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Abstract

A rigorous mathematical formulation is presented for the problem of optimal design under uncertainty. This formulation involves a nonlinear infinite programming problem in which an optimization is performed on the set of design and control variables, such that the inequality constraints of the chemical plant are satisfied for every parameter value that belongs to a specified polyhedral region. In order to circumvent the problem of infinite dimensionality in the constraints, an equivalence for the feasibility condition is established which leads to a max-min-max constraint. It is shown that if the inequalities are convex, only the vertices in the polyhedron need to be considered to satisfy this constraint. Based on this feature, an algorithm is proposed which uses only a small subset of the vertices in a multiperiod design formulation. Examples are presented to illustrate the application of the method.

Scope

In the optimal design of chemical processes it is very often the case that considerable uncertainty exists in the value of some of the parameters. For instance, values of transfer coefficients, physical properties or cost data may not be well established at the design stage. Furthermore, one can expect that during the operation of the plant variations will occur in flowrates, compositions, pressures and temperatures of the feedstreams of the process. Therefore, it is clearly very important to consider at the design stage the effect that uncertain parameters can have on both the optitnality and feasibility of operation of the plant.

In order to account for the uncertainties in the values of these parameters, the procedure that is normally used in practice is to assume nominal values for the parameters in the optimal design, and then apply empirical overdesign factors to the resulting sizes of the units. Since this procedure lacks a firm rational basis, a number of different methods have been suggested to account for the uncertainties in a more systematic manner, and a detailed review of these methods can be found in Halemane (1982). The proposed methods differ mainly in the basic design strategies that are postulated, since in principle the problem of design under uncertainty is not well-defined. However, it should be pointed out that the major objectives that one would like to accomplish in this problem are to ensure optimality and feasibility of operation for a given range of parameter values.

It is the purpose of this paper to present for the problem of optimal design under uncertainty, a new mathematical formulation that can ensure rigorously feasibility of operation of the plant for a bounded range of parameter values specified by the designer. The proposed formulation which involves an infinite number of constraints and variables, is very general and yields fundamental insight and understanding of the problem of design under uncertainty. A solution algorithm is proposed to solve this problem for the case when the constraint functions are convex, and its application is presented through two design problems.

Conclusions and Significance

This paper has presented a rigorous formulation for the problem of design under uncertainty. As has been shown, the crucial aspect in this problem is to guarantee the existence of feasible regions of operation for the specified range of parameter values. The max-min-max constraint provides the required mathematical framework to handle this aspect. In addition, this formulation has yielded the following interesting insights and results:

1. For a given design and fixed parameter value the max-min-max problem provides a measure of the size of the feasible region for operation.
2. The critical parameter value corresponds to the one for which the feasible region of operation is the smallest.

3. **In general there can be more than a** single critical point that must be **considered in a design.** This contradicts the usual practice in design **which Is to consider a** single "worst" parameter value.
4. If **the** constraints are convex the critical points must lie at the vertices of the polyhedral region of parameters.

Based on these results an algorithm has been proposed for solving the problem of design under uncertainty. This algorithm leads to an efficient solution procedure as has been shown in the two example problems.

Introduction

In the design of chemical plants there are usually a number of parameters for which there is considerable uncertainty in their actual values. For instance, these parameters can correspond to internal process parameters such as transfer coefficients, reaction constants, efficiencies or physical properties. In addition, the uncertain parameters can also be external to the process such as specifications in the feedstreams, utility streams, environmental conditions or economic cost data.

In order to account systematically for the uncertainties in the parameter values, Grossmann and Sargent (1978) have proposed a design strategy in which the basic objective is to design a flexible plant as follows. Firstly, a design should be selected for which it can be ensured that the design specifications will be satisfied for a bounded region of the parameters. This should be accomplished by suitable manipulation of the control variables for the different realizations of the parameter values. Secondly, the design should be selected so as to optimize the expected value of the investment and operating cost taken over the specified range of parameter values. The basic idea in this strategy is that advantage should be taken from the fact that control variables can be adjusted to satisfy the design specifications during the operation of the plant, as it is only the design of the plant itself that will remain fixed. The strategy clearly reflects one of the main concerns of design engineers, which is to ensure feasible operation of the plant in the region of parameters that has been specified. In addition, the important point is that this is done while simultaneously optimizing the design of the chemical plant. Therefore, this strategy offers the potential of avoiding empirical overdesign for which neither optimality nor feasibility of operation can be guaranteed.

It is the objective of this paper to present for the above cited strategy a new mathematical formulation in which feasibility of operation can be ensured rigorously* This formulation corresponds to a two-stage nonlinear infinite program (NLIP), for which an equivalence has been established through a max-min-max constraint for satisfying the infinite number of inequality constraints. The proposed formulation is more general than the one presented by Grossmann and Sargent (1978) which can fail in some cases to ensure feasibility as shown by Halemane (1982). The paper also presents a solution algorithm for the NLIP problem when the constraint functions are convex, and its application is illustrated with two example problems.

Mathematical Formulation

The variables in the design problem of a chemical plant with uncertainty in parameter values can be partitioned into four categories. The vector d of design variables is associated with the sizing of the units. These remain fixed once the design is implemented, and do not vary with the changes in the operation of the plant. The vector z denotes the control variables that can be manipulated in the operation so as to meet the specifications and also to minimize the operating cost. The vector x corresponds to the state variables which are determined by solving the set of equations representing the process system. Finally, 9 is the vector of independent parameters in the design whose values are subject to uncertainty. Assuming that bounded values of these parameters are specified, the region T that is defined to contain all possible values of these parameters, is given by

$$T \ll I e I 8^L \leq 8 \leq G^U | \qquad (1)$$

where 9^L and 8^U represent given lower and upper bounds on 9.

In order to derive the mathematical formulation it is convenient to consider the design strategy as being composed of two stages: an operating stage and a design stage•

I. Operating stage: Assuming that a given design d has been selected, it is anticipated that the plant will be operated optimally while satisfying the constraints of the process for all possible realizations of the parameters in T. Hence, the objective in this stage is to select for every realization 9 *e* T, a control z which is optimal and feasible.

Clearly, for the given design d and for any value of 9, the state variables can be expressed as an implicit function of the control z from the system of equations of the process,

$$h(d,z,x,9) = 0 \quad \rightarrow x « x(d,z,9) \tag{2}$$

Since the control variable z should be selected so as to satisfy the specifications given by the vector of inequality constraints,

$$g(d,z,x,9) = g(d,z,x(d,z,9),9) = f(d,z,9) \leq 0 \tag{3}$$

the optimal operation of the plant that minimizes the cost will be given by the nonlinear program (NLP)

$$\begin{aligned} &\underset{z}{\text{ndn}}\ C(d,z,9) \\ &\text{s.t. } f(d,z,9) \leq 0 \end{aligned} \tag{A}$$

The solution to this problem defines the cost function C*(d,9) which corresponds to the optimal operation of the plant for fixed values of d_y9. Moreover, if the optimization is performed for every realization 9 e T, the average cost of operation will be given by the expected value $\underset{9€T}{E}$ |c*(d_f9)}.

