Carnegie Mellon University
Research Showcase @ CMU

Department of Chemical Engineering | Carnegie Institute of Technology

1983

An index for operational flexibility in chemical process design. Part I,

Ross Edward. Swaney
Carnegie Mellon University

Ignacio E. Grossmann

Follow this and additional works at: http://repository.cmu.edu/cheme

This Technical Report is brought to you for free and open access by the Carnegie Institute of Technology at Research Showcase @ CMU. It has been accepted for inclusion in Department of Chemical Engineering by an authorized administrator of Research Showcase @ CMU. For more information, please contact research-showcase@andrew.cmu.edu.

NOTICE WARNING CONCERNING COPYRIGHT RESTRICTIONS:
The copyright law of the United States (title 17, U.S. Code) governs the making of photocopies or other reproductions of copyrighted material. Any copying of this document without permission of its author may be prohibited by law.

AN INDEX FOR OPERATIONAL FLEXIBILITY IN CHEMICAL PROCESS DESIGN
PART I: FORMULATION AND THEORY

by

R.E. Swaney fc I.E. Grossmann

December, 1983

DRC-06-54-83

An Index for Operational Flexibility in Chemical Process Design. Part I: Formulation and Theory

Ross E. Swaney and Ignacio E. Grossmann*
Department of Chemical Engineering
Carnegie-Mellon University
Pittsburgh, PA 15213

December, 1983

* Author to whom correspondence should be addressed.

ABSTRACT

One of the key components of chemical plant operability is flexibility - the ability to operate over a range of conditions while satisfying performance specifications. A general framework for analyzing flexibility in chemical process design is presented in this paper. A quantitative index is proposed which measures the size of the parameter space over which feasible steady-state operation of the plant can be attained. The mathematical formulation of this index and a detailed study of its properties are presented. Application of the flexibility index in design is illustrated with an example.

UNIVERSITY LIBRARIES
CARNEGIE-MELLON UNIVERSITY
PITTSBURGH, PENNSYLVANIA 15213

SCOPE

The goal in chemical process design is to produce a plant design which is optimal with respect to cost and performance. Plant performance, though, involves a broad range of criteria. A good process design must not only exhibit an optimal balance between capital and operating costs; it must also exhibit operability characteristics which will allow economic performance to be realizable in a practical operating environment. Operability considerations involve the aspects of flexibility, controllability, reliability, and safety. Although these aspects may appear to be similar, they actually correspond to different technical concepts. Flexibility is concerned with the problem of ensuring feasible steady-state operation over a variety of operating conditions, whereas controllability is concerned with the quality and stability of the dynamic response of the process. On the other hand, reliability is concerned with the probability of normal operation given that mechanical and electrical failures can occur, while safety is concerned with the hazards that are consequences of these failures. Because these operability characteristics are the implicit results of design-stage decisions, they must be given direct attention during the design process if the goal of producing a good design is to be achieved.

Most of the previous methods for process synthesis (see Nishida et al.,1981) and flowsheet optimization (e.g. Edhal et al., 1983; Biegler and Hughes, 1981; Jirapongphan et.al., 1980) consider a singte nominal operating condition in the design of chemical processes. Although these procedures can often provide useful results, there is still a substantial gap between the designs obtained from such procedures and the designs, that are actually implemented in practice. The major reason for this gap is that conventional procedures for synthesis and flowsheet optimization do not explicitly account for those factors which relate to plant operability. Therefore, the common practice is to introduce additional equipment and employ various types of empirical overdesign to improve operability characteristics. However, with this approach it is generally not possible to guarantee either optimality or feasible operation for conditions that are different from the nominal point selected for the design.

It is only recently that new tools are emerging to simultaneously handle both economic and operability aspects in process design (see Grossmann et. al., 1983; Morari, 1983; Grossmann and Morari, 1983). The purpose of this paper is to present a systematic framework for analyzing flexibility in chemical processes. To accomplish this objective an index of flexibility is proposed which provides a measure of the region of feasible operation in the space of the uncertain parameters. This index also provides bounds of the parameters within which feasible operation is guaranteed, and it allows the identification of those "worst-case" conditions that limit the flexibility of the process. The mathematical formulation of the proposed index and its basic properties are presented. Application of the index in process design is illustrated with an example. Efficient algorithms for computation of the flexibility index are given in Part II.

CONCLUSIONS AND SIGNIFICANCE

The problem of quantitatively characterizing the flexibility of a chemical plant design has been addressed in this paper. A flexibility index has been proposed which provides a measure of the size of the region of feasible steady-state operation. This index has a meaningful interpretation in that it corresponds to the maximum scaled deviation of uncertain parameters from their nominal values for which feasible operation can be guaranteed. Furthermore, computation of this index can be used to identify the critical parameter combinations which limit the flexibility of a given design. A rigorous study of the mathematical properties of the index has been presented,, with particular emphasis on the conditions under which it can be guaranteed that the critical points will correspond to extreme values (vertices) of the parameters. Formulations that are useful for the computation of the index have also been presented. Application of the flexibility index has been illustrated in the design of a simple pipe, pump and control valve system. The example shows that the index can be a useful tool for assessing the flexibility of a design, for comparing alternative flowsheets and for establishing proper trade-offs between flexibility and its cost.

INTRODUCTION

The design procedure may be viewed in two stages: 1) choosing the process configuration, and 2) determining the values for the design parameters of the chosen configuration. In both stages the major objective is to arrive at a design that is both economical and operable. While most systematic design tools that have been developed in the past are directed towards the improvement of process economics, they usually neglect the objective of improving plant operability.

An important first step in incorporating operability considerations at the design stage is to provide an adequate treatment of operational flexibility. Flexibility as a design attribute represents the ability of a design to tolerate and adjust to variations in conditions which may be encountered during operation. The sources of these variations may be both external and internal to the process. Examples of external sources of variations include changes in throughput, feed quality, product requirements, battery-limit conditions, and ambient temperature, as well as fluctuations in utilities. Internal sources include variables such as exchanger fouling and catalyst deactivation. The presence of these variations make it the designer's task to provide a design which will exhibit feasible steady-state operation not just for a particular nominal operating condition, but rather for a range of varying conditions.

The conventional procedure to provide for flexibility in a design is to choose a "conservative" set of conditions as the design basis. Additional units are then commonly introduced and empirical overdesign factors are applied to the individual pieces of equipment in the process. While this practice is widely used, it has two major disadvantages. First, since the effects of process interactions on the equipment comprising the process may not be adequately considered, the degree of flexibility actually achieved through this procedure is in general uncertain. Second, since the plant is designed and optimized at a single condition, there is no guarantee that plant performance will be economical over a range of different conditions. Clearly more systematic procedures are desirable.

Recently, Grossmann and Halemane (1982,1983) have developed procedures for

designing optimal chemical plants in which the degree of flexibility is specified either by a finite sequence of discrete operating modes, or by a bounded set of uncertain parameters. This paper addresses the problem of flexibility from a different viewpoint; the objective here is to provide the designer with the capability to:

1. Evaluate the flexibility characteristics of an existing or proposed design in relation to expected operating requirements.
2. Determine the operating conditions which limit the flexibility in a design to identify process bottlenecks.
3. Compare the degrees of flexibility offered by different design configurations.

Since a quantitative characterization of flexibility is required to accomplish these objectives, a scalar index for operational flexibility is proposed in this paper. As will be shown this index provides a measure of the region of feasible operation in the space of the uncertain parameters. This region accounts for the fact that the process can be adjusted depending on the particular realization of parameters. The proposed index also provides parameter bounds for guaranteed feasible operation, as well as information on the "worst" operating conditions that limit the flexibility in a design.

It should be noted that an interesting application of the index of flexibility is that it could be used within a multicritefion optimization framework for minimizing cost and maximizing flexibility as discussed in Grossmann et al. (1983). With this approach trade-off curves for different flowsheets could be obtained as shown in Fig. 1 in order to determine "optimal" degrees of flexibility. This approach circumvents the problem of having to assign economic penalties for infeasible operation as for instance in the method of Weisman and Holzman (1972). Also, it should be noted that as opposed to the resilience index for heat exchanger networks proposed by Saboo et al. (1983), the index of flexibility presented in this paper is applicable to any chemical processes that operate in the steady-state.

Mathematical formulations and basic properties of the index of flexibility are presented here in Part I. The objective is to establish those conditions and properties

that can be exploited to simplify the numerical computation of the index. As will be shown in Part II (Swaney and Grossmann, 1983), efficient algorithms can be developed based on the properties presented in this paper.

AN INDEX OF FLEXIBILITY

Flexibility of a plant design represents the ability to accomodate variations of a set of uncertain parameters θ_j j=1,...p. Since the degree of flexibility is determined by the range of parameter variations that the design can tolerate, a scalar index of flexibility can be constructed to measure the size of the feasible operating region in the space of uncertain parameters θ. The feasible region R shown in Fig. 2 gives the complete description of the flexibility characteristics of the design. Combinations of the uncertain parameters lying inside the region permit adjustment of the process to achieve feasible plant operation, while those parameter values outside of the region do not. In general the actual shape of this region could be rather complex, and since an arbitrary geometry is difficult to treat in a meaningful way, the following approach is proposed.

Firstly, it will be assumed that the uncertain parameters vary independently of each other.[1] It makes sense, then, to analyze the feasible region R by taking feasible nominal parameter values as a base point, and then determining the maximum ranges over which the parameters may vary independently of each other while still remaining inside the feasible region. Geometrically, this approach corresponds to inscribing within the feasible region a hyper-rectangle which is centered at the nominal point θ^N as shown in Fig. 2. The size of the feasible region is then characterized by the lengths of the sides of the rectangle, which in turn define lower and upper bounds for the parameters. The remaining difficulty is that the rectangle is not uniquely determined; trade-offs can result by increasing the ranges of some parameters while decreasing the ranges of others.

In actual practice however, each uncertain parameter θ_j will not vary over totally arbitrary ranges. For example, the temperature of cooling water typically

---

[1] If the set of parameters in the original problem formulation is dependent then principal component analysis may be employed to obtain an independent set

varies between 290K and 305K, whereas throughput may vary by as much as ±30% during normal plant operation. Therefore, if it is assumed that expected deviations or range estimates $A0^{*}_{j}, A0_{\tilde{j}}$, are given in the positive and negative directions for each parameter j, the sides of the rectangle can be scaled in proportion to the expected deviations. This then yields a unique definition of the maximum hyper-rectangle that can be inscribed within the feasible region as is shown in Fig. 3. Using the expected deviations as scaling factors positive and negative variations in the uncertain parameters may be expressed as scaled deviations from a given nominal value:

$$\varepsilon^{+}_{j} = \frac{o_j - e^{**}_j}{\Delta\theta_j} \qquad \varepsilon^{-} = \frac{of - e_j}{\Delta\theta_j} \qquad (1)$$

One may then consider the feasible region expressed in the space of the scaled parameters as shown in Fig. 4. In the scaled space the hyper-rectangle appears as a hypercube, centered at the nominal point (located at the origin). The dimension of the largest hypercube which may be inscribed within the feasible region may then be adopted as the desired measure of the size of the region. The index of flexibility, F, is therefore defined as one-half the length of a side of that hypercube. In that way, any set of scaled parameter deviations which do not exceed the value of F will lie inside the hypercube and therefore permit feasible operation.

Referring back to Fig. 3, in the parameter space *6* the flexibility index determines the maximum hyper-rectangle T that can be expanded around the nominal point with sides proportional to the expected deviations Ad^{*}_{j}, Ad'_{j} This hyper-rectangle then defines the actual lower and upper bounds

$$(\theta^{N} - F\Delta\theta^{-}) \leq \theta \leq (\theta^{N} + F\Delta\theta^{+})$$

over which feasible operation can be guaranteed for the set of uncertain parameters.

It should be noted that in the proposed index of flexibility it is through the expected deviations $A0^{+}_{j}$, AdT_{j} that the designer specifies that part of the feasible region which is of practical interest. Grossmann et al. (1983) present a brief discussion on the statistical interpretation of the expected deviations, and suggest

that an appropriate choice is to use range or variance estimates of the parameters. In actual practice the design engineer could specify these range estimates based on experience, statistical data, or rule-of-thumb target values.

