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by

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RESEARCH REPORT

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OPTIMIZATION STRATEGIES FOR FLEXIBLE CHEMICAL PROCESSES

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Abstract. The objective of this paper is to give an overview of the optimization strategies that are required when designing chemical processes in which the existence of regions of feasible steady-state operation must be ensured in the face of parameter variations. Two major areas are considered: optimal design with a fixed degree of flexibility, and design with optimal degree of flexibility. For the first area the problems of multiperiod design, and design under uncertainty are analyzed. For the second area the problem of deriving an index of flexibility in the context of multiobjective optimization is discussed. As shown in the paper, the major challenge in these problems lies in the development of efficient solution procedures for large scale nonlinear programs which are either highly structured, or otherwise involve an infinite number of constraints.

INTRODUCTION

Flexibility is one of the main concerns in the design of chemical plants. The reason is that for a design to be useful in practice it is essential that the plant be able to satisfy specifications and constraints despite variations that may occur in parameter values during operation. For example, in practice it is quite likely that the amount and quality of the feedstreams to the process will vary during operation. This aspect will be particularly critical when the plant has to process alternate feedstocks as is commonly the case in many chemical processes (see for instance Draaisma and Mol, 1977; Rhoe and de Blingiers, 1979). Other examples of changes that often occur during plant operation include variations in the ambient temperature, deactivation of catalysts, fouling of heat exchangers, and wearout of mechanical equipment such as pumps and compressors. Therefore, it is clear that at the design stage some degree of flexibility must be introduced to ensure that the plant will be able to cope with uncertain parameters during operation.

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The usual approach that is used in practice is to design and optimize chemical plants for nominal values of the parameters. Since considerable uncertainties in these values often exist, empirical overdesign factors are used to provide for flexibility in the operation of the chemical plant (Rudd and Watson, 1968). However, it is clear that with this approach not much insight can be obtained as to the actual degree of flexibility that is being achieved in the design. Also, with this approach, it becomes difficult to justify on economic grounds the extent of the overdesign.

In the context of the theory of chemical process design, the need for a rational method of designing flexible chemical plants stems from the fact that there is still a substantial gap between the designs that are obtained with currently available computer-aids and the designs that are actually implemented in practice. The major reason for this gap is that the computer-aids do not explicitly account for operability considerations at the design stage. This would involve handling simultaneously the aspects of flexibility, controllability, reliability and safety of the chemical plant. It should be noted that although some of these aspects are quite similar, they actually correspond to different technical concepts. For instance, flexibility is concerned with the problem of ensuring feasible regions of operation, whereas controllability is concerned with the quality and stability of the dynamic response of the process (Lennhoff and Morari, 1982). On the other hand, reliability is concerned with the probability of normal operation given that mechanical or electrical failures can occur in the operating units, whereas safety is concerned with the consequences of failures in the form of hazards (Henley and Kumamoto, 1981).

Clearly, one of the first steps in incorporating operability considerations at the design stage would be to develop procedures which ensure that the plant will be able to meet the specifications economically for a given range of parameter values. This paper addresses this problem explicitly for the case when feasible steady-state operations must be guaranteed. Professor Morari (1982) in this Symposium will address the problem when dynamic considerations of operability are included in the design procedure.

If one accepts that flexibility in plant design is concerned with the problem of ensuring the existence of feasible regions of operation for a variety of different conditions, one could conceive of the following two types of design capabilities. In the first one, one should be able to design a chemical plant that has a fixed degree of flexibility at minimum cost. That is, the designer could specify a finite number of different operating conditions and specifications that the design must satisfy. Or more generally, one could specify the varying conditions as a bounded range of parameter values over which the design must be able to meet the specifications. Note that the basic concern would be to ensure that the design is both economical and capable of meeting specifications for the different conditions imposed.

The second type of design capability that can be conceived is one which determines the optimal degree of flexibility that is actually required by a chemical plant. In this procedure the objective would be to establish proper trade-offs between the cost of the plant and its flexibility. This procedure could clearly be regarded as a generalization of the first type of design capability since the degree of flexibility has to be determined. However, the generalization is by no means trivial as it requires a metric or quantitative measure of flexibility. In other words, some kind of scalar index is required which can measure the size of the region of feasible operation for the design. In this way, one could discriminate designs that are more flexible than others in a quantitative way. Furthermore, one could then in principle establish proper trade-offs between cost and flexibility through a multiobjective optimization approach.

It is the purpose of this paper to present an overview of previous and current work relating to the development of procedures for handling the aspect of flexibility in chemical process design. The paper will concentrate on the work that was initiated at Imperial College and that has been performed by our research group at Carnegie-Mellon University over the last three years. As will be shown in this paper the major challenge in these problems lies in developing efficient optimization strategies for solving nonlinear programs that are either of very large scale, but are highly structured, or otherwise involve an infinite number of constraints.

OPTIMAL DESIGN FOR FIXED DEGREE OF FLEXIBILITY

There are two classes of problems that can be considered in the design of chemical plants for which a fixed degree of flexibility is specified. The first one is the deterministic multiperiod problem wherein the plant is designed optimally to operate under various specified conditions in a sequence of time periods. Typical examples are refineries that handle various types of crudes, or pharmaceutical plants that produce several products. The second type of problem deals with the design of chemical plants where significant uncertainty is involved in the values of some of the process parameters. Examples of this case arise when values of feed specifications, transfer coefficients, physical properties or cost data are not well established. In this case the objective is to obtain a design for which both optimality and feasibility of operation of the chemical plant can be guaranteed for a specified bounded range of parameter values. It must be noted that in general the design problem can also be a combination of the above two problems.

Multiperiod Design Problem

One way to introduce flexibility in a chemical plant is to design it for a specified number N of different operating conditions (Grossmann and Sargent, 1979). For example, a plant may be specified to process a variety of feedstocks, produce different products, or operate at different levels of capacity. The goal is then to ensure that the plant will be able to meet the specifications for N successive periods of operation, requiring at the same time that the plant be designed and operated so as to optimize a given objective function, which is typically a combination of the investment and operating costs.

Very little has been discussed in the literature about deterministic multiperiod problems. Loonkar and Robinson (1970), Sparrow, Forder and Rippin (1975), Oi, Itoh and Muchi (1979), Suhami (1981), Suhami and Mah (1982), Knopf, Okos and Reklaitis (1980), Takamatsu, Hashimoto and Hasebe (1981), discuss design procedures that are applicable only to batch/semicontinuous processes. This important class of problems in which scheduling of operations is one of the main issues will be covered in detail in this Symposium by Professor Rippin (1982). Grossmann and Sargent (1979) give a general formulation for designing multipurpose chemical plants which can also be applied to problems described by the deterministic multiperiod model. As shown below, this involves the solution of a large nonlinear program, wherein the main computational difficulty is due to the large number of decision variables involved.

In order to formulate the multiperiod design problem it is assumed that the plant is subjected to piecewise operating conditions in N successive time periods. Also, dynamic effects are neglected, since the lengths of the transients are considered to be much smaller than the time periods for the successive steady states. The optimal design problem is then given by the following multiperiod nonlinear program

$$\min_{\substack{d,z^1,z^2,\ldots z^N\\ t^1,t^2,\ldots t^N}} \quad C = C^0(d) + \sum_{i=1}^{N} C^i(d,z^i,x^i,t^i)$$

$$\text{s.t.} \quad \left.\begin{array}{l} h^i(d,z^i,x^i,t^i) = 0 \\ g^i(d,z^i,x^i,t^i) \le 0 \end{array}\right\} \; i = 1,N \qquad (1)$$

$$r(d,z^1,\ldots z^N,x^1,\ldots x^2,t^1,\ldots t^N) \le 0$$

where

d is the vector of design variables representing equipment sizes

z^i is the vector of control variables in period i

x^i is the vector of state variables in period i

t^i is the length of time for each period i

h^i is the vector of equations in period i

g^i is the vector of inequalities in period i

r is the vector of inequalities that involve variables of all periods

N is the number of periods

It should be noted that the vector of design variables d remains fixed throughout the periods of operation as it represents the sizes of the units. Also, the control variables z^i represent the degrees of freedom in the operation of the plant, and therefore, they correspond to variables that can be manipulated directly or indirectly in the operation of the plant.

Since the dimension of h^i is the same as for x^i, the decision variables for the problem in (1) are given by the design variables d, the control variables z^i, $i=1,2,\ldots N$, and the lengths of periods t^i, $i=1,2,\ldots N$. The main difficulty that arises in the solution of this multiperiod problem is the fact that the number of decision variables can become rather large as the number of periods N increases. This implies that the computational burden that would be required by using current nonlinear programming algorithms could become excessive, and also that the numerical solution could be very difficult to obtain. However, it should be noted that problem (1) has a very special structure. Firstly, the objective function is separable in the design variables and in the N periods of operation. Secondly, since the variables x^i, z^i, t^i, are associated with the corresponding period i, the constraints have a bordered block-diagonal structure, where the coupling variables are given by the vector d, and the coupling constraints by the vector r. Therefore, it is clear that an efficient optimization algorithm ought to take advantage of this structure in order to reduce the computational requirements. As will be shown in the next section algorithms can be developed that accomplish this goal.

Projection-Restriction Strategy

Recently, Grossmann and Halemane (1980) have developed a very efficient decomposition scheme based on a projection-restriction strategy for solving an important particular case of problem (1). Namely, if one assumes that the lengths of the periods t^i are specified by the designer and that the vector of inequalities r only involves the design variables d, the multiperiod design problem is given by

$$\min_{d,z^1,z^2,\ldots z^N} \quad C = C^0(d) + \sum_{i=1}^{N} C^i(d,z^i,x^i) \tag{2}$$

$$\text{s.t.} \quad \left.\begin{array}{l} h^i(d,z^i,x^i) = 0 \\ g^i(d,z^i,x^i) \le 0 \end{array}\right\} \quad i = 1,N$$

$$r(d) \le 0$$

Note that problem (2) also has a block-diagonal structure, but it involves coupling in the variables d only and no coupling in the constraints. Although at first sight this problem appears to be too specific, it turns out to be one of the underlying formulations for solving design problems under uncertainty as will be shown later in the paper. Furthermore, the formulation in (2) still has a wide applicability in deterministic multiperiod design problems.