II. Design Stage: In order to achieve the basic objective of feasibility of operation in the region of parameters T, the design variable d must be chosen so as to ensure that for every value of 9 the control variable z in the operating stage can be selected to satisfy the constraints in (4).

Note that an improper selection of d can lead to infeasible operation for some realizations of θ in which case no selection of the control z will exist so as to satisfy the inequality constraints in (4). Furthermore, in order to achieve the optimal design, the design variable d must be selected so as to minimize the expected value of the optimal cost function $C^*(d,\theta)$ over the entire region T.

This strategy can then be expressed mathematically as

$$\begin{aligned} &\underset{d}{\text{minimize}} \ \underset{\theta \in T}{E} \left\{ C^*(d,\theta) \right\} \\ &\text{s.t.} \quad \forall\theta \in T \left\{ \exists z (\forall j \in J [f_j(d,z,\theta) \leq 0]) \right\} \end{aligned} \tag{5}$$

where $J = \left\{1,2,\ldots,m\right\}$ is the index set for the components of vector f. The constraint in (5) is denoted as the feasibility constraint, because the existence of a feasible region of operation in the region T can be ensured if and only if this constraint is satisfied. In fact, this logical constraint states that for every point $\theta \in T$, in the space of parameters, there must exist at least one value for the vector z of control variables, that gives rise to non-positive values for all the individual constraint functions. Qualitatively, this means that irrespective of the actual values taken by the parameters, the proposed design d of the plant can be operated to satisfy the specifications.

Since the objective function in (5) is itself determined through the NLP in (4), the problem of optimal design under uncertainty can be formulated in its final form as a two-stage programming problem:

$$\begin{aligned} &\underset{d}{\text{minimize}} \ \underset{\theta \in T}{E} \left\{ \min_{z} C(d,z,\theta) \ \middle| \ f(d,z,\theta) \leq 0 \right\} \\ &\text{s.t.} \quad \forall\theta \in T \left\{ \exists z (\forall j \in J \ [f_j(d,z,\theta) \leq 0 \ ]) \right\} \end{aligned} \tag{6}$$

Note that since there are infinite numbers of possible realizations for the values of the parameters θ, and since the optimal operation of the plant i8 implicitly dependent on 0, the overall number of decision variables involved in problem (6) is infinite. This is because for every value of 8 an optimal value of the control variables z is being chosen. Also, note that the feasibility constraint represents an infinite set of constraints since the inequalities in (4) are defined for the infinite set of values GcT. Therefore, problem (6) corresponds to a two-stage nonlinear infinite program, it should be noted that Malik and Hughes (1979) have also presented a similar two-stage programming formulation, but without including explicitly the feasibility constraint.

<u>Simplification of the NLIP</u>

The nonlinear infinite program in (6) that represents the mathematical formulation of the design problem under uncertainty, poses great computational difficulties for numerical solution, and in fact has a more complex structure than the semi-infinite programs treated in the literature (see Hettich, 1979). A first step in simplification so as to make the problem more tractable, is to perform a discretization over the parameter space in order to approximate the expected cost by a weighted cost function (Grossmann and Sargent, 1978), which reduces (6) to

$$\underset{d,z^x,z^-,\ldots z^n}{\text{minimize}} \quad \sum_{i«l}^{n} w^1\, C(d,z^i,e^i)$$

$$\text{s.t.}\quad f(d,z^i,0^i) \text{ £ } 0\ ,\quad i«l,2,\ldots,n \qquad (7)$$

$$\forall\theta\epsilon T\ \{\exists z\,(\forall j\epsilon J[\,f_j(d,z,\theta)\le 0])\}$$

where the weights w^i correspond to discrete probabilities for the selected finite number of parameter points G^T, i=l,2,...n. With this simplification the number of decision variables in (7) is finite, since optimization is performed over the vector d of design variables and the finite number of vectors $z^1,*^2,\ldots\wedge^{11}$ of control variables. The control variables z^1 are selected to satisfy the corresponding constraints $f(d,z^1,0^1) \wedge 0$, so as to result in an optimal feasible operation at the point 9^i of the parameter space. Note that

despite this discretization, the feasibility constraint is still imposed so **as to restrict** the choice on the design d to guarantee feasible operation for every **point GeT.** Thus, the formulation in (7) is a nonlinear semi-infinite program (NLSIP), with a finite number of decision variables and infinite number of constraints.

It is interesting to note that if the feasibility constraint is excluded in (7), the resulting structure of the problem is equivalent to that of a deterministic multi-period problem, where the plant operates in each period with the parameter value 8^{i}, and with the length of period proportional to v^{i}, As discussed by Grossmann and Halemane (1982), this class of multi-period design problems can be solved very efficiently with the projection-restriction strategy that they have proposed. The question that immediately arises then is whether a finite number of points in 0-space can be selected, so that by ensuring feasibility of the design for those points, one can guarantee that the feasibility constraint in (7) will be satisfied. If such a choice of finite number of parameters values were possible one could clearly solve problem (7) as an equivalent deterministic multi-period design problem. In order to answer this question, it is essential to first reformulate the feasibility constraint in (7) in a more amenable form for analysis.

Reformulation of the Feasibility Constraint

The logical constraint

$$\forall \theta \in T \left\{ \exists z \left(\forall j \in J \left[f_j(d,z,\theta) \le 0 \right] \right) \right] \qquad (8)$$

which ensures overall feasibility of the design is the major source of computational difficulty in numerical solution of the design problem represented by the NLSIP in (7). The reason is that it involves an infinite number of inequality constraints for which feasibility has to be tested.

The following theorem provides a possibility for circumventing this problem.

Theorem 1

The **logical** constraint (8) and the max-min-max constraint,

$$\max_{\theta \in T} \min_{z} \max_{j \in J} f_j(d,z,\theta) \le 0 \qquad (9)$$

are exactly equivalent.

Proof

The theorem can be proved in two parts, namely, (8) $\Rightarrow$ (9) and (9) $\Rightarrow$ (8), as given by Polak and Sangiovanni-Vincentelli (1979) and Halemane and Grossmann (1981). An alternative proof which is simpler and more direct is given here. By the definition of the terms and relationships used in (8) and (9), the following equivalences apply by considering global max and min operators:

$$\forall \theta \in T \{\exists z [\forall j \in J (f_j(d,z,\theta) \le 0)]\}$$

$$\Leftrightarrow \forall \theta \in T \{\exists z (\max_{j \in J} f_j(d,z,\theta) \le 0)\}$$

$$\Leftrightarrow \forall \theta \in T \{\min_{z} \max_{j \in J} f_j(d,z,\theta) \le 0\}$$

$$\Leftrightarrow \max_{\theta \in T} \min_{z} \max_{j \in J} f_j(d,z,\theta) \le 0$$

From these steps the equivalence of the first and last relations is established, which is exactly the one stated in the theorem. QED.