Mathematical Formulation

Having defined qualitatively the index of flexibility, the mathematical formulation to determine this index will be presented. Consider the physical performance of the chemical plant to be described by the following set of constraints

$$h(d,z,x,0) = 0 \qquad (2)$$

$$g(d,z,x,0) \pounds 0$$

where h is the vector of equations (such as mass and energy balances or equilibrium relations) which hold for steady-state operation of the process, and g is the vector of inequalities (typically physical operating limits or product specifications) which must be satisfied if operation is to be feasible. The set of all variables is partitioned according to the following scheme: d is the vector of design variables that define equipment sizes. These are fixed at the design stage and remain constant during plant operation. *0* is the vector of uncertain parameters referred to previously. The vector of state variables x is a subset of the remaining variables having the same dimension as h. The vector z of control variables represents the degrees of freedom that are available during operation, and which can therefore be adjusted for different realizations of *8.*

For a given plant design d, and for any realization of *6* during operation, the state variables may be expressed as an implicit function of the control z using the equalities from (2)

$$h(d,z,x,0) * 0 \;=\hat{}\; x = x(d,z,0)$$

which allows elimination of the state variables, so that the process may be described by the following reduced inequality constraints:

$$g(d,z,x(d,z,\theta),\theta) = f(d,z,\theta) \leq 0. \tag{3}$$

The inequalities in (3) determine feasibility or infeasibility of operation for a chosen control z when d and θ are given. However, since the control variables represent degrees of freedom that may be adjusted during operation to suit prevailing conditions, feasibility for a given d and θ requires only that <u>some</u> z exist for which $f(d,z,\theta) \leq 0$. Correspondingly, R, the region of feasibility in θ-space, is defined by

$$R = \left\{\theta \mid \left[\exists z \mid f(d,z,\theta) \leq 0\right]\right\}. \tag{4}$$

Evaluation of the flexibility index F corresponds to inscribing within region R a scaled hyper-rectangle T (see Fig. 3) which may be expressed in terms of the non-negative scalar variable δ as

$$T(\delta) = \{\theta \mid (\theta^N - \delta\Delta\theta^-) \leq \theta \leq (\theta^N + \delta\Delta\theta^+)\} \tag{5}$$

The flexibility index, F, for a given design d, is then given by the maximum value of δ in the semi-infinite programming problem

$$\begin{aligned} F &= \max \delta \\ \text{s.t. } &\forall \theta \in T(\delta) \left\{\exists z \mid f(d,z,\theta) \leq 0\right\} \\ T(\delta) &= \{\theta \mid (\theta^N - \delta\Delta\theta^-) \leq \theta \leq (\theta^N + \delta\Delta\theta^+)\} \end{aligned} \tag{6}$$

where the first constraint imposes the condition that operation be feasible for all θ values that lie within the hyper-rectangle $T(\delta)$. Halemane and Grossmann (1983) have shown that the feasibility condition is mathematically equivalent to

$$\max_{\theta \in T(\delta)} \min_{z} \max_{i \in I} f_i(d,z,\theta) \leq 0. \tag{7}$$

Therefore, an equivalent formulation for the flexibility index is

$$F = \max \delta \tag{8}$$

$$\text{s.t.} \quad \max_{\theta \in T(\delta)} \min_{z} \max_{i \in I} f_i(d,z,\theta) \leq 0$$

$$T(\delta) = \{\theta \mid (\theta^N - \delta\Delta\theta^-) \leq \theta \leq (\theta^N + \delta\Delta\theta^+)\}.$$

The direct solution of the problem in (8) is in general very difficult since it involves the max-min-max constraint, which as discussed in Grossmann et al. (1983) can lead to a non-differentiable global optimization problem. Before attempting to devise a solution procedure for this problem, it is first necessary to establish some mathematical properties of the flexibility index. In the next three sections, two alternate descriptions of the feasible region R are developed. The first is used to establish conditions under which the solution to (8) will occur only at a vertex (corner-point) of the hyper-rectangle T. The second representation provides the foundation for the solution algorithms presented in Part II.

MATHEMATICAL PROPERTIES

Conditions for a Vertex Solution

As shown in the example of Fig. 3, the maximum hyper-rectangle that can expanded around the nominal parameter point touches the boundary at a vertex of the hyper-rectangle. This vertex can be regarded as a critical point (or "worst-case" operation) for the design since it is the one that limits the maximum flexibility of the plant (i.e. the size of the maximum hyper-rectangle). In the general case there is the possiblity of having more than one critical point, since there may be more than one set of conditions which will reach the flexibility limits of a design. Although intuitively one might think that a critical point must lie at a vertex, this may not always be the case as shown in Fig. 5, where the maximum hyper-rectangle touches the boundary at one of the faces of the hyper-rectangle. Therefore, a crucial question that arises is, what is the nature of the constraint functions for which the critical points will only lie at vertices? For cases where this property holds true the computation of the index of flexibility could be simplified considerably, as then only the finite number of directions from the nominal point to the vertices would have to be analyzed to determine the maximum hyper-rectangle.

In order to answer the above question, it is convenient to define the following function which provides a measure of feasibility for a design d at the parameter realization *6* (see Kalemane and Grossmann, 1983):

$$yid.d) * \min_{u,z} \quad u \tag{9}$$

$$\text{s.L} \quad f_i(d,z.0) \text{ £ } u \ , \ i\text{GI}$$

Values of *6* for which f(d,0) £ 0 are thus feasible and lie within the region R, which as shown in Appendix I may then also be expressed as

$$R = \left\{ \theta \ \middle| \ \psi(d,\theta) \leq 0 \right\}. \tag{10}$$

Note that the boundary of R is determined implicitly by the equation *f(d,d)* = 0(see Fig. 3). Also, the function *f(d.d)* can be incorporated into problem (8) by rewriting it as

$$F \text{ « } \max \ a \tag{11}$$

$$\text{s.t.} \quad \max_{\theta \in T(\delta)} \psi(d,\theta) \leq 0$$

$$f\{d,0) = \min_{z} \max_{i6I} f.(d,z,0)$$

$$T(\delta) = \{0 \ | \ (tf^N - \&Ad\sim) \text{ £ } 6 \text{ £ } (6^N + \delta\Delta\theta^+)\}$$

One first has to determine the properties of the function *f(d,0),* which defines the boundary for feasible operation in the parameter space. The following properties, proven in Appendix II, hold for the function *fid,6):*

<u>Property 1</u>. If f_i(d,z,0), i€I, are continuous functions in z and *8.* then f(d,0) is a continuous function in *6.*

<u>Property 2</u>. If **, *d** is a bounded solution of (11), and f_i(d,z0), iGI, are continuous in z and *8.* then *?(d,6*)* = 0.

Although this second property is rather obvious from Figs. 3 and 5, its rigorous

proof is important in that it shows that continuity of the constraint functions is a sufficient condition for the solution of (11) to be at the boundary of region R, $\gamma(d,\theta) = 0$.

The next point to be considered concerns the nature of the function *f(d,0)* for which the solution of problem (11) will lie at a vertex of the hyper-rectangle T. Fig. 3 would suggest that a sufficient condition is that *f(6.d)* define a convex feasible region. However, this condition is too stringent, since Fig. 6 shows a nonconvex region for which the solution still lies at a vertex. On the other hand, the region shown in,Fig. 5 is also nonconvex, but in this case the solution does not lie at a vertex. As will be shown below, a less stringent condition than requiring convexity of *f(6. 6)* is that this function be one-dimensional quasi-convex (1-DQC).

<u>Definition 1</u>. *fid,6)* is a one-dimensional quasi-convex function in *6* if and only if for 0^1, 6^2 G R, where $0^2 = 0^1 \bullet Xe'$, X is a non-zero scalar, and e^j is a coordinate direction given by the j'th column of the identity matrix I (dim p x p), the following condition holds:

$$maxif(d.e\backslash f(d.d^2)\} \ * \ ?(d,*0Mi\text{-}a)0^2) \qquad Va\in[0,1].$$

Qualitatively what this definition means is that one-dimensional quasi-convexity requires that the function *f(6.8)* be quasi-convex only along directions parallel to the coordinates. Therefore, this leaves the possibility that *f{6,6)* be not quasi-convex along a direction different from the coordinates. To give a geometrical interpretation of this property it is convenient to define what a one-dimensional convex region is and how it relates to a 1-DQC function.

<u>Definition 2</u>. R is a one-dimensional convex region if and only if for 0^1, 0^2 G R, where $0^2 = 0^1 \bullet Xe^j_{\#}$ X # 0. the point *6 « a6f(\-a)6*$_z$ G R for all *a* G [0,1].

<u>Theorem 1</u>. If *f(d.6)* is 1-DQC then the region R is one-dimensional convex.

In the example shown in Fig. 6 one can see that the region R is one-dimensional convex since by taking any two points belonging to the region and that

lie parallel to the coordinates (e.g. points A and B), the line connecting these points also lies inside the region R. However, Fig. 5 shows an example for which some points in the line connecting a similar pair of points A and B lie outside the region R. Since in the former case the largest hyper-rectangle T touches the boundary at the vertex, it would seem that 1-DQC in the function *f(d,0)* is a sufficient condition for this to happen. This property is proved in the following theorem.

<u>Theorem 2</u>. If *f(6,8)* is continuous and 1-DQC in 0, then the solution *0** of problem (11) must lie at an extreme point of the hyper-rectangle *1(6%*

The significance of this theorem is that it establishes rigorous sufficient conditions under which critical points will correspond to extreme points, or vertices, in the parameter space. However, since this theorem is expressed in terms of requirements for the function *f(6.8),* the next relevant question is, what class of constraint functions will lead to a 1-DQC *f(d.0)7* One could be tempted to think that joint 1-DQC of the parameters *0* and controls z in the constraint functions is all that is required. This would be a very desirable property since for instance functions that are monotone in z and *6,* whether convex or concave, are also 1-DQC. Unfortunately, as shown in the theorem below a somewhat stronger condition must be imposed on the constraint functions to ensure that f(d,0) is 1-DQC.

<u>Theorem 3</u>. If the constraint functions f_i(d,z,0), iGI, are jointly quasi-convex in z and one-dimensional quasi-convex in *0* then the function *f{d,6)* is one-dimensional quasi-convex in *0.*

The geometrical interpretation of this result is that the constraint functions must define a convex region in the space of the controls and each parameter, taken one at a time. If this is the case, then from Theorem 2 it can be guaranteed that the critical point of the hyper-rectangle will lie at a vertex. If, on the other hand, a convex region does not exist for one parameter and all the controls, then the critical point may not lie at the vertex of the hyper-rectangle. An example of this case is shown in Fig. 7, where for constant *0-* the constraint functions define a non-convex region in z and $\$_{19}$ and the critical point 0* does not lie at one of the extreme points of the line defined by *d₁" - i*A0~₁ £ 0^ £ 0*f + &*A0₁*.*

Summarizing the results of this section, the solution i*, 0* of problem (8) for the flexibility index is located at the boundary of the feasible region R since f(d,0*)=O. Furthermore, if the constraint functions f_i(d,z,0) are jointly quasi-convex in z and 1-DQC in *6.* then *d** corresponds to a vertex of the hyper-rectangle TU*). Also, since in this case the maximization of *f(d,d)* in the parameter space involves a 1-DQC function, there will be in general more than one local maximum of f(d,0). Consequently, any algorithm for determining the flexibility index in (8) which assumes the class of functions described above will in principle have to examine all the vertex directions. It is important to point out that the above results apply also to the case where the constraints f_i(d,z,0) are jointly convex in z and *6* (which includes, for instance, constraints that are linear in z and *6)* since joint convexity is a particular case of one-dimensional quasi-convexity. Also, it should be mentioned that although for practical design problems it might not be possible to establish whether in fact the actual constraints belong to the class of functions described above, the theoretical results presented here describe precisely the class of problems for which the critical points for feasible operation correspond to vertices or extreme values of the parameters.

