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Abstract

This paper addresses the problem of how to evaluate and optimize the probability of feasible operation for a design that is described by a nonlinear model. This property, which is denoted as the Stochastic Flexibility, represents the cumulative distribution over the feasible region in the space of the uncertain parameters. It is shown that the evaluation problem, which requires a sequence of optimization problems, can be formulated as a single nonlinear programming model which can be extended to design optimization problems for maximizing the stochastic flexibility subject to a cost constraint. A solution method based on Generalized Benders Decomposition is proposed to effectively solve this problem. A comparison with Taguchi's method for minimizing quadratic loss is also presented to point out that the use of a reward function can lead to more sensible designs. Finally, several process design examples are presented to illustrate the determination of trade-offs between cost and flexibility.

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1. Introduction

An inherent part in the design of a chemical process involves accounting for uncertainties. Uncertainties can be of two basic types: those that are characterized by continuous probability distributions (continuous uncertainties) and those characterized by discrete probability distributions (discrete uncertainties). Examples of the first type would include feed flowrates, rate constants and product demands. Equipment availability would be an example of an uncertainty characterized by a discrete distribution. Both types of uncertainties can have a significant impact on the feasibility of operation for a process.

Numerous methods have been developed to account for uncertainties. The most well known is reliability, which measures the probability that a process is available given only discrete uncertainties (see Dhillon 1984). When the process contains only continuous uncertainties, several different flexibility metrics have been developed which characterize the ability of a process to tolerate the uncertainties for feasible operation. Examples of these types of metrics can be found in Swaney and Grossmann (1985), Kubic and Stein (1988) and Straub and Grossmann (1990). The latter authors have proposed a measure known as the Stochastic Flexibility that corresponds to the probability of feasible operation, but whose solution has been restricted to linear systems. Until recently no work had been reported on systems containing both types of uncertainties, but Straub and Grossmann (1990) and Pistikopoulos et al. (1990) have developed a framework for their integration. While these metrics have been aimed at measuring capabilities for feasible operation, Taguchi methods in terms of quadratic penalties, have been aimed at measuring capabilities for consistent performance in the face of continuous parameter uncertainties. Furthermore, Taguchi concepts have emerged as a major design tool in many industrial applications.

The goal of this paper is twofold. The first is to develop solution methods for the Stochastic Flexibility (SF) metric for nonlinear systems. Methods for both evaluation and optimization will be presented. The secondary goal of the paper is to discuss the similarities and differences between the SF and Taguchi methods that are based on the quadratic loss function which have motivated the development of a new Taguchi metric in terms of a reward function. A number of different examples will be presented to illustrate the application of the proposed methods and their scope in the evaluation and optimization of systems design.

2. Review of Stochastic Flexibility

The stochastic flexibility, SF, is a probabilistic measure of a system's ability to tolerate continuous uncertainties. It is defined as the probability that a given design will operate feasibly. The concept of the stochastic flexibility is shown in Figure 1. The triangle represents the feasible region of operation for the system in the space of the continuous uncertainties, 0j and 02- Each of the continuous uncertainties is described by a probabilistic distribution. In this case, *Q* and 02 are independent parameters characterized by normal distributions, which gives rise to a joint distribution whose contours are circles. The stochastic flexibility is the cumulative probability of the joint distribution that lies within the feasible region; that is, the integral of the joint distribution over the shaded region.

The systems of interest are modeled mathematically with a set of equality and inequality constraints:

$$h(d,z,x,0)=O$$
$$g(d,z,x,0)<£O$$

These equations can be linear or nonlinear. The variables in these equations are classified as follows:

d	design variables that define the capacity or sizes of units
z	control variables representing degrees of freedom which can be adjusted to compensate for changes in 0
x	state variables
0	uncertain continuous parameters

In this model the continuous uncertain parameters 0_m (m=l,...,M) are characterized by a joint probability distribution function j(0). This distributions that compose j(0) may or may not be independent. Typical distributions include normal, uniform, and triangular. These distributions are modified with additional constraints, called sigma bounds to reflect the fact that after a certain point the cumulative probability exhibits negligible changes. For example, if 0 is characterized by a normal distribution, sigma bounds limiting the range of 0! from $0^{MIN}=0_1^{n0m}-3a$ to $0^{MAX}=0_1^{nom}+3a$ would be introduced, where Qf^{om} corresponds to the mean value of the parameter. These bounds prevent the integration over insignificant portions of the joint distribution. They also insure a closed feasible region which prevents difficulties with numerical integration schemes.

3. Evaluation and Optimization of SF for Nonlinear Systems

The fundamental idea of the proposed integration scheme of (1) is similar to the one described by Straub and Grossmann (1990). The integral for the SF will be represented as follows:

$$SF = \int_{Q_1} \int_{\theta_2(\theta_1)} \dots \int_{\theta_M^L(\theta_1,\theta_2,\dots,\theta_{M-1})}^{\theta_M^U(\theta_1,\theta_2,\dots,\theta_{M-1})} j(\theta)\, d\theta_M \dots d\theta_2 d\theta_1 \tag{1}$$

where θ_1^L, θ_1^U, $\theta_2^L(\theta_1)$, $\theta_2^U(\theta_1)$... describe the boundary of the feasible region.

For the sake of clarity in the presentation, we will restrict ourselves to two-dimensional problems, since the extension of the proposed ideas to higher dimensions is straightforward. As shown in Figure 2, lower and upper bounds θ_1^L, θ_1^U on θ_1 are determined first. Quadrature points θ_1^{q1} are then generated for a fixed choice of Q1 nodes, q1=1,...Q1.

The next step is then to determine lower and upper bounds θ_2^{Lq1} θ_2^{Uq1} for θ_2 at each point θ_1^{q1}. Finally, quadrature points θ_2^{q1q2} are generated in θ_2 space for a fixed choice of Q2 nodes, with which one can then apply a Gaussian quadrature formula (see eqn. (3) below) to estimate the multiple integral. Figure 2 shows how the placement of the quadrature points might appear in a two dimensional case. Note that all the quadrature points are located within the feasible region. Because of this feature the quadrature scheme has proven to be very accurate.

4. Sequential Approach

For fixed design d, the simplest approach to determine the bounds described above is to solve a sequence of optimization problems. Again, for clarity in presentation only the inequality constraints over a two dimensional parameter space will be shown in the equations below. The sequence of optimization problems is as follows. First, the lower and upper bounds of Q_x are given by,

$$\theta_1^L = \arg\left[\min\ \theta_1 \mid g(d,z,x,\theta_1,\theta_2) \le 0\right\} \quad \theta_1^U = \arg\left\{\max\ \theta_1 \ g(d,z,x,\theta_1,\theta_2) \le 0\right\} \tag{2a}$$

The quadrature points in Q_x space are then determined from

$$e_1^{ql}= 0.5\ [eV\ o+vf)+ eV\ a\text{-}v?^1)\ ] \qquad qi=i,...Qi \qquad (2b)$$

where the $v^{\wedge 1}$ correspond to the location of the quadrature points in the [-1,1] interval (see Carnahan et al. 1969). The lower and upper bounds of 8_2 at each quadrature point can then be obtained as follows,

$$\theta_2^{Lqi}\text{-arg}\left\{ \min\ 62!\ \ g(d,z,x,6_1^{ql},e_2)\leq 0 \right\} \qquad qi=l,...Qi$$

$$6_2^{Uql}=\text{arg}\ \{ \max\ 6_2|\ \ g(d,z,x,\theta^{ql},e_2)\leq 0 \} \qquad qi=l,...Qi \qquad (2c)$$

Having the bounds on 6_2, the quadrature points in 8_2 are determined as follows:

$$6?^{qz}= 0.5\ [<\#*\ (l+vjO+ eV^{qi}\ d\text{-}v5^2)\ ] \qquad qi\text{-}l....Qi \quad q_2=l,...Q_2 \qquad (2d)$$

Finally, the estimation of the SF is given by,

$$SF=\frac{\theta_1^U-\theta_1^L}{2} \sum_{q1=1}^{Q1} w_1^{q1} \frac{(\theta_2^{U\,q1}-\theta_2^{L\,q1})}{2} \sum_{q2=1}^{Q2} w_2^{q2}\ j\,(\theta_1^{q1},\theta_2^{q1,q2}) \qquad (3)$$

where $w^{\wedge 1}$, w_2^{q2} are the weights corresponding to each quadrature point (see Carnahan et al-1969). It should be noted that the above equations can be readily generalized to higher dimensions of the parameter space 0.

For the linear case the problem of solving the $2(1+QP_1(1+QP_2(...\text{-}(1+QP_{M-1}))))$ optimization problems in (2a),(2b) and (2c) was circumvented by Straub and Grossmann (1990) by using an inequality reduction scheme in which constraints are successively projected into lower dimensions of the uncertain parameters, with which bounds and quadrature points can be computed analytically. While this is an elegant scheme, it has two drawbacks: first it is limited to a modest number of constraints as it relies on identification of active sets; secondly, it cannot be easily extended to the optimization of the design variables d. Also, extending the inequality reduction scheme to nonlinear constraints is not straightforward. Therefore, a simultaneous approach that embeds the equations of (2) into a single optimization problem will be considered.

5. Embedded Approach

We can implicitly embed the sequential optimizations in (2), and the evaluation of the SF as given in (3), into one single the NLP model in which the bounds and quadrature points are selected to maximize the SF. The formulation is given by:

$$
\begin{aligned}
\max\ SF = {} & \frac{\theta_1^U-\theta_1^L}{2}\sum_{q1=1}^{Q1} w_1^{q1}\frac{(\theta_2^{U\,q1}-\theta_2^{L\,q1})}{2}\sum_{q2=1}^{Q2} w_2^{q2}\, j\,(\theta_1^{q1},\theta_2^{q1,q2}) \\
\text{s.t.}\quad & g_1^L(d,z^{(\cdot)},x^{(\cdot)},\theta_1^L,\theta_2^{(\cdot)})\le 0 \\
& g_1^U(d,z^{(\cdot)},x^{(\cdot)},\theta_1^U,\theta_2^{(\cdot)})\le 0 \\
& \theta_1^{q1}=0.5\,[\theta_1^U(1+v_1^{q1})+\theta_1^L(1-v_1^{q1})] \qquad q_1=1,\dots Q_1 \\
& g_2^{L\,q1}(d,z^{(\cdot)},x^{(\cdot)},\theta_1^{q1},\theta_2^{L\,q1})\le 0 \qquad q_1=1,\dots Q_1 \\
& g_2^{U\,q1}(d,z^{(\cdot)},x^{(\cdot)},\theta_1^{q1},\theta_2^{U\,q1})\le 0 \qquad q_1=1,\dots Q_1 \\
& \theta_2^{q1\,q2}=0.5\,[\theta_2^{U\,q1}(1+v_2^{q2})+\theta_2^{L\,q1}(1-v_2^{q2})] \qquad q_1=1,\dots Q_1\ \ q_2=1,\dots Q_2 \\
& \theta_1^{MIN}\le\theta_1^L\le\theta_1^U\le\theta_1^{MAX} \\
& \theta_2^{MIN}\le\theta_2^{L\,q1}\le\theta_2^{U\,q1}\le\theta_2^{MAX} \qquad q_1=1,\dots Q_1 \\
& \theta_2^{MIN}\le\theta_2^{(\cdot)}\le\theta_2^{MAX}
\end{aligned}
\qquad \text{(NLP1)}
$$

In (NLP1) the notation $z^{(\cdot)}, x^{(\cdot)}, \theta_2^{(\cdot)}$, denotes variables that are associated with each set of constraints since they must be chosen independently to determine the lower and upper bounds θ_1^L, θ_1^U, and $\theta_2^{L\,q1}$, $\theta_2^{U\,q1}$, $q_1=1,\dots Q_1$. For instance, in the first two constraints different z, x, and θ_2 values must be chosen for determining the bounds θ_1^L and θ_1^U. Also note that in (NLP1), θ_i^{MIN} and θ_i^{MAX} correspond to the sigma bounds that limit the range of the distributions.

