stage Output $X_{r-1} = h_r(X_r, d_r)$

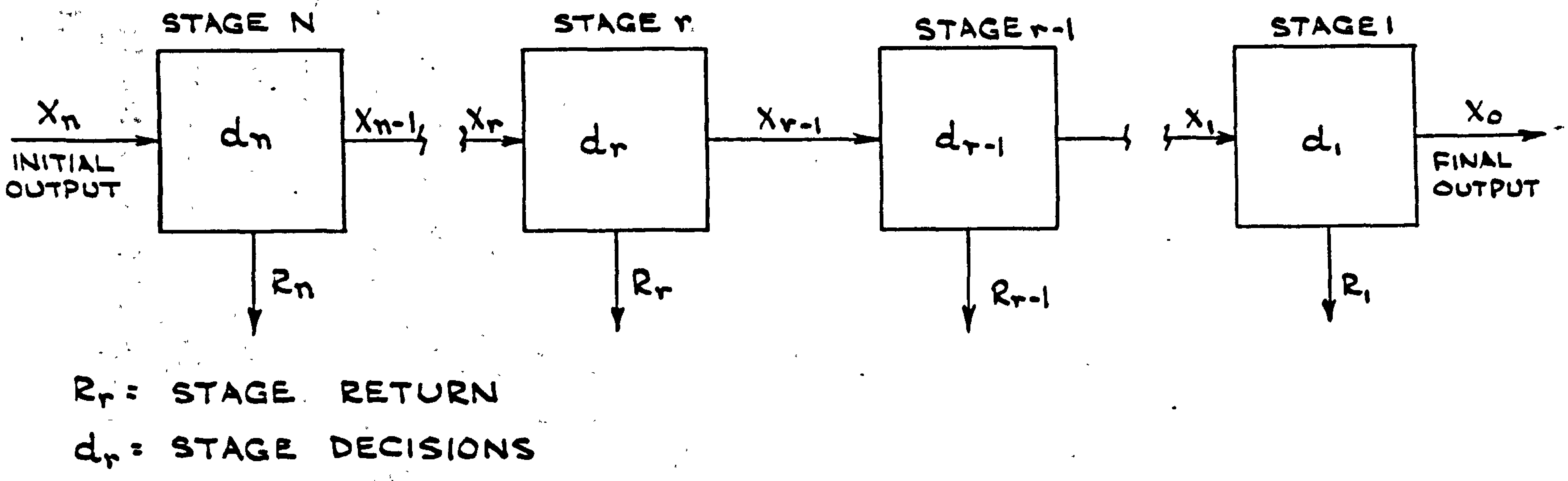
Stage Return $R_r = g_r(X_r, d_r, X_{r-1}) = g_r(X_r, d_r)$

The analysis is based on the repeated application of the functional relationships

$$Q_r(X_r, d_r) = g_r(X_r, d_r) + f_{r-1}(X_{r-1}) \quad (A1.1)$$

where $X_{r-1} = h_r(X_r, d_r)$ and $f_0(X_0) = 0$

and
$$f_r(X_r) = \max\left[Q_r(X_r, d_r)\right] \quad (A1.2)$$



OUTLINE OF SIMPLE MULTISTAGE PROCESS

Fig. A1.1

for all $r = 1,2 \ldots N$ over all feasible values of the inputs X_r. In these equations :-

(i) $f_r(X_r)$ is the maximum (optimal) return from the r stage process consisting of stages 1 through r.

(ii) the expression $f_r(X_r)$ reflects the obvious fact that the maximum return from a process depends on the input X_r to the process

(iii) the quantity $Q_r(X_r, d_r)$ is the combined return from stages 1 to r and consists of the stage r return $g_r(X_r, d_r)$ plus the maximum return $f_{r-1}(X_{r-1})$ from stages 1 to n-1.

Equation (A1.1) is a formal statement of the principle of optimality :-

> No matter what the input (X_r) and the decision (d_r) and the resulting output (X_{r-1}) at stage r may be, the decisions $(d_1 \ldots . d_{r-1})$ must be made in such a way as to yield the maximum return from the r-1 stage process with input X_{r-1}.

Equation (A1.2) states that corresponding to each feasible value of the input (X_r) there is an optimal stage r decision $\left[\text{e.g. say } d_r^* = d_r^*(X_r)\right]$ which maximizes the combined r stage return $Q_r(X_r, d_r)$.

(ii) Note on Application of Dynamic Programming to Simple Systems.

Some investigations were carried out using dynamic programming on the economic optimization of two and three stage systems. A number of decision alternatives were given for each stage. The purpose of the work was to observe the effect on the optimal configuration of the whole system caused by the application of different economic criteria. The criteria applied were:-

(i) Gross Profit over 5 years.

(ii) Percentage Return on Investment.

(iii) Venture Profit.

(iv) Venture Worth.

(i) Gross Profit over 5 years: For all stages except the last stage, or alternatively any in-process stage producing a saleable product, the gross profit is negative. The criterion is additive and may be applied easily.

(ii) Percentage Return on Investment: (see section 2.2): If we write the percentage return on investment for a stage r we have,

$$R_r = \frac{P_r}{I_r}$$

where P_r = profit from stage r and I_r = total capital investment for the stage. For an in-process stage, the numerator will consist of the total annual costs and will be negative. If we consider a two stage process and apply dynamic programming to the last stage (i.e. stage 1), we can write:-

$$R_1^{max} = MAX\left[\frac{P_1}{I_1}\right]$$

where R_1^{max} = the maximum % return from the last stage. Applying dynamic programming over the two stages:-

$$R_2^{max} = MAX\left[R_2, R_1^{max}\right]$$

$$= MAX\left[\frac{P_2 + P_1}{I_2 + I_1}\right] \qquad (A1.3)$$

or alternatively $R_2^{max} = MAX\left[\frac{R_2 I_2 + R_1^{max} I_1}{I_2 + I_1}\right]$ (A1.4)

It is clear from equations (A1.3) and (A1.4) that the functional relationship involved will necessitate some additional calculations compared with additive criteria. As with gross profit, negative values will be obtained for all stages except the last (stage 1).*

(iii) and (iv) <u>Venture Profit and Venture Worth (V.W.):</u>
The Venture Profit (V.P.) was handled in a similar fashion to V.W. in the manner described fully in section 2.6. It

* i.e. FOR THE USUAL CASE WHERE ONLY THE PRODUCT FROM THE LAST STAGE CONTRIBUTES TO THE GROSS PROFIT.

may be noted that under the assumptions given in Chapter 2, the V.W. is equivalent to the Venture Profit, summed and discounted over the project lifetime.

No difficulty was experienced in optimizing the systems which were of the straight-through, separating branch or combining-branch form. The amount of computation increased rapidly with the combining-branched systems. As was expected, in virtually all the cases studied, different optimal plant configurations were arrived at using the different criteria. The exceptions were the Venture Profit and Venture Worth criteria both of which resulted in the same optimum configuration for the various systems investigated. This result was due in part to the simplifications made in the V.W. equation and partly to the assumed economics of the system.

The Venture Profit equation (zero salvage value assumed) may be written

$$V.P. = (1-t)R - i_m I_w - \left[i_m + \frac{i}{(1+i)^n - 1} - dt \right] I \qquad (A1.5)$$

The V.W. as given by equation (2.11) for zero salvage value is

$$V.W. = (1-t)RZ - i_m I_w Z - \left[i_m Z + \frac{iZ}{(1+i)^n - 1} - dtY \right] I \qquad (A1.6)$$

where $Z = \frac{(1+i)^n - 1}{i(1+i)^n}$, $Y = \frac{(1+i)^r - 1}{i(1+i)^r}$ and the remaining notation that of Chapter 2. If the terms in the square brackets in equations (A1.5) and (A1.6) are evaluated for the assumptions made in the investigations i.e.

$i_m = 0.15$, $i = 0.10$, $n = 10$ yrs., $r = 5$ yrs., $t = 0.50$ and $d = 0.20$

$$\left[i_m + \frac{i}{(1+i)^n - 1} - dt \right] = 0.11275$$

$$\left[i_m Z + \frac{iZ}{(1+i)^n - 1} - dtY \right] = 0.927$$

If equation (A1.5) is multiplied by the constant Z and equation (A1.6) rearranged, we obtain

$$V.P. \times Z = \left[(1-t)R - i_m I_w \right] Z - 0.692\ I \qquad (A1.7)$$

$$V.W. = \left[(1-t)R - i_m I_w \right] Z - 0.927\ I \qquad (A1.8)$$

It may thus be seen that the Venture Profit, under the assumptions made, is equivalent in all but the last term to a constant times the Venture Worth. It might be expected therefore that the application of either criteria would in many instances result in the same optimal system, particularly when R is large.

(iii) Recent Developments in Replacement Models.

The early work of Terborgh has already been described in section 1.4 and, in his later work, the inferiority gradient concept, has been retained - although the treatment is different. In the first studies the replacement decision was on the basis of a cash figure comparison at present time between the adverse minimum of the defender and that of the challenger. It has been pointed out that the adverse minimum of the challenger (i.e. C_M) had two components (a) a capital recovery cost component and (b) a component representing the present worth of the advantage of replacing with the next year challenger and its successors, rather than with the currently available challenger. In order to calculate C_M it is necessary to know both the inferiority gradient and the economic life. In figure 1.5 the gradient = £50 and the economic life = 8 yrs. An equation for C_M given is

$$C_M = I\left[\frac{i(1+i)^n}{(1+i)^n - 1}\right] + \frac{g}{i} - \frac{ng}{i}\left[\frac{i}{(1+i)^n - 1}\right] \qquad (A1.9)$$

where I = initial capital cost; i = interest rate; g = inferiority gradient; n = economic life.