An Alternate Formulation

In this section a parametric description of the boundary of the feasible region R is developed which leads to an alternate formulation for the flexibility index that is of direct use when developing the solution procedures for problem (8) presented in Part II. The first step is to adopt the following parametric description for *0:*

$$6 \ll 0^H \cdot \text{iff} \tag{12}$$

The vector *$* represents a direction of displacement from the nominal point 0^N, With *i* a non-negative scalar distance (see Fig. 8a). By substituting (12) into (5), the hyper-rectangle T may be expressed in terms of simple bounds for *&,* i.e. a constant set T:

$$T * \{ y \mid -A0\sim <> df \pounds A0^+ \} \tag{13}$$

The boundary of the feasible region may then be described parametrically as

the scaled distance *&*(&)* from the nominal point to the boundary in the direction *V.* The function *&*(3)* is given by

$$S^*(\&) * \max 3$$

$$\text{s.t. } f(d,z,0) * 0 \qquad (14)$$

$$0 * 0^N + \delta\theta$$

subject to the following assumption:

<u>Assumption 1</u>. The solution specified by (14) is taken to be that solution 3* with the property that

$$\left\{ \exists z \mid f(d,z,(\theta^N+\delta\theta)) \le 0 \right\} \quad ¥ \; S \; e \; [0,3^*] \qquad (15)$$

This assumption provides that the entire path from the nominal point to the boundary at distance 3* is feasible; i.e. if (14) has multiple local solutions, the solution with the smallest value for 3 is chosen. One may note that since the nominal point (5=0) is by definition feasible, (14) is feasible for all *V,* and *&*(&)* £ 0.

Figures 8a and 8b illustrate the use of (12) and *b*(8)* in describing the feasible region. As may be seen, the function *&*(&)* will not necessarily provide a description of all points on the boundary of region R. Parametric description of the entire boundary would require convexity of R along all radial directions emanating from the nominal point 0^N, a condition which would also guarantee the validity of Assumption 1. However, this convexity restriction is by no means neccessary for the purpose at hand, since for any direction V_9 *b*(&)* will elways describe any point on the boundary of R which could touch the surface of the inscribed hyper-rectangle T. Consequently, the utility of the function 3*(3[r]) may be seen from the following simple expression for the flexibility index:

<u>Theorem 4</u>. If Assumption 1 holds, then the formulation

$$F * \min_{\theta \in T} 3^*(\wedge) \qquad (16)$$

is equivalent to problem (6), where *&*(8)* is defined in (14).

Geometrically, solving (16) consists of finding the direction *9* for which the distance *&*(&)* to the boundary of R is shortest *{&** in Fig. 8a). This then defines the largest hyper-rectangle T(<5*) that can be inscribed within region R. Note that if the properties of the previous section are met, the solution *ff** will correspond to a vertex direction, i.e. *V** € *{&^{k}.* k=1,...,2^p}, where the components V^*_j are particular choices of either $A0^+_j$ or $-A0^-_j$.

<u>Properties of *y[d.d)* and *h*(8)*</u>

The functions *y(6.6)* and *&*(8)* provide two different means of analyzing the feasible region R. Below, some properties of these functions are presented and the relation between them is established. The objective is to determine those properties that can be exploited to produce an efficient solution procedure.

First, for convenience *fid.d)* may be reformulated in terms of *ff* and *&:*

$$f^*ii.ff) = \min_{u,z} u \qquad (17)$$

$$\text{s.t. } f_i(d,z,0) - u \le 0, \quad i \in I$$

$$e - e^H - sdf^* o.$$

Solving subproblem (17) corresponds to. determining feasibility at a particular *8* location (i.e. for a particular distance *&* in direction *9);* on the other hand, subproblem (14) defining *S*(&)* determines the distance *S** to the boundary of region R along direction *V.* In the following, the two subproblems are compared for a given direction *&=&^{k}* (e.g. a vertex direction).

In order to establish the properties of the solutions to (17) and (14), it is convenient to formulate the following pair of problems which illustrate the close relation between the two:

PI: $u^*(\delta) = \min u$

s.t. $f_i\{d,z,0) - u$ £ 0 . $i \in I$

$0\text{-}0'' \quad - \delta\tilde{\theta}^k$ ** 0

P2: $\delta^*_u(u) = \max_{\delta,z} b$

s.t. $f_i(d.z,0) - u$ £ 0 , iGI

$e - \theta^N - \delta\tilde{\theta}^k = 0$

Note from P1 and (17) that u*(3) * *f'ii.if*).* and from P2 and (14) that «*$_u$(0) = 5*{^^{k}). We will make the following two assumptions for problems PI and P2:

1) Joint quasi-convexity of f_i(d,z,^) over the subspace spanned by z and the ray *0 * 0^N * iFK*

2) Linear independence of the gradients in z of the active constraints.

These assumptions provide that when a solution to P1 or P2 exists, it is determined by the unique solution to the corresponding Kuhn-Tucker conditions (Bazaraa and Shetty, 1979, Theorems 4.3.6 and 4.3.7). The Kuhn-Tucker conditions for P1 may be written:

$$1 - \sum_i \lambda_i = 0 \tag{18a}$$

$$\lambda^T \nabla_z f^T(d,z,\theta) = 0^T \tag{18b}$$

$$\lambda^T \nabla_\theta f^T(d,z,\theta) + v^T = 0^T \tag{18c}$$

$$\lambda \geq 0 \tag{18d}$$

$$\lambda_i[f_i(d,z,\theta) - u] = 0 \quad , i \in I \tag{18e}$$

$$f_i(d,z,\theta) - u \leq 0 \quad , i \in I \tag{18f}$$

$$\theta - \theta^N - \delta \tilde{\theta}^k = 0 \tag{18g}$$

and those for P2:

$$1 + v^T \tilde{\theta}^k = 0 \tag{19a}$$

$$\lambda^T \nabla_z f^T(d,z,\theta) = 0^T \tag{19b}$$

$$\lambda^T \nabla_\theta f^T(d,z,\theta) + v^T = 0^T \tag{19c}$$

$$\lambda \geq 0 \tag{19d}$$

$$\lambda_i[f_i(d,z,\theta) - u] = 0 \quad , i \in I \tag{19e}$$

$$f_i(d,z,\theta) - u \leq 0 \quad , i \in I \tag{19f}$$

$$\theta - \theta^N - \delta \tilde{\theta}^k = 0 \tag{19g}$$

Here λ and v are vectors of multipliers for the inequality and equality constraints respectively. Analysis of (18) and (19) provides the following conclusions:

<u>Property 3</u>: Let the dimensions of the vectors z and θ be n_z vand n_θ respectively. Then n, the number of inequality constraints which are active with non-zero multipliers at the solution to P1 or P2, is given by $n = n_z + 1$.

<u>Property 4</u>: The solutions to both $\delta_u^*(0)$ in P2 and $u^*(\delta_u^*(0))$ in P1 are characterized by the same set of active constraints and specify identical values for z, θ, u, and δ.

Property 3 implies that a solution to $\gamma^*(\delta,\tilde{\theta}^k) = u^*(\delta)$ or $\delta^*(\tilde{\theta}^k) = \delta_u^*(0)$ is

completely determined by solving the system of equations corresponding to the appropriate set of n_z+1 active constraints for z and u or 5. Property 4 shows that the solutions to (17) and (14) become identical at the boundary of the feasible region, and that $f^*(\&.ff^k) = 0$. These properties in the form presented depend on linear independence of the z-gradients of the active constraints and on the assumed uniqueness of the solution to the n_z+1 active set equations. Both of those assumptions may be relaxed. In the event that there are more control variables than linearity-independent active constraints, the excess degrees of freedom in z may be specified arbitrarily (e.g., set $z_j = z_j^{\wedge}$ for those z_j with dependent gradients if their values are not fixed by the stationarity requirements in (18b, 19b)). When degeneracies occur, uniqueness of the solution may not hold, but the equivalency of solutions to P1 and P2 remains.

The significance of these results is that the subproblem in (14) can be used to locate the boundary of the region R along a vertex direction to determine the maximum feasible deviation from the nominal point. Then, assuming the solutions to (8) lie at the vertices of T, problem (16) may be formulated more simply as $F = \min_k\{6^*\{\&^k\}$. On the other hand, problem (17) can be used to check for feasibility at a given deviation 5 for any vertex k. These subproblems form the basis of the direct search procedure presented in Part II. The example in the next section demonstrates the application of the -flexibility index, and provides geometric illustration of the mathematical properties established in this paper.

EXAMPLE

Illustration of the flexibility index is provided by the simple example shown in Fig. 9. There a centrifugal pump must transport liquid at a flowrate m from its source at pressure P_1 through a pipe run to its destination at pressure P^*_2 Both the flowrate m and the pressure P_2^* are expected to vary significantly during operation. The actual pressure $?_2$ must remain within a tolerance e of the desired pressure P_2^* and is controlled with a valve on the pump discharge. The design variables to be selected are the pipe diameter D, the pump head H, the driver power W, and the control valve size $C_v^{\wedge}$. The control variable z is the valve coefficient C_v, the uncertain parameters 6_y and $\$_2$ are P_2^* and m respectively, and P_2 is a state variable.

The nominal value for P_2^* is 800 kPa with expected deviations of +200 and -550 kPa. The nominal value of m is 10 kg/s with expected deviations of +2 and -5 kg/s. P_y is fixed at 100 kPa. The problem consists then of determining the flexibility index for different designs that could be proposed for this system, as well as developing the trade-off curve of cost versus flexibility.

The equations and constraints describing the above system are as follows:

a) Energy balance

$$P_1 \cdot \rho H \frac{m^2}{l>C_v^2} \cdot km^{1-84}D^{\sim 5*16} - P_2 = 0 \qquad (20)$$

b) Outlet pressure tolerance

$$P_2^* - € £ P_2 £ P_2^* \cdot € \qquad (21,22)$$

c) Pump driver power limit

$$\frac{mH}{f} £ \hat{W} \qquad (23)$$

d) Control valve range

$$rC_v^{MAX} \leq C_v \leq C_v^{MAX} \qquad (24,25)$$

where the constant k describes pressure drop in the pipe, the ratio r describes the control valve range, and the liquid density /> and pump efficiency *rj* are treated as constants. The values of the constants in (20) - (25) are given in Table 1.

The reduced inequalities f(d,z,0)£O may be obtained by elimination of the state variable P_2 from (20), yielding

$$(P_1 + \rho H - \frac{m^2}{l>C_v^2} - km^{184}D^{\sim 5,16}) - P_2^* - « * 0 \qquad (26)$$

$$-<^{p}i * P^{H} \frac{m^2}{5''} * km^{1-84}D^{\sim 5,16}) + P! - c £ 0 \qquad (27)$$

$$mH - {}_v\hat{W} £ 0 \qquad (28)$$

$$C_y - C j * \wedge \wedge 0 \qquad (29)$$

$$rC_v^{MAX} \_ c \wedge 0 \qquad (30)$$

For a given design d * ($\hat{W}$,H,D,C^AX). these inequalities may be rewritten in terms of z • C_y, $f Pj*. 0_2* m. and constants a_t - a_Q:

$$a_{+} - \frac{e^2}{4} - a_{\_} \wedge_{\_}^{84} - 6_{,} \pounds 0 \qquad (31)$$

$$-a_{3} + \frac{A^2}{Ar} \cdot a_{\_} *_{2}^{'84} * 0_{,} \pounds 0 \qquad (32)$$

$$*_{2} - a_{4} \pounds 0 \qquad (33)$$

$$z - a_{\_} \pounds 0 \qquad (34)$$

$$a_{6} - 2 \wedge 0 \qquad (35)$$

Since Property 3 applies for this problem, the boundary of the feasible region f(d,0)=O may be constructed by considering the appropriate pairs of constraints in (9) with u=0 and eliminating z between each pair to yield contours in 0-space. Region R is then the intersection of the individual feasible regions for each pair as shown in Fig. 10, where the boundary is determined by the constraint pairs (27),(29); (26),(30); and (26),(28) or (27),(28). It is interesting to note that in this example the conditions of Theorem 3 are not met, since the constraint function in (31) is not jointly quasiconvex in z and each 6_j. However, for this problem the function *f(6.6)* is one-dimensional convex in *6* in spite of this. Theorems 1 and 2 apply, so that the region R is one-dimensional convex as seen in Fig. 10.