With this alternative and equivalent formulation of the feasibility constraint the optimal design problem in (7) can be rewritten as

$$\min_{d, z^1, z^2, \ldots, z^n} \sum_{i=1}^{n} w^i \, C(d, z^i, \theta^i)$$

$$\text{s.t.} \quad f(d, z^i, \theta^i) \le 0, \quad i = 1,2,\ldots,n$$

$$\max_{\theta \in T} \min_{z} \max_{j \in J} f_j(d,z,\theta) \le 0 \qquad (10)$$

In order to describe qualitatively the significance of the max-min-max constraint in (10), note that the inequality constraints are satisfied for non-positive values of the functions $f_j(d,z,\theta)$, $j \in J$. Hence, the 'worst constraint' function is that which is most likely to be violated, and is denoted by the index $\bar{j}$ which corresponds to the maximum valued function $f_{\bar{j}}(d,z,\theta)$ for given d,z,θ. The control $\bar{z}$ that minimizes this function $f_{\bar{j}}(d,z,\theta)$ for any given d,θ, corresponds to the 'most feasible' operation for the worst constraint. Then, the critical parameter value θ^c is that for which the worst constraint $f_{\bar{j}}$ is maximized while having the control $\bar{z}$, for a given design d. Therefore, if for a design d a control variable $\bar{z}$ can be chosen to satisfy the constraints at the critical parameter value θ^c, then the design d can be guaranteed to have feasible operation at every $\theta \in T$.

In the formulation given by (10) the max-min-max constraint provides the possibility of circumventing the problem of simultaneously handling the infinite number of inequality constraints. The reason is that the max-min-max constraint determines a point θ^c for which the inequalities are most likely to be violated, while requiring that these inequalities be satisfied at that point. However, this constraint involves solving the subproblem,

$$\max_{\theta \in T} \; \min_{z} \; \max_{j \in J} \; f_j(d,z,\theta) \tag{11}$$

which in general is very difficult to solve (Polak and Sangiovanni-Vincentelli, 1979). Furthermore, it is not clear under which circumstances the solution of this subproblem is unique since in Theorem 1, global max and min operators had to be assumed for the proof. Therefore, it is desirable as a next step to examine the properties and interpretation of the max-min-max constraint so as to gain a better insight and understanding from it.

Interpretation and Properties of the Max-Min-Max Constraint

The ntx-min-max constraint can be written as a constrained max-min problem, by introducing an extra variable u:

$$\max_{9 \in T} \min_{z} \left\{ u \mid u \geq f_j(d,z,0),\ \forall j \in J \right\} \leq 0 \qquad (12)$$

It then follows that for a given point 9eT the value 4(d,6) determined by

$$\bullet(d,e) = \min_{z} \{u \mid u \geq f_j(d,z,S),\ \forall j \in J\} \qquad \mathbf{(13)}$$

indicates the extent of (in)feasibility of operation of the design d for that single point 0. A negative value of t(d,0) indicates a finite region of feasibility and a positive value indicates infeasibility. Thus, the value $\psi(d,e)$ can be interpreted to be a good measure of (in)feasibility of operation at the chosen point $0_e T$. Since the constraint in (12) leads to a point 0^C which maximizes ^(d,0), 0° corresponds to critical point in the parameter space for which the design d has either the smallest degree of feasibility (if $t(d,0^C) \wedge 0$), or the largest degree of infeasibility (if $t(d,9^C) > 0$).

To illustrate these ideas consider the following set of two constraints which involve one control variable z and one parameter 0:

$$f_l = -z + 0 \leq 0$$

$$f_2 = z - 20 + 2 - d \wedge O \qquad (14)$$

Figure la shows a plot of the feasible region on z-0 space, for a design corresponding to d = 0.5. As can be observed in the figure, the size of the feasible region increases as 0 increases, with 0 = 1 being infeasible, 0-1.5 being feasible at one point of z, and 0 = 2 having a finite region of feasibility* f(d,0) is determined by solving for d = 0.5, 1 £ 0 £ 2, the problem

$$t(d,\theta) \equiv \min_z u$$

$$\text{s.t.} \quad u \geq f_1 = -z + \theta$$

$$u \geq f_2 = z - 2\theta + 2 - d \qquad (15)$$

and its results are plotted in Figure lb. Note that f = 0 for 0 = 1.5 which has a single point of feasibility as shown in Figure la. Also, negative values of *if* correspond to finite regions of feasibility as for instance at 9 = 2, and positive values of *if* are associated with infeasibility as in 6 = 1, which is the critical point where the maximum of f is attained. Note also that f decreases monotonically with increasing 0, since the feasible region gets expanded. From these observations it is clear that -{ can be interpreted as a measure of the size of the feasible region for operability. This region corresponds to the projection of the actual overall feasible region in the d-z-9 space onto the z-space for fixed values of d and 0.

To study the effect of changes in d, the region of feasibility of (14) is shown in Figure 2a for d = 1, and the corresponding values of f are shown in Figure 2b. By changing d from 0.5 to 1.0, overall feasibility has been achieved for all values of 0 in the specified range 1 ^ 0 £ 2. Again, it is clear from Figure 2a that 0 * 1 is a critical point, since it corresponds to the smallest size of feasible region in the z-space for the specified range 1 £ 0 £ 2 . Thus, the design d = 1, which is feasible for the critical point 0 = 1 is found to be also feasible for the entire range 1 * 0 ≤ 2.

The example above would suggest that feasible operation in the design can be guaranteed by considering one single critical 0-point. In fact, this may not be true in the general case, as is easily observed if a third constraint is considered together with the two others in (14) to give:

$$f_1 = -z + 9 \quad £ \; 0$$

$$f_2 = z - 29 + 2 - d \quad £ \; 0$$

$$f_3 = -z + 69 - 9d \quad £ \; 0 \tag{16}$$

$$1 \leq 9 \leq 2$$

The feasible region for this set of constraints is shown in Figure 3a for d = 1, and the corresponding function f is shown in Figure 3b. Note that f is nondifferentiable at 0 = 9/5, and that it exhibits two local maxima at 9 = 1 and 0 = 2. It is clear from Figure 3a that the size of the feasible region decreases at both extreme points, 0 = 1 and 0 = 2 , and gets enlarged towards the interior point 0 = 9/5. Thus, there are in this case two critical points to be considered for design, which are in fact the two extreme points of the specified range 1 € 0 £ 2. This observation on the location of critical points can be generalized for the case of a set of nonlinear convex constraint functions through the following theorem.

<u>Theorem 2</u>

If the constraint functions $f_j(d,z,0)$ are jointly convex in z and 9, then the problem

$$\max_{0 \in T} \; \min_{z} \; \max_{j \in J} \; f_j(d,z,0) \tag{17}$$

has its global solution 0^c at an extreme point of the polyhedral region $T = \{e \mid 0^L * 0 £ e^U\}$.

<u>Proof</u>;

This theorem is proved in three parts as follows -

<u>Property *1*</u>. If for every jej, $f_j(d,z,0)$ is jointly convex in z and 0, then $4(d,z,0) = \max_{j \in J} f_j(d,z,0)$ is also jointly convex in z and 0.