As shown in the Appendix A, the sequential optimization and calculation of the quadrature points (2) are equivalent to (NLP1) provided a sufficiently large number of quadrature points is selected. Qualitatively the idea is that for a sufficient number of quadrature points, the bounds θ_1^L, θ_1^U, and $\theta_2^{L\,q1}$, $\theta_2^{U\,q1}$, $q_1=1,\dots Q_1$ will be placed on the boundary of the feasible space so as to evaluate the approximation of the integral for the SF. Although problem (NLP1) is potentially large in size, it has two attractive features. The most significant is that (NLP1) can easily be extended to design optimization problems in which the design variables are selected to maximize SF subject to an upper limit **a** of a cost function, cost(d), over a set D for the design variables. This is shown in (NLP2).

$$
\begin{aligned}
\max\ SF = {} & \frac{\theta_1^U - \theta_1^L}{2} \sum_{q1=1}^{Q1} w_1^{q1} \frac{(\theta_2^{U\,q1} - \theta_2^{L\,q1})}{2} \sum_{q2=1}^{Q2} w_2^{q2}\, j(\theta_1^{q1}, \theta_2^{q1,q2}) \\
\text{s.t.}\quad & g_1^L(d, z^{(\cdot)}, x^{(\cdot)}, \theta_1^L, \theta_2^{(\cdot)}) \le 0 \\
& g_1^U(d, z^{(\cdot)}, x^{(\cdot)}, \theta_1^U, \theta_2^{(\cdot)}) \le 0 \\
& \theta_1^{q1} = 0.5\,[\theta_1^U (1+v_1^{q1}) + \theta_1^L (1-v_1^{q1})] \qquad q_1=1,\ldots Q_1 \\
& g_2^{L\,q1}(d, z^{(\cdot)}, x^{(\cdot)}, \theta_1^{q1}, \theta_2^{L\,q1}) \le 0 \qquad q_1=1,\ldots Q_1 \\
& g_2^{U\,q1}(d, z^{(\cdot)}, x^{(\cdot)}, \theta_1^{q1}, \theta_2^{U\,q1}) \le 0 \qquad q_1=1,\ldots Q_1 \\
& \theta_2^{q1\,q2} = 0.5\,[\theta_2^{U\,q1} (1+v_2^{q2}) + \theta_2^{L\,q1} (1-v_2^{q2})] \qquad q_1=1,\ldots Q_1 \quad q_2=1,\ldots Q_2 \\
& \mathrm{cost}(d) \le \alpha \\
& \theta_1^{MIN} \le \theta_1^L \le \theta_1^U \le \theta_1^{MAX} \\
& \theta_2^{MIN} \le \theta_2^{L\,q1} \le \theta_2^{U\,q1} \le \theta_2^{MAX} \qquad q_1=1,\ldots Q_1 \\
& \theta_2^{MIN} \le \theta_2^{(\cdot)} \le \theta_2^{MAX} \\
& d \in D
\end{aligned}
\qquad \text{(NLP2)}
$$

The second feature of (NLP1) is that it provides a single model for evaluating the SF, although there is a trade-off between solving one large NLP or a sequence of $2(1+QP_1(1+QP_2(\ldots(1+QP_M.i))))$ smaller NLP's. Finally, also note that by solving (NLP1) one can determine sensitivity information for the design variables. That is,

$$
\frac{\partial SF}{\partial d} = \sum_k \frac{\partial SF}{\partial g_k} \frac{\partial g_k}{\partial d} = \sum_k \lambda_k \frac{\partial g_k}{\partial d} \qquad (4)
$$

where λ_k are the Kuhn-Tucker multipliers of (NLP1), assuming the Lagrangian is written as the objective function minus the constraint terms.

6. Remarks

With regard to the application of the sequential optimizations in (2) or (NLP1) to nonlinear feasible regions, several points can be made. First, if the region is convex then the method will place all of the quadrature points inside the feasible region. This is important since the quadrature scheme is then an appropriate approximation to (1). When the region is nonconvex the quadrature scheme will still approximate (1) correctly if the feasible region is 1-d convex in each parameter θ_M m=1,...M (see Swaney and Grossmann, 1985; and Figure 2). On the other hand, if this is not true, then the quadrature scheme may or may not correctly integrate over the feasible region. In this case portions of the feasible region may be excluded from the integral while portions of the infeasible region may be included. It should be noted that the problem with nonconvex regions is less important the larger the SF is. When the SF is large we are essentially integrating over the region bounded by the distribution constraints, not the system bounds. Thus, in this case, the influence of nonconvexities is small.

There are several ways to reduce the complexity of the integration scheme to evaluate and optimize the SF. These include modifications to the integration method and also the solution techniques for the NLP problem. The simplest technique is to determine if an uncertain parameter is bounded on only one side. For example, if the activation energy in an adiabatic CSTR is uncertain, decreases from the nominal value will not cause infeasibilities in many cases. Thus, in the formulations (NLP1) and (NLP2) the lower bound on the activation energy can be fixed to the value of the corresponding distribution constraint instead of being a variable in the NLP. Obviously it is to our advantage to place the uncertainties with fixed bounds last in the integration scheme, since this will have the largest effect on the size reduction.

Another simple change is to integrate apriori over one parameter 6_M (last uncertain parameter) and write the cumulative distribution, $F(0_M^L\ 0M^UX$ as a function of the bounds. This eliminates the need for quadrature points in 0_M space, further reducing the size of the NLP. In the two-dimensional case the objective takes the following form with this modification:

$$\max SF = \frac{\theta_1^U - \theta_1^L}{2} \sum_{Q''}^{Q1} w_1^{q1}\ j(\theta_1^{q1})\, F(\theta_2^{L\,q1}, \theta_2^{U\,q1}) \tag{5}$$

Note that this simplification assumes that 0_M is independent of 0I,...6M-I- Finally, even with the above provisions, problems (NLP1) and (NLP2) may become very large. The next section addresses this issue for the design optimization problem (NLP2).

7. A Benders Decomposition Procedure

As discussed earlier, one of the advantages of the nonlinear programming formulation in (NLP1) is that the evaluation problem can be embedded into a single NLP. This allows us to easily extend the evaluation problem to a design optimization problem given by (NLP2). This NLP though, may become too large to solve in a reasonable amount of time. In order to be able to solve these larger problems we propose a computational scheme based on Generalized Benders decomposition.

The basic idea behind Benders decomposition (Geoffrion 1972) is to partition the variables into two sets: complicating and non-complicating variables. By fixing the former, the problem yields a subproblem whose solution yields a lower bound (maximization case); the complicating variables are then updated with a master problem that accumulates Lagrangian approximations of previous iterations and whose solution yields an upper bound. This upper bound decreases monotonically as the sequence of iterations proceeds. The procedure is then to repeatedly solve the subproblems and master problems until the lower and upper bounds converge within a specified tolerance. It will be assumed here that the reader is familiar with the details of Generalized Benders decomposition. A recent review can be found in Sahinidis and Grossmann (1991).

In applying Benders decomposition to (NLP2) we designate the design variables d to be the complicating variables. The subproblem then corresponds to problem (NLP1), and the master problem is defined in terms of the design variables d. Although this decomposes the problem somewhat, we are still left with a large NLP in the subproblem. The way around this is to decompose this subproblem into a sequence of NLFs similar to (2). Each of these NLP's is significantly smaller than NLP1. For reasons that will become apparent, it is convenient to determine the lower and upper bounds for each 6 with a single NLP. That is for 8j, instead of obtaining the bounds from

$$9V\text{=arg} \{ \min 8i \mid g(d,z,x,9i,92)\leq 0 \} \quad 9i^{U}\text{=arg} \{ \max 9i \mid g(d,z,x,9i,92)\leq 0 \} \tag{2a}$$

we solve the NLP problem:

$$\begin{aligned} \max \quad & eF\text{-}e\}\text{-} \\ \text{s.t.} \quad & g_1^L(d,z^{(\cdot)},x^{(\cdot)},\theta_1^L,\theta_2^{(\cdot)})\leq 0 \\ & g_1^U(d,z^{(\cdot} \\ & \theta r \leq \theta \leq \theta \leq \theta^{c} \\ & 0_2^{MIN}\leq e£^{)}\leq e2^{MAX} \end{aligned} \tag{NLP3}$$

It is easy to show that the Kuhn-Tucker conditions for (NLP3) are identical to the combined Kuhn-Tucker conditions for (2a). We can proceed in a similar manner for finding the lower and upper bounds for $9\wedge^{1}$ qx=l,...Qi. The subproblem then consists of sequentially solving the following NLPs for a fixed d^k,

1) Solve (NLP3) for $d=d^k$.

2) For qi=l,...Qi, solve

$$\begin{aligned} &\max\ (\theta_2^{U\,q1} - \theta_2^{L\,q1}) \\ &\text{s.t}\quad g_1^{q1}(d^k,z(\cdot),x(\cdot),\theta_1^{q1},\theta_2^{L\,q1}) \le 0 \\ &\qquad g_2^{U\,q1}(d^k,z(\cdot),x(\cdot),\theta_1^{q1},\theta_2^{U\,q1}) \le 0 \\ &\qquad \theta_2^{MIN} \le \theta_2^{L\,q1} \le \theta_2^{U\,q1} \le \theta_2^{MAX} \end{aligned} \tag{NLP4}$$

Based on the results of these two steps, the lower bound for the SF_L, corresponding to d^k, can be calculated using equation (3). Having solved the problems in (NLP3) and (NLP4) the master problem can be formulated. However, the multipliers %, of these problems do not correspond to the ones for problem (NLPl) for the fixed *dK* For instance, the vector of multipliers for the first constraint in (NLP3) correspond to ^' = d(8₁ᵘ-8₁ᴸ)/9giᴸf while the vector of multipliers for the first constraint in (NLPl) correspond to A^^SF/dgxk The two multipliers can easily be related with the following correction factors obtained by comparing the Kuhn-Tucker conditions of (NLPl) and (NLP3), (see Appendix B):

$$CF_1^L = \frac{1}{2}\sum_{q1=1}^{Q1} w_1^{q1}\frac{(\theta_2^{U\,q1}-\theta_2^{L\,q1})}{2}\sum_{q2=1}^{Q2} w_2^{q2}\, j(\theta_1^{q1},\theta_2^{q1,q2})$$
$$+\sum_{q1}\left\{\frac{\theta_1^U-\theta_1^L}{2} w_1^{q1}\frac{(\theta_2^{U\,q1}-\theta_2^{L\,q1})}{2}\sum_{q2=1}^{Q2} w_2^{q2}\frac{\partial j(\theta_1^{q1},\theta_2^{q1,q2})}{\partial\theta_1^{q1}} - \lambda_2^{L\,q1}\frac{\partial g_2^{L\,q1}}{\partial\theta_1^{q1}} - \lambda_2^{U\,q1}\frac{\partial g_2^{U\,q1}}{\partial\theta_1^{q1}}\right\}((-1/2)(1-v_1^{q1}))$$

(6a)

$$CF_1^U = \frac{1}{2}\sum_{q1=1} w_1^{q1}\frac{(\theta_2^{U\,q1}-\theta_2^{L\,q1})}{2}\sum_{q2=1}^{Q2} w_2^{q2}\, j(\theta_1^{q1},\theta_2^{q1,q2})$$
$$-\sum_{q1}\left\{\frac{\theta_1^U-\theta_1^L}{2} w_1^{q1}\frac{(\theta_2^{U\,q1}-\theta_2^{L\,q1})}{2}\sum_{q2=1}^{Q2} w_2^{q2}\frac{\partial j(\theta_1^{q1},\theta_2^{q1,q2})}{\partial\theta_1^{q1}} - \lambda_2^{L\,q1}\frac{\partial g_2^{L\,q1}}{\partial\theta_1^{q1}} - \lambda_2^{U\,q1}\frac{\partial g_2^{U\,q1}}{\partial\theta_1^{q1}}\right\}((-1/2)(1+v_1^{q1}))$$

(6b)

Hence, for problem (NLP3), the corrected multipliers for the two constraints are

$$\lambda_1^L = CF_1^L\,\hat{\lambda}_1^L,\qquad \lambda_1^U = CF_1^U\,\hat{\lambda}_1^U. \tag{7}$$

Similarly in relating the problems in (NLP4) with (NLPl), the corrected multipliers are given by