Also depicted in Fig. 10 is the rectangle T(<5*) inscribed within R around the nominal point. As shown, the one-dimensional convexity of region R provides that TU*), the solution to problem (8), touches the boundary of R at a vertex. Note that Property 3 applies, and therefore n s n^+1 * 2, since *6*(&^{k})* at the limiting vertex 1 is determined by the combination of constraints (27) and (29). Vertex 2 illustrates a case of degeneracy. Since *&*{V^k)* for vertex 2 is determined by constraint (28), which has a zero z-gradient, linear independence of the gradients is lost. The consequence here is that z is not uniquely determined, and may vary between the limits implied by (26) and (27). However, a valid solution to (14) may still be characterized by a set of n_z+1 active constraints by choosing either (26) or (27) in conjunction with (28).

The resulting feasible regions R corresponding to three different proposed designs are depicted in Fig. 11. The first design d° is a "minimal" design, which has been optimized at the nominal operating point. Since the nominal point lies at the

boundary of the feasible region R for d°, no rectangle of finite size can be expanded, and therefore the flexibility index for this design is zero. Design d^1 is more conventional; pump head />H has been increased by 230 kPa to reflect the expected 200 kPa increase in P_2^* and to provide an extra 30 kPa for flexibility in the control valve. Driver power W is sized at the resulting head and the expected high value for m of 12 kg/s. The index of flexibility for d^1 is illustrated in Fig. 11 by the rectangle inscribed within the d^1 region. The critical point for this design lies at the vertex which simultaneously maximizes P_2^* and m, for which 5_k=0.62. Thus d^1 has a flexibility index of F-0.62 which implies that the maximum variations this design can handle are +1.24 and -3.1 kg/s for the flowrate, and +124 and -341 kPa for the delivery pressure. Therefore, in spite of the chosen overdesign allowances the condition P_2^*=1000 kPa, m=12 kg/s remains infeasible. Nor is d^1 the least expensive design possessing a flexibility index of 0.62, since the driver size could be reduced somewhat without influencing F. Design d^2 shown in Fig. 11 is one for which the flexibility targets are exactly met, i.e. F=1.0, at minimum cost as given by the data in Table 1. Note that in this case the region R is modified in such a way so as to exactly contain the rectangle whose sides correspond to the specified expected deviations, +2 and -5 kg/s for the flowrate and +200 and -550 kPa for the delivery pressure. Also note that in this design, three vertices of the rectangle are critical points. This behavior results because the design optimization tries to include the desired rectangle within the smallest possible feasible region, which causes as many vertices to touch the boundary as possible.

As illustrated in Fig. 11, the proposed flexibility index provides a systematic measure of the size of that region of feasible steady-state operation which is of interest to the design engineer. Furthermore, this index is very easy to interpret since values that lie between 0 and 1 denote the fraction of the range of expected deviations which can be handled. Values of the index greater than 1 denote designs for which it is possible to exceed the expected deviations and still have feasible operation.

Finally, Fig. 12 shows the trade-off curve between cost and flexibility for this

system. This curve was generated by optimizing the system for various levels of flexibility (i.e. €-constraint method as in Haimes et al., 1975). The cost function considered is the annualized investment and operating cost which was evaluated at the nominal point condition. As can be seen from this curve, for values of flexibility that lie within 0 and 1.3 only a moderate linear increase is experienced in the cost function. However, for flexibility values greater than 1.3 a rather sharp increase in the cost is experienced since the system becomes more inefficient to operate. Analysis of this trade-off curve will permit the designer to select an appropriate point in the curve, and so establish the degree of flexibility considered to be optimal.

Acknowledgement

The authors would like to acknowledge financial support provided by the National Science Foundation under grant CPE-8121665, and to the Exxon Industrial Fellowship.

References

Bazaraa, M.S. and CM. Shetty. *Nonlinear Programming,* John Wiley & Sons, New York (1979).

Edhal, R.H., M.H. Locke and A.W. Westerberg, "Improved Successive Quadratic Programming Optimization Algorithm". *AIChE J..* 29, 871 (1983).

Biegler, LT. and R.R. Hughes, "Infeasible Path Optimization with Sequential Modular Simulators", paper presented at the AIChE Annual Meeting, New Orleans (1981).

Evans, J.P. and F.J. Gould, "Stability in nonlinear programming". *Operations Research.* 18 (1970).

Grossmann, I.E. and K.P. Halemane, "Decomposition Strategy for Designing Flexible Chemical Plants", *AIChE J..* 28, 686 (1982).

Grossmann, I.E., K.P. Halemane and R.E. Swaney, "Optimization Strategies for Flexible Chemical Processes", *Computers and Chem. Eng..* 7, 439 (1983).

Grossmann, I.E. and M. Morari, "Operability, Resiliency and Flexibility- Process Design Objectives for a Changing World", paper presented at the 2nd International Conference on Foundations of Computer-Aided Process Design, Snowmass (1983).

Haimes, Y.Y., W.A. Hall and H.T. Freedman, *Multiobjective Optimization in Water Resource Systems: the Surrogate Worth Tradeoff Method.* Elsevier Scientific Publishing Co., Amsterdam (1975).

Halemane, K.P. and I.E. Grossmann, "Optimal Process Design Under Uncertainty", *AIChE J..* 29, 425 (1983).

Jirapongphan, S., J.F. Boston, H.I. Britt and L.B. Evans, "A Nonlinear Simultaneous Modular Algorithm for Process Flowsheet Optimization", paper presented at the AIChE Annual Meeting, Chicago (1980).

Morari, M., "Flexibility and Resiliency of Process Systems", *Computers and Chem. Eng.* , 7, 423 (1983).

Nishida, N., G. Stephanopoulos and A.W. Westerberg, "Journal Review: Process Synthesis", *AIChE J..* 27, 321 (1981).

Polak, E. and A. Sangiovanni-Vincentelli, "Theoretical and Computational Aspects of the Optimal Design Centering, Tolerancing and Tuning Problem", *IEEE Trans, on Circuits and Systems.* CAS-26, 795 (1979).

Saboo, A.K., M. Morari and D.C. Woodcock, "Design of Resilient Processing Plants: A Resilience Index for Heat Exchanger Networks", submitted to *Chem. Eng. Sci.* (1983).

Swaney, R.E. and I.E. Grossmann, "An Index for Operational Flexibility in Chemical Process Design. Part II: Computational Algorithms", submitted to *AIChE J.* (1983).

Weisman, J. and A.G. Holzman, "Optimal Process System Design Under Conditions of Risk", *Ind. Eng. Chem. Proc. Des. Dev.*. 11, 386 (1972).

APPENDIX 1 - Equivalence for Region Representation

Theorem. The regions R'= \d | [3^z | ttd.z.O) £ Ojj and R*= {# I fid.6) ^ 0 j are equivalent.

Proof. Firstly, by definition

$$R' \ll \{0 \mid [\, 3^* \mid f(d.z.^*) * 0]\} = \{d \mid [\, 3z \mid V\ 161.\ VdAW * 0]\}$$

By applying global max and min operators, the following equivalences hold:

$$R' = \{\theta \mid [\, 3^* \mid V\ 16I.\ fjfo.z.0) \wedge 0]\}$$

$$\Longleftrightarrow \{\theta \mid [\, 3^* \mid \wedge_{161} x\ f.(d,z.0) < 0]\}$$

$$\Longleftrightarrow \{\theta \mid \min_{z} \max_{i \in I} f.(d.z,0) <> 0\}$$

$$\Longleftrightarrow \{\theta \mid [\, \min_{z} u \mid u \wedge f.(d_f z \wedge) \,] \wedge 0\}$$

$$\Longleftrightarrow \{\theta \mid \psi(d,\theta) * 0\} = R''$$

which then proves that R'≡R*. QED.

APPENDIX II - Proofs of Properties and Theorems

Proof of Property 1.

The proof of this property can be found in Evans and Gould (1970) and in Polak and Sangiovanni (1979). In Theorem 4.13 of Evans and Gould it is shown that if *f[d.z,0)* = $\max_{i \in I}$ f.(d,z,0), then the function *?{d.z,8)* is continuous in z and *8.* Polak and Sangiovanni show that if ^(d,z,0) is continuous in z and *6* then *f{d,6)* = $\min_{z}$ *f(d,z,O)* is continuous in *0.*

Proof of Property 2.

Assume that 3*, *d** is a solution of (11) but that *fid.d*)* < 0. Since for any *&'* > *i*. T(&*)* C *T(&')* it follows that

$$\max_{\theta \in T(\delta^*)} \psi(d,\theta) = \psi(d,\theta^*) \leq \max_{\theta \in T(\delta')} \psi(d,\theta) = \psi(d,\theta') \tag{A1}$$

Since from property 1. $\psi(d,\theta)$ is a continuous function in θ this implies that there exists $\epsilon > 0$ and a $\delta^{\bar{}}$ in the neighborhood of δ^* such that

$$| \psi(d,\theta^*) - \psi(d,\theta^{\bar{}}) | < \epsilon$$

where $\psi(d,\theta^{\bar{}}) = \max_{\theta \in T(\delta^{\bar{}})} \psi(d,\theta)$. The above inequality and the hypothesis imply

$$\psi(d,\theta^{\bar{}}) - \epsilon < \psi(d,\theta^*) < 0$$

which for an arbitrarily small selection of ϵ yields

$$\psi(d,\theta^{\bar{}}) < 0 \tag{A2}$$

But since $\delta^{\bar{}}$ can be selected arbitrarily close to δ^*, and such that $\delta^{\bar{}} > \delta^*$, (A1) and (A2) would imply that $\delta^{\bar{}}$ is a feasible solution of (11) for which

$$\psi(d,\theta^*) \leq \psi(d,\theta^{\bar{}}) < 0$$

which in turn contradicts the assumption that δ^* is the solution to problem (11). Hence $\psi(d,\theta^*) = 0$ at the solution of problem (10). <u>QED</u>

<u>Proof of Theorem 1.</u>

Consider θ^1, θ^2, $\theta^2 = \theta^1 + \lambda e^j$, $\lambda \neq 0$ and such that θ^1, $\theta^2 \in R$. Assume that $\psi(d,\theta)$ is 1-DQC, but that the region R is not one-dimensional convex. This then implies that there exists an $\bar{\alpha} \in (0,1)$ such that for $\bar{\theta}=\bar{\alpha}\theta^1+(1-\bar{\alpha})\theta^2$, $\psi(d,\bar{\theta}) > 0$. But since $\psi(d,\theta)$ is 1-DQC we have $\psi(d,\bar{\theta}) \leq \max\{\psi(d,\theta^1), \psi(d,\theta^2)\}$.

Furthermore, since θ^1, $\theta^2 \in R$ implies $\psi(d,\theta^1) \leq 0$, $\psi(d,\theta^2) \leq 0$, it follows from the above inequality that $\psi(d,\bar{\theta}) \leq 0$, which is a contradiction. Therefore, if $\psi(d,\theta)$ is 1-DQC then the region R is one-dimensional convex. <u>QED</u>.

<u>Proof of Theorem 2.</u>

Assume that the solution θ^* is a non-extreme point, in which case we can select θ^1, θ^2, $\theta^2 = \theta^1 + \lambda e^j$, $\lambda \neq 0$, θ^1, $\theta^2 \in T(\delta^*)$, and a scalar $\bar{\alpha} \in (0,1)$ such that

*0** * S0Mi-S)0^2. Since *f[d,0)* is 1-DQC this implies that *f{6.0*) £ max{f[d,O*).* f(d,0^2)}. But from property 2, *yid.O*)* = 0, which would imply that *n\axlf{d.d^y). f[d.6^2))* * 0.

Clearly, if the equality holds we have a degenerate solution. If the strict inequality holds this would imply that either *f{d,d^y)* > 0 or *f{d,6^2)* > 0, which leads to a contradiction. Therefore, *0** must be an extreme point. QED.