Proof:

Let $0 \le \lambda \le 1$, $z^3 = (1-\lambda)z^1 + \lambda z^2$, $\theta^3 = (1-\lambda)\theta^1 + \lambda\theta^2$. Since for every $j \in J$ $f_j(d,z,\theta)$ is jointly convex in z and θ,

$$(1 - \lambda)\ f_j(d,z,^1,\theta^1) + \lambda\ f_j(d,z^2,\theta^2) \ge f_j(d,z^3,\theta^3)\ \forall j \in J$$

Taking the summation over the index set J and replacing the functions at each of the three points by the maximum valued function,

$$m(1 - \lambda) \max_{j \in J} f_j(d,z^1,\theta^1) + m\lambda \max_{j \in J} f_j(d,z^2,\theta^2) \ge m \max_{j \in J} f_j(d,z^3,\theta^3)$$

where $m = |J|$. Cancelling out the common factor m and using the definition of the function $\phi(d,z\ ,\theta\ )$,

$$(1 - \lambda)\phi(d,z^1,\theta^1) + \lambda\phi(d,z^2,\theta^2) \ge \phi(d,z^3,\theta^3)$$

from which it is clear that the function $\phi(d,z,\theta) = \max_{j \in J} f_j(d,z,\theta)$ is jointly convex in z and θ.

Property 2. If $\phi(d,z,\theta)$ is jointly convex in z,θ, then, $\psi(d,\theta) = \min_z \phi(d,z,\theta)$ is convex in θ.

Proof:

Let $\psi(d,\theta^3) = \min_z \phi(d,z,\theta^3) = \phi(d,z^3,\theta^3)$.

Let θ^1, $\theta^2 \in T$ be two distinct points that are different from θ^3, and $0 < \lambda < 1$ such that $\theta^3 = (1 - \lambda)\theta^1 + \lambda\theta^2$.

Let $\psi(d,\theta^1) = \min_z \phi(d,z,\theta^1) = \phi(d,z^1,\theta^1)$

and $\psi(d,\theta^2) = \min_z \phi(d,z,\theta^2) = \phi(d,z^2,\theta^2)$.

Since $\phi(d,z,\theta)$ is jointly convex in z and θ,

$$(1 - \lambda)\phi(d,z^1,\theta^1) + \lambda\phi(d,z^2\theta^2) \ge \phi(d,z^{12},\theta^3),$$

where $z^{12} = (1 - \lambda)z^1 + \lambda z^2$.

But,

$$\phi(d,z^{12},\theta^3) \ge \min_z \phi(d,z,\theta^3) = \phi(d,z^3,\theta^3)$$

therefore,

$$(1 - X)\ rfCd.z^{1\wedge1}) + Xrf(d,z^2,e^2) :\geq\ 4(d,z^3,8^3)$$

or,

$$(1 - X)\ tcd.e^1) + xu<i,e^2) * t(d,e^3)\ \bullet$$

Noting that $9^3 = (1 - X)9^1 + X9^2$, it is clear that t(d,9) is convex in 9.

<u>Property 3</u>, If t(d,9) is convex in 9, then every <u>local</u> solution 0° of the problem

$$\max_{9eT} t(d,9)$$

lies at an extreme point of the convex region T.

<u>Proof</u>;

Assume that 0° is a non-extreme point of the region T, and let 9^1, 0^2cT be two distinct points in the neighborhood of 9° and 0 < X < 1 such that $G° - (1 - X)©^1 + X®^2$- Since $(d,8) is convex in 9,

$$(i - X)\ \bullet(d,©^1) + \lambda\phi(d,\theta^2) \geq \phi(d,\theta^o).$$

That is, $x[t(d,e^2) - tC\wedge e^1)] * *(d,e°) - \phi(d,\theta^1)$.

Since 8^1 and 0^2 can be chosen in the neighborhood of 0° so as to make the left-hand side negative, the above inequality gives

$$t(d,0°) - tCd,©^1) * 0$$

which is a contradiction since 0^o maximizes locally the function o(d,0). Hence, the assumption that 0° is a non-extreme point of the region T must be incorrect, and this proves the result stated above.

<u>Property 4</u>, If the region T is a polyhedron defined as in (1), the global solution 0^C must lie at a corner point (vertex) of this polyhedron, unless the solution is degenerate.

This result is obvious from the fact that the vertices are the only extreme points for a polyhedral region, and that all boundary points (as well as the interior points) can be expressed as a convex combination of the extreme points (vertices). Therefore, any local solution to the problem (18), and hence its global solution 0°, must lie at a vertex of the polyhedral region T. Thus, the result stated in Theorem 2 is proved. QED.

Discussion

Since there are a finite number of vertices for the polyhedron T, Theorem 2 provides an answer to the question as to whether a finite number of points can be considered for design to ensure feasibility for all the points in the polyhedron T. It follows from Theorem 2 that if the constraints are convex, feasibility of operation for every value of 0€T can be guaranteed by considering in the design all the vertices of the polyhedron T, since any of them will correspond to the critical parameter 8°. Also, since (17) represents a maximization of a convex function as shown in Property 3 of Theorem 2, there can be multiplicity of local solutions for (17), and hence a number of different critical points. This result contradicts the common practice in design of considering only a single "worst" parameter value.

It should also be clear that the assumption of convexity on the constraint functions in Theorem 2 is a sufficient condition for the location of critical points at the vertices of the polyhedron T. Therefore, there can also be cases when even if nonconvex constraint functions are involved, the critical points correspond to vertices. However, it is clear that this will not always necessarily be true.

Solution Algorithms

In solving the design problem (10) it is essential to satisfy the max-min-max constraint in order to guarantee feasibility of operation of the plant for every 0€T. As was proved in Theorem 2, if the inequality constraint functions are convex, then the critical points must lie at any of the vertices of the polyhedron T. Since there are a finite number of vertices in T, a design obtained by considering all these vertices will be feasible for any other point in the polyhedron. This would then suggest the following algorithm:

Algorithm I

Step 1. Include all the vertices in the set T_o « {G^i j 0^i is a vertex of T, i = 1,2,...,N}

Step 2. Solve the problem

$$\begin{aligned} &\underset{d,z^1,z^2,\ldots,z^N}{\text{minimize}} \quad C^\circ(d) + \sum_{i=1}^{N} w^i\, C(d,z^i,\theta^i) \\ &\text{s.t.} \quad f(d,z^i,\theta^i) \le 0 \quad i=1,2,\ldots,N \\ &\qquad\qquad \theta^i \in T_0 \end{aligned} \tag{18}$$

with the projection-restriction strategy (Grossmann and Halemane, 1982) so as to obtain the design d°.

Since T_0 includes all N vertices of the polyhedron T, every critical point θ^c corresponding to the above design d° will also be included in T_0. Therefore the design d° will be feasible for its critical points, and hence it will also be feasible for every $\theta \in T$.