λ^ ' ‡Cl ¹ ^ ¹ ¹ ¹ , λ₂U I ='C^ ¹ * ^ ¹ ql=l,...Ql. **(8)**

where

$$CF_2^{L\,q1} = \frac{\theta_1^U-\theta_1^L}{2} w_1^{q1} \left(\frac{1}{2}\right) \sum_{q2=1}^{Q2} w_2^{q2}\, j(\theta_1^{q1}, \theta_2^{q1,q2})$$
$$+\sum_{q2} \left\{ \frac{\theta_1^U-\theta_1^L}{2} w_1^{q1} \frac{(\theta_2^{U\,q1} - \theta_2^{L\,q1})}{2} w_2^{q2} \frac{\partial j(\theta_1^{q1}, \theta_2^{q1,q2})}{\partial \theta_2^{q1,q2}} \right\} (-1/2)(1-v_2^{q2}) \qquad q1=1,\dots Q1 \qquad (9a)$$

$$CF_2^{U\,q1} = \frac{\theta_1^U-\theta_1^L}{2} w_1^{q1} \left(\frac{1}{2}\right) \sum_{q2=1}^{Q2} w_2^{q2}\, j(\theta_1^{q1}, \theta_2^{q1,q2})$$
$$-\sum_{q2} \left\{ \frac{\theta_1^U-\theta_1^L}{2} w_1^{q1} \frac{(\theta_2^{U\,q1} - \theta_2^{L\,q1})}{2} w_2^{q2} \frac{\partial j(\theta_1^{q1}, \theta_2^{q1,q2})}{\partial \theta_2^{q1,q2}} \right\} (-1/2)(1+v_2^{q2}) \qquad q1=1,\dots Q1 \qquad (9b)$$

Given different values of the design variables d^k, k=l,...K, that yield a corresponding stochastic flexibility SI* k=l,...K, one can then define the master problem as follows:

$$SF_B^K = \max_{d} \beta_B$$
$$\text{s.t. } \beta_B \le SF^k - (\lambda_1^L)^k g_1^L(d,u_1^{Lk}) - (\lambda_1^U)^k g_1^U(d,u_1^{Uk}) - \sum_{q1=1}^{Q1} \left[(\lambda_2^{L\,q1})^k g_2^{L\,q1}(d,u_2^{Lq1k}) + (\lambda_2^{U\,q1})^k g_2^{U\,q1}(d,u_2^{Uq1k}) \right] \qquad k=1,\dots K$$
$$\text{cost}(d) \le a$$
$$d \in D \quad \beta_B \in \Re^1$$

(NLP5)

where SF_B^K is the predicted upper bound and u_1^{Lk}, u_1^{Uk}, $U2^{L<}i^{lk}$ and $U2^{U(*lk}$ correspond to the optimal values of z,x and 0 in the subproblems (NLP3) and (NLP4) for a given design d^k. It should be noted that SF_B^K is only guaranteed to be a rigorous upper bound if the inequalities g(0 are convex and the integral in (1) is quasi-concave (see Geoffrion, 1972). Also, note that (NLP5) reduces to an LP if the design variables d appear in linear form in the constraints.

Summarizing, the steps involved in the Benders decomposition scheme are as follows:

1) Select an initial design d^1. Set the lower bound SF_L=-©°, K=l, and select a tolerance e.

2a) Solve (NLP3) to obtain 0_X^L, 0 ^. *ftf* and *ftf* and calculate e ^ ^{1}, ql=l,...Ql with (2b).

2b) For ql=l,...Ql, solve (NLP4) to obtain G^1, Q_2^{Vql}> A^1. $A?^1$ and calculate $e_2*^{1}*^{2}$ with (4.2d).

2c) Calculate SF with (3) and update the lower bound, SF_L=max{SF,SF_L}

3a) Calculate CF^1, CF^1 ql=l,...Ql and CF*f, CF^ as in (9) and (6) to obtain the contacted multipliers \\, Xp and X^\ X^{ql}_2 for ql=l,...Ql as in (7) and (8).

3b) Solve the master problem in (NLP5) to obtain a new design d^{K+1} and an upper bound SF_B^K.

4) If SF_B^K£SF_L+e, stop; the solution is the design d^K with stochastic flexibility SF_L. Otherwise, set K=K+1 and return to step 2.

It should be noted that in the above procedure it is assumed that the NLP subproblems in step 2 are feasible. In our experience we have not found computational difficulties with infeasibilities provided the initial design d^1 has a non-empty feasible region. Furthermore, we have also found that the number of major iterations is quite modest (typically 3 to 7 iterations). We attribute this to the fact that most of the inequalities in (NLP3) and (NLP4) are always active by which the Lagrangians in the master problem yield good approximations. Also note that the programs solved in the subproblem are nearly identical. This is significant because the information generated during the solution of the first NLP is used to aid in the solution of the second NLP, and so on. This helps to reduce the total CPU time necessary to perform each subproblem.

In practice the correction factors are occasionally negative. This is the result of roundoff errors in the large number of numeric computations required to calculate the correction factors. Based on our experience, the magnitude of the negative correction factors are much smaller than the magnitude of the positive correction factors, thus, the optimal solutions are not effected.

A Small Design Optimization Problem

A small example will be presented to illustrate the proposed method. The system is given by 3 inequality constraints and a cost constraint involving two uncertain parameters 9_1,0_2 and two design variables d_x and d_2:

•g^-3-djSO **(10a)**

g_2=25-$d_r e_1$*e_2≤0 (10b)

g_3=e_2-d_2*(i-exp(-e_1))≤o (ioc)

cost(d)=d!+d_2≤16 (lOd)

The uncertain parameters are assumed to be described by normal distribution functions; N(6,1.5) for B_x and N(6,l) for 6_2. The goal of this problem is determine the values of d_x and d_2 that maximize the stochastic flexibility subject to the cost constraint in (lOd).

Two different solution techniques were used to solve the problem with 5 point quadrature for each parameter (Ql=5, Q2=5). The initial point selected for the design variables was dj=7, d_2=7. The first technique was to directly solve the model in (NLP2), that is the entire problem embedded as a single NLR This NLP has 64 equations and 47 variables and required 2.23 CPU seconds on an IBM RS/6000 using GAMS/MINOS, The optimal solution was d ^ . 0 9 d_2=8.91 resulting in SF=0.968. The feasible regions for the initial and final designs are shown in Figures 3 and 4.

The problem was also formulated using the Benders decomposition scheme described in the previous section. Here the subproblems in step 2 involved solving 6 NLFs. The first NLP (NLP3) has 7 equations (a feasibility constraint requiring $Q_l^L \leq 9_1^v$ and (10a) (10b) (10c) repeated for both the lower and upper bounds) and 4 variables ($0J^1$-, 6 ^, $6_2^{\#1}$,$6_2^{\#2}$) The remaining 5 NLFs (NLP4) each had 5 equations (feasibility and (10b) (10c) repeated for both the lower and upper bounds) and 2 variables ($6_2^{Lc*1}0_2^{U<*1}$). The master problem, containing (K+l) constraints and 3 variables, was an LP since the constraints are linear in d for fixed 0. The modified Benders scheme required 7 major iterations to reach the optimal solution within a tolerance of 0.0001 for the lower and upper bounds. The convergence of the bounds is shown in Figure 5. The subproblems required a total of 3.30 CPU seconds and the master 0.46 CPU seconds for a total of 3.76 CPU seconds. The optimal solution was essentially the same as the full NLP. In this small example no computational savings were obtained. As will be shown later in the paper in Example 2 this trend is reversed in larger problems.

8. Taguchi Quadratic Penalty Methods

The purpose of this section of the paper is to demonstrate how Taguchi's design method based on quadratic loss functions can be accommodated with the methods presented in this paper, and how the resulting method compares with the SF. The fundamental element of Taguchi's methods is the quadratic loss function that penalizes deviations from targets under conditions of uncertainty. In practice, signal-to-noise ratios are used to determine the optimal design variables to minimize the effect of uncertainty (Kackar, 1985). The relationship between the signal-to-noise ratios and the quadratic penalty function has been established by Leon et al. (1987)- The relationship is exact under special circumstances, that is when the system model is of the following form:

$$x=f_1(d,z)*f_2(d,9) \tag{11}$$

We now wish to proceed in the direction of directly applying the quadratic penalty to design problems. We will refer to the resulting metric as the the Taguchi metric (TG).

In the context of the process model given described by the equality and inequality constraints, the Taguchi design approach associates a penalty with one of the state variables x. Other penalties associated with the inequality constraints are not considered. The allowable penalties on the single x variable take one of the three forms shown below:

a) A target value is desired for x, $x=x^T$which leads to the penalty $c'\wedge x-x^1)^2$.
b) The smallest possible value is desired for x, in terms of upper bounds, $x\leq x^u$
which leads to the penalty $c^u(x/x^u)^2$.
c) The largest possible value is desired for x, in terms of lower bounds, $x\geq x^L$
which leads to the penalty $cKx^L/x)^2$.

where c^T, c^u and c^L are specified cost coefficients. The above is rather restrictive if there are several output variables of interest, or if we wish to impose penalties on the values of other variables or combinations of variables. In most design problems we will often require multiple penalties and also satisfaction of the inequality constraints. In order to allow for multiple penalties we can simply redefine the penalties shown above as follows:

a) $q^T(Xj-x\wedge for xpx\wedge$ i € T
b) $c_i^u(x_i/x_i^u)^2$.for $Xi\leq Xi^U$ i *e* U.
c) $c\wedge Cx\wedge/Xj)^2$ for $Xi\geq Xj^L$ i € L.

where q^7 q^u and q^L are cost coefficients. The overall penalty can then be defined as follows:

$$P(x)=\sum_{ieT} c?(xi-x?)^2+\sum_{ieU} cF(xi/xP)^2 \sum_{ieL} c_i^L(x_i^L/x_i)^2 \tag{12}$$

Penalties can, of course, be defined with other norms as discussed in Feldmann and Director (1991).

The goal in the design problem is to minimize the expected value of this penalty, the TGP metric, which takes the form shown below

$$TGP=\int_{\theta_1^{MIN}}^{\theta_1^{MAX}} \cdots\int_{\theta_M^{MIN}}^{\theta_M^{MAX}} P(x(G))\ j(i\theta)\ d\theta_M....d\theta_2\, d\theta_1 \tag{13}$$

where x(6) is determined by the equality constraints and 0^{MIN} and G^{MAX} represent the limits of the distribution values or sigma bounds. While (13) allows us to have multiple penalties on the state variables it does not allow penalties involving inequality constraints in terms of d,z,6. One way to handle this is to treat these inequalities constraints as soft constraints; that is we introduce the non-negative variable y such that

$$g(d,z,x,9)\leq y \tag{14}$$

One could then include a penalty for 7>0 in (12). While this may be appropriate for some problems, in others the inequalities need to be hard constraints, strictly less than or equal to zero. This would involve an infinite penalty for y>0 if we were to penalize violations in a manner similar to the soft constraints A rigorous way to impose these constraints is to have them restrict the bounds on the variables, similar to the SF formulation in (1); that is,

$$TGP=\int_{\theta_1^L}^{\theta_1^U}\int_{\theta_2^L(\theta_1)}^{\theta_2^U(\theta_1)} \cdots\int_{\theta_M^L(\theta_1,\theta_2,\ldots,\theta_{M-1})}^{\theta_M^U(\theta_1,\theta_2,\ldots,\theta_{M-1})} P(x(0))\ j(0)\ d0M....d02\ dGi \tag{15}$$

where the lower and upper bounds are defined by the feasible region exactly as in the SF case, see (2). The problem with (15) is that it may assign zero quadratic penalty to 0 that lie outside the feasible region. Since both choices, infinite penalty or zero penalty are not acceptable we have to modify the formulation. The easiest way to do this is to create a reward function as shown below

$$R(x)=C-P(x) \tag{16}$$

where C must be sufficiently large such that R(x)≥0 V d G D. The objective of the design formulation is now given by

$$TGR=\int^{\theta_1^U}\int^{\theta_2^U(\theta_1)} \cdots\int_{\theta_M^L(\theta_1,\theta_2,\ldots,\theta_{M-1})}^{\theta_M^U(\theta_1,\theta_2,\ldots,\theta_{M-1})} R(x(6))\ j(6)\ d0M....dG2\ d0i \tag{17}$$

Naturally **the** metric is dependent on the choice of C. However, this formulation is more appropriate **and** can be easily accommodated in the model (NLP1) for evaluation and model (NLP2) for optimization. Furthermore, a Benders decomposition scheme can also be **applied that** is virtually identical to **the** one for the SF metric. In the next section a small example will be presented to clarify the points of the this section and to show how (13) and (17) relate to the SF metric.