Proof of Theorem 3.

a) In the first part, it will be proved that *f(6.z,d)* = $\max_{i \in I}$ f_i(d,z,0) is jointly quasi-convex in z and 1-DQC in *0.* Assume the negation of this statement, which would then imply that there exists an 5 6 (0,1) such that for z\ z^2, and 0^1, *6^2. d^2* = 0^1 + Xe^j, X * 0, the following inequality applies:

$$\wedge(d,SyMi\text{-}S)y^2) > \max\{f>(d,y^1),\ f>(d,y^2)\} \quad \text{where } y * \begin{bmatrix} z \\ \theta \end{bmatrix}.$$

This in turn implies that there exists a constraint T, *f{d,z,d)* = *t$_i$Ad,z,8)* such that

$$f_i\{d,\bar{a}y\wedge d\text{-}SJy^2) > \max\{\max_{i \in I} f_i td.y^1),\ \max_{i \in I} f_i(d,y^2)\} \wedge \max(f\wedge y^1),\ f\wedge y^2)\}$$

But this contradicts the assumption that the function *U$_i$* is jointly quasi-convex in z and 1-DQC in *6.* Therefore, *f(d.z,d)* is jointly quasi-convex in z, and 1-DQC in *e.*

b) It will be proved that *fkd.d)* is 1-DQC. Let *6^3*= S0Mi-2)0^2 where 5 6 (0,1) and e\ *0^2* are defined as above. Also let *f{d,0^k)* = min ^(d,z,0^k) - ^(d,z^k,0^k), k= 1,2,3. Since *f(d.z.ff)* is jointly quasi-convex in z, and 1-DQC in *B.* and z^3 is the global minimizer of *f(d,z,0^3)*

$$\max\{\phi(d,z^1,\theta^1),\ \phi(d,z^2,\theta^2)\} \geq \phi(d,\ 5z^1*(1\text{-}5)z^2,\ 0^3)\ Z\ f(d,z^3.e^3)$$

or equivalently,

$$maxif(d.0\backslash\ f(d.d^2)\}\ *\ f\{d,0^3)$$

which proves that *f(6,0)* is 1-DQC in *6.* QED.

Proof of Theorem 4.

Consider that (6) may be rewritten as

$$F^{s} \max i$$

$$\text{s.t. } TU) \subset R \qquad \text{(A3)}$$

Let *V** be the solution to (16) with *&*$*)* = $\hat{S}$. For all *i* > $\hat{i}$. *1(5)* will contain the point *6* = 0^N + *b$**. which is infeasible for (14) and thus outside of region R. Consequently, F £ 3. Next, consider that all points contained in T(<5) may be expressed as

$$T(3) = \{ e \mid e * e^N \cdot \delta\tilde{\theta},\ \tilde{\theta} \in \tilde{T},\ \delta \in [0, \hat{\delta}] \}$$

Assumption 1 provides that *6* = 0^N • *bV* is feasible for all *&E[0.&*{&)].* and the minimization in (16) provides that $\hat{5}$ = 3*(^*) ^ *&*(&)* for all 9^€T. Consequently, $T\hat{U}$) C R, $\hat{j}$ is the maximizer for (A3), and F=$\hat{3}$ may be determined by solving (16). QED.

Proof of Property 3.

Since the gradients in z are assumed to be linearly independent, this implies from (18b) that the number of non-zero multipliers $X._1$ in P1 is n > n_z, since (18a) provides that there exists at least one non-zero multiplier. Similarly, from (19b) the number of non-zero multipliers $X._1$ in P2 is n > n_z, since from (19a) v # 0, which implies in (19c) the existence of at least one non-zero multiplier. Furthermore, since the complete set of active constraints contained in (18f),d8g) and (19f),(19g) form a system of (n + n^) equations in (n^ + 1 + n^) variables, for this sytem to have a solution in general will require n £ n_z + 1. Therefore, n « n_z • 1. QED.

Proof of Property 4.

Let (z*, *6*.* u\ *b*.* $X^{<2>}$, $v^{(2)}$) denote the solution to P2, where u* is a specified

value. Also let c = ^ x!$^{2)}_{i}$. Since (z*. *d**. u\ *i**. $X^{(2>}$. $v^{l2)}$) is a solution to the system (19a) - (19g), it can be shown by algebraic substitution that (z*, *6**. u*, *&**. $X^{(1)}$. $v^{(1>}$) will be a solution to (18a) - (I8g) by letting $X^{(1)} = X^{(2)}/c$ and $v^{<1>} = v^{(2)}/c$. Since solutions to P2 and P1 are unique, their values for z*, *0**. u*, and *b** are thus identical. Futhermore, since $X^{(1)} = X^{(2)}/c$ and c > 0, both solutions are characterized by the same active set. The proof of this property is completed by setting u* = 0 in P2. and *b** = $3^*_u(0)$ in PI. <u>QED</u>.

Table 1. Data for example

Pump efficiency	$\eta = 0.50$
Liquid density	$\rho = 1000\ kg/m^3$
Control valve range	$r = 0.05$
Pressure drop constant	$k = 9.101 \times 10^{-6}\ (kPa)(kg/s)^{-1.86}(m)^{3.16}$
Inlet Pressure	$P_1 = 100\ kPa$
Outlet pressure control tolerance	$\leq 20\ kPa$
Annualized cost	$C = c_1 D + c_2 W^{.86} + c_3 W^N$
	$W^N = \frac{m^N H}{\eta}$
	$c_1 = 5.6 \times 10^5\ \$/m$
	$c_2 = 482.84\ \$/(kW)^{.86}$
	$c_3 = 500\ \$/kW$

[Captions for Figures]

Fig. 1: Trade-off curves of cost vs. degree of flexibility for alternative design configurations.

Fig. 2: Feasible region in 0-space and inscribed hyper-rectangles.

Fig. 3: Maximum scaled hyper-rectangle T inscribed within feasible region.

Fig. 4: Feasible region and inscribed hypercube in scaled parameter space.

Fig. 5: Region with non-vertex critical point.

Fig. 6: One-dimensional convex region.

Fig. 7: Non-convex subspace for 2 and parameter 0_y.

Fig. 8a: Parametric description of region R using *i* and *V.*

Fig. 8b: Corresponding function *S*{ff).*

Fig. 9: Pump and pipe run example.

Fig. 10: Construction of region R and rectangle TU*) for pump example.

Fig. 11: Feasible regions and flexibility indices for designs d°, d\ d^2.

Fig. 12: Cost vs. flexibility for pump example.