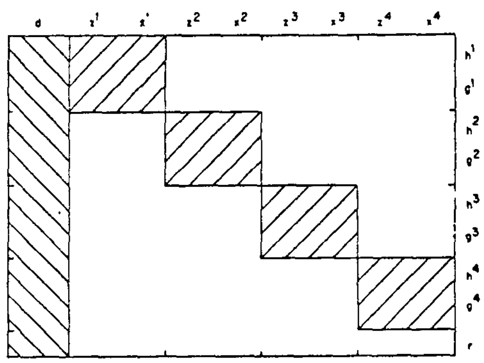


Fig. 1. Block-diagonal structure of the constraints in problem (2).

The decomposition technique proposed by Grossmann and Halemane (1980) exploits two basic features in this design problem. The first one is the block-diagonal structure in the constraints which is shown in Fig. 1. Since the objective function C is separable in the N periods, this implies that if the vector d is fixed, the optimization problem decomposes in N uncoupled subproblems, each having as decision variables the control variables z^i, i=1,2,...N. The second feature that is exploited, and which is strictly heuristic in nature, is that many of the inequality constraints become active at the solution. Clearly, this feature cannot be expected to hold necessarily for any arbitrary mathematical problem. However, in the context of multiperiod chemical plant design this condition seems to hold true in general. The main reason for this is that cost functions tend to be monotonic, and therefore, the optimal solutions commonly lie at the boundary of the feasible region (Westerberg and Debrosse, 1973). Another important reason is that in the formulation of multiperiod problems it is necessary to treat most of the output variables of the process in the form of inequalities in order to introduce a positive number of degrees of freedom (see Grossmann and Sargent, 1979). Since these output variables (e.g. production rates, purity specifications, target temperatures and pressures) are normally fixed for the single period problem, they will have a high tendency to become active at the solution. In fact, the observation that many inequalities do become active at the solution has been confirmed numerically in a number of example problems (see Grossmann and Halemane, 1980).

The main steps involved in the projection-restriction strategy, which is based on some ideas proposed by Grigoriadis (1971) and Ritter (1973) for linearly constrained problems, are as follows:

Step 1 - Find a feasible point d, z^i, x^i, i=1,2,...N, for problem (2).

Step 2 -
(Projection) Fixing the values of the vector d, solve the N subproblems

$$\min_{z^i} \; C^i(d,z^i,x^i) \tag{3}$$

$$\text{s.t.} \quad h^i(d,z^i,x^i) = 0 \qquad i = 1,2,\ldots N$$

$$g^i(d,z^i,x^i) \le 0$$

Step 3 -
(Restriction) (a) For each subproblem i, convert the n_A^i inequality constraints g_A^i that are active in Step 2 into equalities and define

$$h_R^i = \begin{bmatrix} h^i \\ g_A^i \end{bmatrix}, \quad g_R^i = g_I^i \quad i=1,2,\ldots N \tag{4}$$

where h'_R, g'_R are the redefined sets of equality and inequality constraints, and g'_I are the sets of inequality constraints that are not active in Step 2.

(b) Eliminate n'_A variables z'_A from the vector

$$z' = \begin{pmatrix} z'_A \\ z'_I \end{pmatrix} \text{, so as to define}$$

$$z'_R = z'_I \,, \quad x'_R = \begin{pmatrix} x' \\ z'_A \end{pmatrix} \,, \quad i=1,2,...N \tag{5}$$

where z'_R is the *redefined* vector of control variables which results from eliminating the vector z'_A of n'_A elements, and x'_R is the expanded vector of state variables.

Step 4 - Solve the restricted problem:

$$\underset{d,z^1_R,z^2_R,...z^N_R}{\textit{minimize}} \quad C = C^0(d) + \sum_{i=1}^{N} C^i(d,z^i_R,x^i_R)$$

$$\text{s.t.} \quad \left.\begin{matrix} h^i_R\,(d,z^i_R,x^i_R) = 0 \\ g^i_R\,(d,z^i_R,x^i_R) \le 0 \end{matrix}\right\} \quad i = 1,2,...N \tag{6}$$

$$r(d) \le 0$$

Step 5 - Return to Step 2 and iterate until no further changes occur in the values of the variables d and in the active set of constraints.

Note that in Step 4 the projection-restriction strategy really consists in solving problem (2) simultaneously for all variables, but in general with a much smaller number of decision variables, since many of these get eliminated by the active constraints determined in Step 2. Clearly, the effectiveness of this strategy relies heavily on the number of inequality constraints that actually become active at the solution.

Also, it should be noted that for effective implementation of this procedure it is necessary to find an initial feasible point in Step 1 efficiently, and to ensure nonsingularity in the redefined system of equation h'_R in Step 3. For the first point Grossmann and Halemane (1980) have suggested an alternate optimization scheme of design and control variables in which the sum of squares of violation of constraints is minimized. For the second point, they perform an analysis on the reduced jacobian of the system of equations to determine its maximum rank. This scheme allows one to incorporate only those active inequalities that lead to a non-singular system of equations (see Halemane and Grossmann, 1981b).

The results that have been obtained with the projection-restriction strategy are extremely encouraging. Grossmann and Halemane (1980) and Avidan (1982) have found that with the proposed projection-restriction strategy the computer time varies only linearly in the number of periods. This is in great contrast with the polynomial increase (second to third degree) of computer time that is experienced when no decomposition is performed. The reductions in computer time that have been obtained in an example of a reactor with cooler and an example of a flowsheet that involves a reactor, compressor and two separators are of at least one order of magnitude.

In order to substantiate the claims of computational efficiency theoretically, Grossmann and Halemane (1980) have developed a model that represents the computation time required with the decomposition scheme and without it. With this model it was found that if all the control variables are eliminated in the restriction step, one can indeed prove that the computer time has to be linear in the number of periods. For the case when not all the control variables are eliminated it is not possible to obtain a theoretical solution in closed form. However, it is possible to perform a parametric study which shows the interesting result that as the number of periods increases, the fraction of control variables that must be eliminated to ensure reduction in computer time with the projection-restriction strategy decreases exponentially. In other words, as long as some fraction of the inequalities becomes active at the solution (which is almost always the case) very substantial savings in computer time can be achieved with the projection-restriction strategy.

Recently Avidan (1982) has implemented the projection-restriction strategy in the general purpose computer package FLEXPACK using as the optimizer the variable-metric projection method by Sargent and Murtagh (1973). One interesting point that emerged from his work was the fact that further reductions of computer time in the decomposition strategy are possible if the vector of design variables d is partitioned in the capacity variables d_c (e.g. volumes vessels, power of compressors) and in the fixed design variables d_f (areas of exchange, number of plates) as discussed in Grossmann and Sargent (1979). Since the variables d_c are defined by expressions of the form $d_{cj} = \max\{c_{ij}\}$, where c_{ij} is the j'th capacity required for period i, the standard procedure is to replace them by inequalities to avoid discontinuous derivatives. However, since in problem (2) the lengths of the time periods are fixed it is very common that a given period i will define the bottleneck for a given capacity variable d_{cj}. Since by solving the projection step the periods where the bottlenecks occur can be identified, one can replace each design variable d_{cj} by the dominant capacity, which in turn reduces the problem size in the restriction step, particularly if the majority of the design variables are capacity variables. However, it is clear that this procedure will only work if the periods where bottlenecks occur remain the same in the restriction step, and therefore caution should be exercised when using this procedure.

Future directions. It is clear that the next step in the area of multiperiod design problems would be to derive a decomposition strategy for problem (1) which involves the coupling constraints r. This would be an important development since that structure would fit the multiproduct batch plant design problem (Grossmann and Sargent, 1979). It is interesting to note that if only a few variables occur in the constraint r, for instance the lengths of periods t_i, one could still apply the projection-restriction strategy if those variables are treated as design variables. However, this would increase the number of decision variables in the restriction step, and therefore, an extension of the projection-restriction strategy for this case would seem to be worth exploring.

Design under Uncertainty

In chemical plant design 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.

The general form of the problem of design under uncertainty is given by

$$\begin{aligned} \min_{d,z} \quad & C(d,z,x,\theta) \\ \text{s.t.} \quad & h(d,z,x,\theta) = 0 \\ & g(d,z,x,\theta) \le 0 \end{aligned} \qquad (7)$$

where d,z,x, are the vectors of design, control and state variables, and θ is a vector of p parameters for which there is significant uncertainty in their values.

There have been several approaches to the problem of design under uncertainty reported in the literature. They differ from each other in terms of problem formulation as well as solution strategies, since in principle the problem of design under uncertainty is not well-defined. Some authors consider the probability distribution of the parameters as either known or predictable, and minimize the expected value of cost. Another approach consists in transforming the problem into a deterministic one, assuming that the parameters vary within bounded ranges of values that are specified by the designer or by a statistical analysis. As it will be shown in the next section, this latter approach can be regarded as a generalization of the multiperiod problem if the control variables are allowed to be adjusted for the different parameter realizations in order to achieve feasible operation. However, it is worthwhile to first present a brief review on the extensive previous work that has been published on the problem of design under uncertainty.

In the earlier work, the stochastic approach was the one that was most frequently used. For instance, Kittrel and Watson (1966) assume that probability distribution functions of the parameters are available, and propose to select the decision variables in the design so as to minimize the expected value of cost. Wen and Chang (1968) define the 'relative sensitivity' of the cost as the fractional change in the cost function from its nominal value. In selecting the optimal design they minimize either the expected value or the maximal probable value of this relative sensitivity. Weisman and Holzman (1972) incorporate a penalty in the cost function involving the probability of violation for individual constraints, and perform an unconstrained minimization of the expected value of the cost. Although they made an attempt to minimize the probable violation of the constraints, their formulation does not ensure a lower limit on the probability of failure of any given constraint, which in fact could be achieved by using the formulation suggested by Charnes and Cooper (1959) for chance constrained optimization. Lashmet and Szczepanski (1974) apply Monte Carlo simulation for determining overdesign factors for distillation columns. They perform a series of statistical experiments by choosing random values of the parameters (within the specified range), and in each case determine the number of stages in the column needed to meet the specifications. From these data the overdesign factor is determined as the additional number of stages corresponding to 90% cumulative distribution over that for nominal design. Freeman and Gaddy (1975) define dependability as the fraction of time that the process can meet the specifications, and use it as a criterion for selecting the optimum design. They perform a stochastic simulation and determine the optimum values of the decision variables for different values of the parameters chosen randomly. The expected value of the cost corresponding to any given dependability level that minimizes the expected cost is chosen for the optimum design.