The drawback in this algorithm is that the number of vertices N to be considered for design increases exponentially with the number of parameters p, since $N = 2^p$. Thus, for a problem involving ten uncertain parameters ($p = 10$), the design problem has to consider $2^{10} = 1024$ vertices, which would lead to an extremely large problem in (18). Because of this fact, it is desirable that the above algorithm be modified so as to reduce the number of vertices that have to be considered in Step 2. An algorithm that can be used for this purpose is as follows:

Algorithm II

Step 1. Set $k = 0$. Choose an initial set T_0 consisting of N_0 vertices where $N_0 < 2^p$.

This can be achieved by analyzing the signs of the gradients of each of the individual constraint functions with respect to the parameters at initial values of d and z, as suggested by Grossmann and Sargent (1978). If the constraints are monotonic in the parameters, these vertices correspond to maximization of individual constraint functions (Grossmann and Sargent, 1978).

Step 2. Solve the problem

$$\underset{d,z}{\text{minimize}} \quad C^{\circ}(d) + \sum_{i \in T_k} w^{i} \, C(d, z^{i}, \theta^{i}) \tag{19}$$

$$\text{s.t.} \quad f(d, z^{i}, \theta^{i}) \le 0 \quad i=1,2,\ldots N_k$$

so as to obtain the design d^{k}.

Step 3. Determine the critical parameter value $\theta^{c,k}$, by solving for every vertex θ^{i} not included in T_k, the problem

$$f(d^{k}, \theta^{i}) = \min_{u} \{ u \mid u \ge f_j(d^{k}, z, \theta^{i}),\ j \in J \} \tag{20}$$

The vertex that gives rise to the maximum value of f is then determined and is denoted by $\theta^{c,k}$. If $f(d^{k}, \theta^{c,k}) \le 0$, stop; otherwise go to step 4.

Step 4. Define $T_{k+1} = T_k \cup \{\theta^{c,k}\}$, $N_{k+1} = |T_{k+1}|$.

Set $k = k+1$ and iterate from Step 2.

Note that at the termination of this algorithm the design will necessarily be feasible for all values of parameters, because it will be feasible for the critical parameter values. Also, the algorithm has to terminate in a finite number of iterations since there are only a finite number of critical parameter points to be considered. The initial vertices predicted in Step 1 by the method of Grossmann and Sargent (1978) will often yield very good guesses for which only one iteration in Algorithm II may be required. Similarly as in Algorithm I, problem (19) in Step 2 can be solved with the projection-restriction strategy (Grossmann and Halemane, 1982). Also, note that the minimizations in (20) may not have to be performed until completion for all vertices, as they can be stopped when f reaches a negative value in which case the existence of a non-empty feasible region is detected. Thus, by the above considerations Algorithm II will provide in general a much more efficient method of solution than Algorithm I.

However, there are two features in Algorithm II which would require further investigation. One of them is the number of parameter points considered for design, which in turn determines the size of problem (19) in Step 2. This number will increase at each iteration since a new parameter point will be added. The question is whether this number can be kept small throughout by eliminating some of the previous points while adding new ones. This elimination can probably be performed on the basis of the value of J. A second question is whether it is possible to determine the critical parameter point in Step 3 without explicitly analyzing each of the individual vertices and solving for f. If this were possible, it would certainly enhance the efficiency of the above solution strategy when dealing with a large number of parameters.

To illustrate the application of Algorithm II described above, two example problems are presented below.

<u>Example 1</u>

In this example the heat exchanger network 4SP1 of Lee et al. (1970) with outlet temperatures specified as inequalities is considered (see Grossmann and Sargent, 1978). The flowsheet consists of five heat exchangers, one of which is a steam heater and another being a cooler using cooling water, and with two hot streams and two cold streams as shown in Figure 4. Table I gives the data for the problem. The overall heat transfer coefficients U_i, $i = 1,2,\ldots 5$, were considered to be the parameters with $\pm$ 20% uncertainty in their nominal values. The design problem then consists in selecting the areas A_i, $i = 1,2,\ldots 5$ so that irrespective of the actual values of the heat transfer coefficients (within the $\pm$20% range), the specifications on the outlet stream temperatures should be satisfied by suitable choice of the cooling water outlet temperature T_{i5} and the steam temperature T^. Apart from the equality constraints representing the heat balance and design equations for the network, the following inequality constraints on the temperatures of various streams have to be satisfied.

$$
\begin{aligned}
T_3 &\le 534 \\
T_6 &\le 434 \\
T_{10} &\ge 411 \\
T_{12} &\ge 367 \\
T_5 - T_8 &\le 0 \\
T_3 - T_{13} &\ge 0.55 \\
T_{11} - T_5 &\ge 0.55 \\
T_7 - T_2 &\ge 0.55 \\
T_9 - T_6 &\ge 0.55 \\
T_9 - T_{15} &\ge 0.55
\end{aligned}
\qquad (22)
$$

Here the first four constraints correspond to specifications on the outlet temperatures, and the last five on the minimum temperature approach. Table 2 gives the initial set of vertices considered for design, which were obtained by analyzing the signs of gradients of individual constraints as suggested by Grossmann and Sargent (1978). Note that this set consists of the nominal point and four extreme points. The design corresponding to these five parameter points was found to be feasible for all the 32 vertices. The results are given in Table 3, from which it is clear that the values of f are non-positive at all the vertices, thus ensuring feasibility. Note that the actual value of p is dependent on the scaling factors used for the constraint functions, which are given in Table 1 for this problem. Although the choice of these scaling factors is arbitrary, it does not affect in detecting the (in)feasibility of a given design. The total CPU-time required to solve this problem was only 34.7 sec (DEC-20). Optimization was performed in each case with the variable metric projection algorithm of Sargent and Murtagh (1973). In this example problem the optimal feasible solution to the design problem was obtained with a single iteration through Algorithm II, without the need for considering additional vertex points. This may not always be the case as can be seen from the second example below.

<u>Example 2</u>

Figure 5 shows the flowsheet consisting of a reactor and a heat exchanger, used to handle a first-order exothermic reaction A-B, for which the problem data is given in Table 4. The parameters considered to have uncertainty in their values are: (i) F_o, the feed flow rate ($\pm$10%), (ii) T_o, the temperature of the feed stream ($\pm$2%), (iii) T_{w1}, the inlet temperature of cooling water ($\pm$3%), (iv) k_R, the Arrhenius rate constant ($\pm$10%), and (v) the overall heat transfer coefficient for the heat exchanger U ($\pm$10%). Among these five parameters, the first three are associated with inlet streams to the units while the latter two correspond to internal parameters of the process. The conversion is specified to be not less than 90%, and the temperature of the reactor must be lower than the specified upper bound, 389°K. The design problem consists in selecting the optimal sizes for the reactor and heat exchanger so that the specifications can be satisfied by suitable choice of the temperatures T_1, T_2, T_{w2}, in Figure 5, irrespective of the actual values of the parameters. The material and heat balance equations and design equations for the reactor and heat exchanger represent the equality constraints of the design problem, and are given in Grossmann and Halemane (1982). Other specifications to be satisfied are expressed by the following inequality constraints:

$$
\begin{array}{ll}
\text{(a)} & \hat{V} \geq V \\
\text{(b)} & (C_{Ao} - C_{A1})/C_{Ao} \geq 0.90 \\
\text{(c)} & 600 \leq T_1 \leq 389 \\
\text{(d)} & T_1 - T_2 \geq 0 \\
\text{(e)} & T_{w2} - T_{w1} \geq 0 \\
\text{(f)} & T_1 - T_{w2} \geq 11{\cdot}1 \\
\text{(g)} & T_2 - T_{w1} \geq 11{\cdot}1
\end{array}
\tag{23}
$$