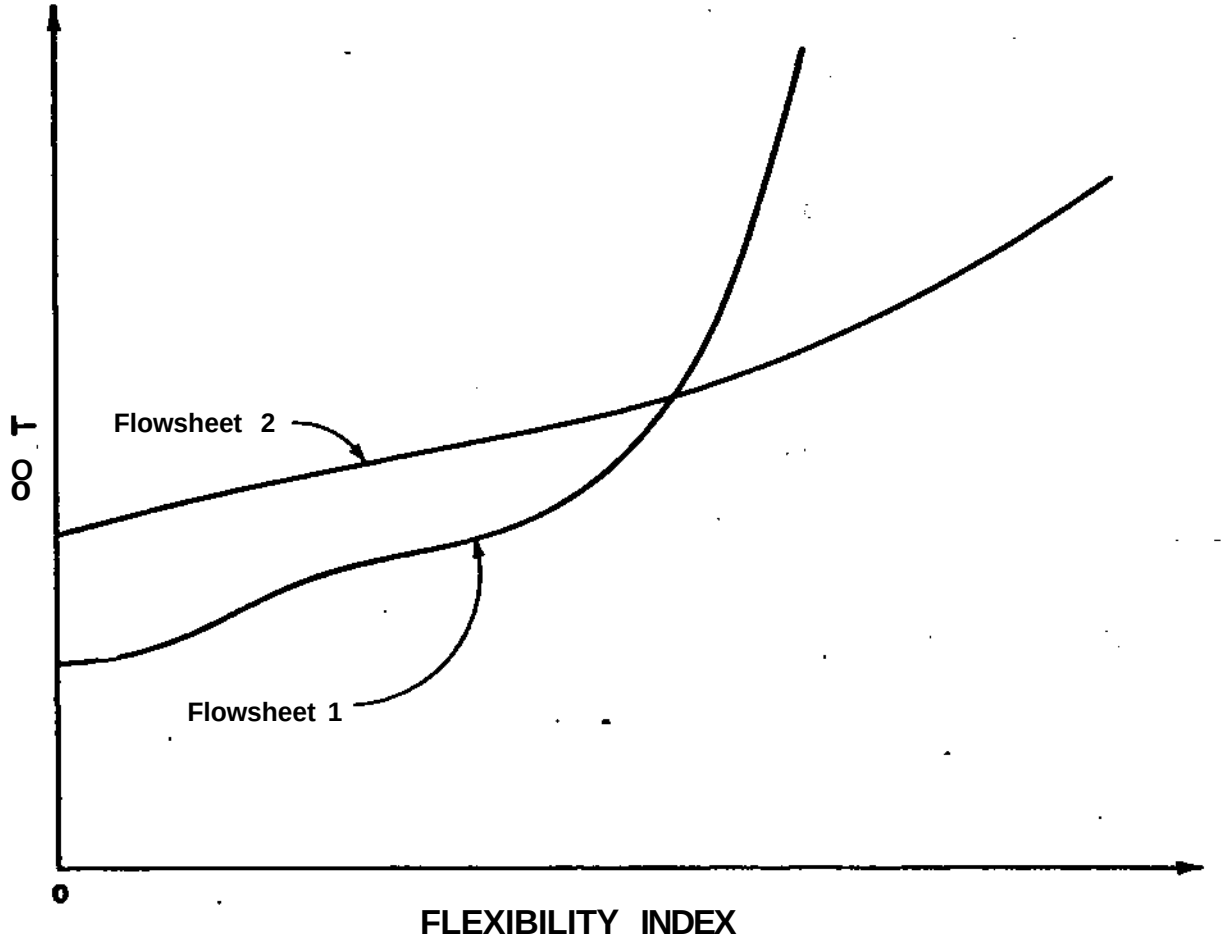


Fig. 1

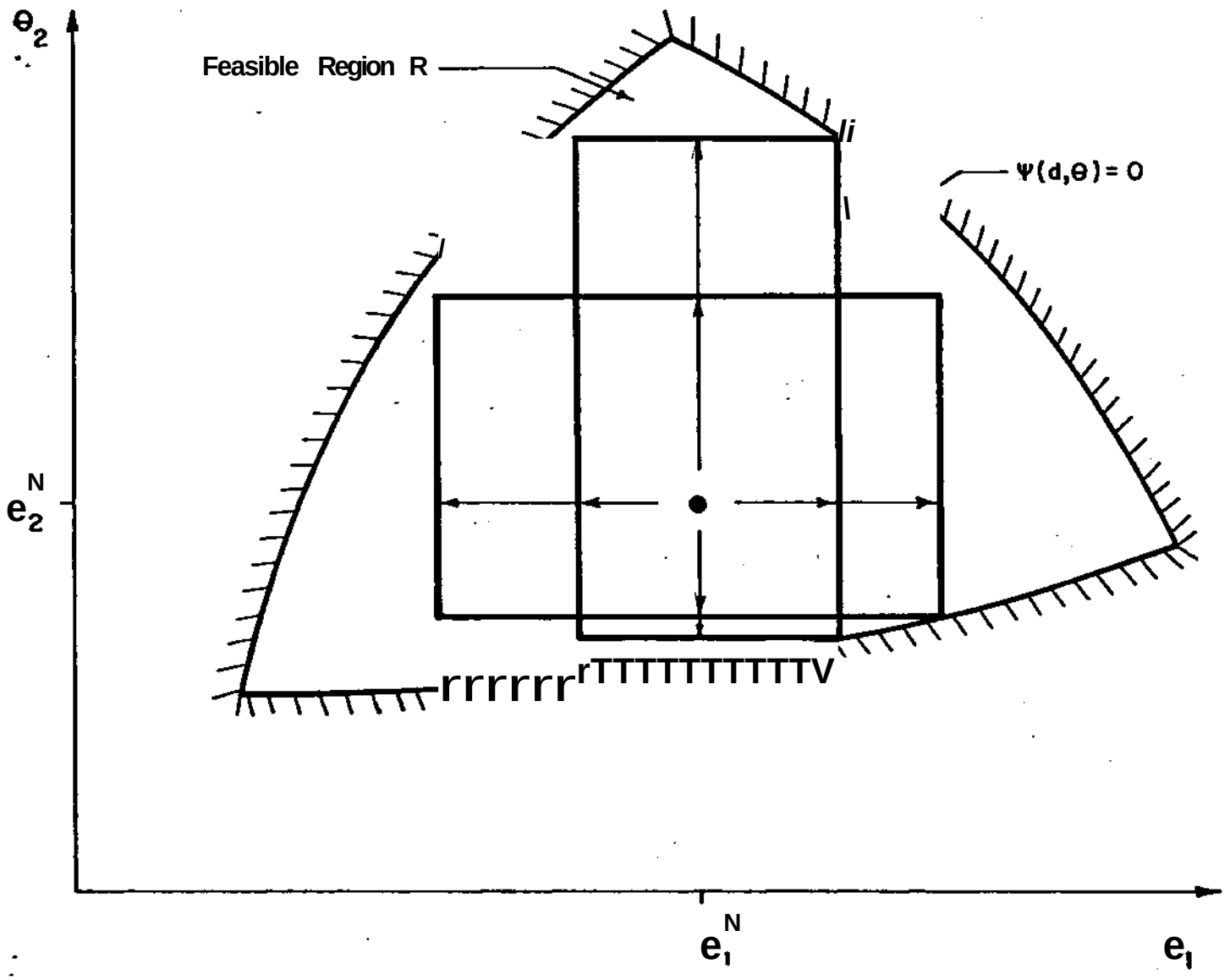


Fig.2

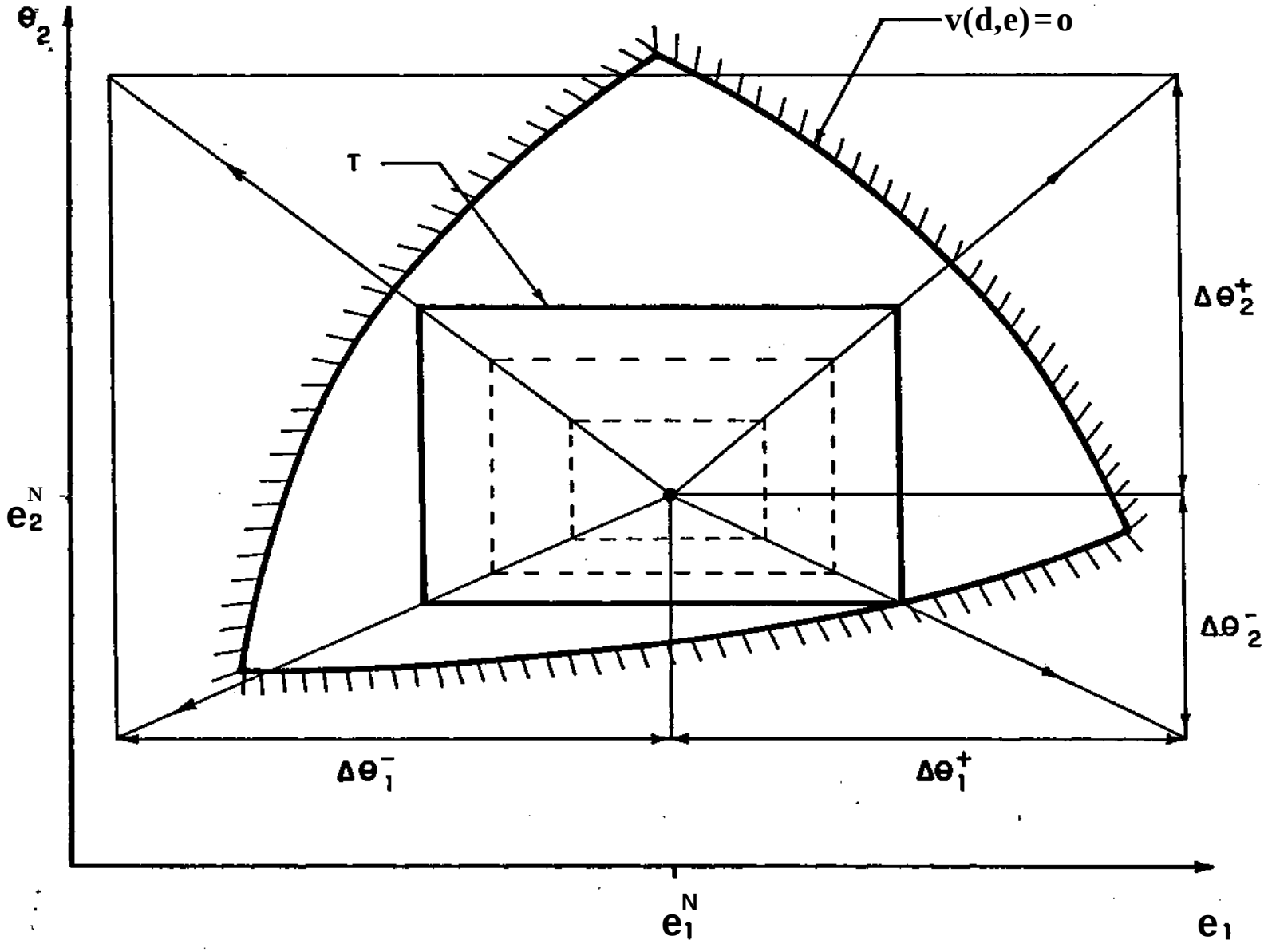

e_2
v(d,e)=o
T
$\Delta\theta_2^+$
e_2^N
$\Delta\theta_2^-$
$\Delta\theta_1^-$
$\Delta\theta_1^+$
e_1^N
e_1