It is to be noted that in the above methods no distinction is made between the two types of decision variables in the problem of optimal process design. The design variables, representing for example the sizes of equipment, get their values assigned in the design stage, and remain unaltered during the operation of the plant. The control variables represent the variables of the plant that can be adjusted in the operation after the plant is installed. For any given design, the optimal plant operation itself can be considered as a means for meeting the specifications while minimizing the operating cost. Therefore, it requires an appropriate choice for the values of control variables depending on the values of the parameters being realized. In a realistic strategy for optimal process design under uncertainty, it is important to incorporate this basic difference between design and control variables into the mathematical formulation.

The following researchers have made a distinction between design and control variables. Watanabe, Nishimura and Matsubara (1973) apply the concept of statistical decision theory by considering the problem of optimal process design as a two-person statistical game between Nature and the designer. They minimize a utility function which is a convex combination of the expected value and the maximum probable value of cost. That is, they follow a strategy which is intermediate between minimax strategy (maximal probable value of cost is minimized) and Bayes' strategy (expected value of cost is minimized). Nishida, Ichikawa and Tazaki (1974) proposed a minimax strategy wherein the maximum value of the cost function, as obtained at the worst parameter value in a specified range, is minimized by selecting the appropriate design. They view the design strategy as a game, wherein the uncertainty in parameter values is considered to result in the maximization of cost, whereas the objective of the designer is to minimize it. It is important to note that the design they come up with actually corresponds to the optimum solution for a particular (namely, the economically worst) value of the parameters, and therefore the design cannot be claimed to be optimal in an overall sense when the parameters do take on different values. Also, the feasibility of this design for other values of the parameters cannot be guaranteed, since this aspect is not explicitly considered in the problem formulation.

Takamatsu, Hashimoto and Shioya (1973) assumed that the parameters vary within specified bounds, and minimize the deviation of the objective function from its value at the nominal solution, while satisfying the constraints linearized around their nominal values. They evaluate each constraint with a separate parameter value that would result in the worst violation of that constraint. In this way they seek a design that would meet the specifications with a single and common operating condition for all the bounded parameter values. This approach will tend to give conservative designs since no advantage is taken of the fact that, depending on the values of the parameters being realized, the operation of the plant can be manipulated in order to satisfy the specifications in the most economical way. Dittmar and Hartmann (1976) use a similar approach as Takamatsu, Hashimoto and Shioya (1973), but instead suggest the use of the same extreme value of the parameter for all the constraints. They determine the design margin for each of these extreme values and select the largest design margin so obtained.

Avriel and Wilde (1969) discuss different strategies such as two-stage (here-and-now), wait-and-see, and permanently-feasible programs then consider the feasible region expressed in the space of the scaled parameters as shown in Fig. 8. In the scaled space the 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. Note that this hypercube has the property that for any of the parameter points contained in it, the existence of control variables which meet the design specifications and constraints is guaranteed.

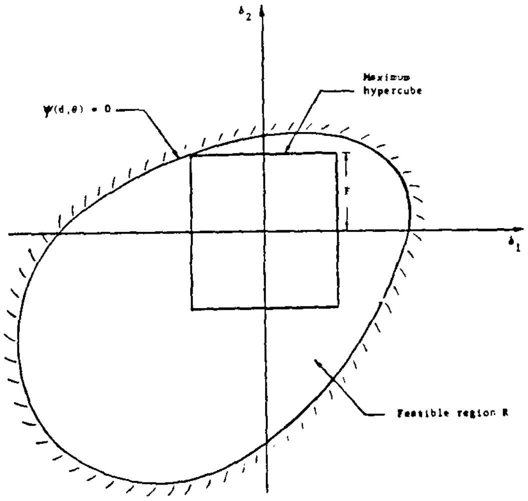


Fig. 8. Maximum hypercube contained in the feasible region R.

The choice of appropriate scaling factors in (32) requires some comment. Arbitrary choice of the scales will of course give unsatisfactory results. For instance, one might consider scaling parameter deviations in proportion to their nominal values, in effect giving equal weight to equal percentage changes for all parameters. To give the same weight, for example, to a percentage change in temperature as to a percentage change in flowrate would in most cases be inappropriate. Referring again to Fig. 6, the flexibility index implies a rectangular region in the space of uncertain parameters inside of which feasible operation is guaranteed for all combinations of parameter realizations. By considering the probability distributions of the parameters one could in theory compute the total probability that parameter realizations will lie within the rectangle by integrating the joint probability density function over the rectangular region. Since it is this probability of feasibility which is the underlying objective of flexibility, it would make sense to define the rectangle in a way which tends to maximize that probability for a given cost. Usually only approximate knowledge of the individual probability distributions will be available, so that a rigorous maximization will not be possible. However, it is reasonable to expect that some estimate of range or variance measure will be available for each parameter, to be specified by the design engineer based on experience, statistical data, or rule-of-thumb target values. An appropriate choice of scaling factors would be to use these variances or range estimates directly; this choice has the following heuristic support.

Consider the problem of defining one corner of a rectangle in a space of two parameters as shown in Fig. 9. Given probability distributions, contours may be constructed representing the locus of corners for rectangles which enclose the same total probability. Since the individual probability distributions will usually be unimodal, these contours will be concave; examples for normal and uniform distributions are shown in the Fig. 9. By invoking the traditional convex cost argument, another contour may be envisioned which represents the locus of corners for rectangles corresponding to designs of constant cost. Since this cost contour will usually be convex, the rectangle which maximizes the probability of feasibility will have its corner located near the "knee" of a constant-probability contour. By scaling in proportion to the square-root of the variance of the individual distributions, the rectangle corner is positioned along a ray which passes through the "knees". By virtue of this the direct use of the variance estimates as scaling factors is deemed reasonable.

Thus, the index of flexibility F represents the size of a scaled hypercube region of guaranteed feasibility, with that size being an approximate representation of the total probability that parameter realizations will be feasible.

In order to evaluate the index of flexibility F, an appropriate mathematical formulation is necessary. Assuming that the state variables x are eliminated as in equation (9), the specifications and constraints for a fixed design d are given by the vector of inequalities $f(d,z,\theta) \leq 0$, where the control vector z is to be adjusted for different realizations of the vector when applied to design problems that correspond to geometric programs. In a two-stage stochastic program, the designer selects values for the design variables (first stage), then observes the actual realization of the uncertain parameters, and accordingly chooses the appropriate values for the control variables (second stage). While selecting the values for design variables in the first stage, it is essential to ensure feasibility of the second stage sub-program, namely that values of control variables can be chosen to satisfy the constraints. The objective is to minimize the expected value of cost while selecting a feasible and optimal design, which appears to be one of the most suitable representations for the problem of chemical process design under uncertainty. In the wait-and-see strategy, the designer waits for an observation of the uncertain parameters and then chooses the optimal values for both design and control variables. Here, each new value of the parameters results in a corresponding optimal design; or in other words, all decision variables are treated as control variables. In the permanently-feasible program, the designer selects (a single set of) values for both design and control variables which will be feasible for every possible realization of the uncertain parameters. Unlike the wait-and-see strategy, here the values of neither design nor control variables change with the variations in the values of the uncertain parameters. That is, in the permanently-feasible program, all decision variables are treated as design variables. Avriel and Wilde (1969) suggest a procedure for obtaining the optimal design, which consists of bounding the objective function value that would be obtained at the solution of the two-stage program by solving the wait-and-see program and permanently feasible program. However, they restrict their approach only to geometric programming formulations. Malik and Hughes (1979) apply a similar approach for general process design problems, although there is no guarantee on the feasibility of the design. Also, the stochastic programming method they propose, based on Monte Carlo simulation, requires great computation effort. Johns, Marketos and Rippin (1976) outline a design strategy in which parameter uncertainty is considered in addition to the possibility of expansions through a two-stage multiperiod formulation. However, they did not address the problem of deriving an efficient solution procedure for handling these problems.

Among the more general purpose formulations for optimization problems with uncertainty, Friedman and Reklaitis (1975a,b) deal with the case of linear programming problems that have uncertainties in the coefficients of the constraints. They show that this formulation can be applied to problems such as planning future operation policies for large interacting systems, production scheduling, resource allocation and determining optimum blending schemes. They incorporate the required flexibility in their system by allowing for possible future additive corrections on the current decisions, and optimize the system by applying an appropriate cost-for-correction in the objective function. It is interesting to see that they were able to identify the need for different corrections for different outcomes of the uncertain coefficients in order to make the problem feasible, and devise a procedure to achieve this in their computations. One obvious drawback with their approach is that it is applicable only to linear systems. A second limitation with their approach is that it cannot be applied directly to the problem of optimal design of flexible chemical plants, because in this case no additive corrections can be applied on the design variables. Instead, it is only the control variables that can be manipulated, so as to meet the specifications in spite of the variations in the values of the uncertain parameters. Kilikas and Hutchison (1980) use a linear process model wherein the coefficients are considered to be varying within specified bounds. Their approach, however, would tend to select the optimum value of their decision variables so as to satisfy their constraints for only one set of parameter values.

