Integrated Statistical Metric of Flexibility for Systems with Discrete State and Continuous Parameter Uncertainties

by

David A. Straub, I. E. Grossmann

EDRC 06-76-89

Integrated Statistical Metric of Flexibility for Systems with Discrete State and Continuous Parameter Uncertainties

David A. Straub and Ignacio E. Grossmann*
Department of Chemical Engineering
Carnegie Mellon University
Pittsburgh, PA 15213

November 1989

Paper 165c. Annual AIChE Meeting, San Francisco

'Author to whom correspondence should be addressed

Abstract

This paper addresses the problem of developing a quantitative measure for the flexibility of a design to withstand uncertainties in the continuous parameters and discrete states. The metric is denoted as the expected stochastic flexibility, E(SF). For a given a linear model, a joint distribution for the parameters and probabilities of failure for the discrete states, the proposed metric predicts the probability of feasible operation of a design.

A novel inequality reduction scheme is proposed to aid in performing the integration over the feasible region characterized by inequalities. A bounding scheme is also proposed to avoid the examination of a large number of discrete states when determining the E(SF). An example problem is presented to demonstrate the fact that the proposed measure provides a framework for integrating flexibility and reliability in process design.

Introduction

The operation of chemical plants is subject to uncertainties in the parameters and in the reliability of its design components. The uncertain parameters typically include such items as flowrates, temperatures, and kinetic rate constants, while design uncertainties include the availability of equipment. Note that these uncertainties are of two types: continuous and discrete, respectively. The types of uncertainties are distinguished by the values they take. Continuous uncertainties may take on a range of values while discrete uncertainties take on only specific values. Because the feasible operation of a chemical plant is clearly dependent upon these uncertainties, it is important to be able to quantitatively determine the effect of these uncertainties on plant operation.

This has been done for two cases, processes with only continuous parameter uncertainties-flexibility (Swaney and Grossmann 1985, Saboo and Morari 1984, Pistikopoulos and Mazzuchi 1989) and processes with only discrete state uncertainties-reliability, (Tzafestas 1980, Shooman 1968, Dhillon 1988). Neither of these two problems, however, fully captures the nature of uncertainties in chemical processes. There is obviously a great need to handle both types of uncertainties together, since they show strong interactions in defining the feasible operation of a plant.

The goal of this paper is to develop a stochastic metric for feasible operation in systems that can be represented by a linear model, and where we can simultaneously account for both types of uncertainties. The proposed metric represents the probability of feasible operation for given probabilities in the discrete states and for given joint distribution functions of the continuous uncertain parameters. For the latter, a novel inequality reduction scheme is proposed that allows the efficient numerical integration of the joint distribution function over the feasible region for a given state. Since the proposed metric requires the enumeration of a large number of discrete states, an effective bounding scheme is proposed that exploits the structure found in reliability problems. Application of the proposed metric is illustrated with an example problem which shows that flexibility and reliability can be integrated within a common framework.

Motivating Example

The most common example of a process containing both discrete and continuous parameter uncertainties is a continuous chemical process with redundant equipment.

In continuous chemical processes there are typically uncertain continuous parameters such as flowrates, product demands, and thermodynamic constants. There are also uncertainties in the discrete states corresponding to the availability of equipment. For example pumps, compressors, or reactors may experience failure modes and become inoperable. An example of this type of system is shown in Figure 1.

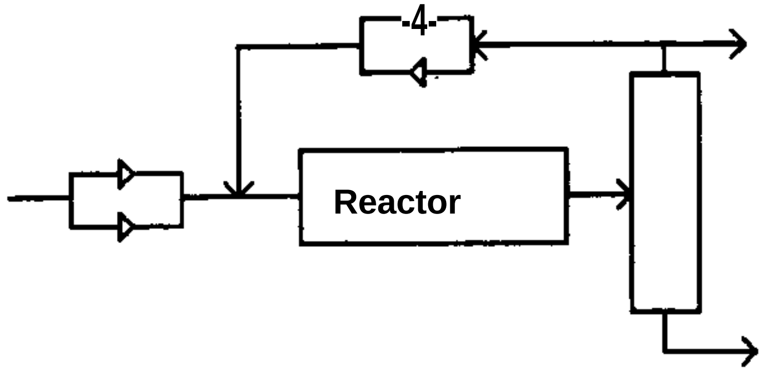

Figure 1. Process flowsheet with redundant chemical equipment

In this process there are redundant compressors in both the feed and recycle lines to increase the reliability, given that the availability of the compressors is uncertain. The continuous uncertainties in this process might include the flowrate of the feed and the kinetic rate constants. The interaction between the types of uncertainties can take several forms. For instance, if all the equipment is available for operation then some of the redundant or back-up equipment can be used to compensate for increases in the flows. At the other extreme, if some of the equipment including its redundant units fail, then the process becomes inoperable. Thus, it is clear that since the flexibility and the reliability of a process are related, one must consider both aspects simultaneously for predicting the expected capability of a process to have feasible operation.

Basic Concepts

The metric which will be proposed to characterize systems with discrete and continuous uncertainties will be denoted as the Expected Stochastic Flexibility, E(SF). The stochastic flexibility, SF, is a measure of a systems ability to tolerate continuous uncertainties for a given discrete state. The discrete uncertainties are taken into account when determining the expected value of the stochastic flexibility.

The concept of the stochastic flexibility is shown in Figure 2. The triangle represents the feasible region of operation for the system in the space of the continuous uncertainties. Each of the continuous uncertainties is described by a probabilistic distribution. In this case e_1 and e_2 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. Thus, mathematically, the stochastic flexibility is the integral of the joint distribution over the shaded region.

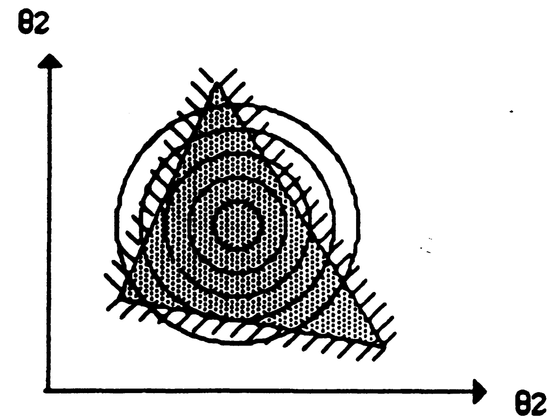

Figure 2 Diagram showing the stochastic flexibility of a feasible region

The discrete uncertainty involves changes in the state of a design which result in different feasible regions. The effect of a design change is shown in Figure 3. Here normal operation is represented by State 1 and results in the outer triangle. State 2 represents the process in which some redundant equipment has failed. Intuitively, when equipment fails the size of the feasible region gets smaller and may not exist at all.

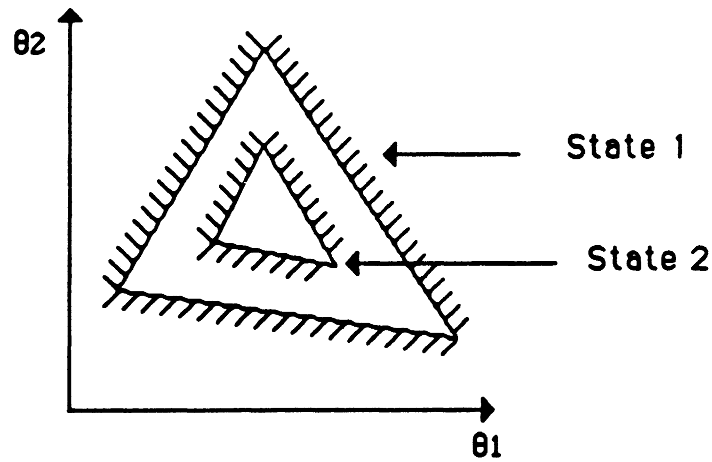

Figure 3 Effect of the discrete uncertainty

The expected stochastic flexibility is calculated by summing up the products of the probability for each state and its corresponding stochastic flexibility. In this way, the E(SF) represents, qualitatively, the probability of feasible operation that we can expect on average over a large time horizon.

Mathematical Description of System

The systems of interest are modeled mathematically with a set of equalities and inequalities, which are assumed to be linear in this paper:

a) performance equations	$A_1x+A_2z+A_3e$-a	(1)
b) specifications	B_1X4B_2z^B_3e^b	(2)
c) capacity constraints	Cjx-^z+C^esd*Iy	(3)

The variables in these equations can be classified as follows:

- d vector of L design variables that define the capacity of units
- e vector of M uncertain continuous parameters
- x vector of state variables
- z vector of control variables as degrees of freedom which can be adjusted to compensate for changes in 9
- y vector of Boolean variables defining the availability of the L pieces of equipment

In this model the continuous uncertainties 9_m (m«1,...,M) are characterized by probability distribution functions. These distributions may or may not be independent. Typical distributions would include normal, beta, uniform, and triangular. The model is rcrciified according to the distributions being used with additional constraints. The constraints reflect the fact that after a certain point the cumulative probability exhibits negligible changes. For example, it 9 was characterized by a normal distribution sounds limiting the range of 8 from 9_1^{nDm}-4a to 9_1^{nom}+4a could be introduced. These bounds prevent the integration over insignificant portions of the joint distribution. They **also** prevent unbounded feasible regions which create difficulties with a quadrature integration scheme.

The discrete uncertainties corresponding to the availability of the L units in a process are represented by the Boolean variables y/, /«1.....L, that determine whether the corresponding /th unit with capacity d/is available. When a discrete uncertainty is active, its Boolean variable y/will be set equal to 1. Otherwise, it will have a value of 0. Therefore based on the way (3) has been written, y/-1 will represent the case when the / th piece of equipment is available.

Each Boolean variable y/ is associated with a probability of being active, p/. That is, P{y/«1}«$P/_f$ and P{y/-0}«1-p/. The determination of p/in the context of availability is explained in Appendix A.

The Boolean variables give rise to different system states Sj and an associated state probability. Each state Sj represents a different combinations of the 0-1 values for the vector y. Specifically Sj-fY^} where Y_1^i-{/|$y^i_/$-i}. For example, with two Boolean variables there are 4 states (0,0)=> SH*)' (0.1)=> S_2-{2}. 0.0)=> S_3-{1}, and (1,1)=> S_4-{1,2}. For each state there is a corresponding state probability P(Sj). Assuming independent probabilities p/, the state probability can be defined as follows:

$$P(S_i) = \prod_{\ell \in Y_1^i} p_\ell \prod_{\ell \in Y_0^i} (1-p_\ell) \qquad i=1,\ldots 2^L$$

where Yo'-f/ly'z-O} and $Y^{\wedge}=\{\ell \mid y^i_\ell = 1\}$ (4)

This probability can be interpreted as the fraction of time that a process is expected to operate in state Sj, for a large horizon time.