Fig. 3

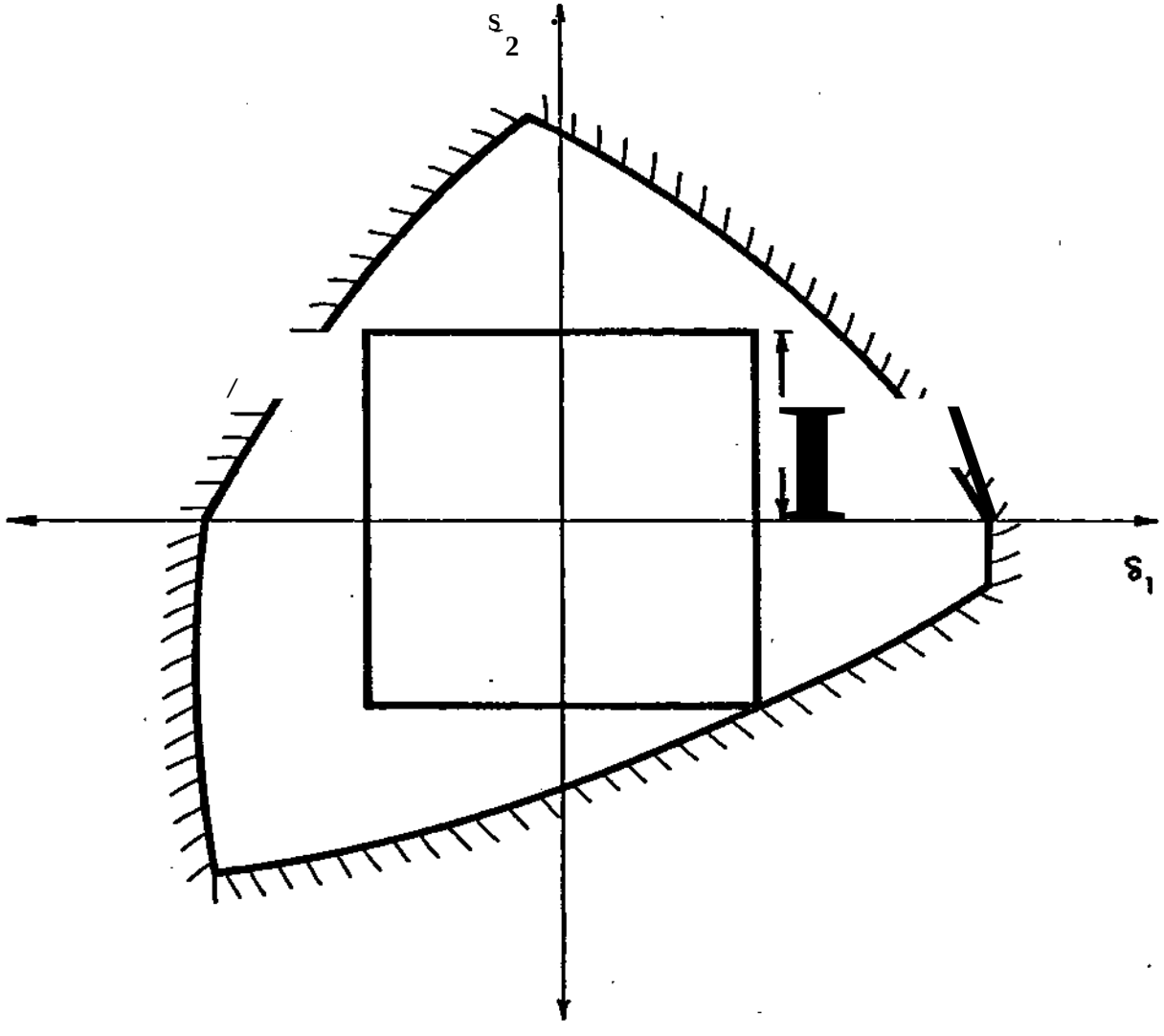


Fig. 4

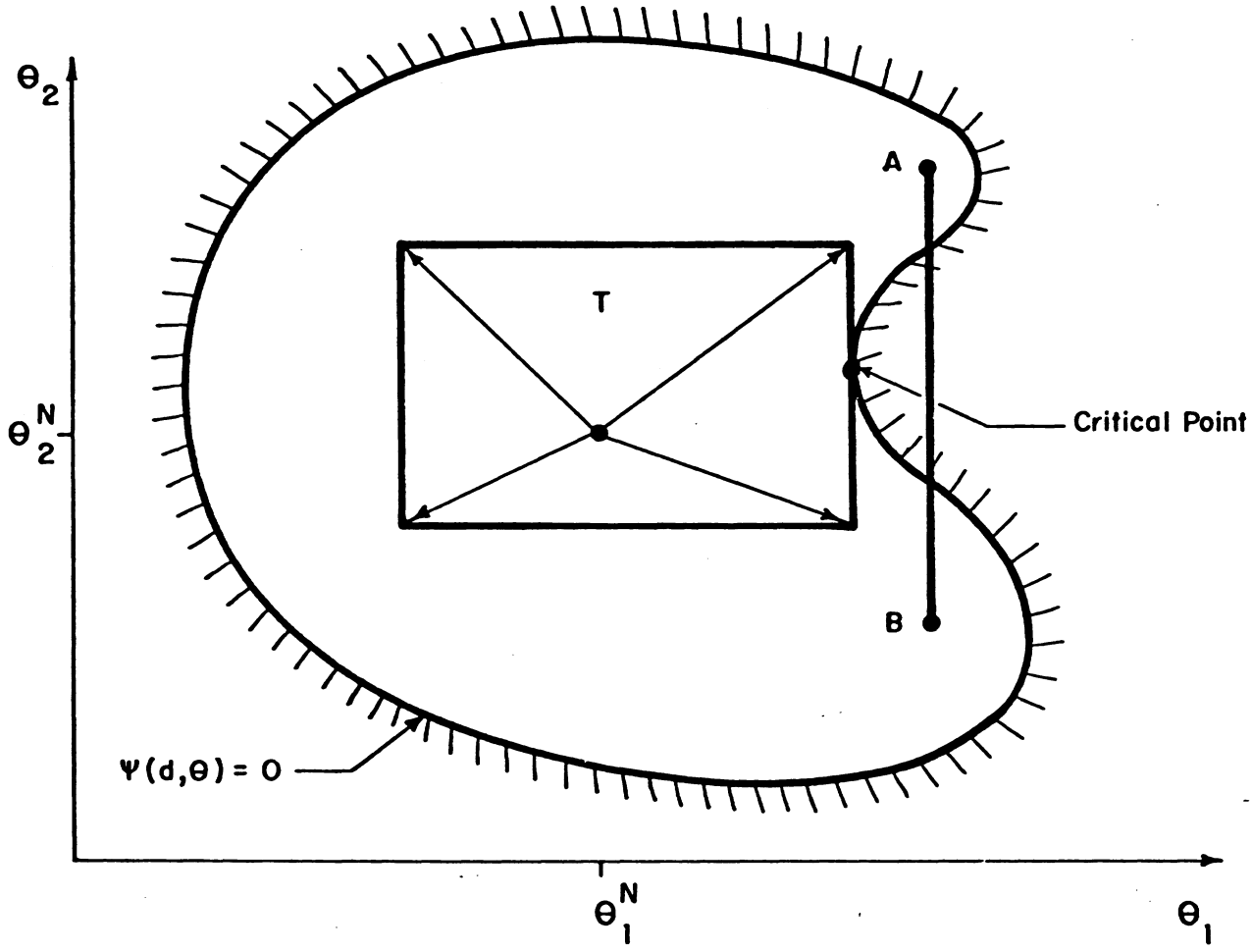

Θ_2
Θ_2^N
A
T
Critical Point
B
$\Psi(d,\Theta) = 0$
Θ_1^N
Θ_1

Fig. 5

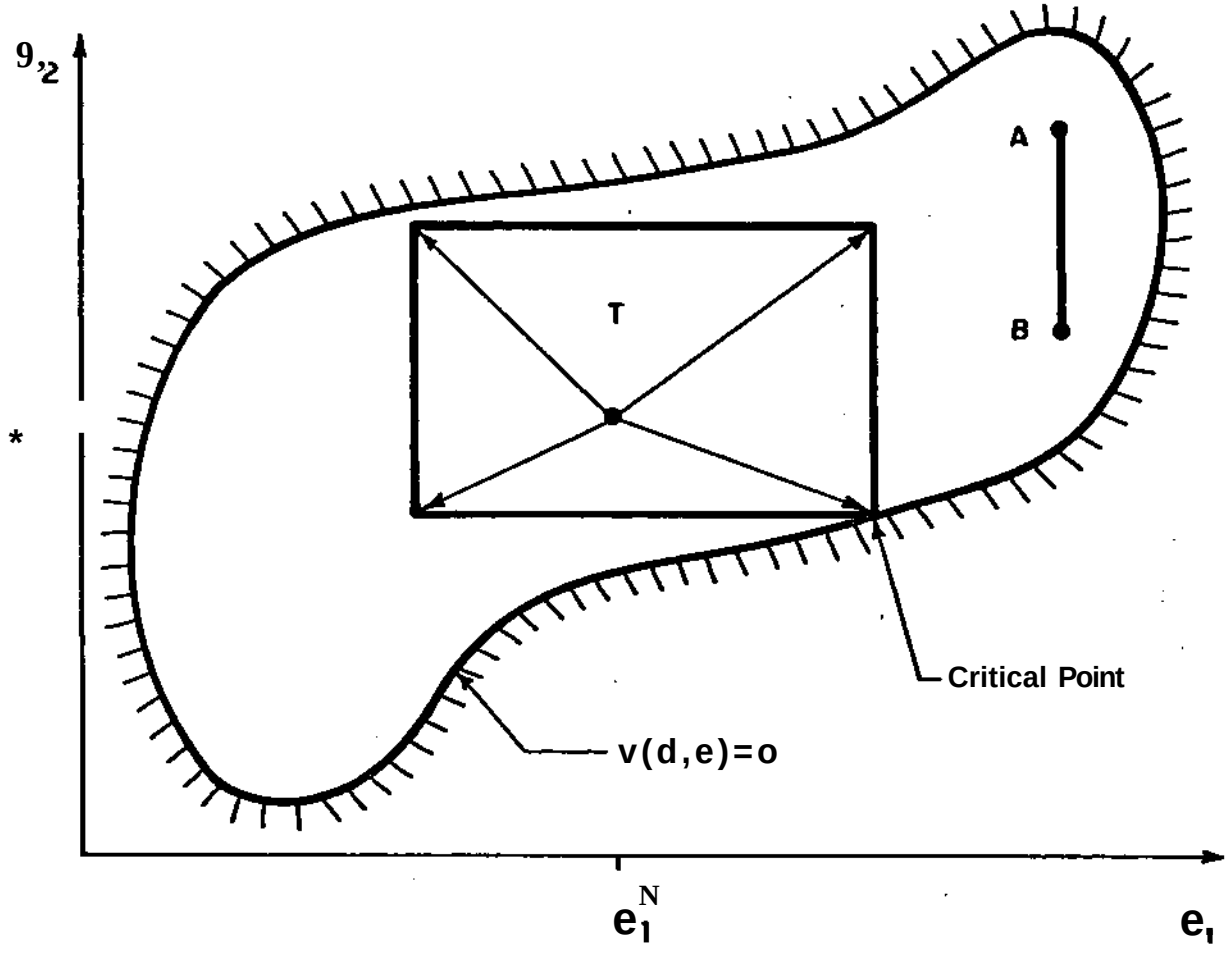


Fig. 6

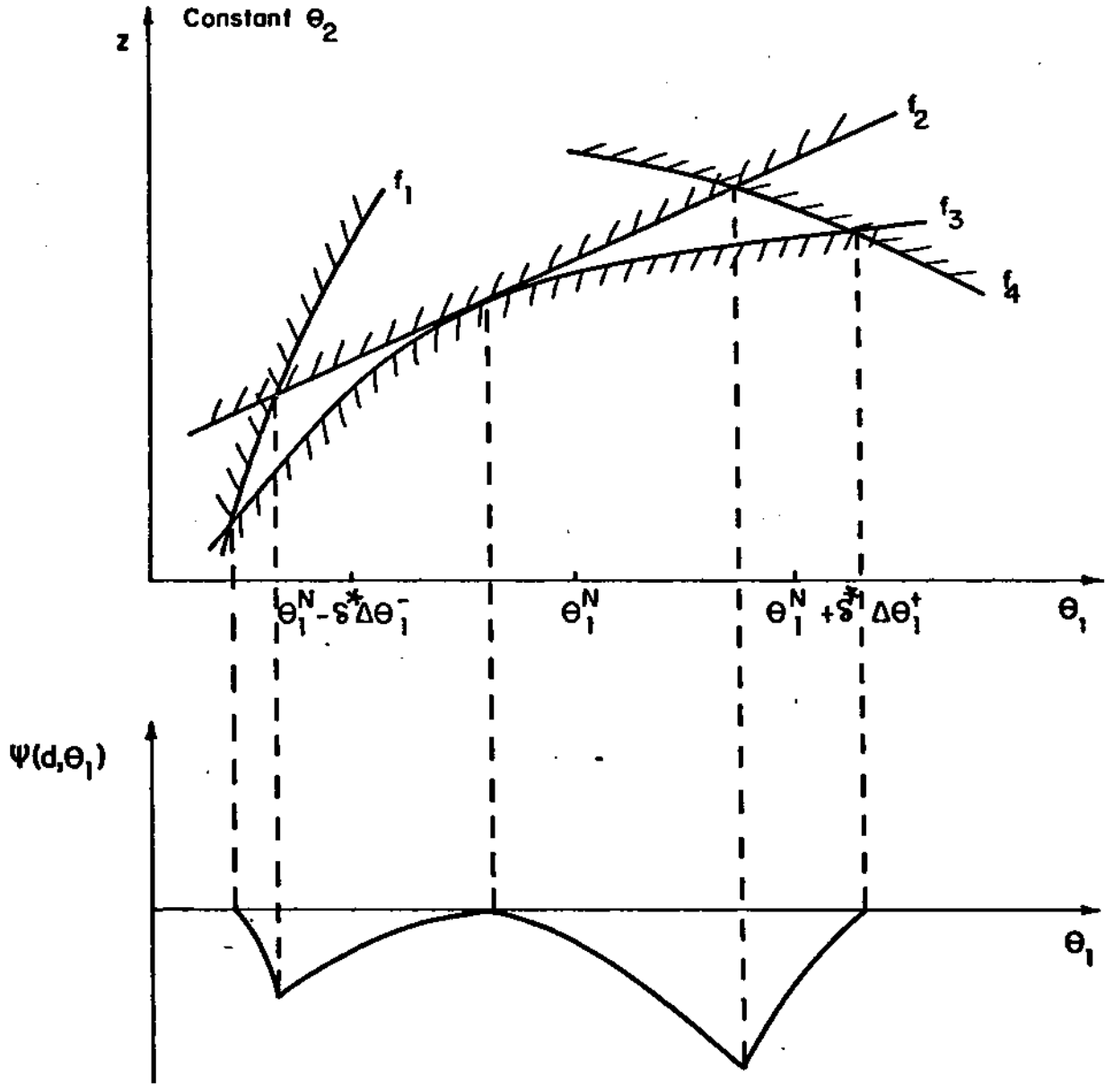
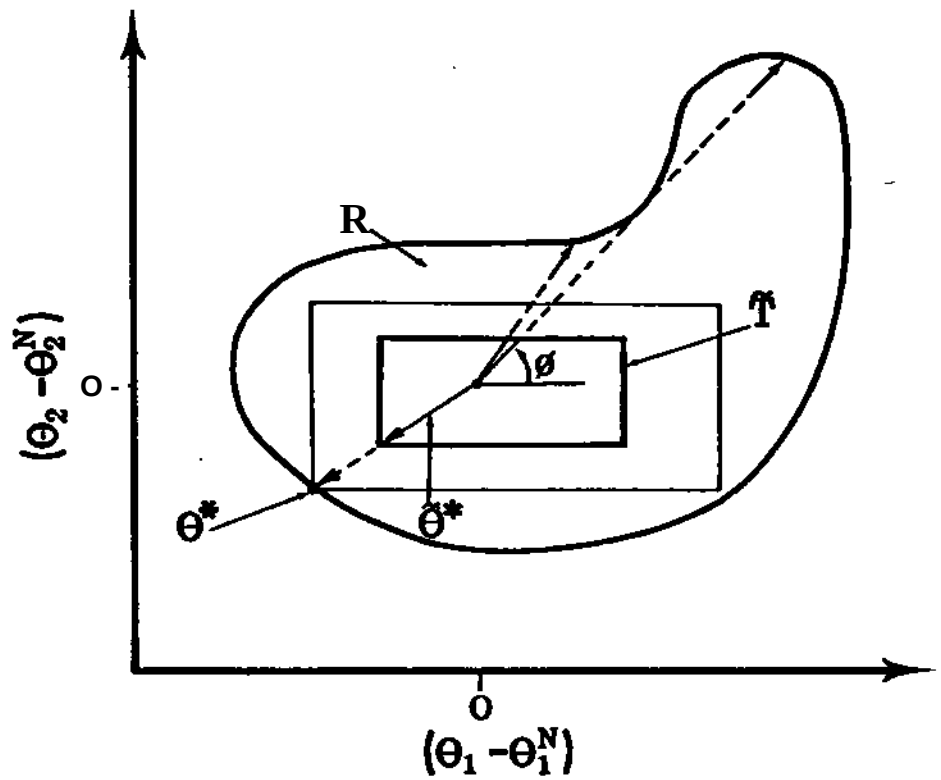

Constant Θ_2
z
f_1
f_2
f_3
f_4
$\Theta_1^N - \delta^* \Delta\Theta_1^-$
Θ_1^N
$\Theta_1^N + \delta^{*1} \Delta\Theta_1^+$
Θ_1
$\Psi(d,\Theta_1)$
Θ_1

Fig. 7


R
T
ø
θ*
θ̃*
0
$(\theta_2 - \theta_2^N)$
0
$(\theta_1 - \theta_1^N)$

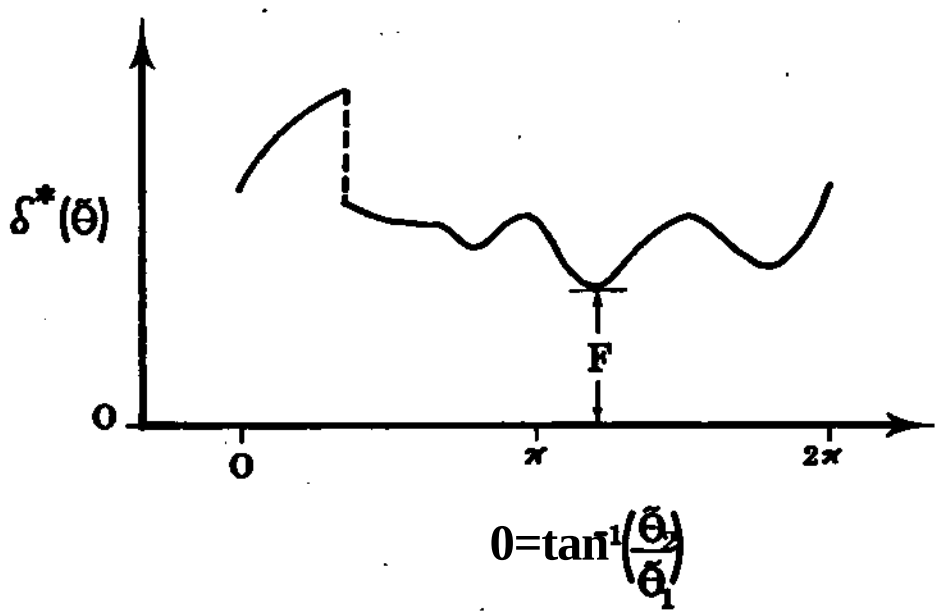

$\delta^*(\tilde{\theta})$
F
0
0
π
2π
$0=\tan^{-1}\left(\frac{\tilde{\theta}_2}{\tilde{\theta}_1}\right)$