With any of the suggested approaches for dealing with parameter uncertainties in process design, one is always faced with the question of whether the designed plant can in fact be guaranteed to operate and satisfy specifications for the entire range of parameter values involved. This question, along with the fact that the problem of optimal process design under uncertainty is not well-defined, requires a systematic procedure in formulating as well as solving such design problems. First of all, it is to be noted that apart from minimizing the cost, the main concern of the design engineer is to ensure feasible steady state operation of the plant for every value of the parameters within specified bounds. Grossmann and Sargent (1978) propose a formulation that tries to incorporate this objective. They approximate the expected value of the cost by a weighted average of a finite number of terms, assuming discrete probabilities for a finite set of parameter values. They select the optimum design by minimizing this expected cost subject to maximizing each of the individual inequality constraints with respect to the parameters. In their solution procedure a small set of extreme values of parameters is selected by analyzing the signs of the gradients of each of the individual inequality constraints, and the optimization is performed for this set of parameter values, in the form of a multiperiod design problem. However, their approach cannot always guarantee that the extreme values that have been selected will ensure feasibility of operation for all the other parameter values. In the next section the formulation proposed by Halemane and Grossmann (1981c) is presented. This formulation is an extension of the work by Grossmann and Sargent (1978), and rigorously ensures feasible operation for the specified set of bounded parameter values.

Two-Stage Programming Formulation

Assuming that bounded values of the uncertain parameters are specified in problem (7), the region T that is defined to contain all possible values of these parameters is given by

$$T = \{\theta \mid \theta^L \le \theta \le \theta^U\} \qquad (8)$$

where θ^L and θ^U represent given lower and upper bounds on θ. Of course the parameters could also be dependent, in which case they would typically be related by linear constraints. However, for the sake of simplicity in the presentation they will be assumed to be independent.

In order to derive the mathematical formulation it is convenient to consider the design strategy used by Halemane and Grossmann (1981c) 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 considered 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 $\theta \in T$, a control z which is both optimal and feasible.

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

$$h(d,z,x,\theta) = 0 \Rightarrow x = x(d,z,\theta) \qquad (9)$$

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

$$g(d,z,x,\theta) = g(d,z,x(d,z,\theta),\theta) = f(d,z,\theta) \le 0 \qquad (10)$$

the optimal operation of the plant that minimizes the cost while satisfying the constraints will be given by the nonlinear program

$$\min_{z} \; C(d,z,\theta) \quad \text{s.t.} \; f(d,z,\theta) \le 0 \qquad (11)$$

The solution to this problem defines the cost function $C^*(d,\theta)$ which corresponds to the optimal operation of the plant for fixed values of d,θ. Furthermore, if the optimization is performed for every realization $\theta \in T$, the average cost of operation will be given by the expected value $E_{\theta \in T}\{C^*(d,\theta)\}$.

II. Design Stage: In order to achieve the basic objective of feasible operation in the region of parameters T, the design variable d must be chosen so as to ensure that for every value of θ the control variable z in the operating stage can indeed be selected to satisfy the constraints in (11). Note that an improper selection of d can lead to infeasible operation for some realization of θ, in which case no selection of the control z will exist so as to satisfy the inequality constraints in (11). 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 for dealing with uncertainties in design can be interpreted qualitatively in the following way. In stage II, the designer selects a design such that if in stage I the operator properly adjusts the controls depending on the realization of the parameter values, feasible and optimal operation of the plant can be achieved within the specified range of parameter values.

Note that the assumption made here is that essentially perfect control of the plant can be achieved, since for instance no noise is assumed in the measurement of the parameters. Although this could clearly be regarded as a limitation of the strategy, it is considered that at the design stage including more detailed information on the control scheme would make the problem virtually unmanageable. Despite the limitation, it is clear that the strong point of the strategy is that it does recognize explicitly that chemical plants can be adjusted during operation to achieve feasibility.

The strategy as stated above can be expressed mathematically as the two-stage programming problem,

$$\begin{aligned} &\underset{d}{\text{minimize}} \ \underset{\theta \in T}{E} \ \{ \min_{z} C(d,z,\theta) \mid f(d,z,\theta) \le 0 \} \\ &\text{s.t.} \ \forall \theta \in T \left\{ \exists z \left(\forall j \in J \left[f_j(d,z,\theta) \le 0 \right] \right) \right\} \end{aligned} \quad (12)$$

where $J = \{1,2,...,m\}$ is the index set for the components of the vector of constraint functions f. The constraint in (12) 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 plant of design d the plant can be operated to satisfy the specifications.

It is interesting to note that since there is an infinite number of possible realizations for the values of the parameters θ, and since the optimal operation of the plant is implicitly dependent on θ, the overall number of decision variables involved in problem (12) is infinite. This is because for every value of θ 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 (10) are defined for the infinite set of values $\theta \in T$. Therefore, problem (12) corresponds to a two-stage nonlinear infinite program.

A first step in simplification to make problem (12) more amenable to solution 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 (12) to

$$\begin{aligned} &\underset{d,z^1,z^2,...z^n}{\text{minimize}} \ \sum_{i=1}^{n} w^i \, C(d,z^i,\theta^i) \\ &\text{s.t.} \ f(d,z^i,\theta^i) \le 0, \ i = 1,2...,n \\ &\forall \theta \in T \left\{ \exists z \left(\forall j \in J \left[f_j(d,z,\theta) \le 0 \right] \right) \right\} \end{aligned} \quad (13)$$

where the weights w^i correspond to discrete probabilities for the selected finite number of parameter points $\theta^i \in T$, $i=1,2,...n$. These weights could be derived from the joint probability distribution function of the parameters, or they could be selected to reflect subjective probabilities assigned by the designer. Note that in the case where a joint distribution function is available, by suitable selection of the parameter bounds one can also define a minimum level of probability of parameter realization for which feasible operation of the chemical plant is guaranteed.

It is important to note that from a practical point of view the simplification for the expected cost as given in (13) does not represent a major limitation. The reason is that by optimizing the design for several parameter values one will obtain designs that in general are not too sensitive in the objective function to changes in parameter values. This has been confirmed with numerical examples reported by Grossmann and Sargent (1978) and by Halemane (1982).

With the simplification in (13) the number of decision variables is finite, since optimization is performed over the vector d of design variables and the finite number of vectors $z^1, z^2,...,z^n$ of control variables. The control variables z^i are selected to satisfy the corresponding constraints $f(d,z^i,\theta^i) \le 0$, so as to achieve optimal feasible operation at the point θ^i of the parameter space. Since the number of decision variables in (13) is finite, but the number of constraints is infinite because the feasibility constraint is still imposed, problem (13) corresponds to a semi-infinite programming problem (see Hettich, 1978; Polak, 1981).

It is interesting to note that if the feasibility constraint is excluded in (13), the resulting structure of the problem is equivalent to that of the deterministic multi-period problem given by (2). This problem could then be interpreted as one where the plant operates in each period with the parameter value θ^i, and with the length of each period being proportional to w^i. Since this problem can be solved very efficiently with the projection-restriction strategy, a very important question that arises is whether a finite number of points in θ-space can be selected, so that by ensuring feasibility of the design for those points, one can guarantee that the feasibility constraint in (13) will be satisfied.

As shown by Halemane and Grossmann (1981a,c), the answer to this problem is given by proving firstly that the feasibility constraint in (13) is mathematically equivalent to the subproblem

$$\max_{\theta \in T} \min_{z} \max_{j \in J} f_j(d,z,\theta) \le 0 \qquad (14)$$

They show that if the constraint functions $f_j(d,z,\theta)$ are jointly convex in z and θ, the global and local solutions to the subproblem in (14) that lead to critical points θ^c must lie at vertices of the polyhedron T in (8) that defines the parameter space. This then implies that if the design can be guaranteed to be feasible at the vertices of T, it can also be guaranteed to be feasible for all other $\theta \in T$.

Halemane and Grossmann (1981c) also show that an interesting interpretation of the constraint in (14) is given if one defines for a fixed d and θ the function

$$\psi(d,\theta) = \min_{z} \{u \mid u \ge f_j(d,z,\theta) \; \forall j \in J\} \qquad (15)$$

Note that this function $\psi(d,\theta)$ provides a measure of feasibility ($\psi \le \theta$) or infeasibility ($\psi > \theta$) for the chosen design d at the parameter value θ. Geometrically, ψ can also be interpreted as the "depth" of the feasible region since it measures the maximum deviation of the constraint functions with respect to the zero bound in (14). Furthermore, since the solution of (14) is given when the function $\psi(d,\theta)$ attains the maximum over the set T, there can in general be a finite number of critical parameter values θ^c for which the degree of feasibility is the smallest. In the convex case, Halemane and Grossmann (1981c) show that these critical points would correspond to some of the vertices of the polyhedron T. These ideas can be illustrated more clearly with the following set of linear constraints

$$\begin{aligned} f_1 &= -z + \theta &\le 0 \\ f_2 &= z - 2\theta + 2 - d &\le 0 \\ f_3 &= -z + 6\theta - 9d &\le 0 \\ & 1 \le \theta \le 2 \end{aligned} \qquad (16)$$

The feasible region for this set of constraints is shown in Figure 2a for d = 1, and the corresponding function ψ is shown in Figure 2b. Note that ψ is nondifferentiable at θ = 9/5, and that it exhibits two local maxima at θ = 1 and θ = 2. It is clear from Figure 2a that the size of the feasible region decreases at both extreme points, θ = 1 and θ = 2, and gets enlarged towards the interior point θ = 9/5. The function ψ plotted in Figure 2b reflects precisely this information, since ψ is strictly negative for 1 < θ < 2, and zero at the two extreme points. Thus, there are in this case two critical points that would have to be considered for design, which are in fact the two extreme points of the parameter θ.

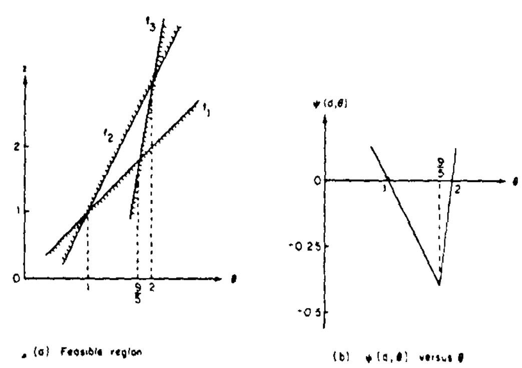


Fig. 2. Feasible region and $\psi(d,\theta)$ for constraints (16) with d = 1.