Finally note that in (1) the vector of state variables, x, has the same dimensions as the equalities. Assuming the the square matrix A_1 is nonsingular, the state variables can be eliminated by solving the equalities for x in terms of z, and 6.

x-fA^-i $[a-A_2z-A_3e]$ % (5)

Substituting into the inequalities yields

$B_1(A_1)^{-1}$ $[a-A_2z-A_3e]+B_2z+B_3e£b$ (6a)

$C_1(A_1)^{-1}$ {a-A2Z-A_3eKC2Z+C3e≤d^t I y^j (6b)

The inequalities in (6) which define the feasibility of operation along with the distribution constraints, can be written in compact form as f(d',z_f6)£0 where d^i»d^t iy' represents the design variables for state S,.

Stochastic Flexibility

Given the model for the system and the probability distributions for the continuous uncertainties the SF for a given state Sj can be calculated. Mathematically the SF takes the form of the integral,

SF(Si)=/ . JO)dB
$^J W^l fi W$ (7)

where y(d^j,6)^0 defines the feasible region of operation in the uncertain parameter space for the fixed design d', that is dependent upon the state S_{jv} and j(6) is the joint distribution of the continuous uncertainties. This integral will be solved using a guassian quadrature scheme described below.

In order to write the integral in quadrature form the order of integration needs to be determined. For this purpose a new parameter x_m (m«1,...,M) will be introduced, in order to relabel the indices of the continuous parameters 8 so that the index of the variable corresponds to the order of integration, which may not neccesarily be the same as the indices of G (e.g. x_1«6_2, $X_2=\theta_1$).

Initially, it is natural to write the integral in the following form

$$SF(S_i) = \int_{\tau_1^L}^{\tau_1^U} \int^{U} \cdots \int^{U} K^*)«(T) \; dr_{Nf} \ldots dx_2 dt_1 \qquad (8)$$

where 8(x)«1 if ytd'.x^O, and 8(x)-0 if v(d^l,t)>0.

Here the integration is performed over a hypercube which encloses the feasible region. This region corresponds to the dashed line in Figure 4. The dots in Figure 4 represent the selected quadrature points for the integration.

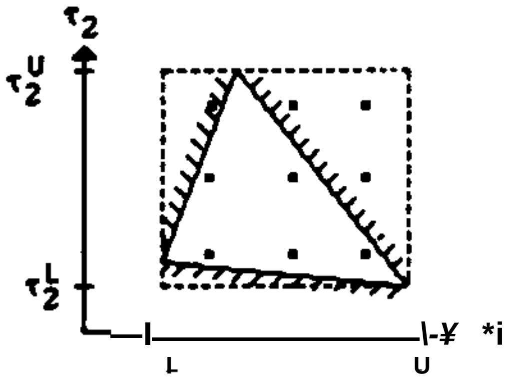

Figure 4 Quadrature points for integral equation 8

The bounds are determined using the following formulations for $m=1,2,..,M$:

$$\tau_m^L = \min_{z,\tau} \tau_m \qquad \tau_m^U = \max_{z,\tau} \tau_m$$
$$\text{s.t. } f_j(d,z,\tau) \le 0,\ j \in J \qquad \text{s.t. } f_j(d,z,\tau) \le 0,\ j \in J$$

It is apparent that this computational scheme has the potential for being very inefficient. First, all the parameter points used to evaluate (8) need to be distinguished as feasible or infeasible. Then for those points which are feasible the value of the joint distribution is evaluated; for those points which are infeasible the integrand is assigned a value of 0. Furthermore, a problem arises in that the resulting approximating function is not smooth. For example, the crossection of a distribution generated in Figure 4 might look like the one shown in Figure 5.

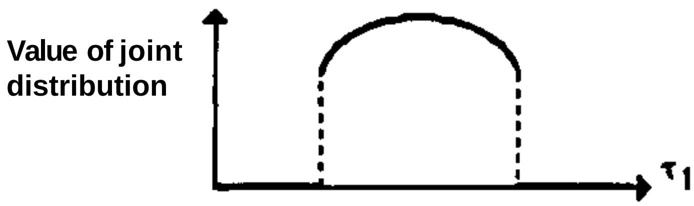

Figure 5 Surface crossection from Figure 4

Although Gaussian quadrature can still be adapted to this discontinuous curve, it will not be efficient and will require a large number of points.

One solution to this problem is to redefine the region of integration as the one that exactly corresponds to the feasible region of operation. In this way the integral takes on the following form:

$$SF(S_i) = \int_{\tau_1^L}^{\tau_1^U} \int_{\tau_2^L(\tau_1)}^{\tau_2^U(\tau_1)} \cdots\cdots \int_{\tau_M^L(\tau_1,\tau_2,\ldots,\tau_{M-1})}^{\tau_M^U(\tau_1,\tau_2,\ldots,\tau_{M-1})} j(\tau)\, d\tau_M \ldots d\tau_2\, d\tau_1 \qquad (10)$$

where $\tau_m^L(\tau_1,\tau_2,\ldots,\tau_{m-1})$ and $\tau_m^U(\tau_1,\tau_2,\ldots,\tau_{m-1})$ are variable lower and upper bounds of parameter τ_m that are evaluated at the parameter values $\tau_1,\tau_2,\ldots,\tau_{m-1}$. These bounds then define the boundary of the feasible region. In order of apply a quadrature formula to estimate this integral the following procedure can be applied.

First determine the upper and lower bounds for τ_1. Then discretize according to a specific quadrature formula over this range. For each discrete point τ_1 determine the maximum and minimum of τ_2. Then discretize over each of these ranges and keep repeating the procedure until all the elements of τ have been discretized. For the two dimensional case shown in Figure 4 the following points would be obtained.

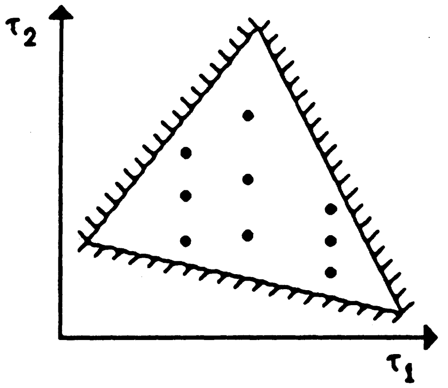

Figure 6 Quadrature points for modified region

This procedure has the advantage that it eliminates infeasible points for the integration. Also by using this procedure the number of quadrature points necessary to get an accurate estimate of the integral is greatly reduced. The price for this simplification is the increase in the number of optimizations (similar to (9)) that have to be performed to determine the bounds. While the scheme depicted in Figure 4 requires 2M optimizations, the scheme in Figure 6 requires $2(1+QP_1(1+QP_2(1+QP_3(\ldots.(1+QP_{M-1})))))$ optimizations where QP_m is the number of quadrature points for parameter m. For the specific example in Figure 6, since $QP_1=3$, $2(1+3)=8$ optimizations are required. This scheme, however, can become very expensive, even for small problems. For a problem with 4 continuous uncertainties each described by 7 quadrature points 800 optimizations are necessary to solve the problem. Fortunately for the case with linear constraints the optimization problems can be greatly simplified. As will be shown in the next two sections, by using an inequality reduction scheme the optimizations can be solved analytically to get the bounds for every uncertain parameter.

Inequality Reduction **Scheme**

The inequality reduction scheme successively eliminates variables from the constraints f(d',2,t)^O. By successively eliminating variables one at a time from the constraints, starting with the control variables we can generate new sets of constraints. Eventually constraints that only depend on x_1 can be obtained. These constraints give us the bounds on x_v Having the bounds on xj we can discretize this range to get the location of the quadrature points in x_1 space. Having the quadrature points in x_1 space the constraints that just depend on x_1 and x_2 can be used to determine the range of t_2 for each quadrature point in x_1 space. This procedure can be repeated until the quadrature points for x_M are obtained using the constraints that depend on x-j, X2,..-1*4.1 •

The scheme will be demonstrated first with an example, and the general mathematical formulation will be presented afterwards.

Example 1

Consider the following 4 constraints involving one control variable and two continuous uncertainties for a given state:

$$f_1«2z+3x_1+x_2+i£0 \quad (11a)$$
$$f_2«-z-3x_1+x_2-0.5£0 \quad (11b)$$
$$f_3--22-2x_1-3x_2-1^0 \quad (11c)$$
$$f_4- \quad x_1+x_2-4^0 \quad (11d)$$

The first step is to eliminate the control variable from the constraints. This is accomplished with the following parametric mathematical program.

$$\psi(d^i,\tau_1,\tau_2)^{1,k} = \min_{zu} u$$
$$\text{s.t. } f_1(d^i,z,\tau_1,\tau_2)\le u$$
$$f_2(d^i,z,\tau_1,\tau_2)\le u$$
$$f_3(d\backslash z,xi,x_2)£u \quad (12)$$

Here $y^{1,k}$£0 defines the first set of reduced constraints. The motivation for this program and the method of solution are explained in Appendix B. There are several solutions to this problem depending upon which constraints are active, that is fj-u. Because there are several possible active sets, the index k is introduced in order to distinguish between solutions generated by the different active sets. The first superscript on y represents the order of reduction. The order signifies the dependence of the constraints, i.e. $v^r»^k«y(d.T_I,T_2,...,T_{M.r}+_1)$. For problem (12) In which the control variables are eliminated r-1.

As shown in Appendix B, the solutions of the problem can be written in term of the active constraints as,

$$\psi^{r,k} = \sum_{j \in J_A^{r,k}} \lambda_j^{r,k} f_j \qquad (13)$$

where Xj'>k are the non-negative multipliers and JA^r,k is the set of active constraints for reduction r and active set k. The multipliers are obtained from the optimality conditions described in Appendix B. Here they lead to the following equations:

^•^•^•I (14a)

2X11-X21-2X31-O (14b)

X|Xj1|-dim{z}+1«2 (14c)

Note that here |X|«0 if X-0 and |X|«1 if X>0. Given that there Is only one control variable z, only two X can be non-zero (dim{z}+1*2). Here there are 2 solutions to these equations: X<|1'1«1/3 X21*1«2/3, and Xi1»2«0.5 X31'2«0.5. Note that only the solutions carry the superscript k, not the defining constraint functions. Given these multipliers the first set of reduced constraints can be generated.

ψ1.1 •0.333 f, + 0.667 f2

« -x<\ +x2 £0 (15a)

ψ1.2 «0.5 f«| + 0.5 f3

«0.5 Xi -x2 ≤0 (15b)

y1,3 «xi+x2-4≤0 (15c)

Note that the fourth reduced inequality (11d) was not included in the mathematical program (12). Since (11d) did not contain the variable being eliminated, it is automatically entered into the set of reduced inequalities.

The resulting constraints define the feasible region in the space of the continuous uncertainties. This feasible region is shown in Figure 7.