9. Example with TG and SF Metrics

In order to understand the relationship between the SF and TG metrics consider the following system which is described by **the** following equation and inequality:

$$x-d_2-d_1\theta = 0 \tag{18}$$

$$40 \leq 5d_r d_2+58 \tag{19}$$

where d_x and d_2 are the design variables, x is the state variable and 6 is the uncertain parameter characterized by a uniform distribution between $9^{MIN}=7$ and $G^{MAX}=13$. Note that in this case there are no control variables. Also, (18) is the equation that describes the system while (19) is a hard constraint that must be satisfied by the chosen design.

Let us assume that the state variable x must lie within specified limits $x^{LO}=15$ and $x^{up}=20$, but that ideally the design should be such that x be as close as possible to a target value of 18; that is $x^T=18$.

In the case of the SF metric, the goal is to choose d_x and d_2 such that the probability that the state x lies within the specified limits $[x^{10}, x^{up}]$ is maximized. By solving (18) for 0^L and G^u in terms of x^{1}-^{0} and x^{up}, the feasible region in 8 space as a function of dj and d_2 can be expressed as,

$$\theta^L \geq (x^{LO}-d_2)/d_1 \tag{20a}$$

$$\theta^U \leq (x^{UP}-d_2)/d_1 \tag{20b}$$

$$\theta^U \leq 1.25d_1 -0.25d_2 +14.5 \tag{20c}$$

$$\theta^{MIN} \leq \theta^L \leq \theta^U \leq \theta^{MAX} \tag{20d}$$

The SF of the design (dj,d_2) is simply the integral of the distribution on 0, $j(0)=1/(0^{max}-0^{min})$, over the feasible region defined by $[0^L> 0^U]$,

$$SF=\int_{\theta^L}^{\theta^U} j(\theta)\, d\theta = \frac{(Q''-e^L)}{(\theta^{MAX}-\theta^{MII}}, \tag{21}$$

where 8^L and 6^U are determined by the constraints in (20). The problem of selecting dj and d_2 to maximize (21) is then given by the following NLP problem that is similar to (NLP1),

$$\begin{aligned}
\max\ & SF=(\theta^U-\theta^L)/(\theta^{MAX}-\theta^{MIN}) \\
\text{s.t.}\ & \theta^L \geq (x^{LO}-d_2)/d_1 \\
& \theta^U \leq (x^{UP}-d_2)/d_1 \\
& 9^U £1.25\ di - 0.25\ d2 + 14.5 \\
& d_1, d_2 \geq 0 \quad e^{MIN} < e^l \wedge e^u < e^{MAX}
\end{aligned} \tag{NLP6}$$

Solving the above NLP, leads to the solution d^O.8 d_2=9,4 with SF=1, which implies that this design can meet the specification $15 \leq x \leq 20$ for all 0 in $7 \leq 0 \leq 13$. The physical meaning is best demonstrated with Figure 6, Here the horizontal axis represents the space 0, while the vertical axis represents the space x. Equation (4.18) represents a line whose slope is the design variable *d* and whose intercept is the design variable d_2. Equation (4.19) represents a constraint in 0 space, as dj decreases and d_2 increases the constraint cuts off more of the 0 space. This figure also clearly demonstrates the concept of projecting the uncertainties from 0 space into the space of x. For a particular 0 go along the vertical axis until the line defined by (4.18) is reached, then go left horizontally to determine the corresponding x. With regard to the SF, as shown in Figure 6 with d ^ . 8 and d_2=9.4, the best design that can be obtained according the the SF metric, the entire distribution of 0 is projected into the feasible space of x. However the distribution on x is widely scattered with $\bar{x}$=17.5 and a=2.08.

Alternatively, consider the Taguchi metric with the quadratic penalty loss, which can be written as,

$$(x-xT)2=(d_2+d_1 0-xT)2 \tag{22}$$

Thus, from (13), the Taguchi metric is the expected value of the loss or,

$$TGP=\int_{-\infty}^{\infty} (d_2+d_1\theta-x^T)^2 j(\theta)\, d\theta = \frac{1}{\theta^{MAX}-\theta^{MIN}}\int_{\theta^{MIN}}^{\theta^{MAX}} (d_2+d_1\theta-x^T)^2\, d\theta \tag{23}$$

Selecting d_x and d_2 so as to maximize the TGP metric above yields d^ d_2=18 with TGP=O. That is, this method predicts a zero violation of the target value x^T=18 with the design d^ and d_2=18. Although this appears to be a superior design than with the SF there is a major problem as seen in Figure 7; namely, for the chosen design variables d ^ , d_2=18, the inequality in (4.19) becomes infeasible for the range 10 £ 8 £ 13. That is, while the distribution on x has $\bar{x}$=18.0 and o=0, the SF=0.5 which is clearly undesirable.

Therefore, the penalty approach for target specifications may produce designs which do not have the capability of meeting as large a range for 6 values as the SF metric does. On the other hand there is a clear trade-off here. The SF design can handle a larger range of variation but then with a higher quadratic loss, while with the TGP metric the opposite trend holds. Nevertheless, on balance it would appear that the designs with the TGP metric are less desirable, and that in any case, the Taguchi metric with the reward function as in (17) provides a more sensible approach.

Formulating the design problem with the reward function in (16) yields the NLP,

$$TGR=\frac{1}{\theta^{MAX}-\theta^{MIN}}\int^{\theta^U} \{c-(d_2+di9-xT)^2)j(e)\ de$$

s.L &≥{jV>-4a)l &\
9"£(xUP-d2)/di (NLP7)
9"≤1.25di- 0.25 d2+14.5
didi≥o $e^{MIN}\le e^L\le e^u\le e^{MAX}$

For a value of C=0 (NLP7) is similar to the TGP metric in (13) except that the inequality (19) is enforced and bounds 0^L and 6^U are variables as in the modified formulation (15). This is not a good metric, however, since, for instance, an optimal solution is given by dj=l d_2=8 with 0L=eu=7# This design does produce zero violation at 9=7 since x=d_1+$d_2$6=18. However, due to the form of the objective with C=0 the sensitivity with the upper bound 6^U has been lost Although the inequality in (19) is satisfied for 6=13, the design is in fact infeasible for 0=13 as then x=21 which exceeds the upper limit for x.

On the other hand a large value of C will make the solution of (NLP7) tend to the one for the SF metric. For instance with C=9 the solution of (NLP7) is d ^ . 7 and d_2=l 1 with 0^L=7 and 6^U=12.623, see Figure 8. In this case the SF=0.938, $\bar{x}$=17.87 and a=1.28, compared to the SF solution, the variance of x has been reduced by sacraficing some feasibility.

In summary, what this example has shown is that the SF metric is in general superior to **the** Taguchi metric, TGP, with quadratic loss since the latter ignores the effect of hard inequality constraints. However, since in general trade-offs might exist between capability for handling ranges (SF metric) and consistent performance (TGP metric), the suggested reward model for the Taguchi metric (TGR) can be used to explore these trade-offs by solving problem (17) for different values of C. Furthermore, in all cases the basic form of the model (NLP2) can be applied to solve these problems.

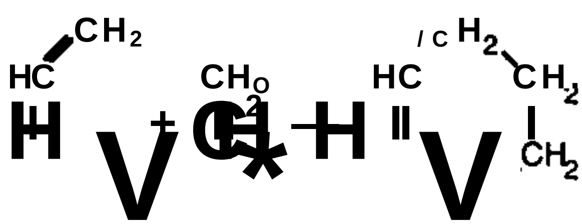
A final difference between the SF and TGR is that the SF has a simple physical meaning. We can say that the difference between design one which has SF=0.7 and design two which has SF=0.9, is that the second design is expected to operate feasibly 20% more of the time. One the other hand the TGR metric might go from TGR=20 to TGR=30, this only tells us that the second design results in a greater centering of the output around the target.

10. **Examples**

In this section two examples will be considered. The first is to illustrate the application of (NLP2) and to show a comparison with the quadratic loss approach.

Adiabatic Reactor Example

The first example involves the following Diels-Alder reaction in an adiabatic plug flow reactor (Hill, 1977).



In this problem the uncertain parameters are the heat of reaction AHr,and the activation energy, AE. The design variable is the space time t. The state variable is the overall conversion, conv. There are no control variables. Note that in this problem the uncertain parameters are not functions of time, simply unknown at the time of design.

The two uncertainties are assumed to be characterized by normal distributions. The heat of reaction AHr has mean -30,000 cal/mol with standard deviation 500 cal/mol. The activation energy has mean 27,500 cal/mol and standard deviation of 400 cal/mol.

The constraints describing the system are shown below (see Hill, 1977),

a) mass balance on reactor

$$T - \int_0^{Conv} \left(\frac{T}{T_o}\right)^2 \frac{(1-f/2)^2}{kC_o(1-f)^2} df = 0 \tag{24a}$$

b) energy balance on reactor:

$$T - T_o - \frac{\Delta H_r f}{57+2.5*f} = 0 \tag{24b}$$

c) rate equation:

$$k - 10^{7.5}\exp(-\Delta E/RT) = 0 \tag{24c}$$

where f is the conversion, To=273 K is the inlet temperature, k is the rate of reaction, C_o is the initial concentration of either species (equimolar feed is assumed), T is the temperature along the reactor and R is the gas constant The first and second constraints result from mass and energy balances on the reactor. The third constraint defines the rate of reaction. Finally, an inequality constraint specifies a lower bound on the conversion;

d) specification:

$$conv^{LB} - conv \leq 0 \tag{24d}$$

The parameter $conv^{LB}$ was chosen to be 0.1, restricting conversions to be greater than or equal to 10%. Five quadrature points were selected for each parameter to evaluate the SF for different alternative designs. To solve problem (NLP1) required 274 variables and 282 equations. The results are shown in Figure 9 which shows the relationship between SF and the design variable x. As shown in this figure, as the space time increases the larger the SF becomes. For instance with a space time of 40 seconds the SF=0.3, while at x=60 the SF=0.82. If costing information were available, that related the value of the design variables to the cost incurred then a trade-off curve could be developed to determine the cost of flexibility.

A second case was also solved in which the output conversion was restricted to be between 8% and 12%. The results of this case are shown in Figure 10. Note that too large a value of the space time will cause the SF to decrease. Clearly the space time has a significant impact on the SF. If we expected the flowrate into the reactor to vary then we would want to regulate this so that the variations are eliminated.

During the solution of the NLPs it was evident that the uncertainty in the activation energy was more significant than the heat of reaction. The bounds on the heat of reaction were nearly always those from the distribution constraints, while the bounds on the activation energy were generated by the conversion constraints. This information can be very useful. For example, if additional experiments were to be done to more accurately determine the parameters then one would obviously investigate the activation energy.

In determining the response curve, the NLPs were solved using GAMS/CONOPT (Drud 1991) as the NLP solver. Each NLP, on average, required 1.22 CPU seconds to solve on an IBM RS/6000.

The Taguchi approach was also applied to this example but with the reward function as in (16) with C=2.5. The target value for the conversion is 0.1. The results of the program are shown in Figure 11, which can be directly compared to Figure 10. Note that the largest TGR value and the largest SF value are in approximately the same location. In determining the response curve, the NLPs were solved using GAMS/MINOS as the NLP solver. Each NLP, on average, required 8.56 CPU seconds to solve on an IBM 6000, which is significantly higher than for the SF.

Reactor Flowsheet Example

The second example involves a plug flow reactor, a fractionator and a recycle stream described by Pistikopoulos and Grossmann (1989). The model is presented in Straub and Grossmann (1992). The flowsheet is shown in Figure 12.