The initial set of parameter points consists of the nominal point and three vertices, obtained by analyzing the gradient of the constraints, as given in Table 5a. The design corresponding to these four points is given in Table 6a. This design is found to be infeasible for eight of the thirty-two vertices as indicated in Table 6b by the positive values of ψ for these eight vertices. Since the value of ψ is found to be the same for all these eight vertices, one among them is chosen to be added to the initial set of vertex points considered in design. This new set of five parameter points is given in Table 5b and the resulting design shown in Table 7a. This design is feasible for all the 32 vertices as shown by the non-positive values of ψ given in Table 7b. Here again, these values of ψ correspond to the scaling factors given in Table 4 for the constraints of the problem. This example illustrates the need for analyzing the max-min-max constraint as a means to achieve feasibility of operation for the specified set of parameter values. The CPU-time needed to obtain the design in each of the two iterations through Algorithm II is also given, in Tables 6a and 7a respectively. Tables 6c and 7c give the CPU-time for checking feasibility and determining ψ for all the vertex points. It took a total of 162 sec (DEC-20) for the complete solution using the variable-metric projection algorithm of Sargent and Murtagh (1973).

Acknovledgment

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Nomenclature

A = Area of heat exchanger, m^2

C = Annual cost, \$/yr

C_A = Concentration of component A, $kgmole/m^3$

C_p = Heat capacity, kj/kgmole K

d = Vector of design variables

E/R = Ratio of activation energy to the gas constant, K

F = Flowrate, kgmole/hr

F_s = Flowrate of steam, kg/hr

F_w = Flowrate of cooling water, kg/hr

FC = Heat capacity flowrate, kj/hr K

f, g = Vector of inequality constraint functions

h = Vector of equality constraint functions

ΔH_{rxn} = Heat of reaction, kj/kgmole

J = Index set for the inequalities

k_R = Reaction rate constant, m^3/kgmole hr

m = Dimension of vector f

N = Number of vertices

T = Region of uncertain parameters

T_i = Temperature of stream i, K

T_w = Temperature of cooling water, K

U = Heat transfer coefficient, kj/m^2 hr K

V_A = Reaction volume for operation, m^3

V = Design volume of reactor, m^3

W_i = Weight for parameter θ

x = Vector of state variables

z = Vector of control variables

θ = Vector of uncertain parameters

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Table 1. **Data** for Example 1

I. **Nominal values** of uncertain parameters.

$U_1 = U_2 = U_3 = U_5 = 3066\ kJ/m^2\ hr\ K$

$U_4 = 4088\ kj/m^2\ hr\ K$

II. Other process parameters

FC_1 =	21,912 kJ/hr K	T_1 =	389 K
FC_4 =	27,461 kJ/hr K	T_4 =	333 K
$FC_?$ =	38,009 kJ/hr K	T_{11} =	434 R
Fc_{u} =	31,674 kJ/hr K	T_{14}	311 R

III. Cost function

$$C = 145.6 \sum_{i=1}^{5} A_i^{0.6} + \sum_{i=1}^{5} w_i(18.5\ F_s^* + 0.923\ F_w^*)$$

$w_t = 0.6,\ v_{\pm} = 0.1,\ i = 2,3,4,5$

IV. Scaling factor for constraints: 1.8

V. Bounds on control variables: $314 \leq T_{1-5} \leq 355$ K; $534 \leq T_{13} \leq 556$ K

Table 2. Parameter Values Considered
For Design in Example 1.

	u_1	u_2	u_3	u_4	u_5
1	N	N	N	N	N
2	U	U	U	U	N
3	L	U	U	U	N
4	U	L	L	L	L
5	L	U	L	U	N

N - Nominal

L - Lower bound

U - Upper bound

Table 3. Results for Example 1.

(a) Heat exchange areas, m^2

A_x	Aj	A_3	A_4	A_5	cost, $/yr.
30.8	62.2	45.58	3-9	2.9	11,758

CPU time (DEC-20) for obtaining the design using the projection-restriction strategy: 16*7 sec

(b) Test for feasibility at the vertices

f(d,8)	Number of vertices
0.0	24
- 0.679	Nominal point
- 2.452	4
- 3.775	4

CPU-time (DEC-20) for checking feasibility and determining f at the vertices: 18*0 sec

(c) Values of **f(d,e)** for individual vertices

f(d,6)	Vertex number v
0.0	0-15, 24-31
- 2.452	20-23
- 3.775	16-19

$$v = \sum_{i=1}^{5} \sigma_i \, 2^{5-i} \quad , \quad \sigma_i = \begin{cases} 0 & \text{if } U_i = U_i^L \\ 1 & \text{if } U_i = U_i^U \end{cases}$$

Table 4. **Data** for Example 2.

I. **Nominal values** of uncertain parameters

k_R = 0.6242 m^3/kgmole hr U = 1635 kJ/m^2 hr K

F_o = 45.36 kgmole/hr T_o = 333 K

T_{wi} = 300 K

II. Other process parameters

E/R = 555.6 K $-\Delta H_{rxn}$ = 23,260 kJ/kgmole

C_{Ao} = 32.04 kgmole/m^3 C_p = 167.4 kJ/kgmole

III. Cost function ($/yr)

$$C = (691.2\,\hat{V}^{0.7} + 873.6\,A^{0.6}) + \sum_{i=1}^{n} w^i(1.76\,F^i + 7.056\,F_1^i)$$

$w^1 = 0.5$, $w^i = 0.5/(n-1)$ $i = 2,3,\ldots n$

IV. Scaling factors for constraints

(a) 3.531 (b) 100 (c) 1.8

(d), (e), (f), (g) 18.0

V. Bounds on control variables

$311 \le T_1 \le 389$ K

$311 \le T_2 \le 389$ K

$301 \le T_{w2} \le 355$ K

Table 5. Parameter Values Considered for Design in Example 2.

	k_R	U	F_0	T_0	T_{wl}
1	N	N	N	N	N
2	L	U	L	L	L
3	U	L	U	U	U
4	U	L	U	U	L
5	L	L	U	U	U

a) Initial set of points: (1), (2), (3), (4)

b) Second set of points: (1), (2), (3), (4), (5)

N - Nominal

L - Lower bound

U - Upper bound

Table 6. Results of Example 2, First Iteration with Algorithm II

(a) **Design** obtained for parameter points given in Table 3a,

$$\hat{V} = 5.3 \text{ m}^3$$

$$A = 10.5 \text{ m}^2$$

$$\text{cost} = 10{,}820 \text{ \$/yr}$$

CPU-time (DEC-20) for obtaining the design using the projection-restriction strategy: 9*2 sec