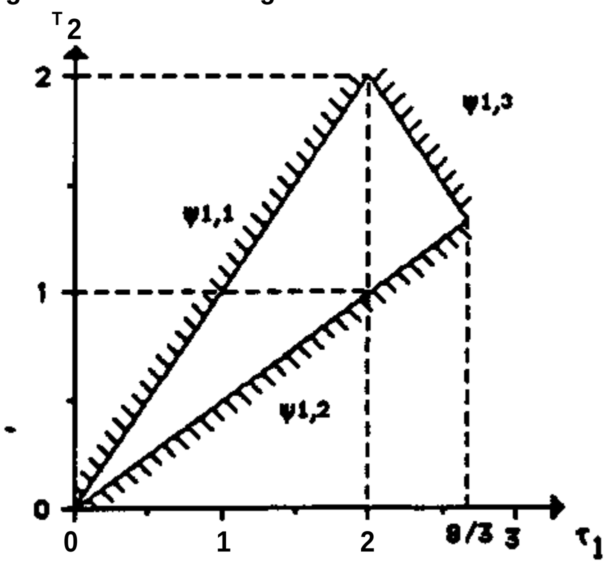

Figure 7. Feasible region for the example problem

Since the goal is to determine the location of the quadrature points in the feasible region, the constraints will be reduced further by eliminating x_2. The formulation for this problem is as follows.

$$\psi(d,\tau_1)^{2Jc}\text{-}\min_{u,\tau_2} u$$

$$\text{s.t. } -\tau_1+\tau_2 \le u$$

$$0.5\ Ti\sim\tau 2 \le u$$

$$t\,l+t\,H^* \qquad (16)$$

Here the multipliers are subject to the following equations.

$$\lambda_1{}^2+\lambda_2{}^2+\lambda_3{}^2=1 \qquad (17a)$$

$$\lambda_1{}^2-\lambda_2{}^2+\lambda_3{}^2=0 \qquad (17b)$$

$$\Sigma|\lambda_j{}^2|=2 \qquad (17c)$$

Again only two multipliers can be nonzero since the elimination of only one parameter is considered. Thus, there are two solutions X«|^2»^{1}«0.5 $X_2{}^2$»^{1}«0.5 and $X_2{}^2$»^{2}«0.5 X3^{2f2}-0.5. From these multipliers the second set of reduced constraints can be generated:

$$y2,1 \quad «0.5(y^{1,1}) \quad +0.5(Y^{1,2})$$
$$-0.25 \quad x\text{^}O \qquad (18a)$$

$$y2,2 \quad -0.5(y^1»^1) \quad +0.5(y^{1,3})$$
$$=0.75\tau_1-2\le 0 \qquad (18b)$$

These constraints lead to the bounds on x_1: 0£ x-| £ 8/3. Now, assume that one of the quadrature points for T-| turns out to be xi«2. Then from the first set of reduced constraints in (15) we get the following bounds on x_2.

$$\tau_2\le\tau_1 \quad \Rightarrow \quad \tau_2\le 2 \qquad (19a)$$

$$\tau_2\ge 0.5\ \tau_1 \quad \Rightarrow \quad \tau_2\ge 1 \qquad (19b)$$

$$\tau_2\le 4-\tau_1 \quad \Rightarrow \quad \tau_2\le 2 \qquad (19c)$$

Thus O^x^ 8/3 , and 1£ x_2^ 2 for x^*2 which are the correct bounds as shown in Figure 7. Having the bounds on x_2 it is clear that one can determine the corresponding quadrature points of x_2 at the value x«j«2.

For the general case the first step of the inequality reduction scheme is to eliminate the control variables z, so that just the uncertain parameters remain. This is accomplished by identifying the possible active ^constraints for the following formulation:

$$\psi(d^i,t) \quad \bullet \min_{zu} u$$

$$f_j(d^i,z,\tau)-u\le 0 \quad j\in J$$

$$(20)$$

The sets of active constraints are obtained from the optimality conditions of the problem:

$$\sum_j \lambda_j = 1$$

$$\sum_j \lambda_j \nabla_z f_j = 0$$

$$\lambda_j (f_j - u) = 0, \lambda_j \geq 0, f_j - u \leq 0 \; j \in J$$

$$\sum_j |\lambda_j| = \dim\{z\} + 1 \tag{21}$$

After determining the possible active sets they are labeled k=1,..,NAS(r). Having determined the active sets, the new constraints $\psi^{1,k} \leq 0$ can be generated using equation (13). The resulting constraints $\psi^{1,k}(d^i,\tau) \leq 0$ are important because they contain only d^i and τ as variables. Since the constraints are linear each $\psi^{1,k}$ can be rearranged into the following form.

$$\psi^{1,k}(d^i,\tau_1,\tau_2,\ldots,\tau_M) \Rightarrow \begin{array}{c} \tau_M \leq \xi_U^{1,k}(d^i,\tau_1,\tau_2,\ldots,\tau_{M-1}) \\ \text{or} \\ \tau_M \geq \xi_L^{1,k}(d^i,\tau_1,\tau_2,\ldots,\tau_{M-1}) \end{array} \quad k=1,\ldots,NAS(1) \tag{22}$$

If $d^i,\tau_1,\ldots,\tau_{M-1}$ are known then the bounds for τ_M can be determined by choosing the largest $\xi^{1,k}{}_L$ and the smallest $\xi^{1,k}{}_U$. In order to get bounds for τ_{M-1} the following formulation is applied by treating τ_M as a "control" variable:

$$\psi(d^i,\tau_1\ldots\tau_{M-1})^{2,k} = \min_{\tau_M u} u$$

$$\text{s.t. } \psi^{1,k}(d^i,\tau) - u \leq 0 \quad k=1,2,\ldots,NAS(1) \tag{23}$$

In this way by solving problem (23) the feasibility constraints $\psi^{2,k}$,k=1,2,...,NAS(2) can be determined, from:

$$\psi^{r,k'} = \sum_{j \in J_A^1(k')} \lambda_j^{r,k'} \psi_j^{r-1,k} \qquad k'=1,\ldots,NAS(r) \tag{24}$$

with r=2 and where the index k denotes the components of the inequalities for the reduction step r-1, and k' is the index of active sets of constraints in step r. Given $\psi^{2,k}$ the bounds on τ_{M-1} can be determined knowing $d,\tau_1,\tau_2,\ldots\tau_{M-2}$. This procedure can be repeated until the bounds for τ_1 are obtained in terms of d^i.

It is important to note that the actual bounds are not determined at this stage, only a set of inequalities for each parameter. The actual bounds are determined in reverse order of the reduction for each of the selected quadrature points. That is the variables are eliminated from M to 1, while the bounds are determined from 1 to M.

Numerical Integration for Determination of Stochastic Flexibility

Having applied the proposed inequality reduction scheme, the quadrature points are determined successively for the parameters $t_{1v}x_2 \ldots x_M$. These quadrature points will be represented in the following form $^{K\%}\backslash\ ^{>T}2$ $\bullet\bullet\bullet\bullet^{fT}M$ ' where q_m-$1_f \ldots {}_f QP_m$ corresponds to the index of the quadrature points for parameter x_m. Only one superscript is necessary to describe the x_1 coordinate of the point. But since the quadrature points for x_2 depend on t_1 that functionality must be expressed when describing the quadrature points for x_2. The quadrature points for x_m depend upon the values of $x_1, \ldots, x_{m-1}$ and thus must have m superscripts.

The indexing is best explained with Figure 8, where as ao example $(x_1^3, t_2^{3,1}$ Represents the first quadrature point for parameter x_2 which is based on the 3rd quadrature point of x_1.

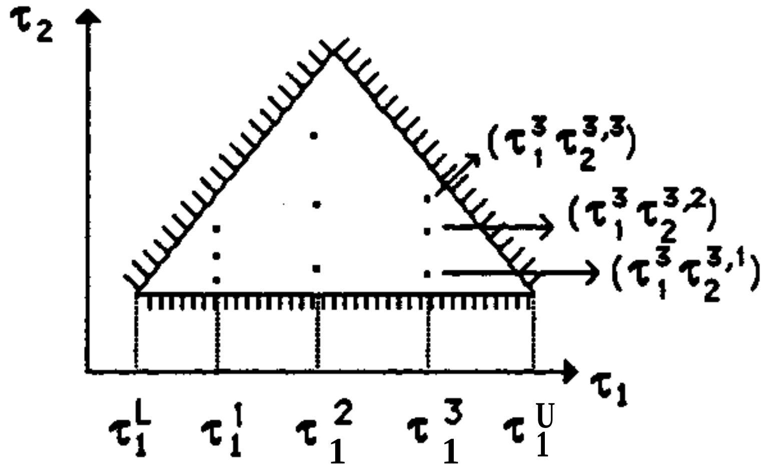

Figure 8 Demonstrating the indexing of the quadrature points.

As mentioned before the bounds $x\text{-}j^L, t_i^u$ are obtained in the last step of the reduction scheme. The quadrature points for t-| are then selected (e.g. $\tau_1^1, \tau_1^2, \tau_1^3$ in Fig. 8). The range of the second parameter is then determined at each discrete point in fusing the reduced inequalities $y^{M};^{1}>$, k«1,2,...,NAS(M-1). For the example in Fig. 7, the bounds for t_2 at the point x^are determined form the inequalities y^1-^{k}k-1,2.....NAS(1) evaluated at t^.

The general procedure for determining the quadrature points can then be summarized as follows:

1) Eliminate the control variables from fsO to yield y^1-^{k}≤;0, k-1.....NAS(1)
2) Eliminate x_M from y^1-^{k}s0 to yield y^2*s0. k-1.....NAS(2).
3) Repeat the elimination procedure until y^M-^{k}£0 k-1,2.....NAS(M) is obtained.

4) Use v^{M}'k£O , k-1,2.....NAS(M), to determine the bounds of x_1: x_1^{L} and x_1^{u} , and generate the discrete points $x^{\wedge 1}$ q1«1,....,QP(1)

5) Using yM-i.k^o , k«1,2.....NAS(M-1), and the discrete points $x^{\wedge 1}$, determine the bounds x_2^{L} $(x^{\wedge 1})$ and x_2^{u} $(T^{\wedge 1})$ of x_2 for each x^and then the discrete points $x_2^{<}i^{1}{}'^{\wedge 2}$ where q^-1......QP(1) and q_2-1.....,QP(2)

6) Repeat until y^{1}»^{k}^0 , k«1,2,...,NAS(1), is used along with $_{Ti}$<$I^{1}{}_{f}x_2$<IM2..... ^{x}Mi$^{q1vq2f,>MqM,,1\ t0}$ determine the ranges of x_M, and discretize each range of x_M.