The design variables in this problem are the reactor volume V, and the limits on the powers of the two pumps, Wj and W_2. The uncertain parameters are the composition of species B in the feed stream, and the forward and reverse rate constants, kj and k_2. The flow into the system and the pressure and temperature of the fractionator act as control variables. The model characterizing the system contains 21 constraints (18 equalities and 3 inequalities) and 27 variables. The goal of this problem is to develop a trade-off curve relating the SF to investment. The modified Benders decomposition scheme was used to determine the optimal design variable values and the corresponding SF for a fixed investment. For each of the 3 uncertain parameters 5 quadrature points were used. The modified subproblem contained 31 NLPs. Each NLP contained 44 equations and 49 variables. In comparison, the NLP corresponding to NLP1 contains 1290 equations and

1484 variables. The master problem contains 4 variables and (K+l) constraints where K is the iteration number. In determining the trade-off curve the modified Benders scheme required an average of 3 iterations to converge to the optimal solution with a tolerance of 0.002. On average each subproblem (31 NLFs) required a total of 42.75 CPU seconds on an HP 9000/835. The master required on average 0.6 CPU seconds. Thus, each optimization problem required on average 130.05 CPU seconds to solve. In comparison the NLP corresponding to NLP1 required 2690 CPU seconds to evaluate the SF for a fixed design. This clearly demonstrates the effectiveness of the modified Benders scheme.

The trade off curve relating SF to investment (a in NLP5) is shown in Figure 13.

As one would expect the more that is invested in the flowsheet the larger the probability of feasible operation. This figure also shows how the price for flexibility increases. The larger the SF is, the more it costs to increase it by a fixed amount. Two other curves are also presented. These curves show the values of the design variables at the optimal SF for a fixed investment. Figure 14 shows the optimal pump capacities versus investment. This curve demonstrates the value of the SF analysis in overdesigning equipment. For a fixed investment it is sub-optimal to overdesign each piece of equipment by a fixed amount As this figure shows, it is not desirable to overdesign the feed pump until an investment of $330,000 is made. On the other hand, the recycle pumps capacity in increased from the start. Figure 15 shows the optimal values of the reactor volume. Note that the reactor volume also increases steadily from the very beginning. The drastic rise at the end is due to the fact that both pumps reach maximum capacity at $390,000. Therefore, when going from an investment of $390,000 to $400,000, all of the capital is invested in the reactor.

11. Conclusions

This paper has presented methods for evaluating and optimizing the stochastic flexibility metric in designs that are described by nonlinear models. For the evaluation problem it has been shown that the procedure based on sequential optimizations can be embedded into a single nonlinear programming model (NLP1) which can then be readily extended as problem (NLP2) in order to optimize the SF under a cost constraint To circumvent the large size of this problem, a Benders decomposition scheme has been proposed which can greatly reduce the computational requirements as was shown in the flowsheet example problem.

This paper has also shown that the Taguchi design approach based on quadratic loss may not yield satisfactory results due to its inability to handle hard constraints. This can have the effect of producing designs that have consistent performance but only over a small parameter range. To avoid this problem a new variant of Taguchi's method has been proposed that incorporates a reward function. The results on a chemical reactor have shown that this metric produces similar designs as the SF metric.

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Appendix A

Proof for Equivalence of Sequential and Embedded Problems

Proposition: The SF predicted by (NLPl), SF^N, is identical to the SF calculated with (3), SF^S, and the sequential optimizations in (2) provided a sufficiently large number of quadrature points is selected

Proof: We will restrict ourselves to the two dimensional case which can be readily extended to higher dimensions.

By construction, SF^S as given by (3) and using the bounds computed in (2) will converge to the multiple integral in (1) within a small error e if a large number of quadrature points Qi , Q2 is selected; that is,

$$SF^s+e = SF= \int_{\theta_1^L}^{U} \int_{\theta_2^L(\theta_1)}^{\theta_2^U(\theta_1)} j(\theta)\, d\theta_2\, d\theta_1 \tag{Al}$$

Let us assume that for the same number of quadrature points, $\hat{Q}i$, $\hat{Q}2$, SF^N predicted by (NLPl) is different from SF^S. This implies that at least one of the lower or upper bounds in (NLPl) is different from the ones in (Al). For definiteness, let us assume that this is the case for only the lower bound of 0_{1f} for which (NLPl) yields $(Qi^L)^N$ * 9^ where $0!^L$ is the lower bound of the integral in (A1).

If $(8!^L)^N < Q_X{}^L{}_9$ this contradicts that 8^ is the smallest lower bound, and hence a solution of the minimization problem in (2a).

If $(0j^L)^N > 6i^L$, we have that for the quadrature points, Qi, Q2, the objective function in (NLPl) is given by,

$$SFN + \delta = SF= \int_{(\theta_1^L)^N}^{U} \int_{\theta_2^L(\theta_1)}^{\theta_2^U(\theta_1)} j(\theta)\, d\theta_2\, d\theta_1 \tag{A2}$$

where 8 is a small error term.

Since the multiple integral in (A2) has a smaller value then the one in (Al) it follows that

$$SF^N + \delta \leq SF^S + e \qquad \text{(A3)}$$

Furthermore, since the integral in (A2) is defined over a smaller domain, for a sufficiently large number of quadrature points, Qi, Q2, the errors are related by 5£e. Hence, $SF^N < SF^S$. The bounds 6^, 0^, Ga^1^^{1}, $G_2^{U(*1}$, ql=l,...$\hat{Q}$i and quadrature points G^^{1}, ql=l,...,$\hat{Q}$i, e_2^{q1q2}, q2=l,...$\hat{Q}$2, of SF^S, however, satisfy the constraints of (NLP1), which contradicts the assumption that SF^N is a solution of the maximization problem in (NLP1). Thus it follows that $SF^N = SF^S$ for a sufficiently large number of quadrature points.

Q.E.D.

Appendix B
Derivation of Correction Factors.

In this appendix the correction factors in (6) and (9) will be derived. This will be done by comparing the Kuhn-Tucker conditions of the embedded optimization problem (NLP1) with those of the sequential problems (NLP3 and NLP4).

The Lagrangian of the embedded problem (NLP1) can be written:

$$\begin{aligned}\mathcal{L}^1 = {} & \frac{\theta_1^U-\theta_1^L}{2}\sum_{q1=1}^{Q1} w_1^{q1}\frac{(\theta_2^{U\,q1}-\theta_2^{L\,q1})}{2}\sum_{q2=1}^{Q2} w_2^{q2}\, j(\theta_1^{q1},\theta_2^{q1,q2}) \\ & -\lambda_1^L g_1^L(\theta_1^L,\theta_2^{(*)}) \\ & -\lambda_1^U g_1^U(\theta_1^U,\theta_2^{(*)}) \\ & -\sum_{q1}\mu_1^{q1}\left\{\theta_1^{q1}-0.5\left[\theta_1^U(1+v_1^{q1})+\theta_1^L(1-v_1^{q1})\right]\right\} \\ & -\sum_{q1}\lambda_2^{L\,q1}g_2^{L\,q1}(\theta_1^{q1},\theta_2^{L\,q1}) \\ & -\sum_{q1}\lambda_2^{U\,q1}g_2^{U\,q1}(\theta_1^{q1},\theta_2^{U\,q1}) \\ & -\sum_{q1}\sum_{q2}\mu_2^{q1q2}\left\{\theta_2^{q1q2}-0.5\left[\theta_2^{U\,q1}(1+v_2^{q2})+\theta_2^{L\,q1}(1-v_2^{q2})\right]\right\}\end{aligned} \tag{B1}$$

Similarly the Lagrangians of (NLP3) and (NLP4), the sequential problems, arc as follows:

$$\mathcal{L}^3 = (\theta_1^U-\theta_1^L) - \hat{\lambda}_1^L g_1^L(\theta_1^L,\theta_2^{(*)}) - \hat{\lambda}_1^U g_1^U(\theta_1^U,\theta_2^{(*)}) \tag{B2}$$

$$\mathcal{L}^4 = (\theta_2^{U\,q1}-\theta_2^{L\,q1}) - \sum_{q1}\hat{\lambda}_2^{L\,q1}g_2^{L\,q1}(\theta_1^{q1},\theta_2^{L\,q1}) - \sum_{q1}\hat{\lambda}_2^{U\,q1}g_2^{U\,q1}(\theta_1^{q1},\theta_2^{U\,q1}) \tag{B3}$$

Having defined the Lagrangians for each of the problems, the Kuhn-Tucker conditions can be compared to determine the relationship between the multipliers. For L^1 we require the following conditions:

$$\frac{\partial\mathcal{L}^1}{\partial\theta_1^L} = -\frac{1}{2}\sum_{q1=1}^{Q1} w_1^{q1}\frac{(\theta_2^{U\,q1}-\theta_2^{L\,q1})}{2}\sum_{q2=1}^{Q2} w_2^{q2}\, j(\theta_1^{q1},\theta_2^{q1,q2}) - \lambda_1^L\frac{\partial g_1^L}{\partial\theta_1^L} - \sum_{q1}\mu_1^{q1}\left\{(-1/2)(1-v_1^{q1})\right\} = 0 \tag{B4}$$

$$\frac{\partial\mathcal{L}^1}{\partial\theta_1^U} = \frac{1}{2}\sum_{q1=1}^{Q1} w_1^{q1}\frac{(\theta_2^{U\,q1}-\theta_2^{L\,q1})}{2}\sum_{q2=1}^{Q2} w_2^{q2}\, j(\theta_1^{q1},\theta_2^{q1,q2}) - \lambda_1^U\frac{\partial g_1^U}{\partial\theta_1^U} - \sum_{q1}\mu_1^{q1}\left\{(-1/2)(1+v_1^{q1})\right\} = 0 \tag{B5}$$

$$\frac{\partial \mathcal{L}^1}{\partial \theta_1^{q1}} = \frac{\theta_1^U-\theta_1^L}{2}\, w_1^{q1}\frac{(\theta_2^{Uq1}-\theta_2^{Lq1})}{2}\sum_{q2=1}^{Q2} w_2^{q2}\frac{\partial j(\theta_1^{q1},\theta_2^{q1,q2})}{\partial\theta_1^{q1}} - \lambda_2^{Lq1}\frac{\partial g_2^{Lq1}}{\partial\theta_1^{q1}} - {}^{q1}\frac{\partial g_2^{Uq1}}{\partial\theta_1^{q1}} - \mu_1^{q1} = 0$$

$q1=1,...Q1$ (B6)

$$\frac{\partial \mathcal{L}^1}{\partial \theta_2^{Lq1}} = \frac{\theta_1^U-\theta_1^L}{2}\, w_1^{q1}\left(\frac{-1}{2}\right)\sum_{q2=1}^{Q2} w_2^{q2}\, j(\theta_1^{q1},\theta_2^{q1,q2}) - \lambda_2^{Lq1}\frac{\partial g_2^{Lq1}}{\partial\theta_2^{Lq1}} - \sum_{q2}\mu_2^{q1q2}(-1/2)(1-v_2^{q2}) = 0$$

$q1=1,...Q1$ (B7)

$$\frac{\partial \mathcal{L}^1}{\partial \theta_2^{Uq1}} = \frac{\theta_1^U-\theta_1^L}{2}\, w_1^{q1}\frac{1}{2}\sum_{q2=1}^{Q2} w_2^{q2}\, j(\theta_1^{q1},\theta_2^{q1,q2}) - \lambda_2^{Uq1}\frac{\partial g_2^{Uq1}}{\partial\theta_2^{Uq1}} - \sum_{q2}\mu_2^{q1q2}(-1/2)(1+v_2^{q2}) = 0$$

$q1=1,...Q1$ (B8)

$$\frac{\partial \mathcal{L}^1}{\partial \theta_2^{q1q2}} = \frac{\theta_1^U-\theta_1^L}{2}\, w_1^{q1}\frac{(\theta_2^{Uq1}-\theta_2^{Lq1})}{2}\, w_2^{q2}\frac{\partial j(\theta_1^{q1},\theta_2^{q1,q2})}{\partial\theta_2^{q1,q2}} - \mu_2^{q1q2} = 0$$