An approximate equation for C_M is

$$C_M = \sqrt{2\, Ig} + \frac{iI + g}{2} \qquad (A1.10)$$

The use of equation (A1.10) to compute C_M overcomes the difficulty that arises when both n and g must be determined. It may be shown that the economic life is a function of the gradient and, conversely, an assumption regarding the economic life implies a value for the gradient. Both these equations are based on the assumption of a zero salvage value and subsequent developments allowed for the possibility of a positive salvage value.

$$C_M = \frac{in\left[Ii + kSa\frac{1}{(1+i)^n}\right] - Sa(1+k)\left[1 + \frac{1}{(1+i)^n}\right]}{in + \frac{1}{(1+i)^n} - 1} \qquad (A1.11)$$

where Sa = estimated terminal salvage value

$$k = \frac{2.3026}{n}(\log I - \log Sa)$$

It will be observed that g does not occur in equation (A1.11). In this instance the estimated economic life and the terminal salvage value, together with the assumption that the decline in salvage value is uniform, enable the gradient to be inferred. For the case where $Sa = 0$, equation (A1.11) becomes

$$C_M = \frac{Ini^2}{in + \frac{1}{(1+i)^n} - 1} \qquad (A1.12)$$

Equations (A1.9), (A1.10) and (A1.12) may be compared, the result from equation (A1.9) being correct. Assume I = 1000 £, $i = 0.15$, $n = 8$ yrs. and $g = £50$

Equation (A1.9)	$C_M = 362$ £
(A1.10)	$= 366$
(A1.12)	$= 342$

The most recent extensions to the model enable after tax comparisons to be made. Furthermore, instead of comparing cash figures, a next-year rate of return is computed. This rate of return is designated the MAPI (Machinery and Allied Products Institute) Urgency Rate and it represents a measure of the current urgency of the project. The basis of the criterion is a comparison between the next year rate of return of the existing asset and the next year rate of return of the challenger. The Urgency Rate as derived constitutes an after tax return on the net investment in the project relative to deferment for one year. The elements which arise in its application and defined in the MAPI context are :-

(i) Net Investment :- the installed cost of the project (i.e. the proposed replacement) less any investment released (salvage value of the replaced assets) or avoided by it.

(ii) Next-Year Operating Advantage :- the sum of (a) the increase in revenue and (b) the reduction in operating costs resulting from the project, as compared with the operating results that would occur next year in its absence.

(iii) Next-Year Capital Consumption Avoided :- the loss of disposal value from holding for a further year the assets that would be replaced by the project plus the next year allocation of capital additions required in its absence.

(iv) Next-Year Capital Consumption Incurred :- the consumption of the project investment itself.

(v) Next-Year Income Tax Adjustment :- the net increase in income tax resulting from the project.

The MAPI Urgency Rate may now be expressed as follows

(a) No Income Tax $\quad \text{RATE} = \frac{(ii) + (iii) - (iv)}{(i)} \cdot 100$

(b) Income Tax Adjustment $\quad \text{RATE} = \frac{(ii) + (iii) - (iv) - (v)}{(i)} \cdot 100$

The complexities of this model prevent its discussion here. The main problem is encountered in estimating the capital consumption incurred by the project and the main MAPI effort has been directed at producing a workable formula to measure this component. Their solution is to substitute patterned projections for capital consumption based on a number of assumptions. The projections are then related in a broad sense to the technological factors of obsolescence and deterioration. Finally a number of mathematical formulae are derived enabling the Urgency Rate to be calculated for the different variants of the 'earnings' projections and for two different methods of depreciation, namely, straight-line and sum-of-digits method.

(iv) Construction of a Pay-off Decision Matrix.

This example indicating the quantification of the logic of decision making is taken from Churchman et ali (19). Two alternative objectives are involved O_1 and O_2 and only two courses of action A_1 and A_2 are possible. Now if the efficiency of each course of action for each objective (for example, this might be the probability of attaining success in some contexts) has been determined along a scale from 0 to 1, the results may be shown in the matrix

	O_1	O_2
A_1	0.8	0.4
A_2	0.2	0.6

In deciding which course of action to select, it is a mistake to select either A_1 or A_2. The decision cannot be made without a knowledge of the relative importance of the objectives. If O_1 is much more important than O_2, A_1 would be selected but if $O_2 \gg O_1$, A_2 would be selected. It is therefore necessary to quantify the relative importance of O_1 and O_2. Suppose that O_1 and O_2 are valued at 0.3 and 0.7, respectively, on a scale from 0 to 1. The efficiency of each course of action may be weighted as follows

	O_1	O_2	TOTAL
A_1	0.3 x 0.8 = 0.24	0.7 x 0.4 = 0.28	0.52
A_2	0.3 x 0.2 = 0.06	0.7 x 0.6 = 0.42	0.48

The sum of the weighted efficiencies (efficiency x relative importance) of a course of action may be called its relative effectiveness and this criterion should be the basis for selecting a course of action. If in the example, the most important objective (O_2) had been chosen and the course of action most efficient relative to it (A_2) followed, an incorrect solution would have been obtained.

APPENDIX 2:

(i) Notes on V.W. Simulation and Programme Details.

(ii) Table of Discounting Factors.

(i) Notes on V.W. Simulation and Programme Details

The equation which was programmed was equation (2.11)

$$V.W. = \left[\frac{(1+i)^n-1}{i(1+i)^n}\right](1-t)R + \left[\frac{(1+i)^r-1}{i(1+i)^r}\right]dtI - \left[\frac{(1+i)^n-1}{i(1+i)^n}\right](i_m-i)$$

$$(I+I_W)-I - \left[\frac{(1+i)^n-1}{(1+i)^n}\right] I_W + \frac{(1-t)Sa}{(1+i)^n} \qquad (2.11)$$

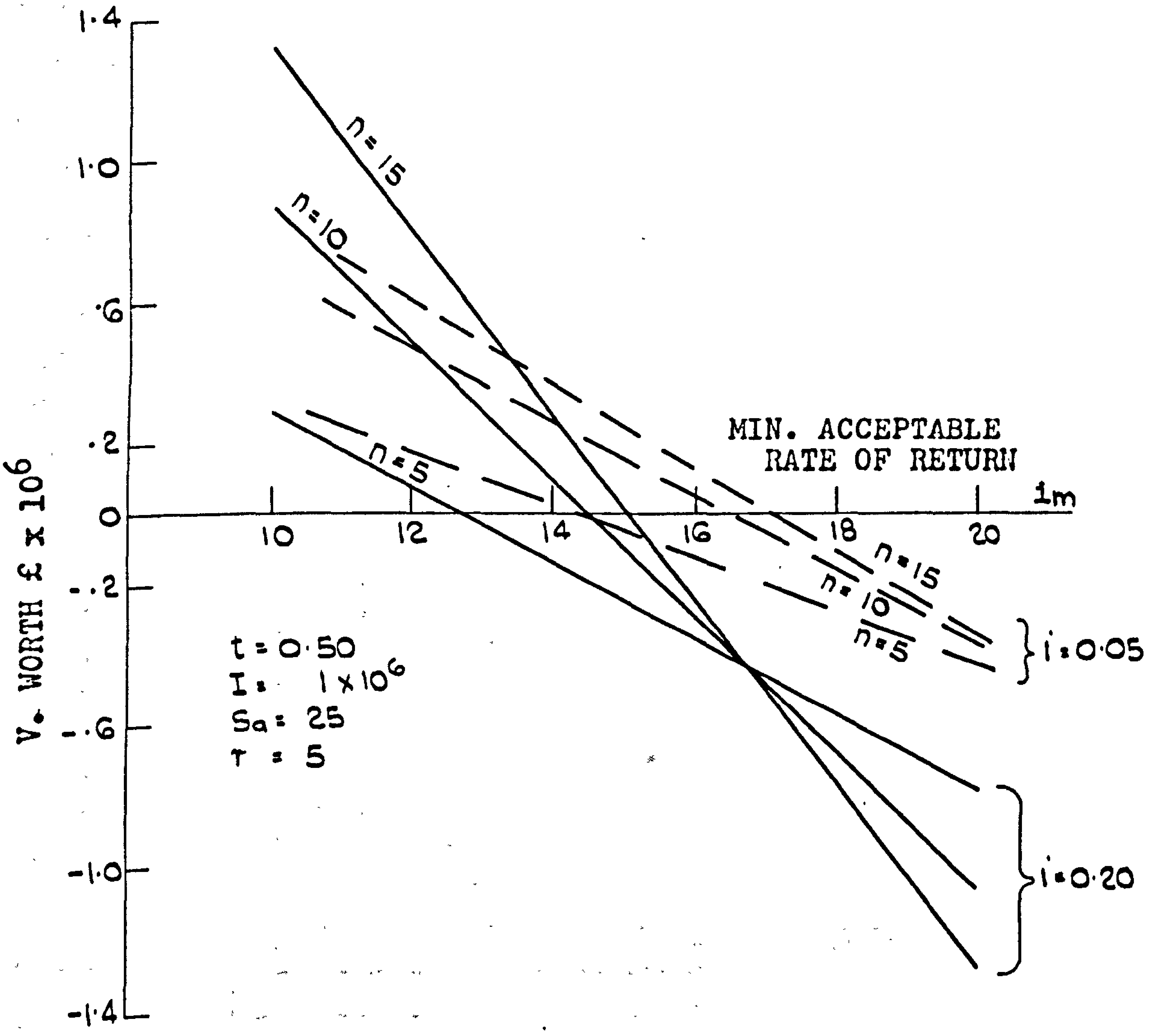
The values given to the parameters in this equation were

t	$= 0.45, 0.50, 0.55$	fraction per yr.
I	$= 5, 10, 15 \times 10^6$	£.
Sa	$= 0, 0.25\ I$	£.
n	$= 5, 10, 15$	yrs.
r	$= 5, 8, 11$	yrs.
i	$= 0.05, 0.20$	fraction per yr.
i_m	$= 0.10, 0.20, 0.30$	fraction per yr.
d	$= {}^1/_r$	fraction per yr.
I_W	$= 0.2\ I$	£
R	$= 0.5\ I$	£ per yr.