After determining all of the quaflrature points the value of the joint distribution can be evaluated at each point and combined according the the quadrature formula, derived in Appendix C.

$$SF(S_i) = \frac{\tau_1 - \tau_1}{2} \sum_{ql=I} w_{1} \frac{\tau_2(\tau_1) - \tau_2(\tau_1)}{2} \sum_{q2=I} w \frac{\tau_3(\tau_1, \tau_2) - \tau_3(\tau_1, \tau_2)}{2} \cdots \sum_{qM=I} w_M\, j(\tau_1, \tau_2, \ldots, \tau_M^{q1,q2,\ldots,qM}) \qquad (25)$$

Remarks

There are several important points about the formulation in (25). First, the number of quadrature points does not have to be the same for each uncertain parameter. For instance the number of points for x_M can be much smaller than the number used for x_{1a} The reason for this is evident if the above procedure is viewed in terms of successively modifying the distributions of the uncertain parameters. This concept is shown in Figure 9. There are 2 continuous uncertainties, both described by normal distributions. The quadrature procedure essentially modifies the distribution of x^ using the feasible region and the distribution of t2- First the feasible region cuts off the distribution at the largest and smallest feasible values of t_1 ($x^{\wedge u}$ and x^). For each discrete point T_1 the integral of x_2's distribution over the feasible region is determined. This value(<1) then becomes a scale factor on x^s distribution. The outer dashed lines extend from the ends of the feasible region down to the representation of x^s distribution. These bounds define the point at which the modified distribution becomes 0. The dashed line in the center shows how a particular point is modified. The dashed line extends down to the value of x_1 at which the integral over x_2 is being determined. The integral value is then used to modify the distribution where the dashed line crosses it.

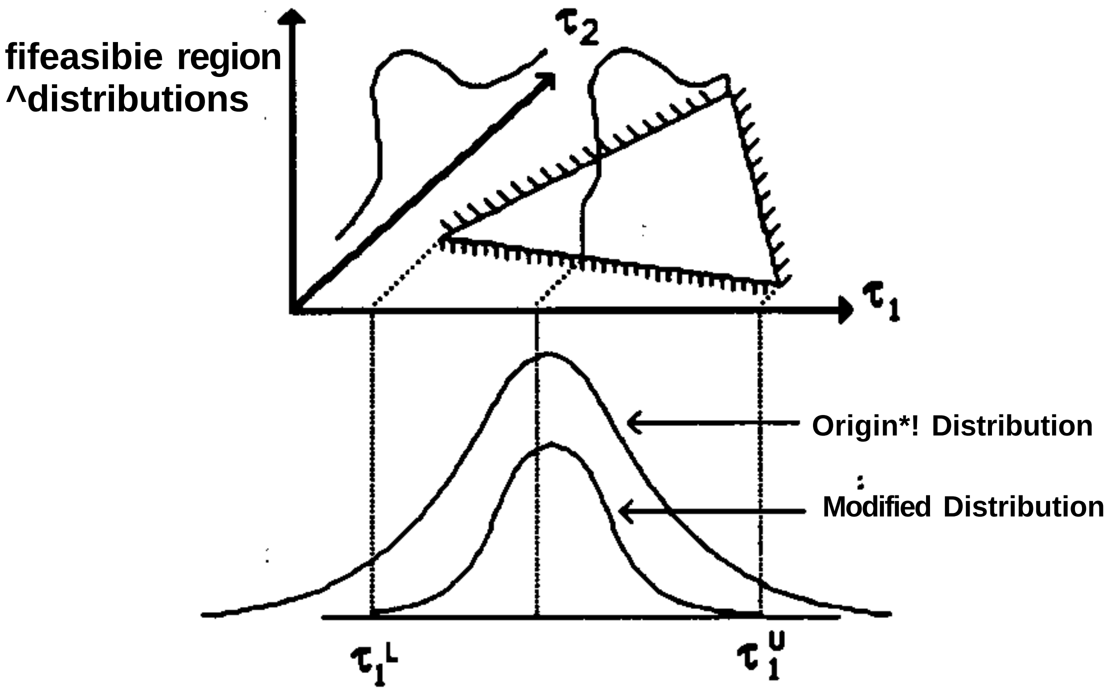

Figure 9 Modification of distribution

The more a distribution is modified the more irregular its shape can become and thus the more quadrature points are necessary to accurately characterize it.

Another important point is that the order in which the 6 are arranged is significant. For example consider the feasible region shown in Figure 10. Here the range of 82 is much smaller than that of e_{1a} Numerically by letting e_2-x_1 we are able to cover more area with the same number of quadrature points. At the present time this topic has not been investigated thoroughly and thus will not be discussed at length.

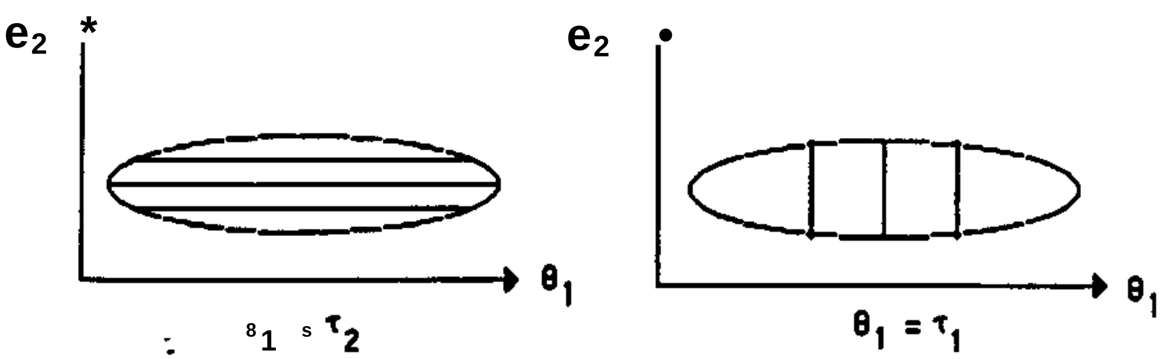

Figure 10 Showing the difference of order makes

This stochastic metric differs from other measures of flexibility in several ways. As opposed to the flexibility index (Swaney and Grossmann, 1985) it takes into account the entire feasible region. It also eliminates the problem of infeasible nominal conditions. Most importantly it takes into account uncertainty in the structure of the process, which is not accounted for in the flexibility index. It does not however, give an explicit range of feasible values like the flexibility index does.

Although other metrics have been developed to measure the integral over a region described by linear constraints, they are limited to continuous uncertainties characterized only by normal distributions (Pistikopoulos and Mazzuchi, 1989). The proposed stochastic flexibility is calculated using a method that allows the continuous uncertainties to be characterized by arbitrary distributions (e.g. normal, beta, uniform, beta).

Example 2

An example will now be presented to demonstrate the calculation of the stochastic flexibility with the proposed procedure. The state variables have already been eliminated resulting in four reduced inequality constraints. There is one control variable, two continuous uncertainties and two design variables.

$$f_1=z-1.6\ \theta_1\ -0.6\ \theta_2\ +d_1-14 \le 0 \tag{26a}$$
$$f_2=z-0.85\ \theta_1-0.925\ \theta_2+d_1+d_2-20\le 0 \tag{26b}$$
$$f_3=z-1.1\ \theta_1-1.4\ \theta_2+d_2-8\le 0 \tag{26c}$$
$$f_4=-z+\theta_1+\theta_2+d_2-7\le 0 \tag{26d}$$

The design variables for the corresponding state are assumed to be given by the values, $d_1=1$ and $d_2=8$. In this example we arbitrarily select $\theta_1=\tau_1$ and $\theta_2=\tau_2$. The continuous uncertainties are described by normal distributions with mean 20 and standard deviation 10: τ_1 N(20,10) and τ_2 N(20,10), they are not correlated. The joint distribution for the continuous uncertainties is shown below.

$$j(\tau_1,\tau_2)=\frac{1}{628.32}\exp\left[\frac{-(\tau_1-20)^2-(\tau_2-20)^2}{200}\right] \tag{27}$$

The first step is to eliminate the control variables from the constraints, eqn (26). Doing this results in 3 reduced constraints:

$$\psi^{1,1}=-0.3\ \tau_1\ +0.2\ \tau_2\ +d_1+0.5\ d_2\ -10.5\le 0 \tag{28a}$$
$$\psi^{1,2}=0.075\ \tau_1\ +0.0375\ \tau_2\ +d_1+d_2-13.5\le 0 \tag{28b}$$
$$\psi^{1,3}=-0.05\ \tau_1\ -0.2\ \tau_2\ +0.5\ d_1\ +d_2\ -7.5\le 0 \tag{28c}$$

These constraints define the feasible region in the space of the continuous uncertainties. The region is shown in Figure 11.

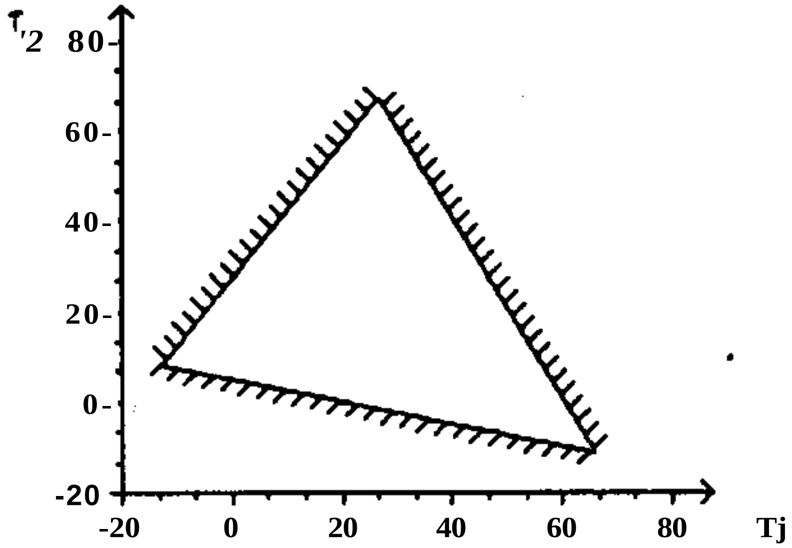

Figure 11 Feasible region

The first set of reduced constraints leads to the following bounds on τ_2, to which distribution constraints have been added to prevent integration over areas where $J(\tau_1,\tau_2)$ is negligible:

$$\tau_2 \geq (0.3\tau_1 - d_1 - 0.5 d_2 + 10.5)/0.2 \quad (29a)$$
$$\tau_2 \leq (13.5 - 0.075\tau_1 - d_1 - d_2)/0.0375 \quad (29b)$$
$$\tau_2 \geq (0.5 d_1 + d_2 - 0.05\tau_1 - 7.5)/0.2 \quad (29c)$$
$$\tau_2 \leq \tau_2^{nom} + 4\sigma_2 \quad (29d)$$
$$\tau_2 \geq \tau_2^{nom} - 4\sigma_2 \quad (29e)$$

Next τ_2 is eliminated from the feasibility constraints (28) using (23) to get the constraints in τ_1 space. The values of the design variables have been substituted into these equations.

$$g_{2,1}(d_1=1, d_2=8) = -0.875\tau_1 - 11.25 \leq 0 \quad (30a)$$
$$g_{2,2}(d_1=1, d_2=8) = 0.875\tau_1 - 57.5 \leq 0 \quad (30b)$$

This leads to the following bounds on τ_1, again adding the distribution constraints:

$$\tau_1 \geq -12.86 \quad (31a)$$
$$\tau_1 \leq 65.71 \quad (31b)$$
$$\tau_1 \leq \tau_1^{nom} + 4\sigma_1 = 60 \quad (31c)$$
$$\tau_1 \geq \tau_1^{nom} - 4\sigma_1 = -20 \quad (31d)$$

These inequalities give the following bounds on 1^.-1$2.86 \le \tau_1 \le 60$.