Solution Procedure

As was shown in the last section, the two-stage programming formulation with the feasibility constraint is given by

$$\begin{aligned} &\min_{d,z^1,z^2,\dots z^n} \sum_{i=1}^{n} w^i C(d,z^i,\theta^i) \\ &\text{s.t.} \quad f(d,z^i,\theta^i) \le 0 \quad i = 1,2,\dots n \\ &\qquad \max_{\theta \in T} \min_{z} \max_{j \in J} f_j(d,z,\theta) \le 0 \end{aligned} \qquad (17)$$

A direct solution procedure for this optimization problem poses great difficulty since it involves the max-min-max constraint, which as has been shown in the example of Figure 2 involves a non-differentiable global optimization problem (see Danskin, 1967; Demyanov and Malozemov, 1974). Therefore, in order to derive a reasonable solution procedure it is best to take advantage of the fact that in the convex case feasibility of this constraint can be guaranteed if the constraint functions are forced to be feasible at the vertices of the polyhedron T. Although this procedure would be strictly valid only for the convex case, it may also be valid in some instances when nonconvex constraint functions are involved.

Given that the objective is to ensure feasibility for all the vertices of the set T, one approach to solve problem (17) would be to reformulate it as a multiperiod problem in which the 2^p parameter vertices are selected as the n points for the design. However, this procedure could clearly become very expensive computationally if the number of parameters p is rather large (e.g. $p \geq 4$). To circumvent this difficulty, Halemane and Grossmann (1981c) have proposed an iterative multi-period design algorithm that is given by the following steps:

Step 1 - Set $k = 0$. Choose an initial set T_o consisting of N_o vertices where $N_o \ll 2^p$.

This can be achieved with small computing requirements using the procedure suggested by Grossmann and Sargent (1978), in which each constraint is maximized individually by assuming monotonicity. The gradients $\partial f_j / \partial \theta_k$ of each of the individual constraint functions f_j, $j=1,2,\ldots m$, with respect to the parameters θ_k, $k=1,2,\ldots p$, are computed at initial values of d and z, and the signs of these gradients are analyzed. If for each individual constraint function f_j, the gradient $\partial f_j / \partial \theta_k > 0$, the upper bound θ^U_k is selected for the parameter θ_k, whereas if $\partial f_j / \partial \theta_k < 0$ the lower bound θ^L_k is selected. Clearly, for zero gradients either choice of the bounds is possible. Since each constraint may lead to a different vertex, the set of vertices obtained for all constraints is finally merged into the smaller set of vertices T_o by using a set covering formulation (see Garfinkel and Nemhauser, 1972). It should be noted that if the constraint functions f_j are monotonic in the parameters θ_k, these vertices will correspond to the maximization of individual constraint functions.

Step 2 - Determine the design vector d^k by solving the problem

$$\begin{aligned} &\underset{d,z^i,i=1,2,\ldots N^k}{\text{minimize}} \quad \sum_{i=1}^{N_k} w_i \, C(d,z^i,\theta^i) \\ &\text{s.t.} \quad f(d,z^i,\theta^i) \leq 0, \; i = 1,2,\ldots N^k \end{aligned} \tag{18}$$

using the projection-restriction strategy for multiperiod-design problems.

Step 3 - Determine the critical parameter values $\theta^{c,k}$ by solving for every vertex θ^i in T, the problem

$$\psi(d^k,\theta^i) = \min_z \{u \mid u \geq f_j(d^k,z,\theta^i),\; j \in J\} \tag{19}$$

The vertex that gives rise to the maximum value of ψ is then determined and is denoted by $\theta^{c,k}$. If $\psi(d^k,\theta^{c,k}) \leq 0$, stop. Otherwise, proceed to Step 4.

Step 4 - Incorporate the new critical point in the design by defining

$$T_{k+1} = T_{k+1} \cup \{\theta^{c,k}\}\;,\; N_{k+1} = |\,T_{k+1}\,|, \tag{20}$$

set $k = k + 1$ and return to 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 can only be a finite number of critical parameter points. 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 global iteration in the algorithm may be required. It is also important to note that the minimizations in (19) may not have to be performed until completion for all vertices, as they can be stopped when ψ reaches a negative value in which case the existence of a non-empty feasible region is detected. Thus, by the above considerations this algorithm should provide in general a more efficient method of solution than the case when all the vertices are included in problem (18). Halemane and Grossmann (1981c) have applied this algorithm to two example problems, each one involving five uncertain parameters: a heat exchanger network and a reactor with a cooler. The computational requirements were modest since no more than two global iterations of the algorithm were required to obtain the optimal and feasible solutions.

The efficiency of the above algorithm could be enhanced further by making use of the following provisions. Firstly, the number of parameter points that must be considered in Step 2 could be kept relatively small at each iteration of the algorithm if some of the vertices are eliminated when new ones are added in Step 3. The obvious criterion would be to discard those vertices that have the smallest negative value of ψ, since they are the ones that are most likely to remain feasible for small changes in the design vector d. However, there is clearly no guarantee that these vertices would become infeasible in the next iteration in which case they would have to be included in Step 2 again.

The second provision would be related to the problem of having to solve problem (19) for each one of the vertices of the set T, which can clearly become a major burden in the computations if the number of parameters p is large. For instance, for p = 10, 1024 vertices need to be analyzed, whereas for p = 20 the number of vertices is 1,048,576. In order to overcome this problem, if one assumes convexity in the constraints, a lower bound on ψ for each vertex i can be computed very efficiently by solving (19) with the constraint functions linearized at the nominal point (z^N, θ^N). That is, the lower bound ψ_L^i at vertex i would be given by

$$\psi_L^i = \min_z u \qquad (21)$$

$$u \geq f_j(d^k, z^N, \theta^N) + \frac{\partial f_j}{\partial z}(z - z^N) + \frac{\partial f_j}{\partial \theta}(\theta - \theta^N) \qquad j \in J$$

where clearly ψ_L^i will yield a rigorous lower bound since the convex functions $f_j(d^k, z, \theta)$ will be greater or equal than the corresponding linearized functions in (21). Note that the computation of these lower bounds involves the solution of a parametric linear programming problem in which only the right hand side is modified at the different vertices. Hence, the solution of the linear program would require very few simplex iterations at the successive vertices (Hillier and Lieberman, 1980). Preliminary numerical results (Swaney, 1982) indicate that the quality of these bounds is very good These bounds could be used either as a heuristic to avoid solving (19) in Step 3, or otherwise they could be used within a rigorous bounding procedure since an upper bound ψ_U^i can be computed by simply evaluating the constraint functions at the control variables z^* predicted by (21). Unfortunately, numerical results have indicated that the quality of these upper bounds is not very good. Further investigation would be required to test the effectiveness of this procedure.

<u>Discussion on locating critical parameter points</u>

Clearly one of the major difficulties involved in the problem of design under uncertainty is the selection of a finite number of critical points whose feasibility will ensure feasibility for the whole set of parameters T. Ideally, one would like a procedure by which the critical parameters could be predicted <u>a priori</u>. At the simplest level one could think of using intuition or engineering judgment to do that, for instance by selecting what would appear to be the "worst" parameter values (e.g. low transfer coefficients, low efficiencies, high flowrates, etc.). However, as has been shown with the heat exchanger network example by Grossmann and Sargent (1978), this selection is not always trivial since in their problem the feasible design is not obtained by selecting the lower bounds for the heat transfer coefficients which would be normally regarded as the "worst" values.

A further complication, as was illustrated in the example of Fig. 2, is that there may be several critical points that may have to be considered for the design. A procedure that can predict several points a priori is the one suggested by Grossmann and Sargent (1978). This procedure predicts the critical points by analyzing the sign of gradients of the constraints, as was outlined in Step 1 of the algorithm. However, although this procedure is very often successful, it may in some cases fail to predict the right set of critical parameter values. In order to gain some insight as to why this may happen, and also to try to understand under which conditions a single critical point exists, consider the following set of three linear constraints that involve two control variables, two parameters and one design variable:

$$
\begin{aligned}
f_1 &= -z_1 + 3\theta_1 - \theta_2 \le 0 \\
f_2 &= -z_2 - \theta_1 + 3\theta_2 \le 0 \\
f_3 &= z_1 + z_2 - \theta_1 - \theta_2 - d \le 0 \\
& 1 \le \theta_i \le 2, \; i = 1,2.
\end{aligned}
\tag{22}
$$

Since these constraint functions are linear, their gradients are independent of the initial point chosen for such calculations; and since they are monotonic in θ, the maximization of each of these functions can be performed by analyzing these gradients. It is clear that the three constraint functions get maximized at the three different vertices $\theta^1 = [2,1]$, $\theta^2 = [1,2]$ and $\theta^3 = [1,1]$ respectively. In order to show that these vertices can lead to designs that may be infeasible, consider problem (15) for establishing the feasibility at a given design d, and parameter θ, which yields

$$
\begin{aligned}
\psi(d,\theta) = \min_z \; & u \\
\text{s.t. } f_1 &= -z_1 + 3\theta_1 - \theta_2 \le u \\
f_2 &= -z_2 - \theta_1 + 3\theta_2 \le u \\
f_3 &= z_1 + z_2 - \theta_1 - \theta_2 - d \le u
\end{aligned}
\tag{23}
$$

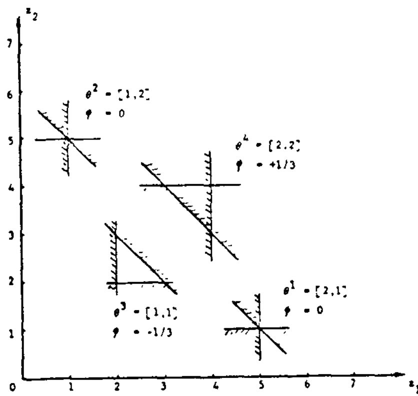


Fig. 3. Feasible region for the constraints in (22) with d = 3.