As was mentioned in section 2.5, it will be observed that this equation is linear with respect to t and also with respect to I, Sa and i_m. Variation in r, n and i on the other hand will result in non-linear changes in the V.W. Figure A2.1 shows how the V.W. varies with changes in the minimum acceptable rate of return. The programme itself was very simple and as may be seen from the schematic diagram in figure A2.2, it consists of seven iterative loops around equation (2.11).

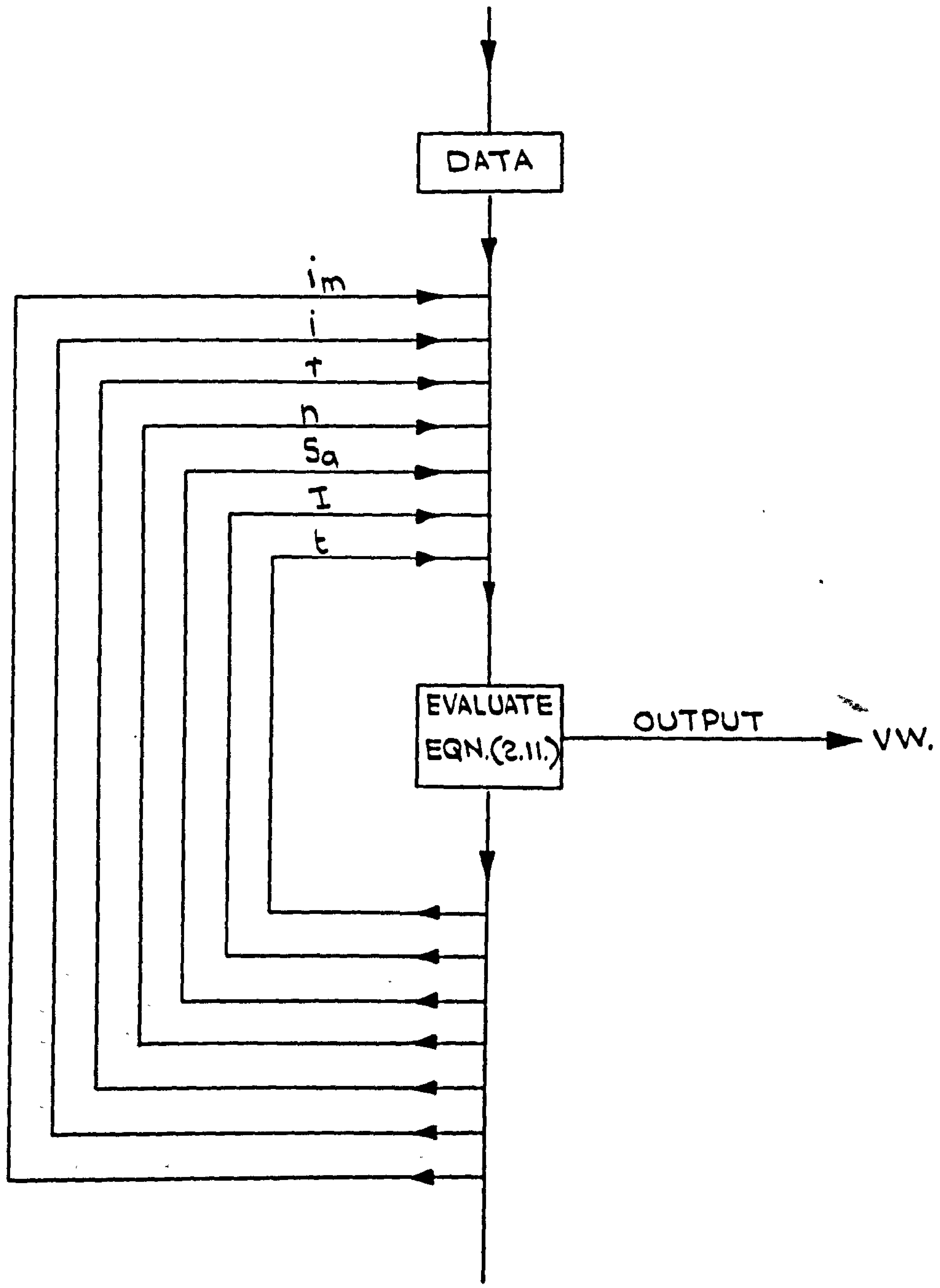
(ii) Table of Discounting Factors

The table below, showing values of the uniform series present worth factor, illustrates the point discussed in section 2.7 regarding the convergence of the discounting factor.



VENTURE WORTH SIMULATION
VARIATION OF i_m.

Fig. A2.1



SCHEMATIC DIAGRAM OF V.W. PROGRAMME.

Fig. A2.2

TABLE A2.1.

CONVERGENCE OF UNIFORM SERIES PRESENT WORTH FACTOR

n \ i	0.05	0.10	0.15	0.20	0.25
5	4.329	3.791	3.352	2.991	2.689
10	7.722	6.144	5.019	4.192	3.571
15	10.380	7.606	5.847	4.675	3.859
20	12.462	8.514	6.259	4.870	3.954
25	14.094	9.077	6.464	4.948	3.985
50	18.256	9.915	6.661	4.999	-
100	19.348	9.999	-	-	-
∞	-	-	6.667	5.000	4.000

$$\sum_{=1}^{k=n} \frac{1}{(1+i)^n} = \frac{(1+i)^n - 1}{i(1+i)^n}$$

This table has been prepared with values taken from Tables E-11, E-16, E-18, E-19, E-22 in Grant (2).

APPENDIX 3:

(i) Derivation of Equation (3.1)

(ii) Parameter Values for $F^* \doteq 50$ and $V^* \doteq 85$

(iii) Schematic Outline of Programme P200.

(i) Derivation of Equation (3.1).

The cost of a distillation column per lb-mole of distillate can be expressed as

$$\frac{C_1 S N}{E h D} \qquad (A3.1)$$

where S = cross-sectional area, ft^2

D = distillate rate, lb.moles/hr

and the other parameters have been defined in section 3.2.

Now

$$S = \frac{V}{Ga} = \frac{D(1+R)}{Ga} \qquad (A3.2)$$

where V = vapour throughput rate, lb.moles/hr. Substituting for S in (A3.1), the first term in equation (3.1) is obtained

$$\frac{C_1 N(1+R)}{E\ h\ Ga} \qquad (A3.3)$$

The condenser and reboiler costs per lb.mole of distillate may be written

$$\frac{C_2 H}{h\ D} \qquad (A3.4)$$

where H = total tubular equipment, ft^2.

But
$$H = \frac{V}{G_b} = \frac{D(1+R)}{G_b} \qquad (A3.5)$$

and substituting for H in (A3.4), the second term in equation (3.1) is obtained

$$\frac{C_2(R+1)}{h\ G_b} \qquad (A3.6)$$

The cost of steam and coolant may be written for the feed at the boiling point as

$$C_3\frac{V}{D} = C_3(R+1) \qquad (A3.7)$$

where C_3 = cost of steam and coolant, to vapourize and condense, respectively, 1 lb. mole of distillate.
The third term in equation (3.1) is given by (A3.7), and it will be seen that the whole equation is the sum of (A3.3), (A3.6) and (A3.7).

(ii) Parameters Values for $F^* \doteq 50$ and $V^* \doteq 85$

The following data, that of Happel, were assumed for the design, operating and cost variables in equation (3.5a).

Payout Time (PT) = 2 yrs.
Steam Cost (C_s) = 0.5 \$/1000 lbs.
Cooling Water Cost (C_w) = 0.2 \$/1000 U.S. gals.

Cooling Water Temperature Differential $(\Delta T_w) = 35\,^{\circ}F$

Incremental Cost of one plate and the necessary section of completed tower $(C_p) = 50$ ¢/ft^2

Incremental Cost (average) for condensers and reboilers (C_T)

$= 3$ ¢/ft^2

$Ga = 15.0$ lb. moles/hr. ft^2

$Gb = 0.10$ lb. mole/hr. ft^2 capacity of condensing and reboiling surface totaled. Corresponding to Mol.Wt.(M) $= 100$ and latent heat (LH) $= 150$ Btu's/lb, assumed.

Maintenance $(m) = 0.05$ fraction/yr. of I.

$h = 8320$ hr. or 95% of total ann. time.

$K = 0.92$ efficiency factor.

The above data may be applied as follows

$$C_1 = C_p\left(\frac{1}{PT} + m\right) = \text{¢/ft}^2\text{. plate. yr.} \qquad (A3.8)$$

where C_1 = amortized incremental unit investment cost of column. The relation for C_2 the amortized incremental unit investment cost of the tubular equipment is

$$C_2 = C_T\left(\frac{1}{PT} + m\right) = \text{¢/ft}^2\text{. yr} \qquad (A3.9)$$

Steam Cost to vapourize 1 lb. mole $= \frac{M \times LH}{L\,H_s} \times \frac{C_s}{1000} = \theta C_s$ ¢/lb.mole

where LH_s = available heat per lb steam.