Having determined the bounds the quadrature can be evaluated. The specific equation that is used is shown below.

$$SF = \frac{\tau_1^U - \tau_1^L}{2} \sum_{q1=1}^{QP1} w_{q1} \frac{\tau_2^U(\tau_1^{q1}) - \tau_2^L(\tau_1^{q1})}{2} \sum_{q2=1}^{QP2} w_{q2} \; j(\tau_1^{q1}, \tau_2^{q1,q2}) \tag{32}$$

Given the range of x_1 the discrete points x ^ 1 can be determined. The discrete points are determined from v_{jf} the points in [-1,1] space, see Appendix C. The conversion to [x<|^L,Xi^u] space is accomplished with equation (33), using the data for five point quadrature shown below (Camahan etc 1969).

Table 1 Quadrature points and weights

	points	weights
qi	v_{a1}	w_{a1}
1	-0.90617	0.23693
2	-0.53846	0.47863
3	0.0000	0.56889
4	0.53846	0.47863
5	0.90617	0.23693

$$\tau_1^{q1} = \{v_{q1}(\tau_1^U - \tau_1^L) + \tau_1^U + \tau_1^L\}/2$$
$$-36.43 \quad v_{q1} + 23.57 \tag{33}$$

The resulting discrete points are shown in Table 2. For each τ_1^{q1} the range of *i<i* can be determined using (29), these ranges are also shown in Table 2.

Table 2 Ranges of x_2 for each τ_1^{q1}

qi	*1<1	V-	τ_2^U
1	•9.44	7.36	13.34
2	3.95	4.01	33.43
3	23.57	•0.89	60.00
4	43.19	-5.80	33.64
5	56.58	-9.15	6.84

Having determined the ranges for t_2 the discrete points can be generated in the same way than those that were generated for x^ The points are shown in Table 3 and also plotted on the feasible region in Figure 12.

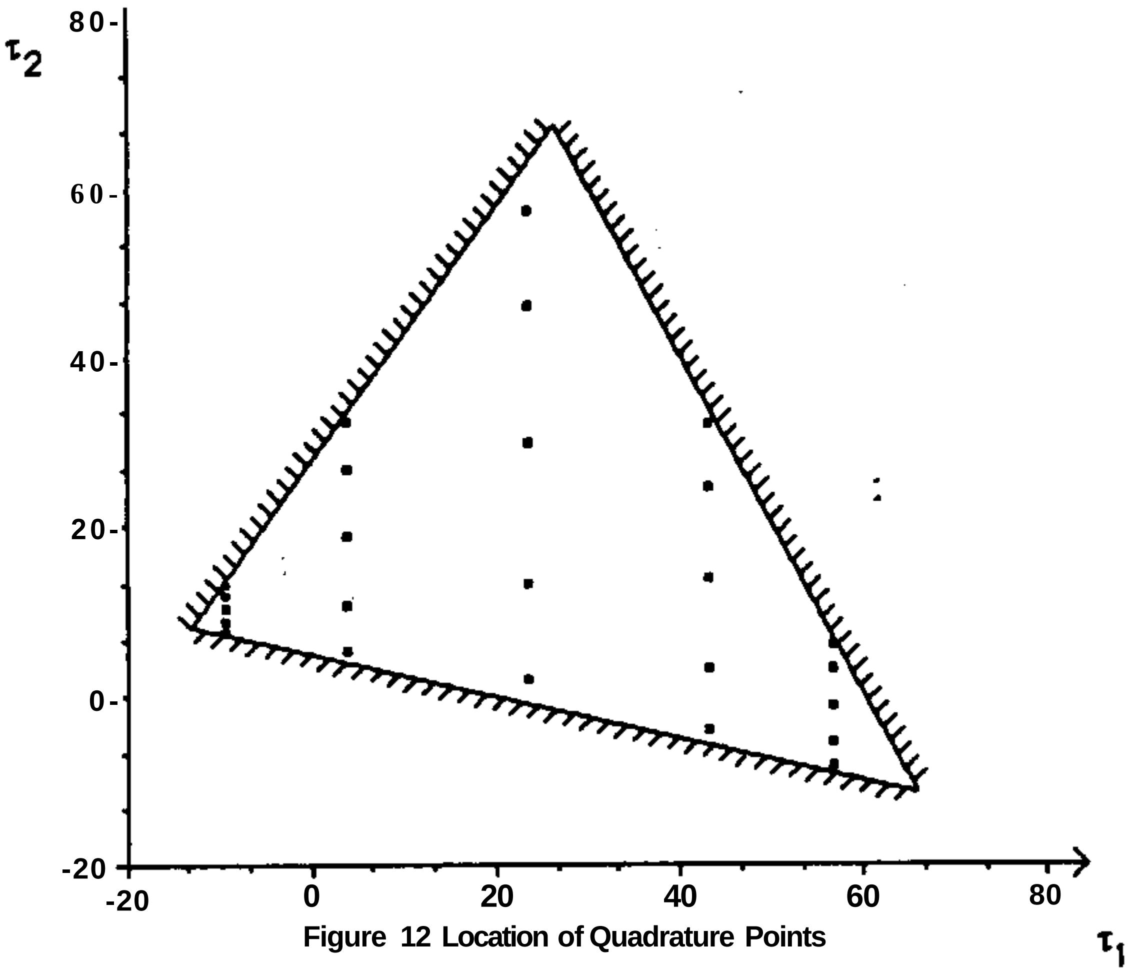

Figure 12 Location of Quadrature Points

Given the location of the quadrature points the joint distribution can be evaluated and then combined according the quadrature formula in (32). The calculations are summarized in Table 3. The first five columns contain the quadrature point data. The sixth and seventh contain the value of the joint distribution and the weights, while the eighth column contains the components of the inner summation. The last column contains the inner sum and is also shown in the second part of the table. The second part of the table contains the components of the outer summation.

Table 3 Summary of Calculations

Point	q1	q2	τ_1^{q1}	$\tau_2^{q1,q2}$	$f(\tau_1^{q1},\tau_2^{q1,q2})$	w_{q2}	w # j	$\sum w*j$ Q2
1	1	1	-9.44	7.64	9.72E-06	0.23693	2.30E-O6	
2	1	2	-9.44	8.74	1.11E-05	0.47863	5.30E-06	
3	1	3	-9.44	10.35	1.31E-05	0.56889	7.45E-06	
4	1	4	-9.44	11.96	1.51E-05	0.47863	723E-06	
5	1	5	-9.44	13.06	1.64E-05	023693	3.89E-06	2.62E-05
6	2I	1	3.95	5.39	1.51E-04	023693	3.58E-05	
7	2!	2	3.95	10.80	2.88E-04	0.47863	1.38E-04	
8	;!	3	3.95	18.72	4.36E-04	0.56889	2.48E-04	
9	2!	4	3.95	26.64	3.52E-04	0.47863	1.69E-04	
10	2I	5	3.95	32.05	2.13E-04	023693	5.03E-05	6.40E-04
11	2E	i	23.57	1.96	2.94E-04	023693	*.96E-05	
12	3;	2	23.57	13.16	1.18E-03	0.47863	5.66E-04	
13	3;	3	23.57	29.55	9.46E-04	0.56889	5.38E-04	
14	3E	4	23.57	45.95	5.15E-05	0.47863	2.47E-05	
15	3E	5	23.57	57.14	1.51E-06	023693	3.57E-07	120E-03
16	AI	1	43.19	-3.95	6.15E-06	023693	1.46E-06	
17	4;	2	43.19	3.30	2.68E-05	0.47863	128E-05	
18	4-	3	43.19	13.92	9.00E-05	0.56889	5.12E-05	
19	4.	4	43.19	24.53	9.77E-05	0.47863	4.68E-05	
20	4\	5	43.19	31.78	5.41 E-05	0.23693	128E-05	125E-04
21	5;	i	56.58	-8.40	3.51 E-08	023693	8.31 E-09	
22	S	2	56.58	-5.46	7.74E-08	0.47863	3.70E-08	
23	Si	3	56.58	-1.15	2.11E-07	0.56889	120E-07	
24	5	4	56.58	3.15	4.78E-07	0.47863	2.29E-07	
25	5	5	56.58	6.09	7.51E-07	0.23693	1.78E-07	5.72E-07

Table 3 continued

$\sum w*j$ q2	U τ_2^L	w_{q1}	Product
2.62E-05	2.988	023693	1.85E-05
6.40E-04	14.709	0.47863	4.51 E-03
120E-03	30.446	0.56889	2.08E-02
125E-04	19.712	0.47863	1.18E-03
5.72E-07	7.991	023693	1.08E-06

Sum- 2.65E-02

$\frac{\tau_1^U - \tau_1^L}{2}$ - 36.43

SF« 0.9641

The value of 0.964 was obtained using 5 point quadrature for both QP1 and QP2. The results for other QP1 and QP2 are shown in Table 4.

Table 4 Comparison of Results for various QP1 and QP2

QP1	QP2	Total Points	SF
3	3	9	1.157
3	5	15	1.200
3	7	21	1.208
5	3	15	0.937
5	5	25	0.964
5	7	35	0.969
7	3	21	0.939
7	5	35	0.950
7	7	49	0.954

These results show that the stochastic flexibility converges to ~0.95 as the number of quadrature points increases. This table also shows that for a fixed number of quadrature points the integral is more accurate if QP1>QP2.

The resulting SF=0.954 can be compared to two other methods of integration. The first being Monte Carlo simulation. Using a 1000 point sample a value of 0.948 was obtained for the stochastic flexibility. An IMSL, DQAND, routine was also adapted to the problem in a manner similar to the way eqn. (8) was written. In this case the upper and lower bounds were [-20, 60] and the absolute and relative errors were specified to be 0.01. The value obtained using this routine was 0.951. The percent difference between the largest and the smallest is only 1.68%. This indicates that the proposed method produces results that are in line with other methods.

Finally it is important to compare the number of function evaluations necessary to solve the problem. This data is shown in Table 5.