$q1=1,...Q1$ $q2=1,...Q2$ (B9)

The relavent Kuhn-Tucker conditions corresponding to $\mathcal{L}^3$ and $\mathcal{L}^4$ are shown below:

$$\frac{\partial \mathcal{L}^3}{\partial \theta_1^L} = -1 - \tilde{\lambda}_1^L\frac{\partial g_1^L}{\partial\theta_1^L} = 0 \qquad \text{(B10)}$$

$$\frac{\partial \mathcal{L}^3}{\partial \theta_1^U} = \qquad \frac{\partial g_1^U}{\partial\theta_1^U} = 0 \qquad \text{(B11)}$$

$$\frac{\partial \mathcal{L}^4}{\partial \theta_2^{Lq1}} = -1 - \lambda_2 \qquad \frac{q1}{\partial\theta} = 0$$

$q1=1,...Q1$ (B12)

$$\frac{\partial \mathcal{L}^4}{\partial \theta_2^{Uq1}} = 1 - \tilde{\lambda}_2^{Uq1}\frac{\partial g_2^{Uq1}}{\partial\theta_2^{Uq1}} = 0$$

$q1=1,...Q1$ (B13)

The first comparison will be between (B7) and (B12), to determine C_2^{Lq1} such that

$$\lambda_2^{Lq1} = C_2^{Lq1}\,\tilde{\lambda}_2^{Lq1}, \qquad q1=1,...Q1. \qquad \text{(B14)}$$

It is clear that if (B12) is multiplied by

$$CF_2^{L\,q1} = \frac{\theta_1^U-\theta_1^L}{2}\, w_1^{q1}\left(\frac{1}{2}\right)\sum_{q2=1}^{Q2} w_2^{q2}\, j(\theta_1^{q1},\theta_2^{q1,q2}) \quad + \sum_{q2} \mu_2^{q1q2}(-1/2)\,(1-v_2^{q2}) \qquad q1=1,\ldots Q1 \qquad \text{(B15)}$$

the resulting equation is identical to (B7), which then defines the correction factor. This equation, however, contains the multipliers of the equations defining the quadrature points, information not available from the sequential problems. This can be overcome by solving (B9) for μ_2^{q1q2} and substituting into (B15), which results in:

$$\begin{aligned} CF_2^{L\,q1} = {} & \frac{\theta_1^U-\theta_1^L}{2}\, w_1^{q1}\left(\frac{1}{2}\right)\sum_{q2=1}^{Q2} w_2^{q2}\, j(\theta_1^{q1},\theta_2^{q1,q2}) \\ & + \sum_{q2}\left\{\frac{\theta_1^U-\theta_1^L}{2}\, w_1^{q1}\,\frac{(\theta_2^{U\,q1}-\theta_2^{L\,q1})}{2}\, w_2^{q2}\,\frac{\partial j(\theta_1^{q1},\theta_2^{q1,q2})}{\partial\theta_2^{q1,q2}}\right\}(-1/2)\,(1-v_2^{q2}) \end{aligned} \qquad q1=1\ldots Q1 \qquad \text{(B16)}$$

Note that this correction factor only requires information on the bounds and quadrature points, which is available from the sequential problems. The same procedure can be used to determine the correction factor for the multipliers corresponding to the upper bound; that is,

$$\lambda_2^{U\,q1} = CF_2^{U\,q1}\,\hat{\lambda}_2^{U\,q1} \qquad q1=1,\ldots Q1 \qquad \text{(B17)}$$

The correction factor is shown below:

$$\begin{aligned} CF_2^{U\,q1} = {} & \frac{\theta_1^U-\theta_1^L}{2}\, w_1^{q1}\left(\frac{1}{2}\right)\sum_{q2=1}^{Q2} w_2^{q2}\, j(\theta_1^{q1},\theta_2^{q1,q2}) \\ & - \sum_{q2}\left\{\frac{\theta_1^U-\theta_1^L}{2}\, w_1^{q1}\,\frac{(\theta_2^{U\,q1}-\theta_2^{L\,q1})}{2}\, w_2^{q2}\,\frac{\partial j(\theta_1^{q1},\theta_2^{q1,q2})}{\partial\theta_2^{q1,q2}}\right\}(-1/2)\,(1+v_2^{q2}) \end{aligned} \qquad q1=1,\ldots Q1 \qquad \text{(B18)}$$

The correction factors for multipliers for constraints corresponding to the bounds on θ_1 can be determined by comparing (B4) and (B10) resulting in,

$$CF_1^L = \frac{1}{2}\sum_{q1=1} w_1^{q1}\,\frac{(\theta_2^{U\,q1}-\theta_2^{L\,q1})}{2}\sum_{q2=1}^{Q2} w_2^{q2}\, j(\theta_1^{q1},\theta_2^{q1,q2}) \quad -\sum_{Q1} \mu_1^{q1}\left((-1/2)\,(1-v_1^{q1})\right) \qquad \text{(B19)}$$

Substituting for the multipliers μ_1^{q1} from (B6)

$$CF_1^L = \frac{1}{2}\sum_{q1=1}^{Q1} w_1^{q1}\frac{(\theta_2^{U\,q1}-\theta_2^{L\,q1})}{2}\sum_{q2=1}^{Q2} w_2^{q2}\, j(\theta_1^{q1},\theta_2^{q1,q2})$$
$$+\sum_{q1}\left\{\frac{\theta_1^U-\theta_1^L}{2}\, w_1^{q1}\frac{(\theta_2^{U\,q1}-\theta_2^{L\,q1})}{2}\sum_{q2=1}^{Q2} w_2^{q2}\frac{\partial j(\theta_1^{q1},\theta_2^{q1,q2})}{\partial\theta_1^{q1}} \quad -\lambda_2^{L\,q1}\frac{\partial g_2^{L\,q1}}{\partial\theta_1^{q1}} - \lambda_2^{U\,q1}\frac{\partial g_2^{U\,q1}}{\partial\theta_1^{q1}}\right\}\{(-1/2)\,(1-v_1^{q1})\}$$

(B20)

Here $X_2^{L_q 1}$ and $X_2^{U_q 1}$ were previously detennined in (B14) and (B17); the corresponding derivatives are detennined analytically. For the upper bound

$$CF_1^U = \frac{1}{2}\sum_{q1=1}^{Q1} w_1^{q1}\frac{(\theta_2^{U\,q1}-\theta_2^{L\,q1})}{2}\sum_{q2=1}^{Q2} w_2^{q2}\, j(\theta_1^{q1},\theta_2^{q1,q2})$$
$$-\sum_{q1}\left\{\frac{\theta_1^U-\theta_1^L}{2}\, w_1^{q1}\frac{(\theta_2^{U\,q1}-\theta_2^{L\,q1})}{2}\sum_{q2=1}^{Q2} w_2^{q2}\frac{\partial j(\theta_1^{q1},\theta_2^{q1,q2})}{\partial\theta_1^{q1}} \quad -\lambda_2^{L\,q1}\frac{\partial g_2^{L\,q1}}{\partial\theta_1^{q1}} - \lambda_2^{U\,q1}\frac{\partial g_2^{U\,q1}}{\partial\theta_1^{q1}}\right\}\{(-1/2)\,(1+v_1^{q1})\}$$

(B21)

Thus the corrected multipliers for the constraints corresponding to the lower and upper bounds on 6j can be obtained as follows:

$$\lambda_L^1 = CF\,\hat{\lambda}_L^1, \qquad \lambda_U^1 = CF\,\hat{\lambda}_U^1.$$

This procedure is readily generalized to higher dimensions.

Captions

Figure 1 Feasible region for evaluating the stochastic flexibility.

Figure 2 Demonstrating the determination of the bounds and quadrature points, for q^ =1,2,3,4, q_2=1,2,3

Figure 3 Feasible region for initial design and contours or distribution.

Figure 4 Feasible region corresponding to optimal solution and contours of distribution.

Figure 5 Convergence of the bounds in the Benders scheme.

Figure 6 System for optimal d from SF problem.

Figure 7 System for optimal d from Quadratic Penalty problem*

Figure 8 System for optimal d from TGR problem.

Figure 9 Results of Example, with lower bound on conversion (0.1).

Figure 10. Results of Example, with lower and upper constraints on conversion [0.8 .12]

Figure 11. Results of Example, quadratic reward problem.

Figure 12 Flowsheet for Example 2.

Figure 13 Trade-off curve relating SF to investment for Example 2.

Figure 14 Pump Capacities for Optimal SF versus Investment for Example 2.

Figure 15 Reactor Volume for Optimal SF versus Investment for Example 2.