Cooling Water Cost to condense 1 lb mole $= \frac{M \times LH}{8.33\ \Delta T_w} \times \frac{C_w}{1000}$

$= \lambda$ \$/lb mole

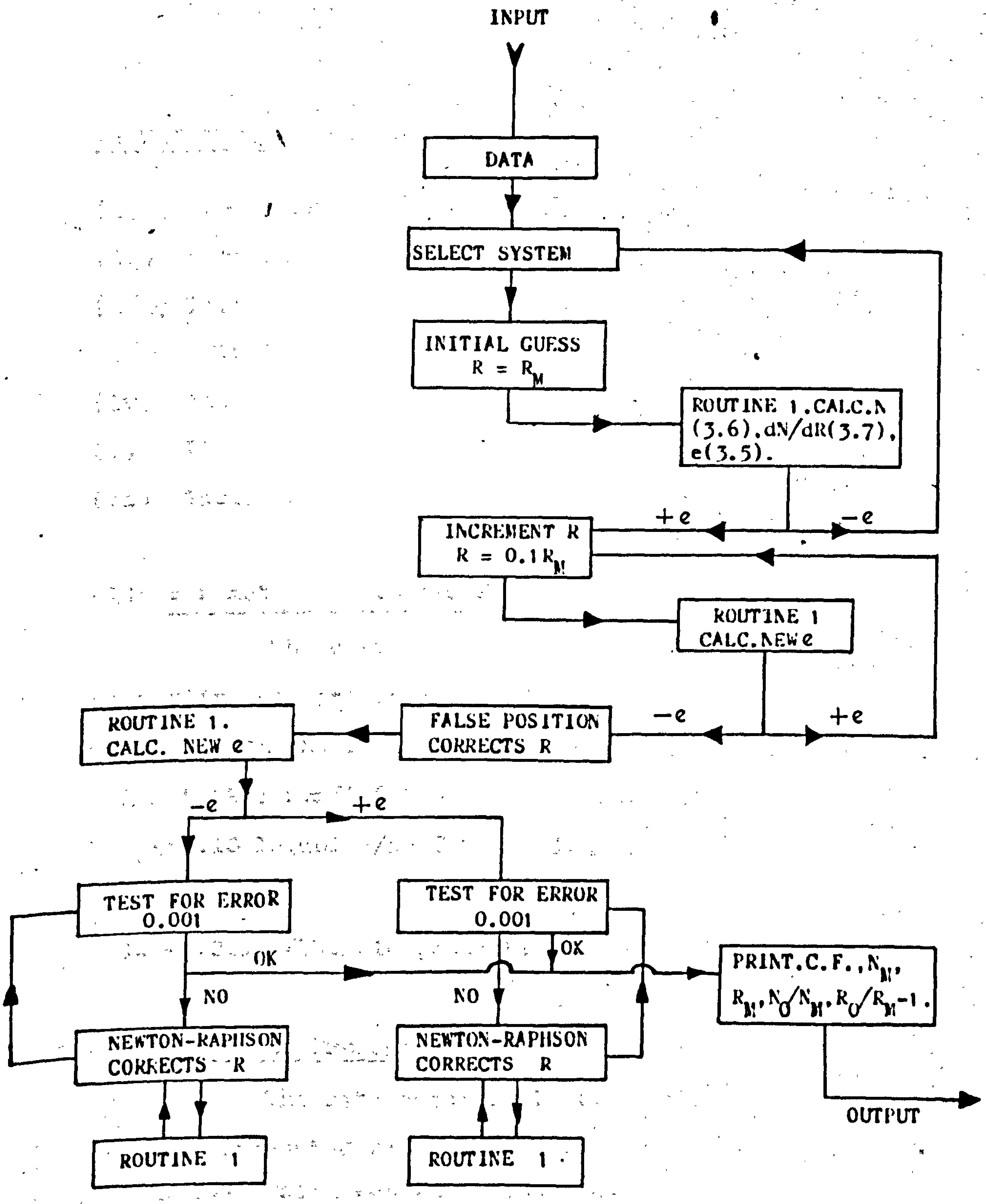
$$\therefore\ C_3 = \theta C_s + \lambda \qquad (A3.10)$$

Now $F^* = K\frac{Ga}{C_1}\left[\frac{C_2}{G_b} + hC_3\right]$ (3.5a)

and the value of F^* obtained using the data given and evaluating equation (3.5a) is $F^* = 47.3$. If V.W. is considered the equivalent cost factor V^* is obtained by means of equation (3.24). In equation (3.24), the nomenclature C_4 and C_5 are equal to C_p and C_T in this Appendix. In order to evaluate V^*, the additional economic variables were assumed to have the values listed at the end of section (3.5). The computed value of $V^* = 84.588$.

(iii) A Schematic Diagram of Programme P200.

The mechanism of this programme has been described in section 3.6 and its pattern may be seen in figure (A3.1).



FLOW DIAGRAM FOR PROGRAMME P200 FIG.A3.1

APPENDIX 4:

(i) Parameter Values for $F^* \div 100$

(ii) Data for Programme P600

(iii) Initial Values for K for Programmes P700, P800, P900, P1000

(iv) Additional Equations Programmed

(v) List of Programmes for Distillation System

(vi) Table A4.1

(i) Parameter Values for $F^* \div 100$

The cost factor $F^* \div 99.9$ used in Programme P400 to verify the optimum solutions obtained from equation (3.5) was based on the following values for the parameters.

$K = 0.92$; $h = 8320$ hrs; $G_a = 15$ lb.moles/hr.ft^2

$G_b = 0.10$ lb.moles/hr.ft^2 ; $C_1 = 20$ \$/ft^2.plate.yr;

$C_2 = 2.0$ \$/ft^2.yr.

$C_3 = 0.015$ \$/lb.mole product.

(ii) Data for Programme P600

The data required in order that equation (3.22) might be evaluated was as follows.

$V = 84.6$ as given in Appendix 3. $D = 50$ lb moles/hr.

$y = 0.9$; $p = 4.0$ \$/lb mol ; $s = 5.0$ \$/lb mol.

(iii) Initial Values of K for Programmes P700, P800, P900, P1000

The initial values, which were chosen for the parameters to evaluate K at the approximate values 0.90, 0.60 and 0.30 for the sensitivity analysis were,

PARAMETER	$K \doteq 0.90$	$K \doteq 0.60$	$K \doteq 0.30$
FA	0.07	0.05	0.12
h_w	4	1.0	0.5
G	1500	850	200
α	3	10	15
$(\mu_L/\rho_L D_L)$	500	250	50
$(\sigma/\mu_L V_g)$	800	400	100

The actual values for K obtained from equation (4.3) were $K \simeq 0.884$, 0.597 and 0.301.

(iv) Additional Equations Programmed.

The following are the equations not given in Chapter 4 for some of the curves plotted.

h_w V F^*

$$\log h_w = -4.15 \log \alpha + 4.15 \log F^* \qquad (A4.1)$$

$$\alpha = \left[\frac{C_2}{G_b} + hC_3\right]\left[\frac{G}{MC_1} \cdot \frac{K}{\frac{0.241}{hw,1}}\right].$$

h_w v V^*

$$\log h_w = -4.15 \log\beta + 4.15 \log V^* \qquad (A4.2)$$

$$\beta = \left[\frac{C_5}{G_b} + hC_3 \frac{\Pi}{\Omega}\right] \left[\frac{G}{MC_4} \cdot \frac{K}{hw_i^{0.241}}\right]$$

FA v F^*

$$\log FA = 3.570 \log\gamma - 3.570 \log F^* \qquad (A4.3)$$

$$\gamma = \left[\frac{C_2}{G_b} + hC_3\right] \left[\frac{G}{MC_1} \frac{K}{FA_i^{-0.28}}\right]$$

FA v V^*

$$\log FA = 3.570 \log\delta - 3.570 \log V^* \qquad (A4.4)$$

$$\delta = \left[\frac{C_5}{G_b} + hC_3 \frac{\Pi}{\Omega}\right] \left[\frac{G}{MC_4} \cdot \frac{K}{FA_i^{-0.28}}\right]$$

G v V^*

$$\log G = -1.0143 \log\zeta + 1.0143 \log V^* \qquad (A4.5)$$

$$\zeta = \left[\frac{C_5}{G_b} + hC_3 \frac{\Pi}{\Omega}\right] \left[\frac{1}{MC_4} \cdot \frac{K}{G_i^{-0.013}}\right]$$

K v F^*

$$K = \left[\frac{MC_1G_b}{C_2G_b + hC_3G_bG}\right] F^* \qquad (A4.6)$$

K v V^*

$$K = \left[\frac{MC_4G_b\Omega}{G_5G\Omega + hC_3G_bG\Pi}\right] V^* \qquad (A4.7)$$

The slope of the K v F^* Curve $=$ 0.01944, and that of the K v V^* Curve is 0.01088, as may be seen in figure 4.12.

(v) List of Programmes for Distillation System.

The following is a full list of the programmes written for this study.

(a) P200: Calculation of R_{opt} by Method of False Position and Newton Raphson. Results shown in figures 4.1, 4.2 and 4.6.

(b) P300: Calculation of R_{opt} by Method of Repeated Plotting. Check programme for the solution of equations (3.5 and (3.26).

(c) P400: Calculation of Unit Cost of Production for $F^* = 100$. Verification of optimum solutions produced by programme P205 through evaluation of equation (3.4). Results are shown in figure 4.4.

(d) P600: Calculation of Venture Worth for $V^* = 85$. Again a verification of the optimum solutions produced by programme P205 through evaluation of equation (3.22). Figure 4.5 shows the results.

(e) P700: Sensitivity of F^* to variations in cost parameters. Results in figures 4.7 and 4.9.

(f) P800: Sensitivity of F^* to variations in design parameters. Results are shown in figures 4.10 and 4.12.

(g) P900: Sensitivity of V^* to variations in cost parameters. Results are shown in figures 4.8 and 4.9.

(h) P1000: Sensitivity of V^* to variations in design parameters. Results are given in figures 4.11 and 4.12.

(vi) Table A4.1

TABLE A4.1.

ECONOMIC OPTIMA AND THE CORRESPONDING REFLUX RATIO FOR SOME TYPICAL SYSTEMS.