Table 5 Comparison of Various Methods

Method	SF	Function Evaluations
Proposed	0.954	49
IMSL	0.951	~1500
MC	0.948	1000
MC	0.952	10,000

It is clear that the proposed method is superior to both Monte Carlo and the adapted IMSL routine. Recall that a function evaluation in the method of this paper only requires the evaluation of the joint distribution at the quadrature point. The other two methods are more complicated in terms of the function evaluation. Both methods generate values of θ^* for which it is necessary it is necessary to determine if θ^* lies within the feasible region. This is accomplished using the same math program that was used in the equality reduction scheme, only here G replaces x (there is no concept of an order of integration for either method):

$$V=\min_{zu} u$$
$$s.t.fj(d\backslash z,e^{*})*u \quad j€j \qquad (34)$$

The solution to this problem indicates the feasibility, if y£0 then $e^{\#}$ lies within the feasible region, otherwise if y>0 then e* lies outside the feasible region. Note that (34) differs from (20) in that e* is known in (34) but t is not known in (20). This makes (34) easier to solve than (20). But it is also important to note that (34) must be solved for each function evaluation whereas (34) is solved only once in the inequality reduction portion of the proposed methods. Thus (20) is not solved for each quadrature point.

Expected Stochastic Flexibility

As mentioned previously in the paper there are two components involved in the calculation of the expected stochastic flexibility: first the stochastic flexibility for a given state that is determined from (25), and second the state probability that is computed from equation (4). Given the state probabilities and the stochastic flexibility for each state the E(SF) can be calculated as follows.

$$E(SF)=\sum_{i=1}^{L} SF(S_i)*P(S_i) \qquad (35)$$

The E(SF) represents the average stochastic flexibility we would measure over the long run.
The summation however may involve a large number of terms even for small number of units, (e.g. 1024 states for L«10 units). In order to prevent the evaluation of the SF for a large number of states, lower and upper bounds can be developed for the E(SF) as follows.

The basis for the bounding procedure is first the fact that the feasible region gets smaller as the number of active states decreases. Or mathematically $SF(S_a)£SF(S_b)$ for S5 c S_a and $n_A(S_a)>n_A(S_b)$ where $n_A(S)$ is the number of active components in system state S-,. The second fact is that for most common systems p/>0.5, which implies that the probability of a unit being available is larger than when it is unavailable. This would then suggest that a reasonably tight lower bound can be obtained by considering a partial summation of (35) that includes those states with the highest number of active of components. A valid upper bound can be obtained by adding to the partial summation the probability of the remaining terms multiplied by a SF_{max} which is larger than any SF in the truncated part of the summation. More specifically assume that the partial summation is evaluated for L, L-1,..., n_A active components. Based on the properties of the SF, the SF with n_A active components bounds the SF for n_A-1 acitve components. But recall there may be more than one state with n_A-1 in the truncated part of the summation, thus there may be a large number of states in level n_A. Thus, to ensure a rigorous upper bound the largest SF in level n_A is used.

To illustrate more clearly the idea behind the proposed bounding scheme, assume that there are four possible states with $n_A(S_1)$-3, $n_A(S_2)$-2, $n_A(S_3)$-2, $n_A(S_4)$-1. The expected stochastic flexibility for this case is as follows.

$$E(SF)-SF(S_1)*P\{S_1)+SF(S2)*P(S2)+SF(S3)^{\#}P(S3)_{+}SF(S_4)*P(S4) \qquad (36)$$

The lower bound for a one term approximation (n_A«3) is obtained by truncating the summation.

$$LB-SF(S_1)*P(S_1) \qquad (37)$$

The upper bound is obtained by selecting for the truncated part of the summation the largest SF in the level n_A-3, that is $SF(S_1)$.

$$UB-SF(S_1)*P(S_1)+SF(S_1)*(P(S_2)+P(S_3)+P(S4)) \qquad (38)$$

Note that the bounds in (37) and (38) only require the evaluation of SFfS^.

The bounds for three terms would then be as follows:

$$LB-SF(S_1)^{\#}P(S_1)+SF(S2)*P(S2)+SF(S_3)*P(S_3) \qquad (39)$$

$$UB-SF(S_1)*P(S_1)+SF(S_2)*P<S_2)+SF(S3)^{\#}P(S3) +P(S_4)*(\max \{SF(S_2),\ SF(S_3)\}) \qquad (40)$$

The bounding procedure can then be stated in general as follows. Let nj be the number of inactive components. Then, there are LI/{(L-n_I)I njl} states that exhibit the same number of active units for fixed rij. Thus, the following bounding scheme can be developed:

1) Set n_r0,Ns«1.
2) Let N-LI/ttL-nj)! n^}
3) Evaluate the stochastic flexibility SF(Sj) for i-Ns.Ns+N-1 .
4) Evaluate the lower and upper bounds:

$$LB=\sum^{N} SF(Si)*P(Sj) \qquad (41a)$$

$$UB=LB+SF_{mmx}» \sum_{i,,N+1}^{2^L} P(S_j) \qquad (41b)$$

where SFmax-max (SF(Sj)} for I-Ns.Ns+N-1

5) If UB-LB<e stop. Otherwise set Ns-N+Ns, $n_r n_{I+}1$, if Ns£2^L go to step 2; otherwise stop.

Several modifications to this procedure are discussed in Appendix D. These modifications allow the upper bound to be tightened significantly by taking advantage of the relationship between the states and substates.

Example 3

In this example the expected stochastic flexibility of a chemical complex will be determined. The system, shown in Figure 6, converts species A to C by two different processes. The first involves plants 1 and 2 (in parallel) for the production of intermediate B, and plant 3 for converting B to C. The second process involves plant 4, producing C directly from A. Uncertainties are assumed in the supply of raw material A (continuous), the demand of product C (continuous) and in the availability of the four processes (discrete).

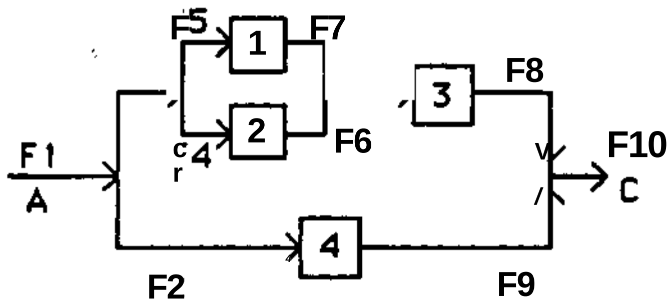

Figure 6 Chemical complex

The variables and parameters used to model this system are given below.

F	Molar flow rates
a	Conversion factors
d	Processing capacity
S	Supply of A
D	Demand for C
y	Boolean variable representing the availability of the plants (1 if available, 0 if unavailable)

The equations used to model the system are as follows.

Mass Balance	Specifications
$F_1 = F_2 \; F_3$	$F_5 \leq d_1 \, y_1$
$F_3 = F_4 + F_5$	$F_6 \leq d_2 \, y_2$
$F_{10} = F_8 + F_9$	$F_3 \leq d_3 \, y_3$
$F_7 = \alpha_1 \, F_5$	$F_2 \leq d_4 \, y_4$
$F_6 = \alpha_2 \, F_4$	$F_1 \leq S$
$F_8 = \alpha_3 \, (F_6 + F_7)$	$F_{10} \geq D$
$F_9 = \alpha_4 \, F_2$	

(42)

The variables are classified as follows

State variables	$F_2, F_4, F_6, F_7, F_8, F_9, F_{10}$
Control variables	F_1, F_3, F_5

Uncertain continuous parameters	D and S
Uncertain discrete states	y

Solving the mass balances for the state variables and eliminating them in the specifications the following set of reduced inequalities is obtained.

$$
\begin{aligned}
f_1:&\quad F_5-d_1\ y_1\leq 0\\
f_2:&\quad F_3-F_5-(d_2/\alpha_1)\ y_2\leq 0\\
f_3:&\quad F_3-d_3\ y_3\leq 0\\
f_4:&\quad F_1-F_3-d_4\ y_4\leq 0\\
f_5:&\quad F_1\ -S\leq 0\\
f_6:&\quad D-\ \alpha_4\ F_1-(\alpha_1{}^*\alpha_3-\alpha_4)\ F_3\leq 0
\end{aligned}
\tag{43}
$$

Table 6 Data for Example 1.

Supply of A	$S^N=12$	$\sigma_A=1\ \Rightarrow$	$N(12,1)$	
Demand	$D^N=7$	$\sigma_D=1\ \Rightarrow$	$N(12,1)$	
Probability of operation	$p_1=0.95$	$p_2=0.95$	$p_3=0.92$	$p_4=0.87$
Mass balance coefficients	$\alpha_1=0.9$	$\alpha_3=0.8$	$\alpha_4=0.7$	
Processing Capacity	$d_1=5$	$d_2=3.5$	$d_3=7$	$d_4=7$

Given this data we can generate the first set of reduced constraints by eliminating the control variables.

$$
\begin{aligned}
&\psi^{1,1}=\ D\leq 13.12\ y_1\ +13.80\ y_2\ +\ 12.75\ y_4\\
&\psi^{1,2}=D\leq 0.36\ \ y_1+0.38\ \ y_2\ \ +21.25\ \ y_3+12.75\ \ y_4\\
&\psi^{1,3}=D-0.85\ \ S\leq 0.36\ \ y_1+0.38\ \ y_2\\
&\psi^{1,4}=D\leq 12.75\ \ y_1+13.42\ \ y_2+0.60\ \ y_3+12.75\ \ y_4\\
&\psi^{1,5}=D\leq 21.85\ \ y_3+12.75\ \ y_4\\
&\psi^{1,6}=D-0.85\ \ S\leq 0.60\ \ y_3\\
&\psi^{1,7}=D\leq D_U\\
&\psi^{1,8}=-D\leq -D_L\\
&\psi^{1,9}=S\leq S_U\\
&\psi^{1,10}=-S\leq -S_L
\end{aligned}
\tag{44}
$$

Note that bounds on the continuous uncertain parameters have been added to this list of constraints. This has been done to prevent unbounded regions. It also prevents quadrature points from being placed where the probability distribution is negligable. The bounds depend on the distribution being used, for example, with a normal distribution the bounds might be the nominal point ± 4 sigma. In this problem $D=\tau_1$ and $S=\tau_2$, thus S should be eliminated from the first set of reduced constraints. All the equations that do not contain S are automatically a part of the second set of reduced constraints, only the inequalities that involve S are part of the inequality reduction scheme.

y2,1- DS13.12 i\ +13.80 y_2 + 12.75 y_4
y2.2-DS0.36 y_{1+}0.38 y_2 +21.25 y_3+12.75 y_4
y2,3=DS12.7K +13.42 y_2+0.60 y_3+12.75 y_4
y2,4=D≤21.85 y_3+12.75 y_4
y2,5-DS0.36 y^O.38 y_2 +0.85 S_U
y2,6-Ds0.60 y_3 +0.85 S_y
y2,7-DsDu
y2,8—DS-D_L (45)

Having both sets of reduced inequalities the E(SF) can be determined. The results using 7 point quadrature for both continuous uncertainties is shown in Table 7.