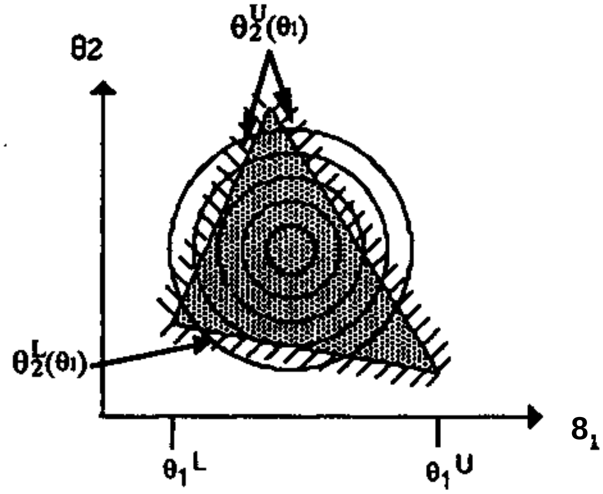

Figure 1

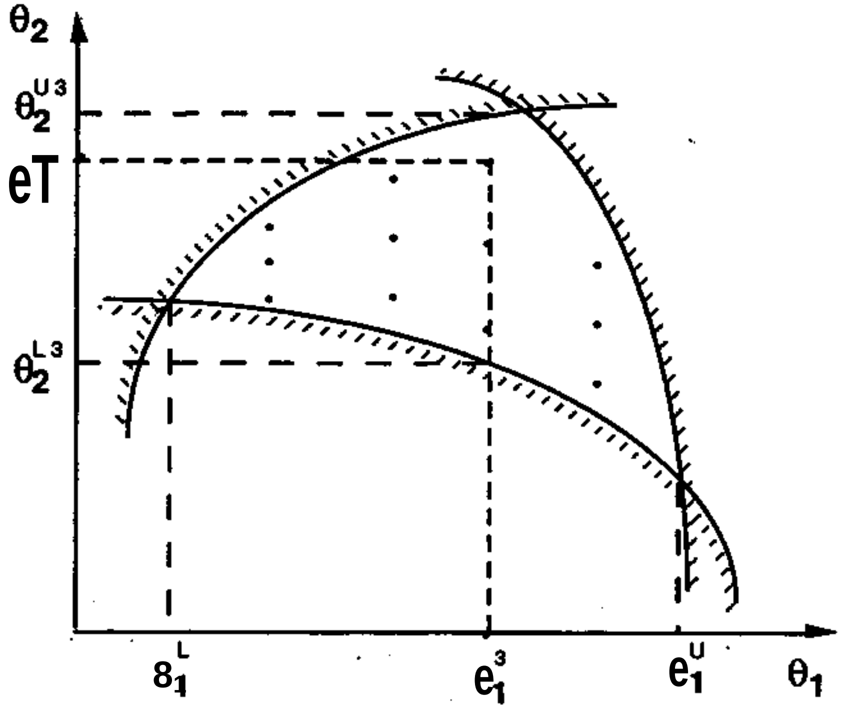

Figure 2

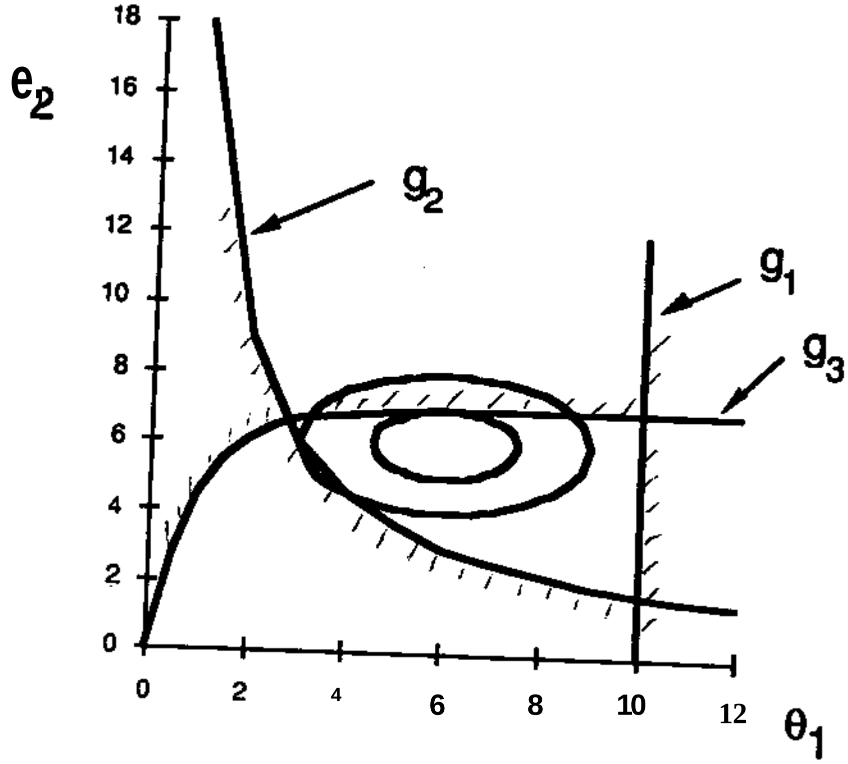

Figure 3

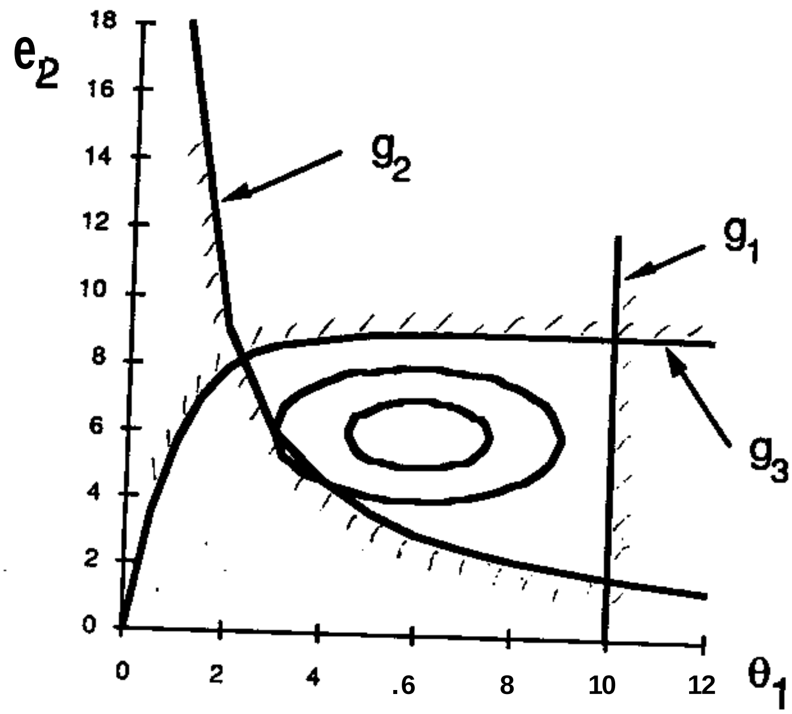

Figure 4

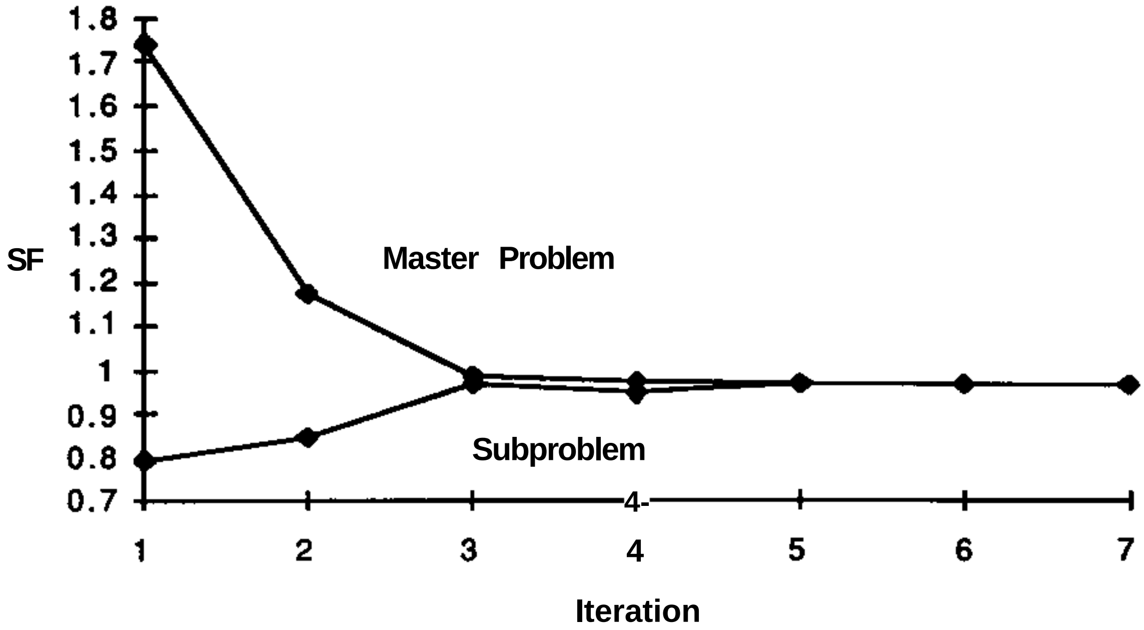

Figure 5

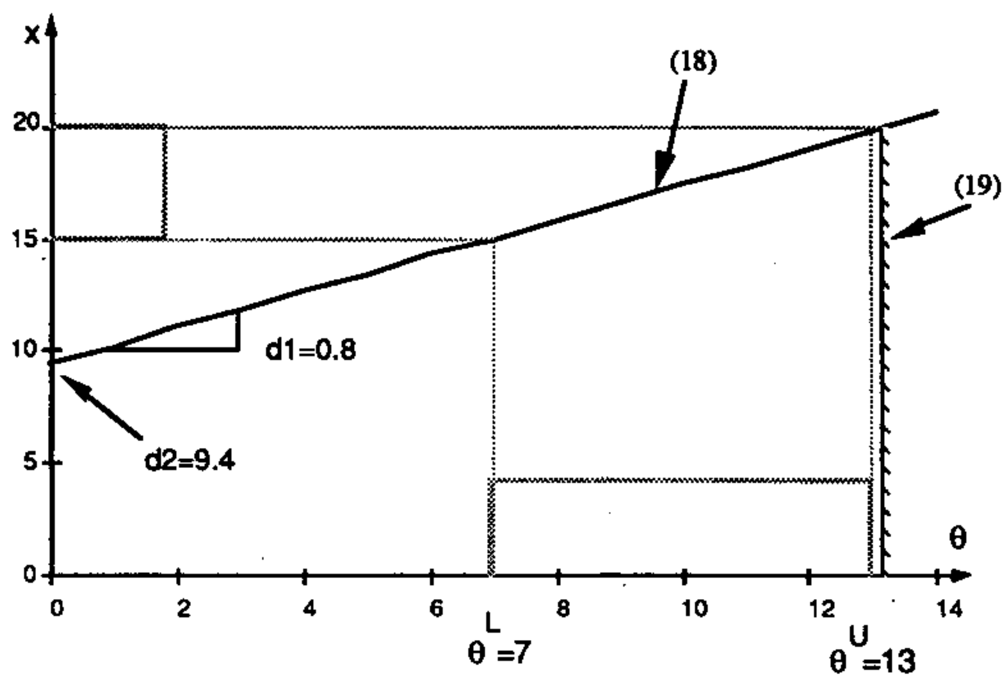

Figure 6

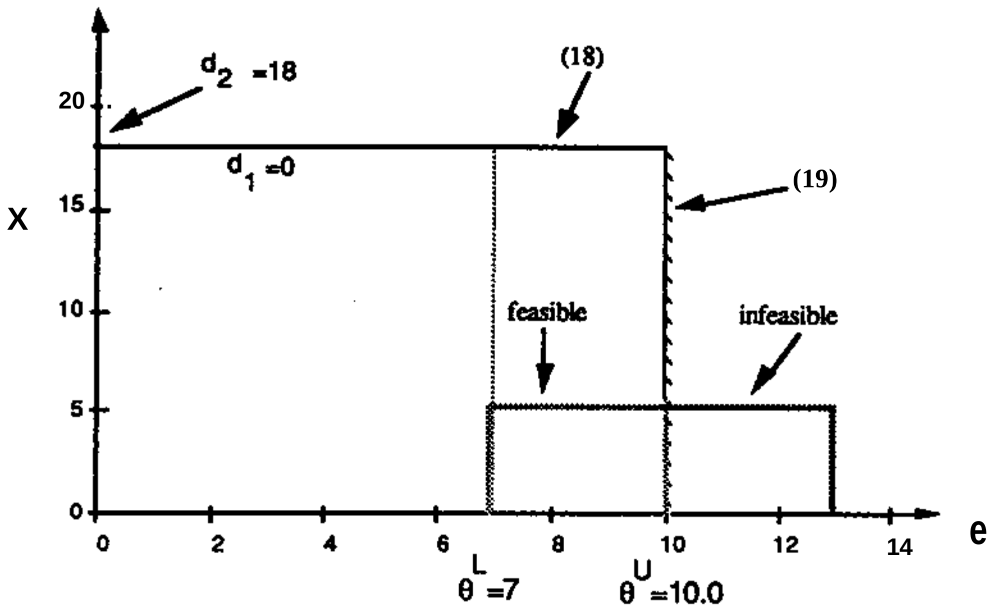

Figure 7

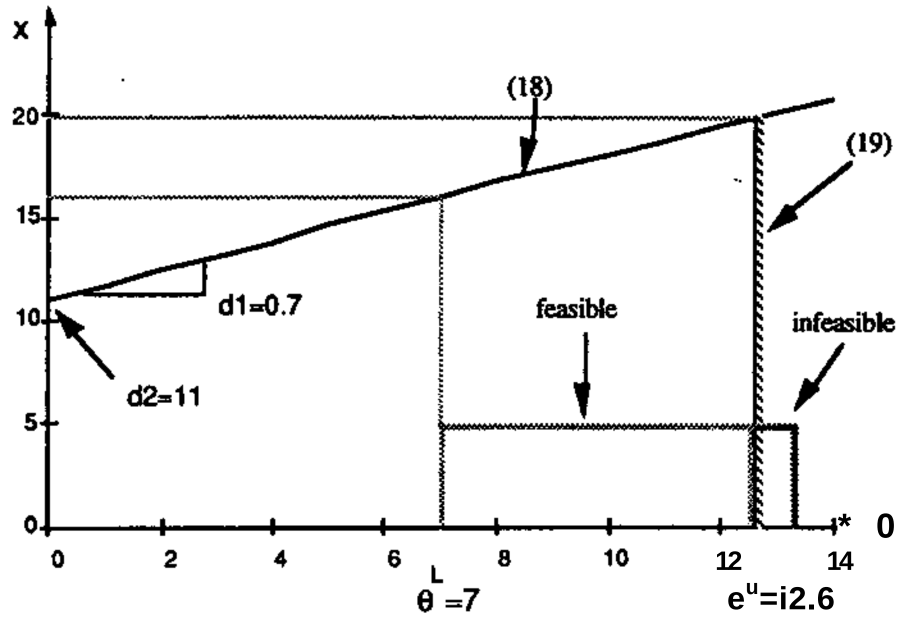

Figure 8

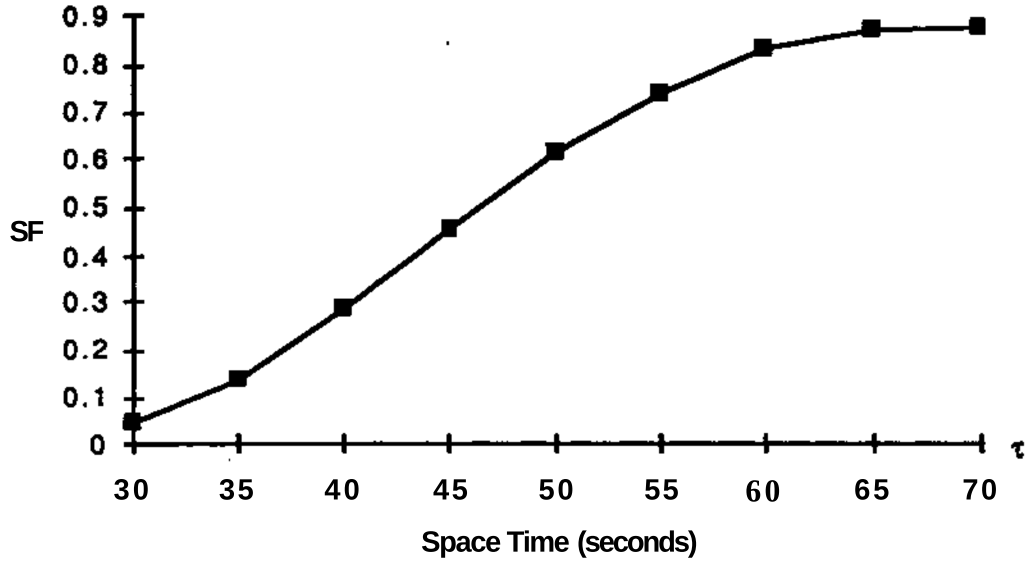
0.9
0.8
0.7
0.6
0.5
SF
0.4
0.3
0.2
0.1
0
τ
30
35
40
45
50
55
60
65
70
Space Time (seconds)