		U.C.x10^{-4} $/lb mol				U.C.x10^{-4} $/lb mol	
R_m	R	$N_m = 20$	$N_m = 30$	R_m	R	$N_m = 20$	$N_m = 30$
0.5	.505	420	495	8.0	8.08	2497	2928
	.510	420	494		8.16	2495	2919
	.515	420	493		(8.24)	(2494)	2912
	.520	420	492		8.32	2495	2907
	(.525)	(419)	492		(8.40)	2497	(2903)
	(.550)	(419)	489		8.8	2519	2905
	(.60)	421	(488)		9.6	2609	2971
	.65	424	489		10.4	2726	3081
	.70	429	492		11.2	2860	3215
	.75	435	497		12.0	3004	3365
	.80	441	502		12.8	3154	3518
	.85	449	509		13.6	3308	3680

TABLE A4.1 Continued:

		V.W.x10 ∅				V.W.x10 ∅	
R_m	R	$N_m = 20$	$N_m = 30$	R_m	R	$N_m = 20$	$N_m = 30$
0.5	.505	31872	31161	8.0	8.08	13963	9844
	.510	31876	31170		8.16	14004	9953
	.515	31879	31178		8.24	14031	10042
	.520	31882	31186		8.32	14045	10114
	.525	31885	31193		(8.40)	(14049)	10169
	(.550)	(31894)	31222		(8.8)	13937	(10255)
	.60	31893	31252		9.6	13300	9828
	(.65)	31874	(31253)		10.4	12371	8978
	.70	31839	31236		11.2	11290	7905
	.75	31796	31204		12.0	10120	6702
	.80	31745	31162		12.8	8892	5416
	.85	31689	31111		13.6	7626	4074

APPENDIX 5:

(i) Set of Equations for System 1 (2^{ND} ORD.)

The following is the set of equations requiring solution when a second order reaction of the type discussed, is occurring in system 1.

$$\frac{dC_A}{dt} = \left[\frac{\eta M_B}{\rho_B}\left(\frac{F}{V_T}\right)C_{A0}\right] C_B - \left(\frac{V_R}{V_T}\right) k_1 C_A C_C + \left(\frac{V_R}{V_T}\right) k_2 C_B C_D \qquad (A5.1)$$

$$\frac{dC_A}{dt} = \left[\frac{\eta M_B}{\rho_B}\left(\frac{F}{V_T}\right) C_{C0}\right] C_B - \left(\frac{V_R}{V_T}\right) k_1 C_A C_C + \left(\frac{V_R}{V_T}\right) k_2 C_B C_D \qquad (A5.2)$$

$$\frac{dC_B}{dt} = -\eta\left(\frac{F}{V_T}\right)C_B + \left(\frac{V_R}{V_T}\right) k_1 C_A C_C - \left(\frac{V_R}{V_T}\right) k_2 C_B C_D \qquad (A5.3)$$

$$\frac{dC_D}{dt} = \left(\frac{V_R}{V_T}\right) k_1 C_A C_C - \left(\frac{V_R}{V_T}\right) k_2 C_B C_D \qquad (A5.4)$$

$$\frac{dC_X}{dt} = \left[\frac{\eta M_B}{\rho_B}\left(\frac{F}{V_T}\right) C_{X0}\right] C_B \qquad (A5.5)$$

$$\frac{d\phi_P}{dt} = \left(\frac{\eta M_B}{\rho_B}\right) F\ C_B \qquad (A5.6)$$

$$\frac{d\phi_R}{dt} = F\left(1 - \frac{\eta M_B}{\rho_B}\right) C_B \qquad (A5.7)$$

(ii) Set of Equations for System 2 (2^{ND} ORD.)

The following are the set of equations for a 2^{nd} order reaction in system 2, where $H = \eta \frac{M_B}{\rho_B}$

$$\frac{dC_A}{dt} = (\frac{F}{VR})C_{Ar} - (\frac{F}{VR})C_A + \left[(\frac{F}{VR})HC_{AO}\right] C_B - \left[(\frac{F}{VR})H\right] C_{Ar}C_B - k_1C_AC_C \quad k_2C_BC_D \qquad (A5.8)$$

$$\frac{dC_C}{dt} = (\frac{F}{VR})C_{Cr} - (\frac{F}{VR})C_C + \left[(\frac{F}{VR})HC_{CO}\right] C_B - \left[(\frac{F}{VR})H\right] C_{Cr}C_B - k_1C_AC_C \quad k_2C_BC_D \qquad (A5.9)$$

$$\frac{dC_B}{dt} = (\frac{F}{VR})C_{Br} - (\frac{F}{VR})C_B - \left[(\frac{F}{VR})H\right] C_{Br}C_B + k_1C_AC_C - k_2C_BC_D \qquad (A5.10)$$

$$\frac{dC_D}{dt} = (\frac{F}{VR})C_{Dr} - (\frac{F}{VR})C_D - \left[(\frac{F}{VR})H\right] C_{Dr}C_B + k_1C_AC_C - k_2C_BC_D \qquad (A5.11)$$

$$\frac{dC_X}{dt} = (\frac{F}{VR})C_{Xr} - (\frac{F}{VR})C_X - \left[(\frac{F}{VR})H\right] C_{Xr}C_B + \left[(\frac{F}{VR})HC_{XO}\right] C_B \qquad (A5.12)$$

$$\frac{dC_{Ar}}{dt} = (\frac{F}{Vs})C_A - (\frac{F}{Vs})C_{Ar} + \left[(\frac{F}{Vs})H\right] C_BC_{Ar} \qquad (A5.13)$$

$$\frac{dC_{Cr}}{dt} = (\frac{F}{Vs})C_C - (\frac{F}{Vs})C_{Cr} + \left[(\frac{F}{Vs})H\right] C_BC_{Cr} \qquad (A5.14)$$

$$\frac{dC_{Br}}{dt} = (\frac{F}{Vs})(1-\eta)C_B - (\frac{F}{Vs})C_{Br} + \left[(\frac{F}{Vs})H\right] C_BC_{Br} \qquad (A5.15)$$

$$\frac{dC_{Dr}}{dt} = (\frac{F}{Vs})C_D - (\frac{F}{Vs})C_{Dr} + \left[(\frac{F}{Vs})H\right] C_BC_{Dr} \qquad (A5.16)$$

$$\frac{dC_{Xr}}{dt} = (\frac{F}{Vs})C_X - (\frac{F}{Vs})C_{Xr} + \left[(\frac{F}{Vs})H\right] C_BC_{Xr} \qquad (A5.17)$$

$$\frac{d\phi_P}{dt} = [FH]\ C_B \qquad (A5.18)$$

$$\frac{d\phi_R}{dt} = F - \phi_P \qquad (A5.19)$$

(iii) List of Programmes for the Reactor Systems.

The following is a list of the programmes written for the reactor study.

(a) P/R 200: Solution of System 1 equations for U.C. Criterion. Solution of equations (5.14), (5.15), (5.16), (5.42), (5.43) and evaluation of equation (5.47).

(b) P/R 300: Solution of System 1 equations for V.W. Criterion. The same set of equations are solved as in P/R 200 but the data is used to evaluate equation (2.11).

(c) P/R 500: Solution of System 2 equations for U.C. Criterion. The set of equations (5.36) to (5.43) are solved and equation (5.47) evaluated.

(d) P/R 600: Solution of System 2 equations for V.W. Criterion. Equations (5.36) to (5.43) are solved and equation (2.11) evaluated.

(e) P/R 800: Solution of System 1 (2^{ND} ORD.) equations for U.C. Criterion. Solution of set of equations (A5.1) to (A5.7) and evaluation of equation (5.47).

(f) P/R 900: Solution of System 1 (2^{ND} ORD.) equations for V.W. Criterion. The same set of equations are solved as in P/R 800 and equation (2.11) evaluated.

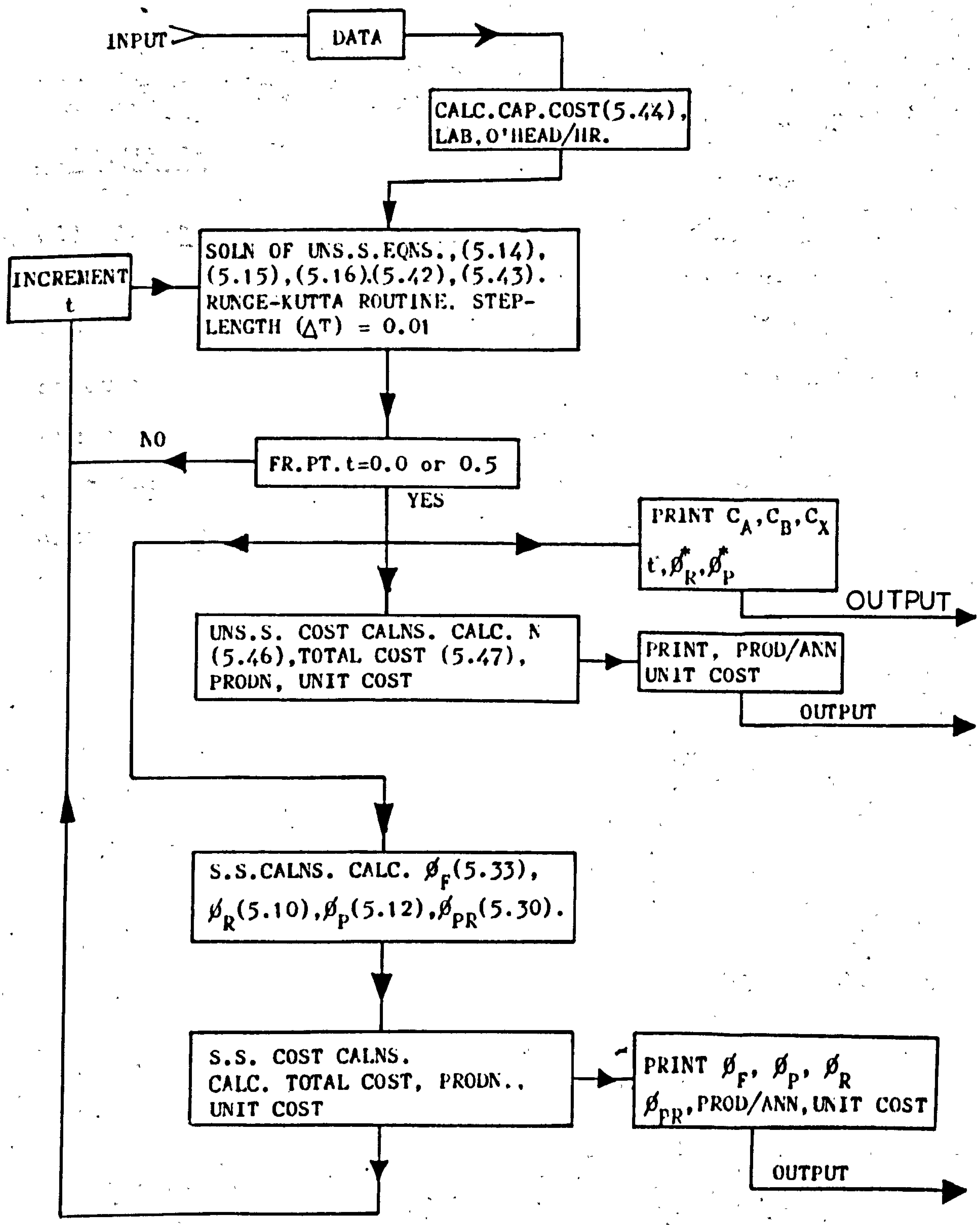
(g) P/R 1100: Solution of System 2 (2^{ND} ORD.) equations for U.C. Criterion. The set of equations (A5.8) to (A5.19) are solved and the data obtained used to evaluate equation (5.47).