Table 7 Summary of results for calculation of Expected Stochastic Flexibility

State	y1	y2	y3	y4	SF(Si)	P(Si)	P*SF
1	1	1	1	1	0.9897	0.7224	0.7149
2	1	1	1	0	0.1894	0.1079	0.0204
3	1	1	0	1	0.1472	0.0628	0.0092
4	1	1	0	0	0.0000	0.0094	0.0000
5	1	0	1	1	0.9891	0.0380	0.0376
6	1	0	1	0	0.0043	0.0057	0.0000
7	1	0	0	1	0.1472	0.0033	0.0005
8	1	0	0	0	0.0000	0.0005	0.0000
9	0	1	1	1	0.9839	0.0380	0.0374
10	0	1	1	0	0.00005	0.0057	0.0000
11	0	1	0	1	0.1472	0.0033	0.0005
12	0	1	0	0	0.0000	0.0005	0.0000
13	0	0	1	1	0.1472	0.0020	0.0003
14	0	0	1	0	0.0000	0.0003	0.0000
15	0	0	0	1	0.1472	0.0002	0.0000
16	0	0	0	0	0.0000	0.0000	0.0000
							0.8209

The expected stochastic flexibility is 0.8209. This means that the chemical complex in Figure 6 has an 82.09% probability of feasible operation.

Although this is a small example assume that it is desired to compute bounds on the expected stochastic flexibility. For example, with nj-0 the following bounds are obtained.

LB=0.9897*0.7224-0.7149 (46a)
UB-0.7149+0.2776*0.9897-0.9897 (46b)

Using nj«1

LB=(0.7224*0.9897)+(0.1079*0.1894)+(0.0628*0.1472)
* +(0.0380*0.9891)+(0.0380*0.9839)
-0.8196 (47a)
UB-0.8196+(0.9891 *(1 -0.9692))
-0.8501 (47b)

Thus after evaluating 4 out of the 16 states the bounds on the E(SF) are fairly tight, 0.8196£E(SF)£0.8501. As discussed in Appendix D, a modified bounding scheme can be used to further tighten these bounds to 0.8199sE(SF)$0.8233.

This example also brings out several important points. First, if only the stochastic flexibility were calculated a value of 0.9897 would have been obtained for the state in which all components are active. On the other hand for the given probabilities for the availability in Table 6. and using the standard equations for reliability (Shooman 1969), the predicted reliability for the system is 0.9893. These two metrics by themselves are somewhat misleading because when the interaction between the continuous and discrete uncertainties are taken into account a much less optimistic probability of feasible operation, 0.8209, is obtained. The reason is that the states in which some equipment has failed do not have enough capacity to meet the demand. This is evident if the E(SF) is compared to the SF for the case when all states are active, 0.8209:0.9897. This dearly indicates that the system has difficulty tolerating the discrete uncertainties.

It is interesting to note that if the capacity of units 3 and 4 are increased from 7 to 10, the E(SF)«0.9356, which is a significant improvement.

Conclusions

This paper has presented a new measure for process operability: the expected stochastic flexibility. This measure provides a framework for integrating flexibility and reliability under a common framework where interactions between these two aspects can be taken into account.

As has been shown, the integration over the continuous parameters can be performed effectively with an inequality reduction scheme whose computational expense is small for linear constraints. Also, a bounding procedure has been suggested that avoids the examination of a large number of states.

Finally, the example problem has shown not only the computational feasibility of the proposed measure, but also the fact that it provides more complete information that when flexibility and reliability are treated as separate measures.

ACKNOWLEDGMENTT

The authors would like to acknowledge financial support for this work under grants NSF:CPE-8351237 and DOE:DE-FG-02-85ER 13396.

REFERENCES

Carnahan, B., Luther, H.A. **and** Wilkes, J.O.,"Applied Numerical Methods." Wiley New York **(1969).**

Dhillon, B. S. **and** Rayapati, S. N., "Chemical-System Reliability: A Review," IEEE **Trans. Rel., Vol. 37.** 199 (1988).

Qrossmann. I. E. **and** Floudas, C. A., "Active Constraint Strategy for Flexibility Analysis in Chemical Processes," **Comp. Chem.** Eng., **Vol.** 11, 675 (1987).

Qrossmann, I.E. **and** Morari, M., "Operability, Resiliency and Flexibility-Process Design Objectives for **a** Changing World"

Henley, E.J. **and** Qandhi, S.L, "Process Reliability Analysis." **AlChE J., Vol. 21,** 677 (1975)

Hwang, C. L, Tillman, F. A. **and** Lee, M. H., "System-Reliability Evaluation Techniques for Complex Large Systems-A Review," IEEE **Trans. Rel.,** R-30, 416 (1981).

IMSL Math/Library, Vol 2 Chapter 4, pp 604-606 (1987)

Lapin, L.L., "Probability and Statistics for Modern Engineering," Brooks/Cole Monterey CA., (1983).

Pistikopoulos, E.N. and Mazzuchi, T.A., "A New Flexibility Index for Processes with Stochastic Parameters," To be presented at Annual AlChE Meeting San Francisco (1989).

Saboo, A.K., and Morari.M., "Design of Resilient Processing Plants-IV," **Chem. Eng.** Sci., **Vol 39,** 579 (1984).

Swaney, R. E. and Grossmann, I. E. "An Index for Operational Flexibility in Chemical Process Design. Part 1 Formulation and Theory," **AlChE J., Vol. 31,** 621 (1985).

Swaney, R. E. and Qrossmann, I. E. "An Index for Operational Flexibility in Chemical Process Design. Part 2 Computational Algorithms," **AlChE J., Vol. 31,** 631 (1985).

Shooman, M. L, Probabilistic Reliability:An Engineering Approach. McGraw-Hill, New York (1968).

Van Rijn, Cyp F.H., "A Systems Engineering Approach to Reliability, Availability and Maintance," Presented at the Conference on Foundations of Computer Aided Operations, FOCAPO, Salt Lake City (1987).

Appendix A Determination of p_ℓ

For each piece of equipment that is to be considered uncertain a probability that the equipment will be available is needed. A simple approach to this is to use mean time to failure (MTTF) and mean time to repair (MTTR) data. Given this data the probability necessary is given by the following expression.

$$p = \frac{MTTF}{MTTF+MTTR} \qquad (A1)$$

This measure is discussed by Van Rijn (1987). He also discusses more complicated models.

Appendix B Reduction of the Constraints

An important part of the integration method is the reduction scheme for the constraints; that is eliminating variables from the constraints while maintaining the same feasible region in the space of those variables that were not eliminated. The variables that will be eliminated are the control variables and the uncertain parameters.

The formulation used to accomplish the elimination is shown below.

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

$$\text{s.t.}\; f_j(d,z,\tau) - u \leq 0 \quad j \in J \qquad \text{(B1)}$$

It is important to note that the parametric solution is not just a term but part of an inequality of the form $y \leq 0$. Although initially it looks as if the optimizations in (B1) are being replaced with equally difficult problems, this is not the case. The optimization shown above can be solved quite simply once the active sets are determined (Grossmann and Floudas, 1987). An active set is the set of indices of the constraints that are active, $f_j = 0$. The active sets are determined from the optimality conditions. The mathematics of the solution will be discussed after motivating the formulation of equation (B1).

The basic idea of the formulation is best described graphically. Consider the feasible region shown in Figure B1. In this system there is one control variable and one uncertain parameter t.

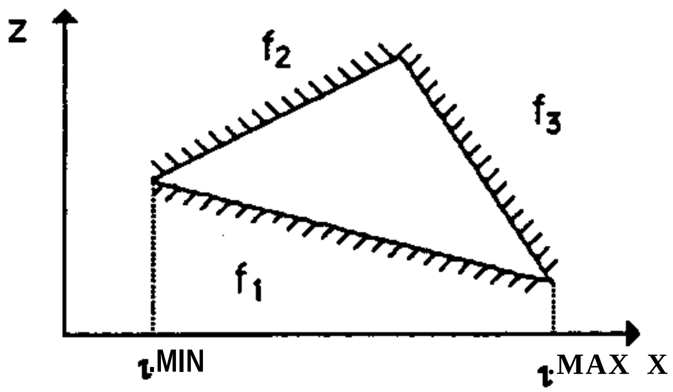

Figure B1 Feasible Region for one control and one parameter

This figure shows the feasible region in z x space. The purpose of the formulation is to eliminate z from the constraints, resulting in reduced constraints that define the feasible region in x space. That is, the reduced constraints would define the following feasible region $x_{min} \leq x \leq x_{max}$.

In order to understand the formulation one must consider the third dimension f, the value of the constraints. Since $f \leq 0$ for feasibility, the feasible region is the interval in which the value of all 3 constraints are less than zero. Outside the feasible region at least one of the constraints is greater than zero. Crossections for a x:T^t_{mjn} and t:t_{mjr}^T5t_{max} are shown in Figures B3 and B4.

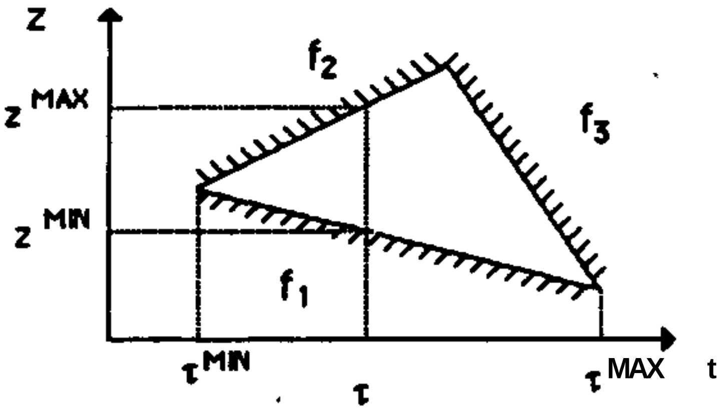

Figure B2 Feasible Region in t-z space.