(b) Test for feasibility at the vertices

f(d,6)	Number of vertices
+1.280	8
0.0	16 + Nominal point
-1.151	8

CPU-time (DEC-20) for checking feasibility and determining f at the vertices: 65*8 sec

(c) Values of **f(d,6)** for individual vertices

if (d,9)	Vertex number v
+1.28	4-7, 12-15
0.0	**0-3, 8-11, 20-23, 28-31**
-1.151	**16-19, 24-27**

$$v = \sum_{i=1}^{5} a_i \, 2^{5-i} \qquad a_i = \begin{cases} 0 & \text{if } \theta_i = \theta_i^L \\ 1 & \text{if } \theta_i = \theta_i^U \end{cases}$$

$$\theta_1 = V, \quad \theta_2 = U, \quad \theta_3 = V, \quad \theta_4 = T_o, \quad \theta_5 = w$$

Table 7. Results of Example 2, Second Iteration with Algorithm II

(a) Design obtained for parameter points given in Table 3b

$\hat{V}$ - 6.5 m^3

A - 9.2 m^2

cost = 10,110 $/yr

CPU-time (DEC-20) for obtaining the design using the projection-restriction strategy: 12*8 sec

(b) Test for feasibility at the vertices

f(d,6)	Number of vertices
0.0	8
-1.220	16 4- Nominal point
-2.323	8

CPU-time (DEC-20) for checking feasibility and determining $ at the vertices: 73*9 sec

(c) Values of f(d,9) for individual vertices

f(d,9)	Vertex number v
0.0	**4-7, 12-15**
-1.22	**0-3, 8-11, 20-23, 28-31**
-2.323	**16-19, 24-27**

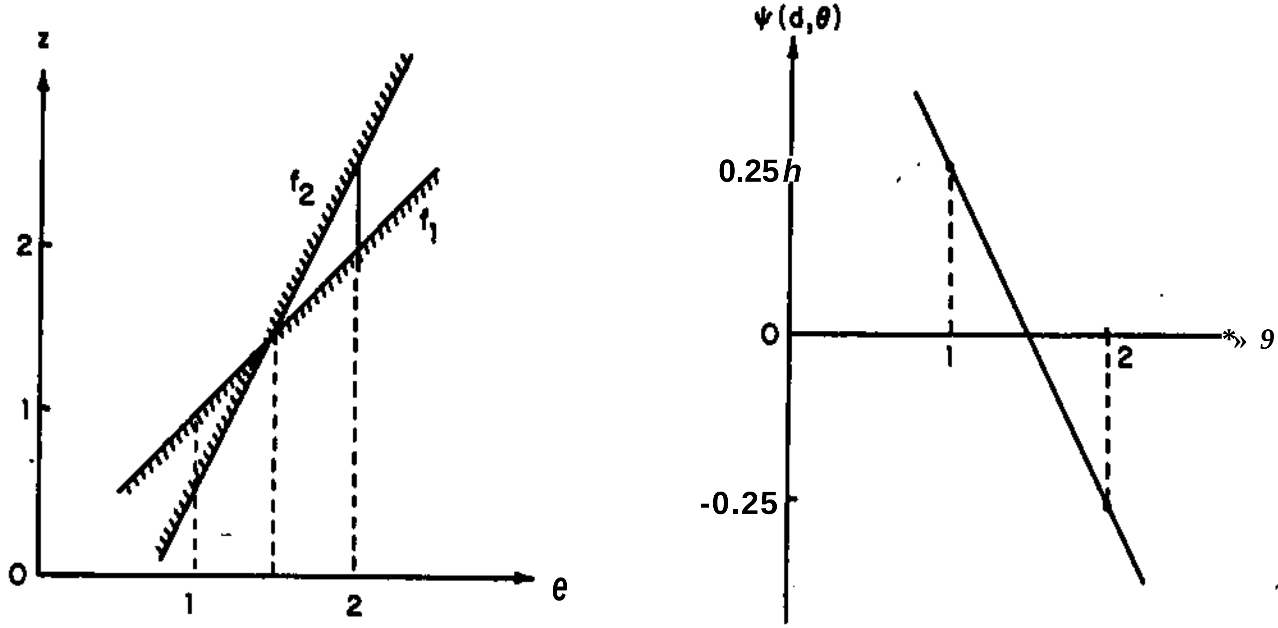
Fig. 1. Feasible region and {(d,e) for constraints (14) with d • 0.5

Fig. 2. Feasible region and {(d,0) for constraints (14) with d - 1

Fig. 3. Feasible region and ^(d,0) for constraints (16) with d • 1

Fig. 4. Heat exchanger network of example 1

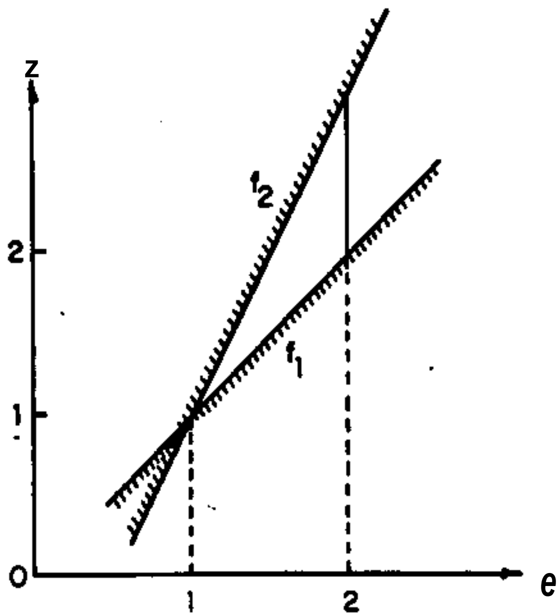
Fig. 5. Reactor-cooler system of example 2