(h) P/R 1200: Solution of System 2 (2^{ND} ORD.) equations for V.W. Criterion. As P/R 1100 except that equation (2.11) is evaluated instead of equation (5.47).

(i) P/T 1: Test of Analytical Solutions. Equations (5.21), (5.22) and (5.23) were programmed and C_A, C_B and C_X evaluated for a series of values of t. The curves obtained were identical within the specified degree of accuracy (i.e. to the third decimal place) to those obtained by the solution of equations (5.14), (5.15) and (5.16) using the INTSTEP routine.

(iv) Schematic Diagram for Typical Programme - P/R 200

Figure A5.1 shows the structure of the programme for P/R 200. The structure of all the P/R programmes was similar.

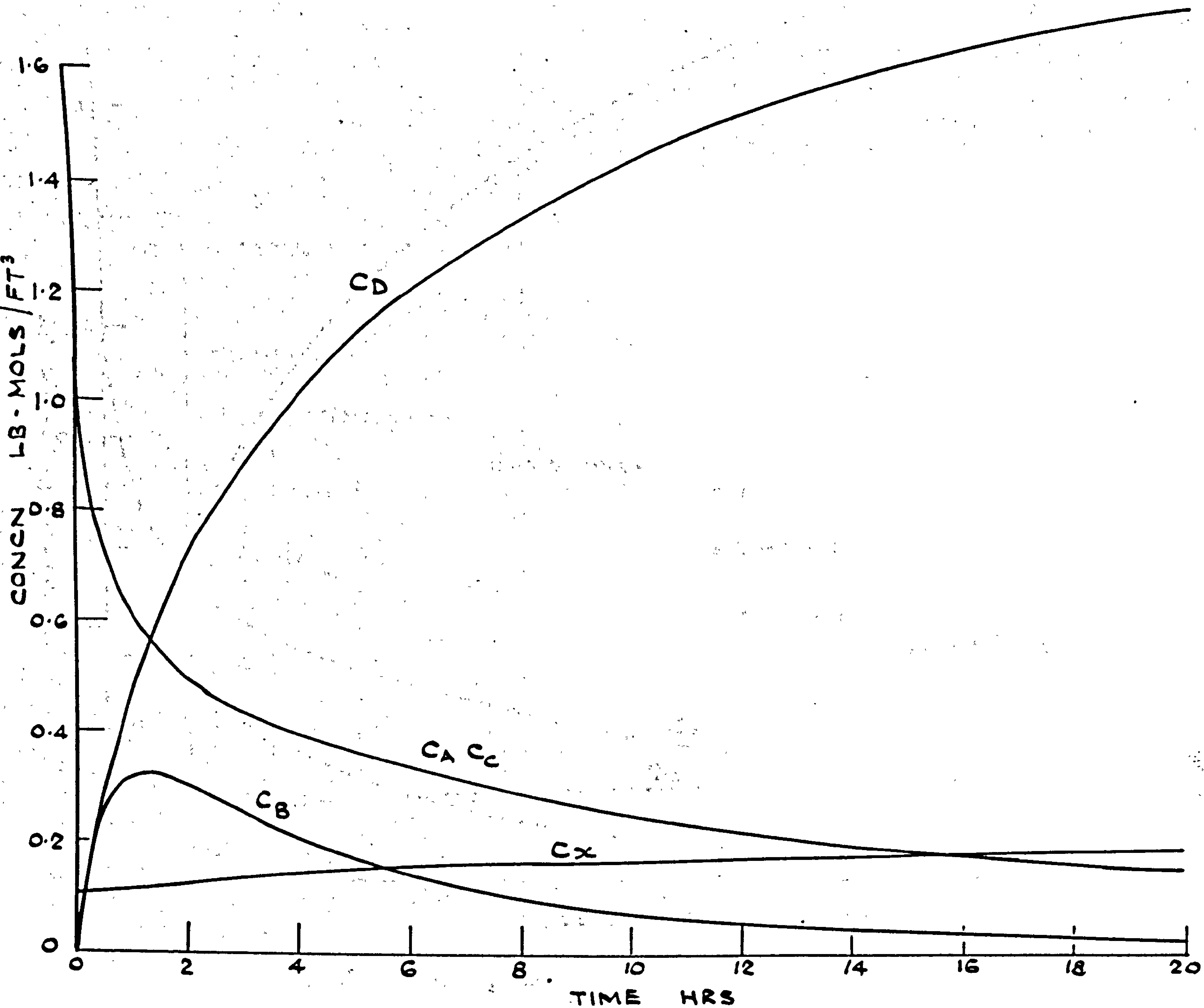


FLOW DIAGRAM FOR PROGRAMME P/R 200 FIG.A5.1

APPENDIX 6:

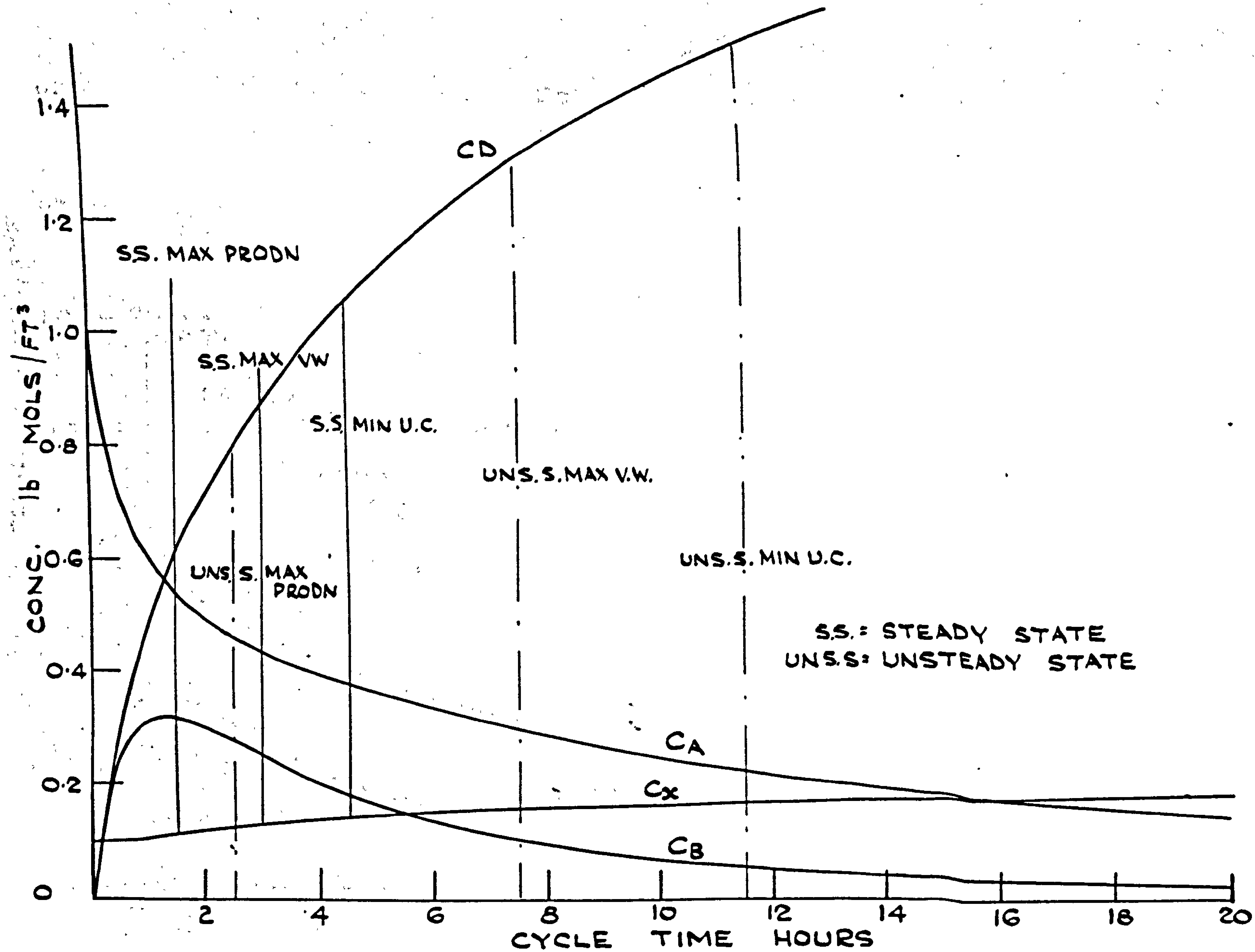
(i) Additional Figures Complementary to Chapter 6.

The figures given in this Appendix need no further discussion beyond that of Chapter 6. With the exception of figure A6.7, they are concerned with 2ND order systems and as has been pointed out, the remarks pertaining to first order systems apply in nearly all cases. Figure A6.7 is discussed in section 6.5.