Figure 3 gives a plot of the feasible region for the set of constraints in (22), with a design d = 3, wherein the values of ψ obtained from (23) are also given for each of the four vertex points of the parameter-space. Since the constraint functions are linear and hence convex, the critical parameter points must lie at a vertex. Clearly, from the values of ψ in Fig. 3, $\theta^4 = [2,2]$ is the critical point, since ψ attains its maximum at this vertex. Also note in Fig. 3

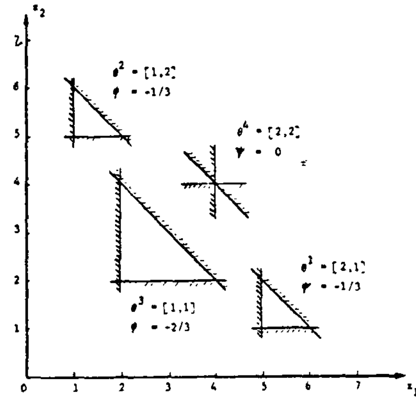


Fig. 4. Feasible region for the constraints in (22) with d = 4.

that the design d = 3 is found to be feasible for the three vertices predicted by maximization of constraints, $\theta^1 = [2,1]$, $\theta^2 = [1,2]$ and $\theta^3 = [1,1]$, whereas it is infeasible for the critical parameter point - namely the vertex $\theta^4 = [2,2]$. To make the design feasible for the critical point as well, consider that the design variable is increased to d = 4. The feasible region and the value of ψ for the four vertices are again shown in Fig. 4 for this value of d = 4, where as it can be seen the design is just feasible for the critical point, whereas a finite region of feasibility exists for all other points in the parameter space. Thus, by ensuring the feasibility of the design for the critical parameter values as predicted by the max-min-max constraint, it is possible to guarantee the overall feasibility of the design for every parameter value within the specified range.

In order to gain some further insight as to why the maximization of individual constraint functions will not always lead to correct critical points, assume that for all $\theta \in T$ the same common (single) set of values z is selected for the control variables. It then follows that the max-min-max constraint reduces to

$$
\max_{\theta \in T} \max_{j \in J} f_j(d,z,\theta) \le 0 \tag{24}
$$

which is equivalent to

$$
\max_{\theta^j \in T} f_j(d,z,\theta^j) \le 0, \; \forall j \in J. \tag{25}
$$

Thus, if for the design d it is possible to select a control z, feasible and common for all $\theta \in T$, then some of the parameter points predicted by maximization of individual constraints will correspond to those (critical points) predicted by the max-min-max constraint. However, it is clear that in general different controls z may have to be selected for different realizations of θ to maintain feasibility and, therefore, by maximization of the individual constraint functions one may not always predict the correct critical points in a design.

Another interesting question about locating critical points is to determine the conditions under which only a single critical point will need to be considered for the design. To analyze this case assume that for a given design d, the set of constraint functions is linear and given by:

$$f_j = \sum_{k=1}^{p} a_{jk}\theta_k + \sum_{k=1}^{n_z} b_{jk} z_k + c_j \le 0, \quad j = 1,2,\dots m \tag{26}$$

The critical point θ^c is given by the solution to the problem:

$$\max_{\theta \in T} \min_{z} u$$

$$\text{s.t.} \sum_{k=1}^{p} a_{jk}\theta_k + \sum_{k=1}^{n_z} b_{jk} z_k + c_j \le u, \ j = 1,2,\dots m \tag{27}$$

Assume that for any $\theta \in T$ the problem

$$\psi(d,\theta) = \min_{z} u$$

$$\text{s.t.} \sum_{k=1}^{p} a_{jk}\theta_k + \sum_{k=1}^{n_z} b_{jk} z_k + c_j \le u, \ j = 1,2,\dots m \tag{28}$$

has the same set of active constraints (e.g. the first r, $r \le m$).

The Kuhn-Tucker conditions for the above minimization problem then yield

$$\text{(a)} \quad 1 = \sum_{j=1}^{r} \lambda_j, \ \lambda_j \ge 0, \ j = 1,\dots r$$

$$\text{(b)} \quad 0 = \sum_{j=1}^{r} \sum_{k=1}^{n_z} \lambda_j b_{jk}, \ k = 1,2,\dots n_z \tag{29}$$

$$\text{(c)} \quad u = \sum_{k=1}^{p} a_{jk}\theta_k + \sum_{k=1}^{n_z} b_{jk} z_k + c_j, \ j = 1,2,\dots r$$

Since the value of u at the minimum determines ψ, it follows that

$$\psi = \frac{1}{r} \sum_{j=1}^{r} \left(\sum_{k=1}^{p} a_{jk}\theta_k + \sum_{k=1}^{n_z} b_{jk} z_k + c_j \right) \tag{30}$$

From this expression it is clear that $\psi(d,\theta)$ is linear and hence monotonic in θ, for the chosen design d. Therefore the maximization of ψ in (30) will lead to a single critical point. Note that in (29) the active constraints are determined by the values of the multipliers λ_j, which are in turn obtained from the subset (a),(b), and since $r \le m$, a necessary condition for having the same set of constraints to be active for every $\theta \in T$ would be: $m \le n_z + 1$. In general, a necessary and sufficient condition would be to have the values of all the multipliers λ_j (j=1,2,...m) uniquely determined by the system (29). Furthermore, if for every k, $\text{sign}(\partial\psi/\partial\theta_k) = \text{sign}(a_{jk})$ for some constraints j, then these constraints are maximized at the point defined by max $\psi(d,\theta)$, and under these conditions the maximization of individual constraints with respect to θ would lead to the critical points.

To illustrate these ideas consider the set of constraints given by (22). The solution to (29 a,b) yields $\lambda_1 = \lambda_2 = \lambda_3 = +1/3$, indicating that the three constraints are active for all θ. Furthermore, from (30) the value for ψ is obtained as $\psi(d,\theta) = 1/3(\theta_1 + \theta_2 - d)$, indicating that $\psi(d,\theta)$ is indeed monotonic in θ, and that maximization of ψ results in the single critical point given by $\theta^4 = [2,2]$. Note that the signs of the gradients $\partial\psi/\partial\theta_1$ and $\partial\psi/\partial\theta_2$ are both positive, whereas there is no constraint in (22) that satisfies this condition. Therefore, in this case since the monotonicity of ψ cannot be related with the monotonicity of the individual constraint functions f_j, the maximization of individual constraint functions does not predict the right critical parameter value. From the analysis presented above, it would be most interesting to investigate whether for nonlinear constraints with special structure the property of monotonicity of ψ also holds when the same set of constraints remains active for all the vertices in T.

Future directions. As has been shown above, it is the aspect of feasibility that greatly complicates the two-stage programming formulation for the design problem under uncertainty. In the case when feasibility can be ensured by considering only the vertices in T, the proposed algorithm provides a reasonable way of tackling the problem. However, there is no question that there is still great incentive to enhance the efficiency of this algorithm and some of the provisions suggested above should be explored further. The greatest challenge, however, would be to devise a procedure that could also handle the nonconvex case for which the critical point may not correspond to a vertex. This would require the solution of the nondifferentiable global optimization problem that is involved in the max-min-max constraint, which at the present time appears to be an extremely difficult problem to tackle.

DESIGN WITH OPTIMAL DEGREE OF FLEXIBILITY

In the first part of the paper procedures were outlined which treat the case of design for a fixed degree of flexibility. In that case the required flexibility is pre-specified, either by a discrete set of required operating conditions or by requiring feasibility of operation when a set of uncertain parameters can vary between fixed bounds. The more general problem is to determine the design which possesses the optimal degree of flexibility. Solution of this problem requires a quantitative characterization of the property of flexibility.

For the flexibility of a design to be "optimal" requires that the economic advantages of flexibility be balanced in relation to its cost. As stated before, flexibility as a design attribute represents the ability of a design to accommodate variations: with a higher degree of flexibility, the range of tolerable variations is greater. The uncertain parameters which describe the variations may be considered as random variables, and conceptually their realizations may be described in terms of their joint probability distribution. It follows then that a design featuring a higher degree of flexibility will have a lower probability of encountering infeasible operation. Since there will be an economic penalty incurred when infeasibilities prevent successful operation, there is strong motivation to provide a design with an adequate degree of flexibility.

Conceptually one could construct a nonlinear program with an objective function which involves the expectation of the composite economic cost, including penalties for infeasibility. In theory the solution to that stochastic program would determine the optimal degree of flexibility. The practical problems of such an approach are two-fold. First, the combined occurrence of the feasibility constraint and the expectation operator make the above program one of great mathematical difficulty. Second, it is doubtful that either the probability distributions of the uncertain parameters or the economic penalties for infeasibility will ever be known very accurately in a practical plant design situation. For these reasons the complex stochastic program as outlined can hardly be justified, and pragmatic simplifications are in order.

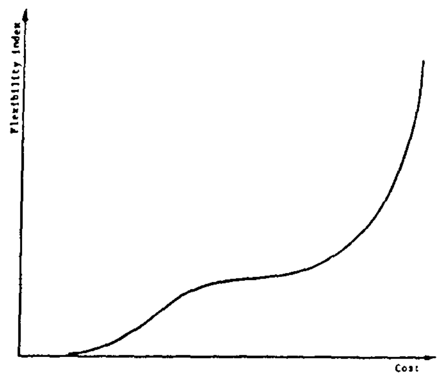


Fig. 5. Trade-off curve for flexibility and cost.

A key step towards simplification is the separation of the composite objective function into two components: minimizing capital and operating costs on the one hand, and maximizing flexibility on the other. The resulting formulation then takes the form of a multicriterion optimization problem, with annualized cost and degree of flexibility as two simultaneous objective functions. The standard procedure would then be to construct a trade-off curve relating flexibility to cost as shown in Fig. 5 (see Clark and Westerberg, 1982). This could be done for instance by using the ϵ-constrained method where one objective is optimized while the other objective is set to the limit ϵ which is varied parametrically (Haimes, Hall and

Freedman, 1975). Examination of the curve would allow the assessment of an appropriate trade-off, thereby establishing an "optimal" degree of flexibility. The principal requirement in such a procedure is that a quantitative measure for the degree of flexibility be available. This need of a metric for flexibility is the motivation for the flexibility index described below.