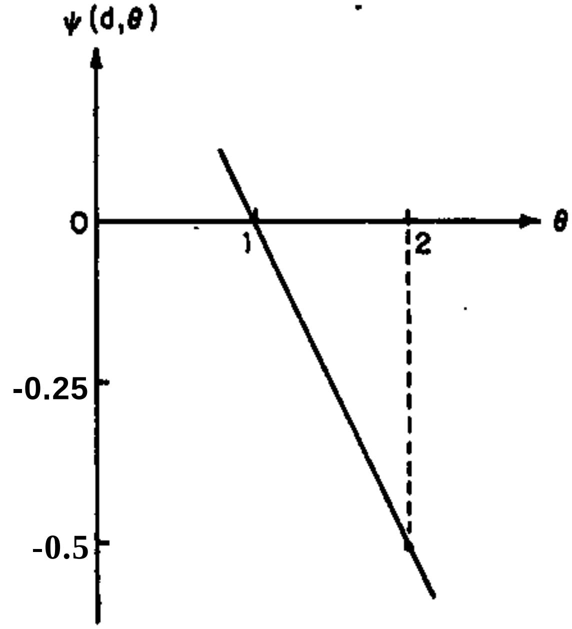
(a) **Feasible region**

(b) ψ(d,θ) versus θ

Fig. 1



(a) Feasible region



(b) ^(d,6) versus 0

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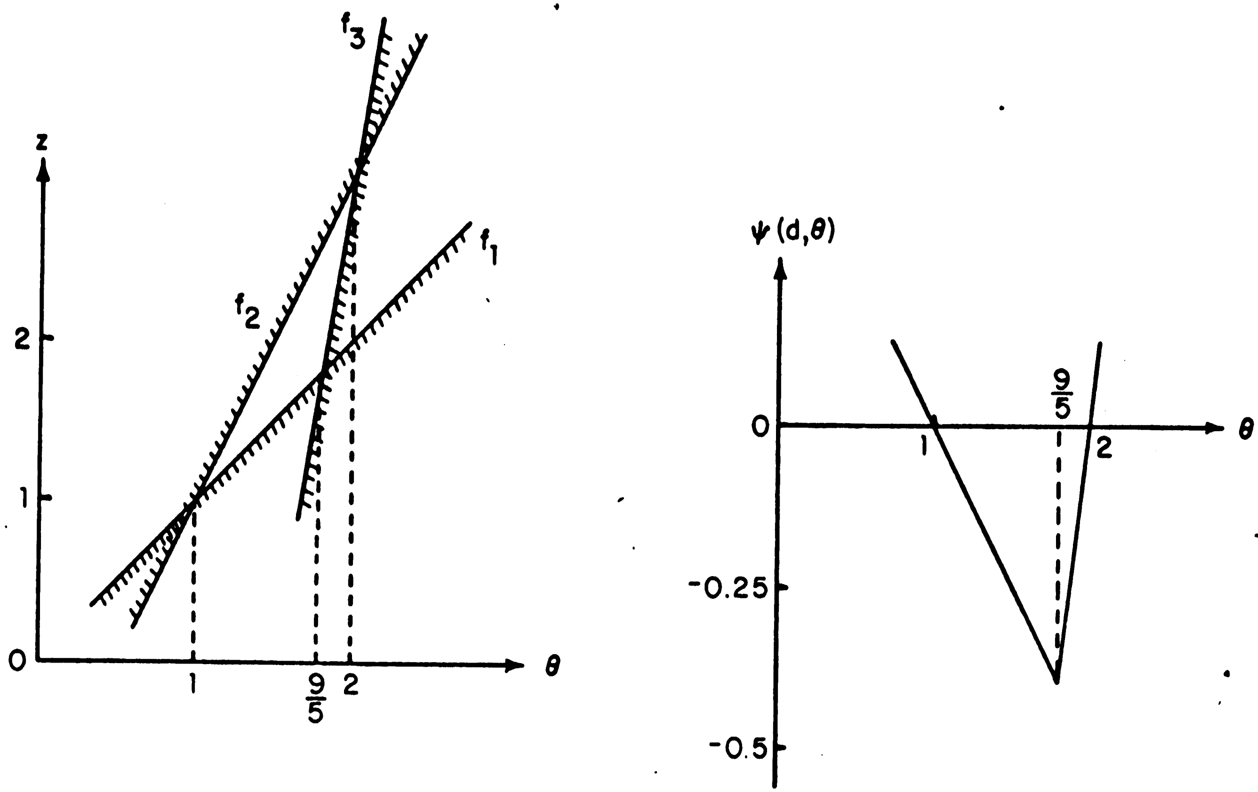
ro



(a) Feasible region

(b) $\psi(d,\theta)$ versus θ

Fig. 3

Fig. 4

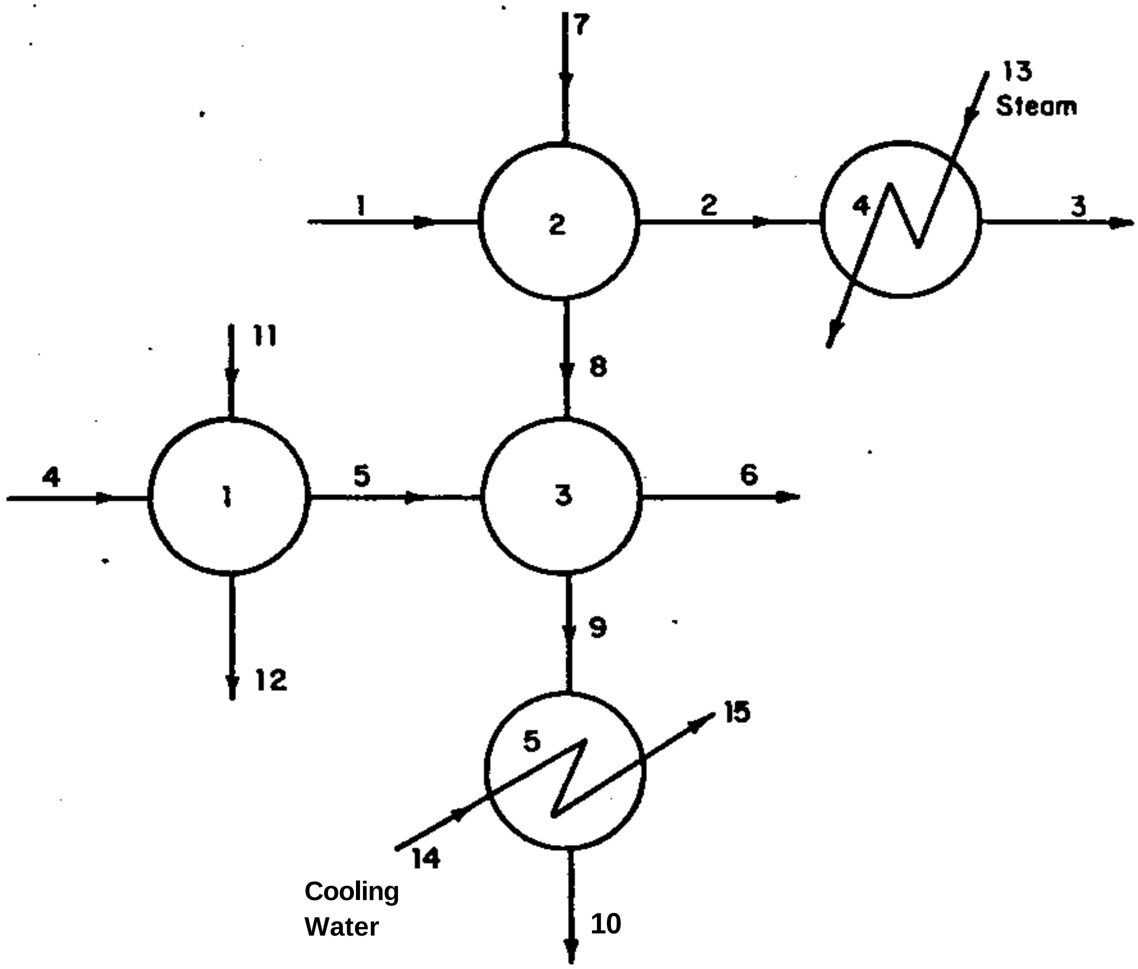


Fig. 5

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