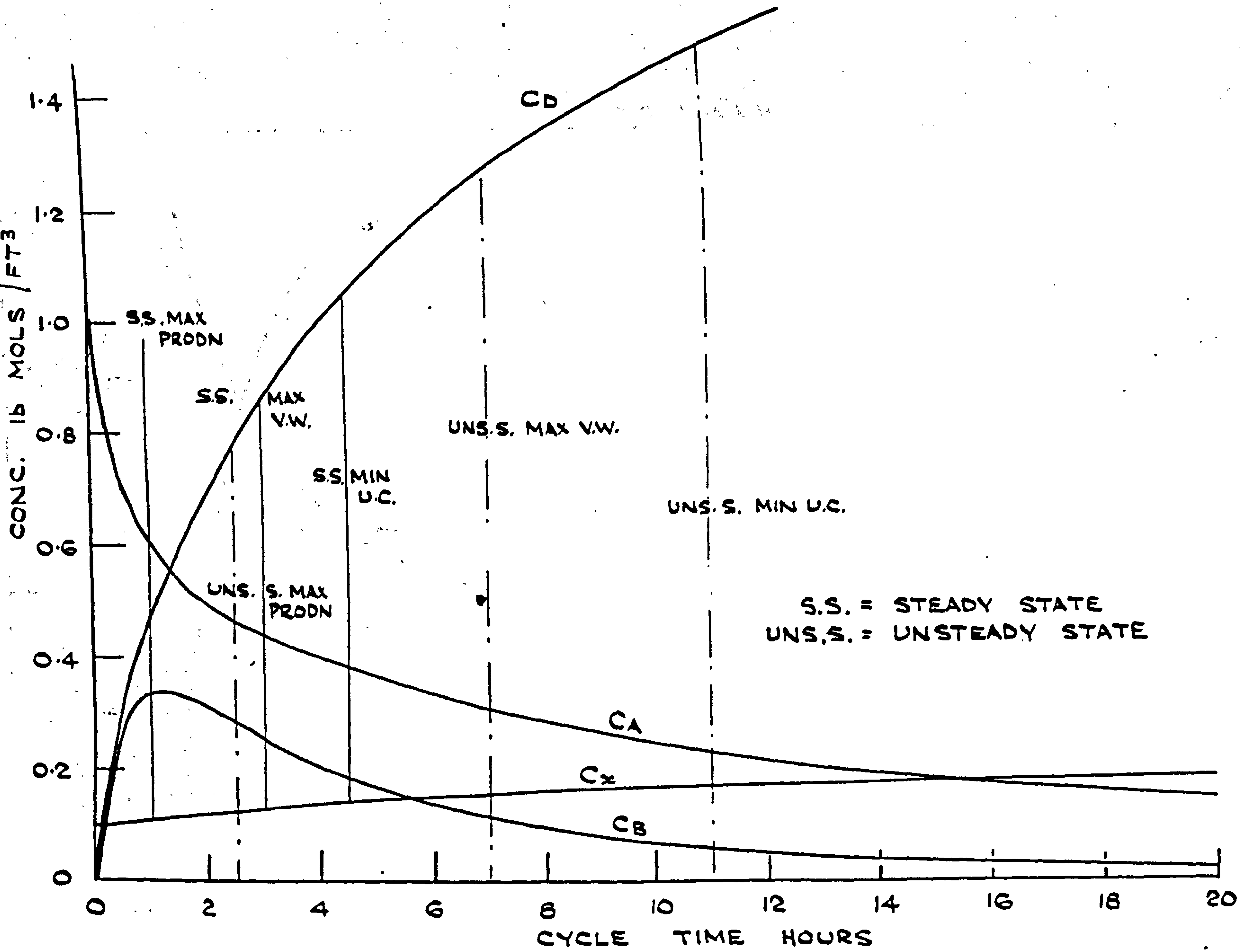


TYPICAL TIME-BEHAVIOUR OF SYSTEM 1 (2nd ORD)