An Index of Flexibility

The problem at hand is to construct a scalar metric whose value for any fixed design characterizes the size of the region of feasible operation in the space of uncertain parameters. Since for each realization of the parameters control variables will be adjusted to attain feasibility of operation (if possible), the feasible region in θ-space may be defined as

$$R = \left\{ \theta \mid \left[\exists z \mid f(d,z,\theta) \leq 0 \right] \right\} \qquad (31)$$

where the vector of inequalities $f(d,z,\theta) \leq 0$ define feasibility in (z, θ)-space. In general the actual shape of this region could be rather complex, being defined by a boundary whose points are determined implicitly by the equation $\psi(d,\theta) = 0$ (see Fig. 6), while the function $\psi(d,\theta)$ is itself the result of the nonlinear program shown in equation (15). A particular example of this region which corresponds to the set of constraints in (22) with d = 4, is shown in Fig. 7.

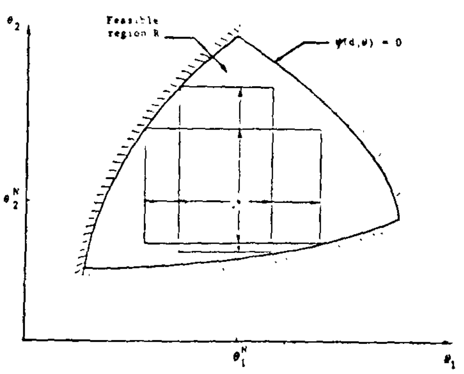


Fig. 6. Hyper-rectangles contained in the feasible region R.

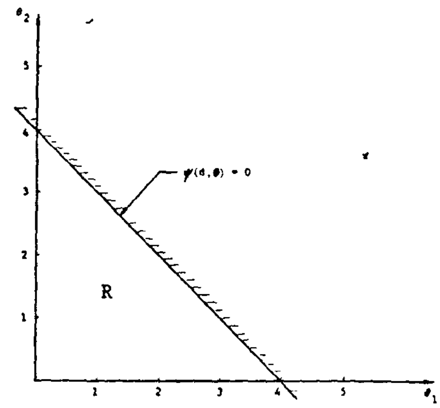


Fig. 7. Plot of region R for the set of constraints in (22) with d = 4.

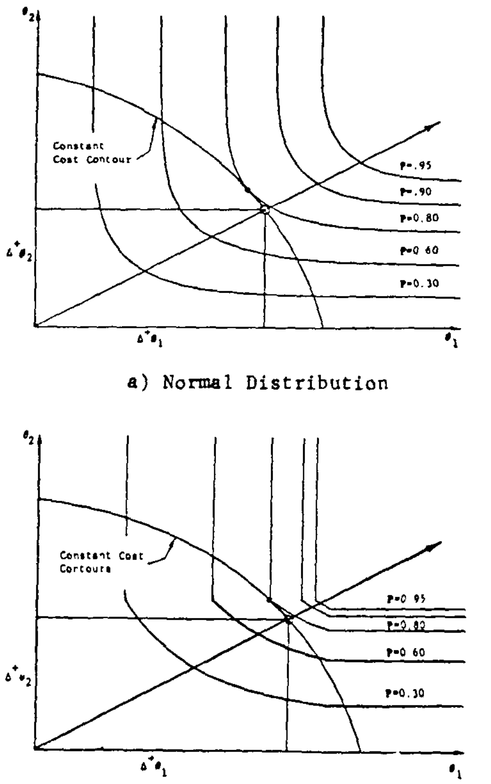
Since in general the geometry of the feasible region as given in (31) is difficult to treat in a meaningful way, the following approach is proposed. It may be assumed that the uncertain parameters will vary independently of each other.[2] It makes sense then to analyze the feasible region R in terms of 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 a hyper-rectangle within the feasible region as shown in Fig. 6. The size of the feasible region is then characterized by the lengths of the sides of the rectangle. The remaining difficulty is that the rectangle is not uniquely determined; trade-offs can result by increasing the range of some parameters while decreasing the range of others.

The solution is to supply a set of scaling factors which in effect determine the proportions of the rectangle. With these factors in hand, positive and negative variations in the uncertain parameters may be expressed as scaled deviations from a given nominal value:

$$\delta_i^+ = \frac{\theta_i - \theta_i^N}{\Delta^+\theta_i}, \quad \delta_i^- = \frac{\theta_i^N - \theta_i}{\Delta^-\theta_i}, \qquad i = 1,\ldots,p \qquad (32)$$

The point θ^N specifies some nominal operation that will be feasible; the scaling factors $\Delta^+\theta_i$ and $\Delta^-\theta_i$, that represent expected positive and negative deviations may well differ from each other, since the nominal values θ_i^N may not lie at the centers of their parameter ranges. One may

[2] If the set of parameters in the original problem formulation are dependent, then principal component analysis may be employed to obtain an independent set.



a) Normal Distribution

b) Uniform Distribution

Fig. 9. Scaling of deviations through distribution functions

of uncertain parameters θ to achieve feasible operation. It is not necessary to introduce the variables δ^+_i, δ^-_i, i = 1,...p explicitly, since a single scalar variable δ may be used to characterize the hypercube of feasible deviations

$$T = \left\{\theta \mid \theta^N_i - \delta\Delta^-\theta_i \le \theta_i \le \theta^N_i + \delta\Delta^+\theta_i, i = 1,...p\right\}. \quad (33)$$

The flexibility index, F, for a given design, d, is then given by the semi-infinite programming problem

$$F = \max \delta$$

$$\text{s.t. } \forall \theta \in T \left\{\exists z \mid \forall j \in J \left[f_j(d,z,\theta) \le 0\right]\right\} \quad (34)$$

$$T = \left\{\theta \mid \theta^N_i - \delta\Delta^-\theta_i \le \theta_i \le \theta^N_i + \delta\Delta^+\theta_i, i=1,...p\right\}$$

where the first constraint imposes the <u>feasibility condition</u> for all θ values that lie within the hypercube T. Using the equivalent formulation for the feasibility condition in (14), this problem may also be formulated as

$$F = \max \delta$$

$$\text{s.t. } \max_{\theta \in T} \min_{z} \max_{j \in J} f_j(d,z,\theta) \le 0 \quad (35)$$

$$T = \left\{\theta \mid \theta^N_i - \delta\Delta^-\theta_i \le \theta_i \le \theta^N_i + \delta\Delta^+\theta_i, i=1,...p\right\}$$

As shown by Swaney and Grossmann (1982), the problem in (35) exhibits two important properties. The first is that if the constraints are jointly convex in z and θ, the maximum of the feasibility constraint lies at one or several of the vertices of the hypercube T given by (33). The second one is that the function ψ given by equation (15) (which provides a measure of feasibility) is zero at these vertices. These properties are illustrated in Fig. 8, where the hypercube touches the boundary $\psi(d,\theta) = 0$ at one of its vertices. Note that this vertex may be interpreted as a critical parameter value which identifies a worst-case condition for the design.

<u>An Efficient Vertex Enumeration Procedure</u>

The formulation in (35) provides the definition of the flexibility index for a chemical plant of fixed design. As in the case of design under uncertainty, the max-min-max constraint is the major source of difficulty when seeking an efficient solution method for (35). However, by assuming that the critical parameter values must occur at vertices of the hypercube, the problem is simplified considerably. Swaney and Grossmann (1982) have recently developed an efficient search method to find the smallest of the maximum tolerable parameter deviations for all vertex directions.

Basically they consider the following subproblems

$$\max_{z,\delta_k} \delta_k$$

$$\text{s.t. } f(d,z,\theta) \le 0 \qquad k \in V \quad (36)$$

$$\theta = \theta^N + \delta_k(\Delta\theta)^k$$

where $(\Delta\theta)^k$ is the vector of deviations that lead to vertex k and V is the set of vertices of the hypercube T. They show that these subproblems define points on the boundary of the feasible region $\psi(d,\theta) \le 0$. The value for F is then taken as $\delta = \min_k \delta_k$.

In order to avoid solving each subproblem in (36) explicitly, the approach suggested by Swaney and Grossmann (1982) takes advantage of the fact that the δ_k value need only be determined for the critical, or worst-case, vertices. Since $\delta_k > \delta$ for those vertices which do not belong to the worst case set, two points may be noted for non-worst-case vertices: 1) The actual value δ_k is unimportant, and 2) The point $\theta = \theta^N + \delta(\Delta\theta)^k$ lies within the feasible region. Therefore, the worst-case set may be identified by testing vertices for feasibility at $\theta = \theta^N + \delta(\Delta\theta)^k$. A procedure may then be constructed wherein the subproblems in (36) for each vertex can usually be replaced by a much easier feasibility test. Basically, the vertices are searched in a sequence; feasibility of each vertex is checked at the point $\theta = \theta^N + \bar{\delta}(\Delta\theta)^k$ where $\bar{\delta}$ is the current upper bound on δ (based on δ_k for the vertices in the current estimate of the worst-case set). If the vertex is infeasible at $\bar{\delta}$, then the value of δ_k is obtained by solving (36), the vertex enters the worst-case set, and the bound $\bar{\delta}$ is updated. If the vertex is feasible at $\bar{\delta}$, the search proceeds to the next vertex.

A good initial estimate for the worst-case vertex direction may be obtained by determining at the nominal parameter θ^N the steepest-ascent direction of the feasibility measure $\psi(d,\theta)$. This would involve the following steps:

Step 1. Determine at θ^N the control z^N such that

$$\psi^N = \min_z u \quad \text{s.t. } u \geq f_j(d,\theta^N,z) \quad j \in J \tag{37}$$

Step 2. For small positive perturbations $\Delta\theta_i$, i=1,2,...p, along each i'th coordinate in the parameter space determine

$$\psi^i = \min_z u \tag{38}$$
$$\text{s.t. } u \geq f_j(d,z^N,\theta^N) + \frac{\partial f_j}{\partial z}(z-z^N) + \frac{\partial f_j}{\partial \theta}\Delta\theta_i \quad j\in J$$

Step 3. Select the vertex direction $\Delta\theta^*$ such that $(\Delta\psi)^T \Delta\theta^* > 0$, where $\Delta\psi^i = \psi^i - \psi^N$, i=1,2...p.