Figure 9

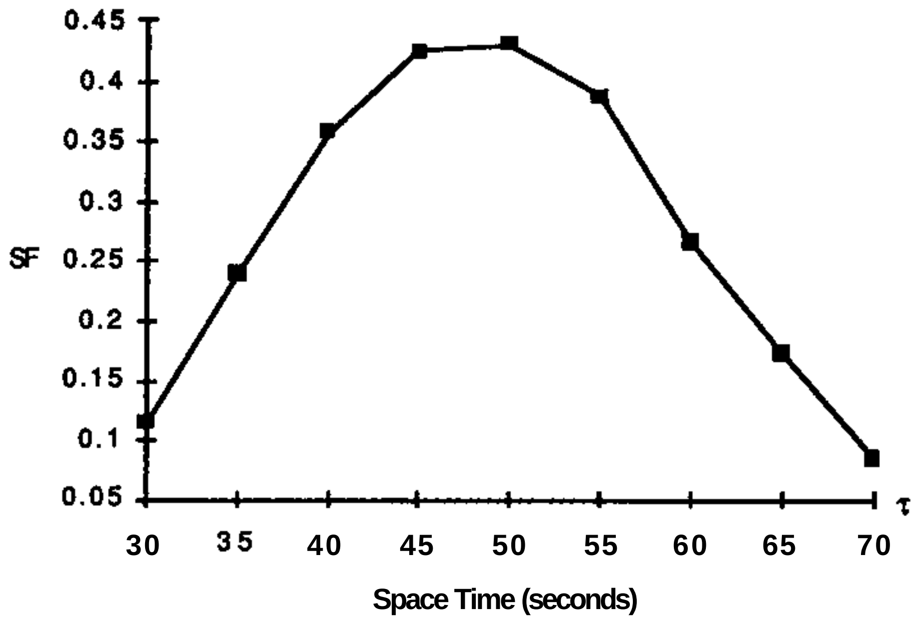

Figure 10.

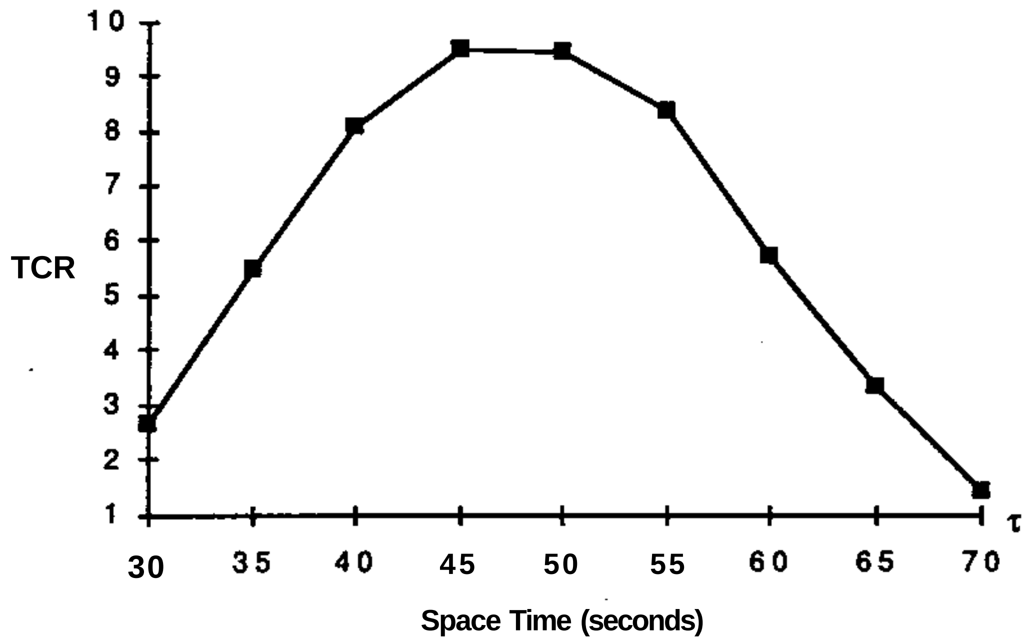

Figure 11.

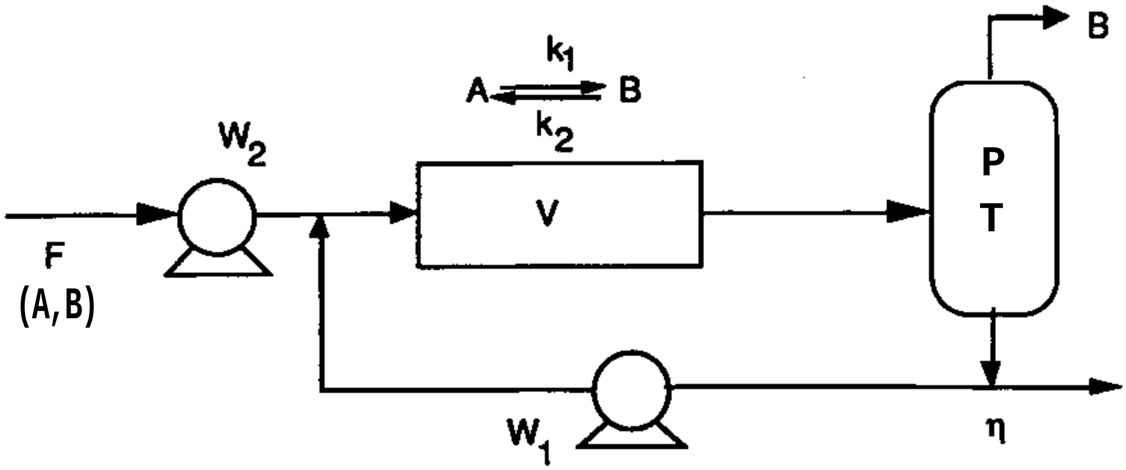

Figure 12

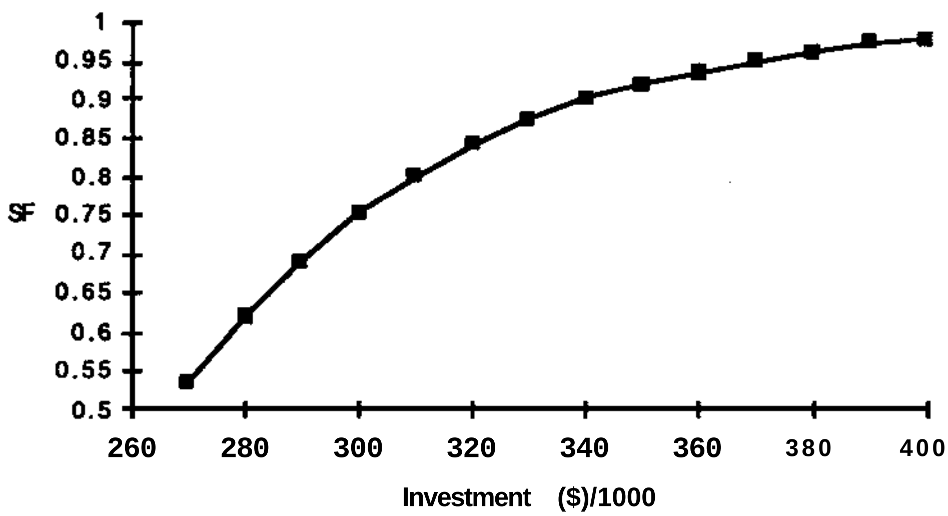

Figure 13

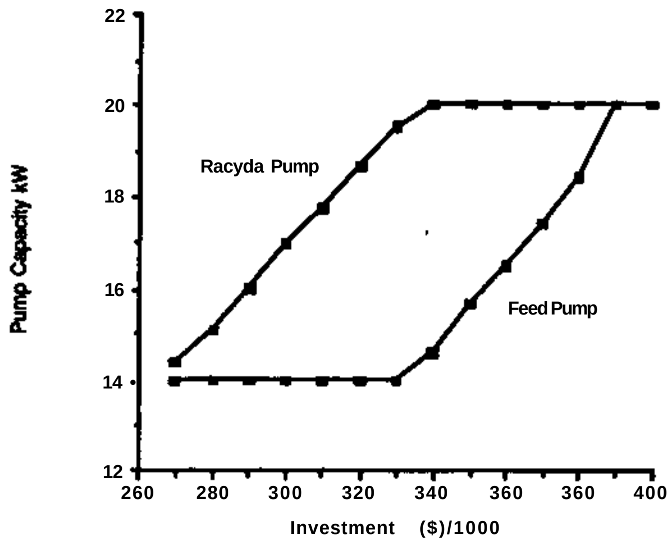

Figure 14

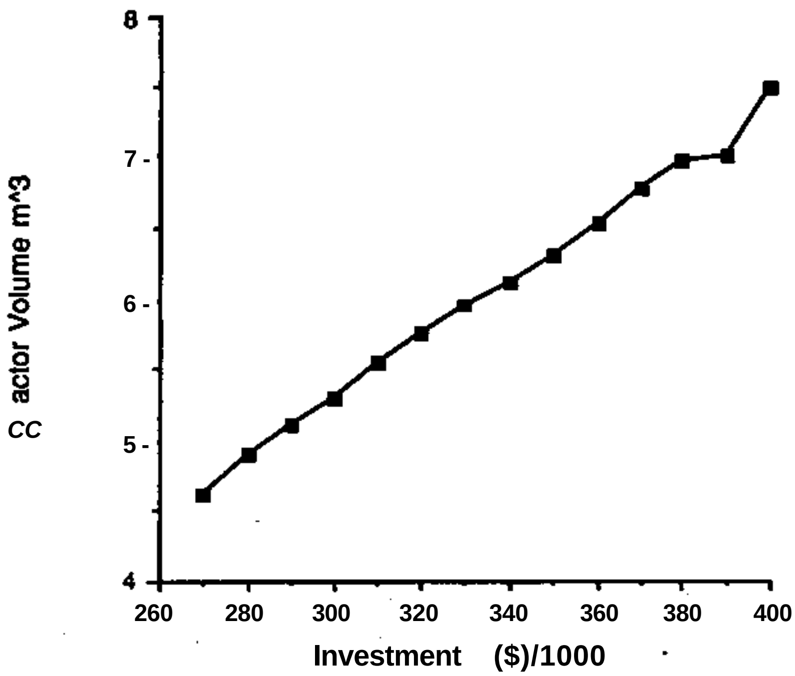

Figure 15