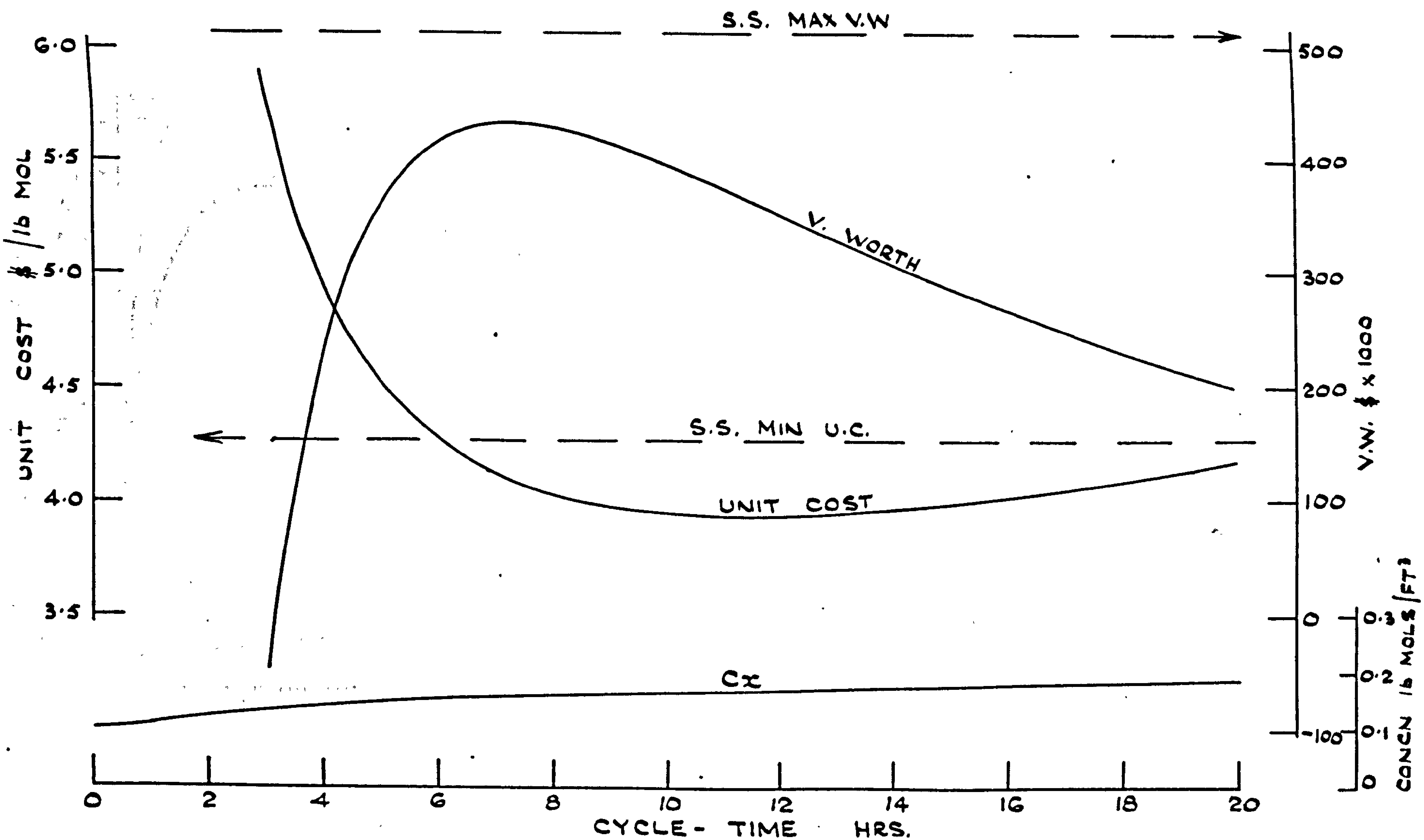
Fig. A6.1



TYPICAL OPTIMUM POINTS OF OPERATION FOR SYSTEM 1 (2nd ORD) Fig.A6.2

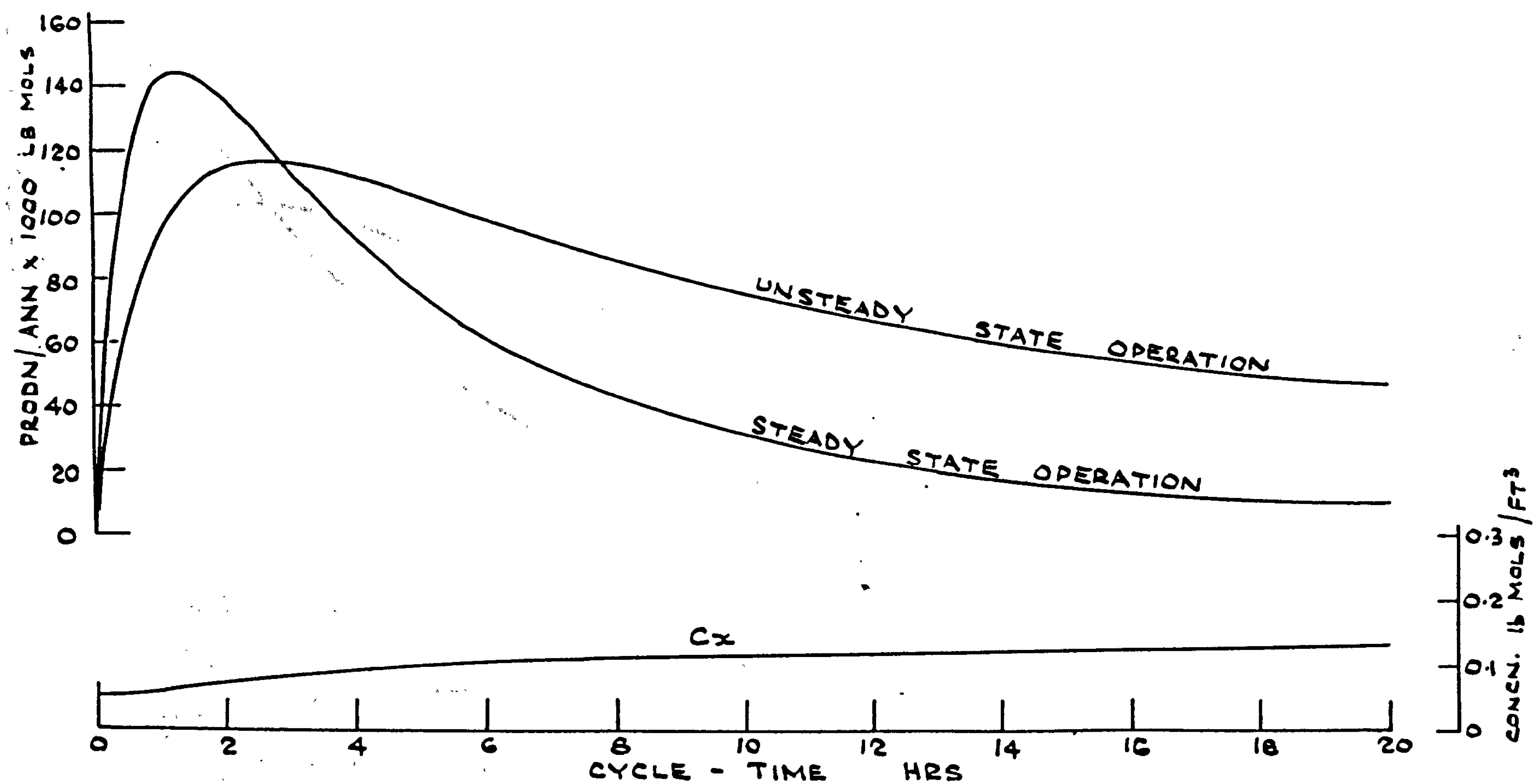


TYPICAL OPTIMUM POINTS OF OPERATION FOR SYSTEM 2 (2nd ORD) Fig. A6.3.



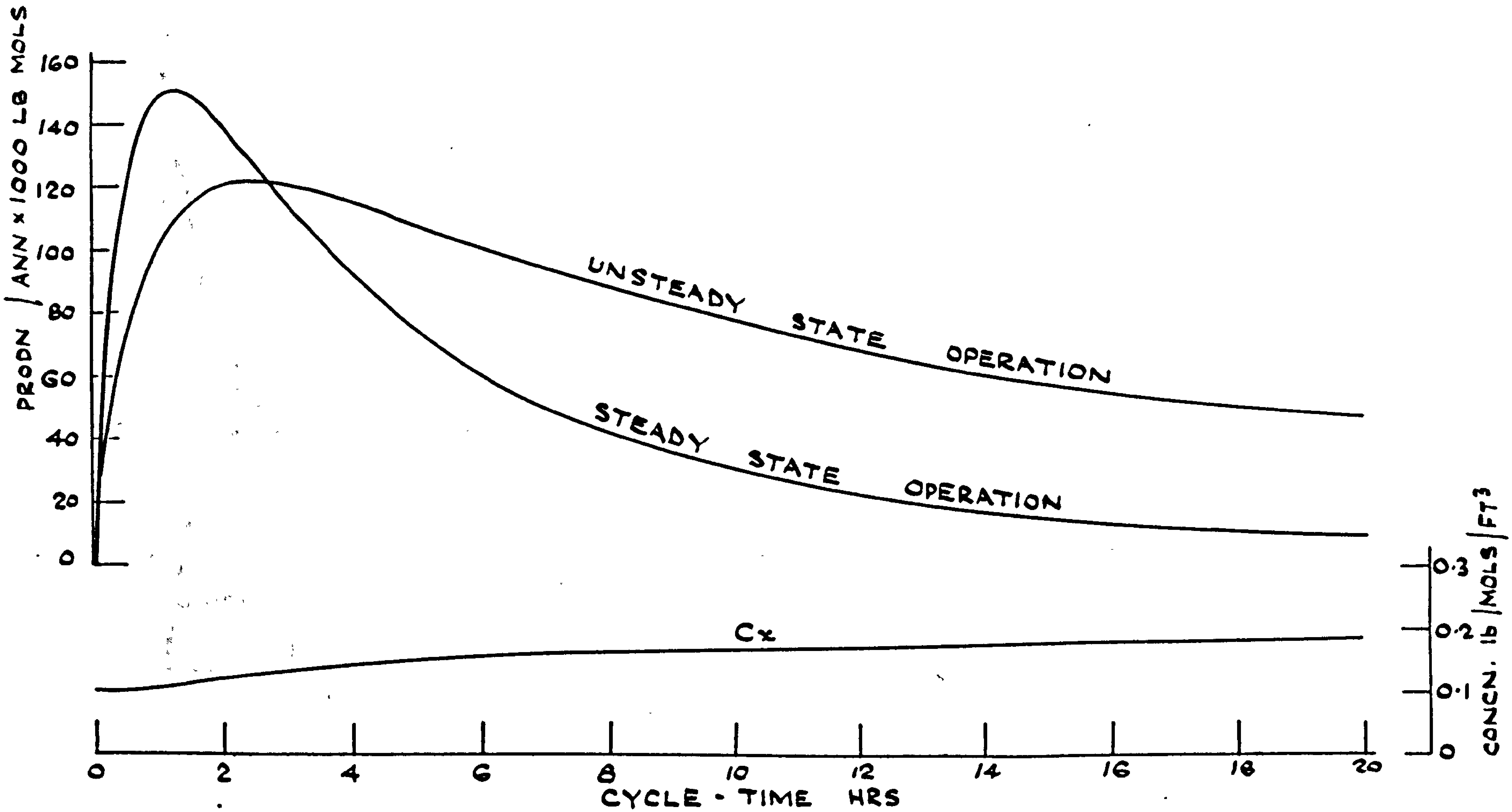
PURGING STRATEGY FOR SYSTEM 1 (2nd ORD)

Fig. A6.4.



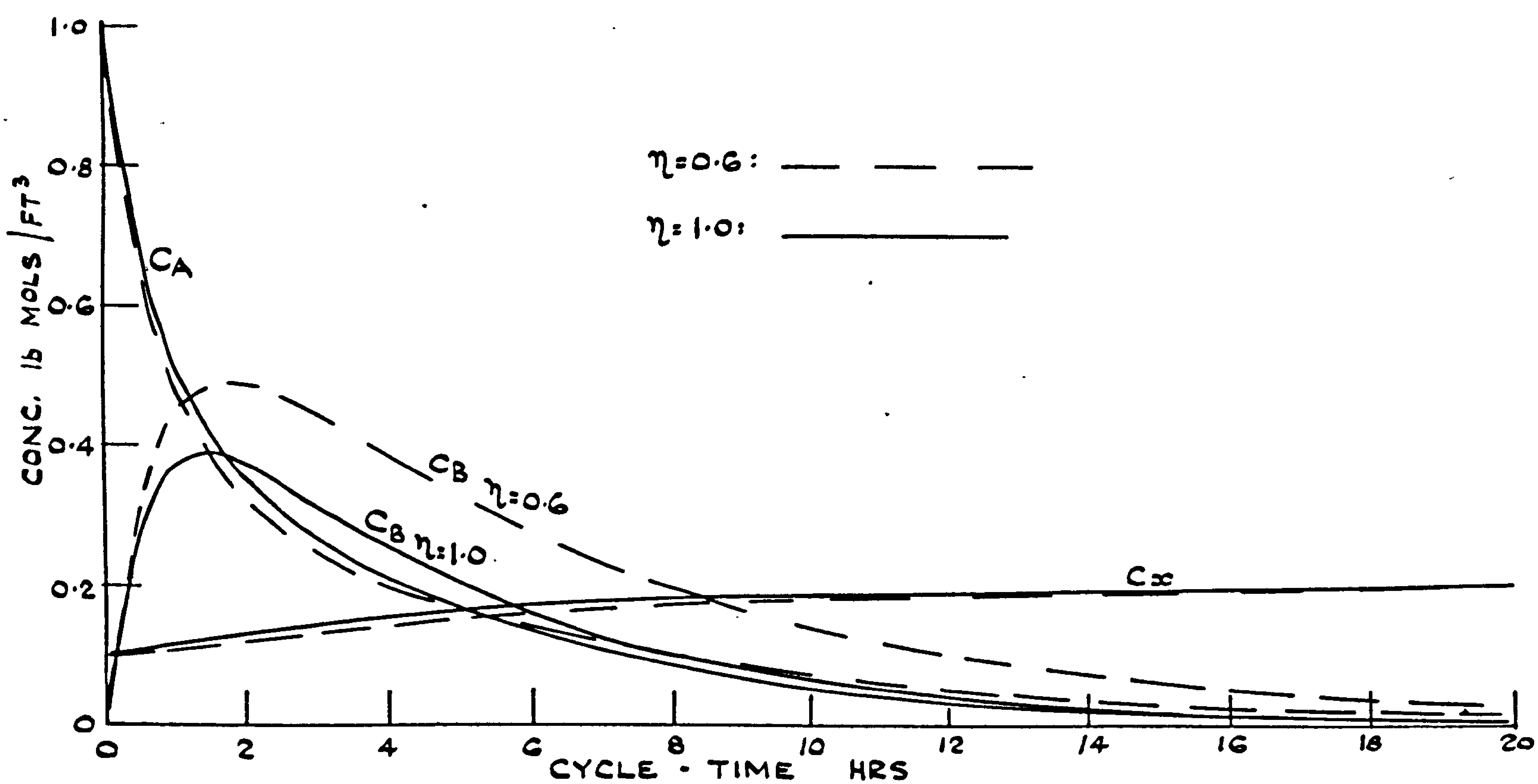
PURGING STRATEGY FOR MAX. PRODN. FROM SYSTEM 1 (2nd ORD).

Fig. A6.5



PURGING STRATEGY FOR MAX. PRODN. FROM SYSTEM 2 (2nd ORD).

Fig. A.6.6



EFFECT OF EFFICIENCY OF SEPARATION ON TIME BEHAVIOUR OF SYSTEM 1

Fig. A6.7