It should be noted that if $\psi(d,\theta)$ is monotonic in θ, the initial estimate will lead to the correct critical vertex for defining the flexibility index F. However, since the property of monotonicity cannot be expected to hold in general, feasibility must be checked for all the other vertices.

To establish feasibility at a given point θ requires only that <u>some</u> z be found for which $f(d,z,\theta) \leq 0$. The z value which solves equation (15) would be a sufficient choice, and a solution procedure applied to (15) will serve as an effective feasible point procedure. However, as was discussed in the algorithm for design under uncertainty it is in general not necessary to find an optimal solution for (15); any point z for which $u \leq 0$ will establish feasibility. The procedure may thus be halted as soon as the condition $u \leq 0$ is obtained, with the result that in many cases feasibility will be established with less work than would be required to solve (15) completely. Clearly, for infeasible vertices, termination with $u > 0$ will result.

Significant economy in performing the feasibility tests may be achieved by taking advantage of the fact that the same set of active constraints will apply to many vertices in the feasibility subproblems. By carefully ordering the sequence of vertex examination, the computational work required to locate a feasible z can be minimized. A heuristic procedure for vertex sequencing which provides an initial sequence, as well as an evolutionary re-ordering method has been developed and is described in Swaney and Grossmann (1982) who apply it to an example problem. It is also interesting to mention that this vertex enumeration procedure could be applied in Step 3 of the algorithm that was presented for design under uncertainty.

<u>A Bounding Procedure</u>

The rigorous evaluation of F requires that the location of the point(s) where the inscribed hypercube touches the boundary of the feasible region be determined. In the above procedure it was assumed that the critical points will lie at vertices of the hypercube, and that they could therefore be identified by searching among the set of all vertices. Unfortunately, if the number of parameters p becomes large the method can become expensive, since the number of vertices to be analyzed increases as 2^p.

The important question that arises, then, is whether a procedure can be derived for evaluating the flexibility index F which does not necessarily require analyzing all of the vertices in the parameter space. Provided one is willing to assume convexity in the feasible region, it is possible to derive a bounding procedure that can accomplish this objective. This bounding procedure is based on two observations. First, a valid upper bound on F is given by a hypercube centered at the origin which contains on at least one of its faces any point belonging to the boundary of the feasible region. Second, if convexity in the region is assumed, a lower bound may be obtained by determining the largest hypercube that can be inscribed in a polytope that is contained within the feasible region, and whose vertices lie on the boundary. This suggests the following procedure whose first three steps are depicted in Fig. 10:

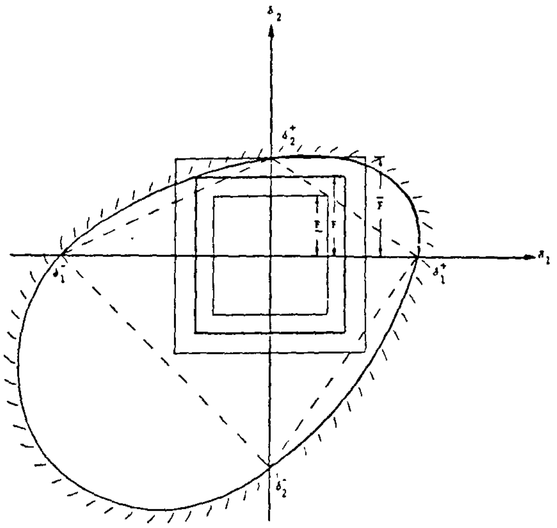


Fig. 10. Lower and upper bounds for maximum hypercube

Step 1. For a fixed value of d, the maximum positive and negative deviations for each parameter are obtained by solving the following 2p subproblems:

$$\max_{z} \ \delta_i^+$$

$$\text{s.t.} \quad f(d, z, \theta_1^N, \ldots, \theta_i^N + \delta_i^+ \Delta^+\theta_i, \ldots \theta_p) \le 0 \qquad i=1,\ldots p$$

$$\max_{z} \ \delta_i^- \tag{39}$$

$$\text{s.t.} \quad f(d, z, \theta_1^N, \ldots, \theta_i^N - \delta_i^- \Delta^-\theta_i, \ldots \theta_p) \le 0 \qquad i=1,\ldots p$$

Step 2. A valid upper bound $\bar{F}$ for the flexibility index is given by the smallest deviation obtained in step 1,

$$\bar{F} = \min_{i=1,\ldots p} \{\delta_i^+, \delta_i^-\} \tag{40}$$

Step 3. A lower bound $\underline{F}$ is obtained by determining the largest hypercube that is contained in the polytope defined by the deviations δ_i^+, δ_i^- $i=1,\ldots p$ obtained in step 1. This hypercube may be determined as follows:

a) For each parameter i calculate

$$a_i = \frac{1}{s_i \min(\delta_i^+, \delta_i^-)} \qquad i=1,\ldots p$$

$$\text{where} \quad s_i = \begin{cases} +1 & \text{if } \delta_i^+ \le \delta_i^- \\ -1 & \text{if } \delta_i^+ > \delta_i^- \end{cases} \tag{41}$$

which will define a vertex k taken in the directions s_i from the nominal point.

b) The equation $a^T\delta = 1$ then describes the hyperplane containing that face of the polytope which is closest to the nominal point (origin).

c) Solve for the lower bound $\underline{F}$ using $a^T\delta = 1$ by setting $\delta_i = \text{sign}(a_i)\underline{F}$.

Step 4. a) An improved upper bound $\bar{F}$ is obtained by solving (36) along the vertex direction which corresponds to the face of the current polytope that is closest to the origin (e.g. in the first iteration the direction is defined by (41)).

b) If $\bar{F} = \underline{F}$, or the bounds are within a specified tolerance, stop. Otherwise go to step 5.

Step 5. a) The polytope contained within the feasible region is expanded by incorporating the additional boundary point found in step 4.

b) The lower bound $\underline{F}$ is updated by inscribing the largest hypercube in the expanded polytope. Return to step 4.

It should be noted that this bounding procedure requires solving at least 2p + 1 optimization subproblems for determining the boundary points. Therefore, it is clear that potential computational gains can only be achieved if the number of parameters p, is strictly greater than two. Also, since there is no guarantee that for some cases (e.g. symmetric regions) all of the vertices will not have to be analyzed, the efficiency of this bounding procedure is unpredictable. Nevertheless, in a number of instances the procedure would require analyzing only a small number of vertices, and if the exact determination of F is not required it could still be a useful tool. Finally, since the assumption of convexity is crucial in establishing the validity of the lower bound, the vertex enumeration procedure presented in the previous section is of more general applicability.

Future directions. It is clear that the flexibility index defined above is only one possible choice. Although this index has the advantage of a meaningful physical interpretation, it might be worthwhile to explore other options which, for instance, do not require the definition of a nominal point. As for the solution procedures, more computational experience is required to test their effectiveness. Also, it would be particularly important to develop an efficient numerical procedure for solving the bicriterion optimization problem of minimizing cost and maximizing flexibility.

GENERAL REMARKS

This paper has attempted to present a unified approach for the problem of design of flexible chemical plants. As has been shown, this area offers a number of very interesting possibilities at both theoretical and practical levels.

On the theoretical side, the problems in flexibility give rise to optimization problems that involve large numbers of decision variables and/or an infinite number of constraints. The distinct feature of these optimization problems is that the major difficulty lies in the feasibility constraints, as opposed to the case where designs are optimized for a single nominal parameter value. It is clear that there is still much work required to derive efficient optimization strategies for solving the challenging problems that arise in flexible design. More research is required to improve the computational efficiency of the methods that have been described in the paper for multiperiod design, design under uncertainty and the flexibility index. Also more work is required to extend these methods, or develop new ones, for handling the nonconvex case. An avenue that is also worthwhile exploring for the development of strategies is the use of computer graphics which can yield interesting insights into the feasibility and movement of constraints (see Arkun and Stephanopoulos, 1979; Etzkorn and Arkun, 1982). It is interesting to note that in the field of electrical engineering very substantial progress has been made in problems related to flexibility, such as in the problem of design centering, tolerancing and tuning of electronic circuits (see Bandler, 1974; Bandler, Lui and Tromp, 1976; Brayton, Director, Hachtel and Vidigal, 1979; Director and Hachtel, 1977; Madsen and Schjaer-Jacobsen, 1978; Polak and Sangiovanni, 1979; Mayne, Polak and Voreadis, 1982). However, it should be noted that the nature of these problems is somewhat different from the ones encountered in chemical process design. The emphasis in the work in electrical engineering has been on manufacturing where the uncertainties arise in the design variables. Another crucial difference in these problems is that in most cases no control variables as considered in this paper are included.

On the practical side, the area of flexibility adds a new important dimension to the field of optimization of chemical processes. The reason is that since in this area the main concern is the feasibility of operation of the plant, there is the possibility of obtaining designs that are not only economically attractive, but perhaps more importantly, sufficiently robust to satisfy design specifications despite uncertainties in the parameter values. Since this would seem to be the overriding concern of design engineers (see Blau, 1981), it is expected that systematic procedures for flexible design could have an important impact in practice. Furthermore, it should be clear that the aim of these procedures is not only to determine rational overdesigns, but also to provide tools that can be used to help close the gap that currently exists between the activities of design and control of chemical plants. It is clear that before performing a detailed analysis on the dynamics and control of a process, it is first of all necessary to determine whether in fact feasible operation over a finite range of parameters can be attained with a proposed design. In principle these tools for flexible design could also be used to synthesize systematically flexible process flowsheets, although there is clearly much more research work required to accomplish this goal.

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