Fig. 8

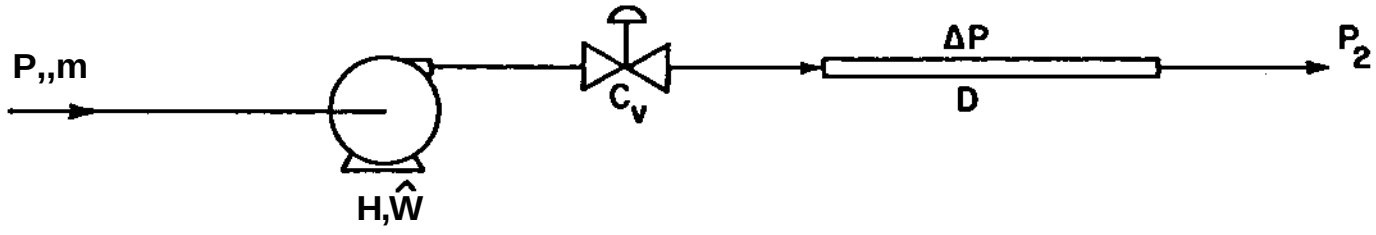


Fig. 9

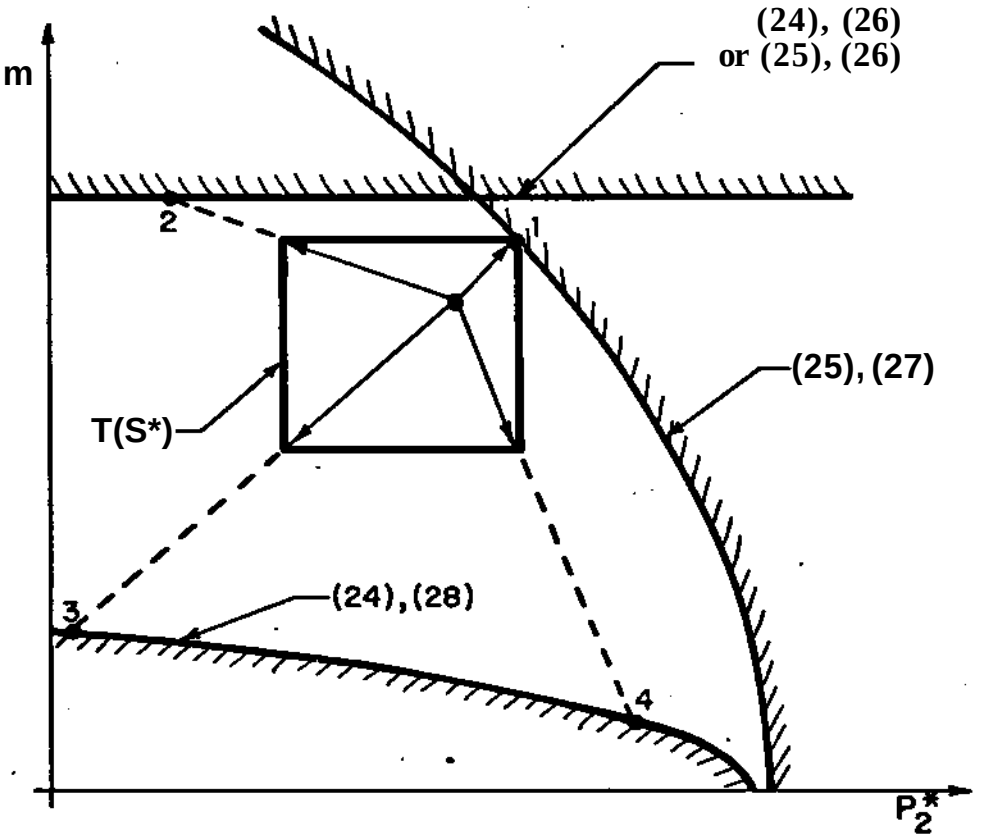


Fig. 10

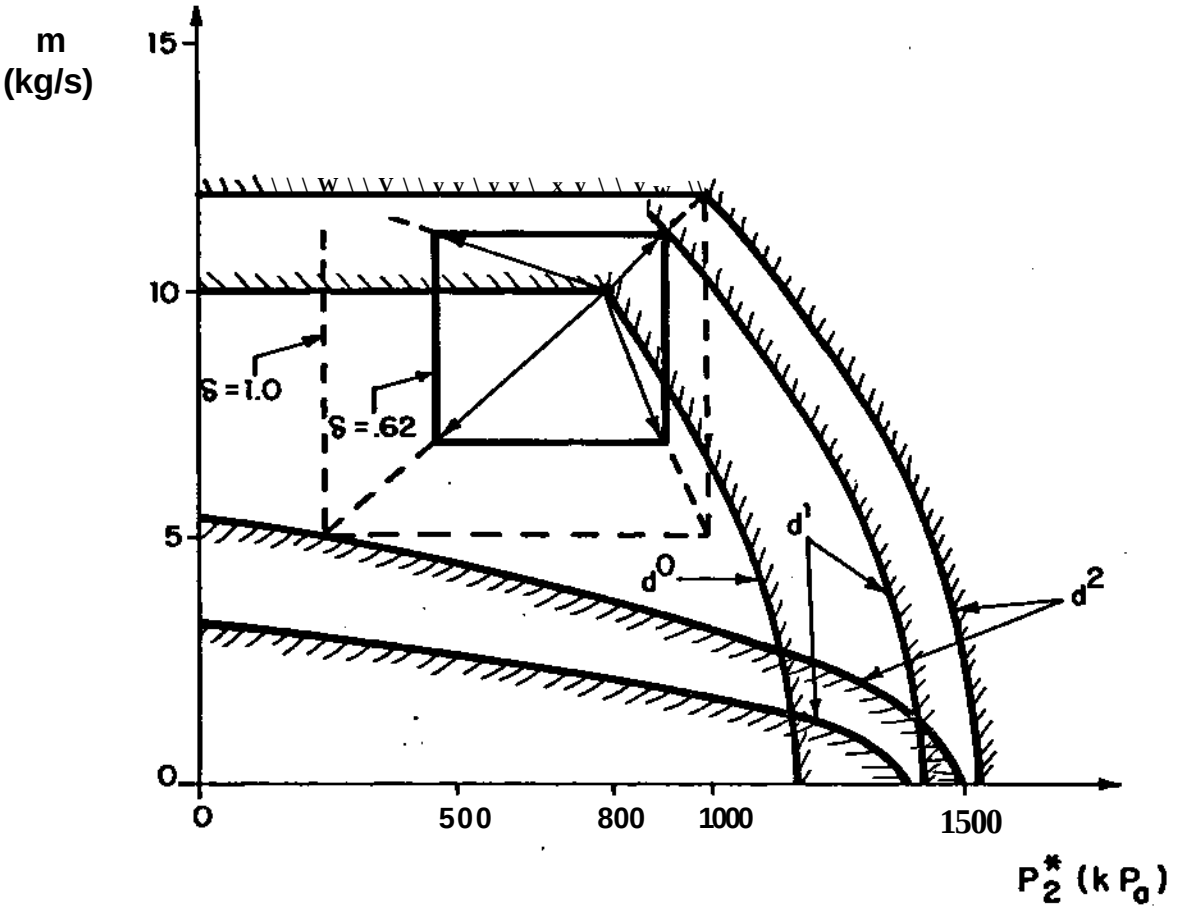


Fig. 11

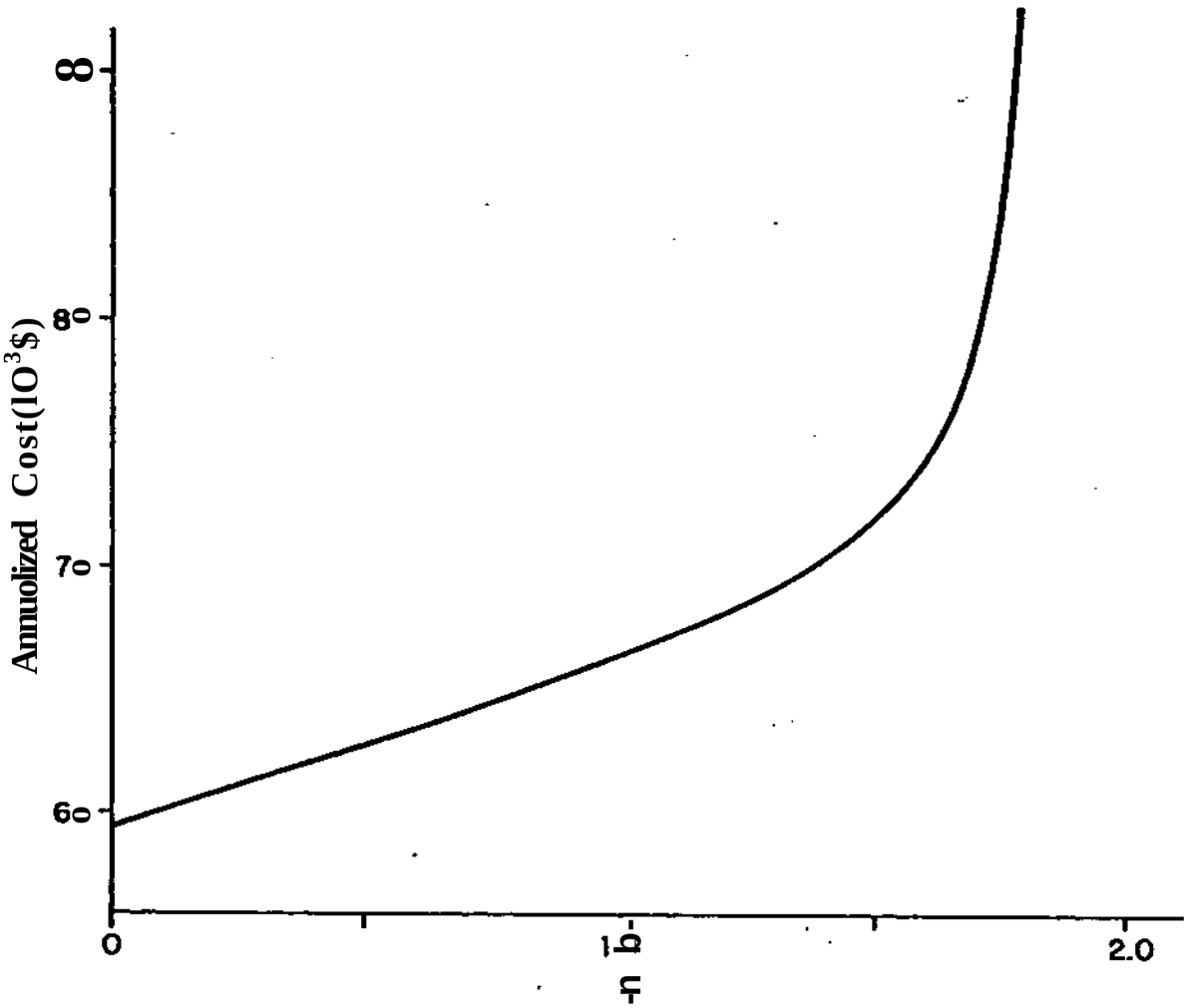


Fig. 12