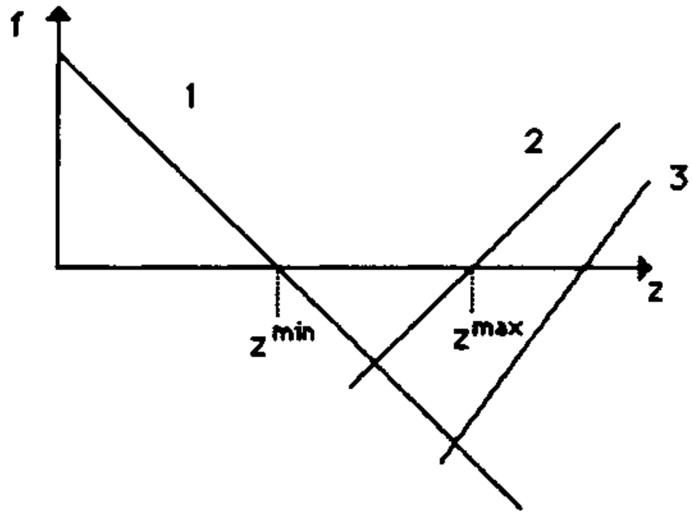

Figure B3 Crossection for $x{:}\tau_{min}\leq\tau\leq\tau_{max}$

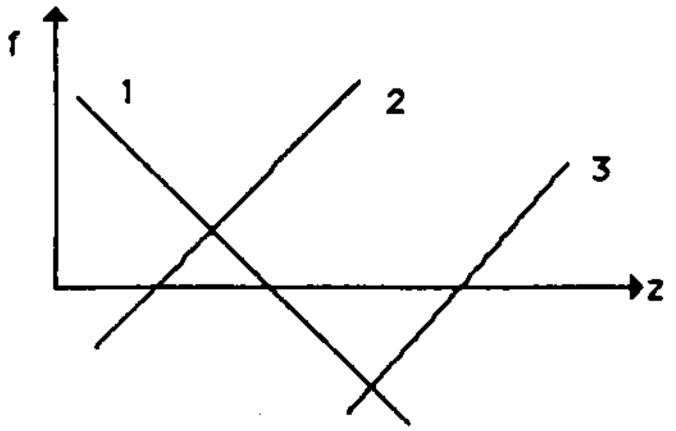

Figure B4 Crossection for x:x£xmjn

In Figure B3 the region between zmin and zmax is a non-empty feasible region since all 3 constraints are less than zero. In Figure B4 there is no feasible region since there is no value of z which results in all 3 constraints being less than zero.

The formulation for the reduced constraints tries to minimize u, the value of the largest constraint. Figure B5 shows the value of u for the crossection in Figure B3.

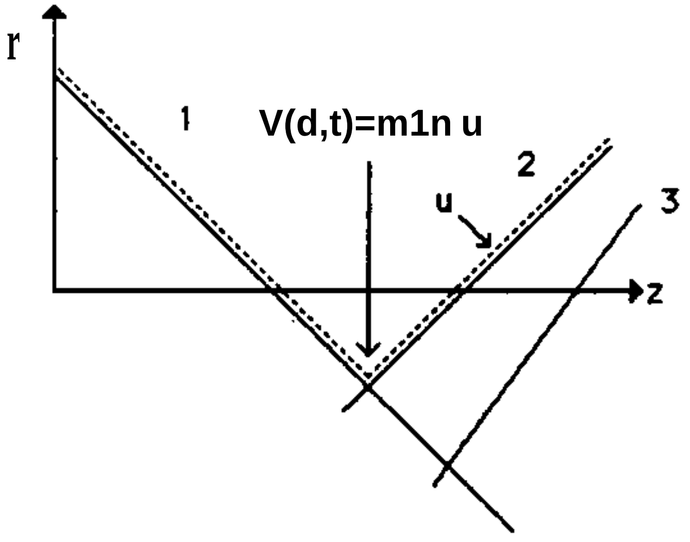

Figure B5 Crossection showing the value of u and the solution y

For given x and d the formulation searches for the smallest value of u along z, the point at which the largest constraint is minimized. This value of u is the solution to the optimization problem at t.
Although a particular! was chosen to demonstrate how y is obtained when solving the problem it is not necessary to choose a particular x. The solution can be generated in terms of x by knowing what

constraints give rise to u, i.e. the active constraints. In this problem there are actually two sets of active constraints, a crossection for τ close to τ_{max} might look like Figure B6.

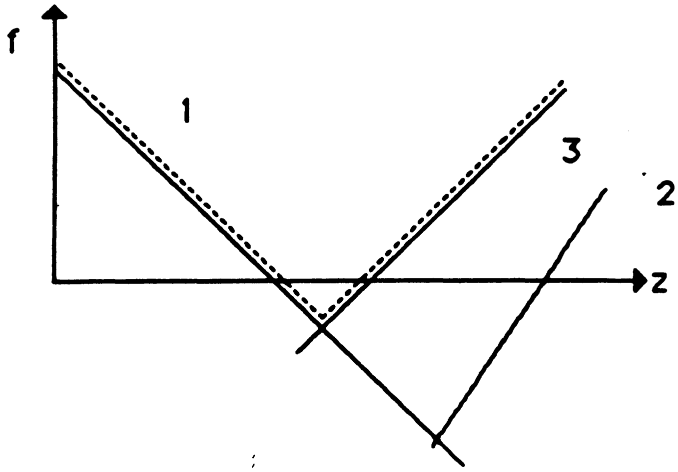

Figure B6 Crossection for τ close to τ_{max}

In this case the active constraints are 1 and 3. For this problem these are the only two active sets. The only other possible combination would be 2 and 3. The problem with 2 and 3 is that the sign of their slope is the same, which would result in $u=-\infty$ for all τ. This means that all τ are feasible, in this case determination of bounds is meaningless.

Each active set (1,2) and (1,3) will give rise to a different function $\psi(d,\tau)$. These two ψ are shown in Figure B7.

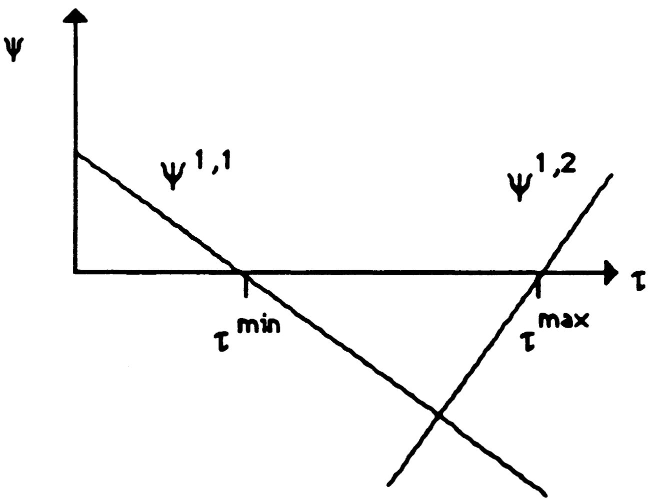

Figure B7 Plot of ψ for the two sets of active constraints

As shown the ψ maintain the same feasible region in the τ space. It might appear that Figure B7 is incorrect since it shows two values of ψ for any value of τ. Actually it is just the larger value that is ψ, the lower value is simply the intersection of the constraints that are not active. For example, the intersection of 1 and 2 in Figure B6 gives rise to the lower values of y in Figure B7 for t to the right of the intersection.

To summarize the control variable z has been eliminated from the constraints while still maintaining the feasible region in t space. Note that the control variable could just as well have been another continuous parameter uncertainty.

Mathematical Formulation

Having motivated the formulation in equation (B1) an outline of the derivation of y will be presented.

For constrained optimization problems the solution (y) can be written in terms of the Lagrangian of the problem. For the general problem in equation (B2);

*

$$\begin{array}{c} \min f(x) \\ \text{s.t.}\, g(x)£0 \end{array} \tag{B2}$$

the lagrangian can be written as follows:

$$L=f(x)+\sum_{j=1}^{m} £x_{j}g_{j} \tag{B3}$$

The multipliers Xj are obtained from the optimality conditions for this problem

$$Vf(x)+5>jV_{gj}(x)=0 \quad j \tag{B4}$$

The derivative is taken with respect to each degree of freedom, the variables over which the optimization is performed. The other optimality conditions are called the complementarity conditions. They specify that only active constraints can have X£0, inactive constraints must have X*0.

*j(gp-O. Xj*O, QjSO, je J (B5)

In equation the function f(x)»u,gj«fj-u, and the degrees of freedom are z and u. Thus the Lagrangian can be written as follows for our problem.

$$L=u+\sum_{i-1} (f_j-u) \tag{B6}$$

The optimality conditions thus yield the following:

$$\nabla_u u+\sum_j \lambda_j \nabla_u (f_j-u)=0 \Rightarrow 1+\sum_j \lambda_j (-1)=0 \Rightarrow \sum_i \lambda_j =1 \tag{B7}$$

$$\nabla_z u+\sum_j \lambda_j \nabla_z (f_j-u)=0 \Rightarrow \mathrm{ZWro}_{i} \tag{B8}$$

$$\lambda_j(f_j - u) = 0$$ (B9)

Using equation (B6) the Lagrangian can be simplified as follows:

$$L = u + \sum_{j=1} \lambda_j (f_j - u)$$

$$= u + \sum_{j=1} \lambda_j f_j - u \sum_{j=1} \lambda_j$$

$$= u + \sum_{j=1} \lambda_j f_j - u$$

$$= \sum_{j=1} \lambda_j f_j$$ (B10)

It can also be shown that the number of X that are active is equal to the number of variables being eliminated +1(see Swaney and Grossmann, 1985), thus:

$$Z|X|-\dim\{z\}+1$$ (B11)

here \\\~*0* if JUO and |X|-1 if X>0.

The solution to the problem can then be written as follows:

$$\psi = \sum_{J} \lambda_j f_j$$ (B12)

the conditions on the multipliers are subject to the following equations:

$$\sum_j \lambda_j = 1$$

$$\sum_j \lambda_j \nabla_z f_j = 0$$

$$\lambda_j (f_j - u) = 0 \quad j \in J$$

$$\sum_j |\lambda_j| = \dim\{z\} + 1$$ (B13)

Appendix C Derivation of Quadrature Formula

The stochastic flexibility is described by the following integral.

$$SF(S_i) = \int_{\tau_1^L}^{\tau_1^U} \int_{\tau_2^L(\tau_1)}^{\tau_2^U(\tau_1)} \cdots \int_{\tau_M^L(\tau_1,\tau_2,\ldots,\tau_{M-1})}^{\tau_M^U(\tau_1,\tau_2,\ldots,\tau_{M-1})} j(\tau)\, d\tau_M \ldots d\tau_2\, d\tau_1 \qquad (C1)$$

Guassian Quadrature will be used to solve the integral. The guassian quadrature formula to be used is shown below.

$$\int_a^b f(x)\, dx = \frac{b-a}{2} \sum_{i=1}^{n} w_i\, f\left(\frac{\gamma_i (b-a)+b+a}{2}\right) \qquad (C2)$$

where γ_i is the location of the quadrature point in (-1,1] space, and w_i is the weight of the quadrature point.

The first step to solve the stochastic flexibility integral is to define the inner integral as a variable that depends on x_1.

$$G(\tau_1) = \int_{\tau_2^L(\tau_1)}^{\tau_2^U(\tau_1)} \cdots \int_{\tau_M^L(\tau_1,\tau_2,\ldots,\tau_{M-1})}^{\tau_M^U(\tau_1,\tau_2,\ldots,\tau_{M-1})} j(\tau)\, d\tau_M \ldots d\tau_2 \qquad (C3)$$

Thus the SF can be written.

$$SF(S_i) = \int_{\tau_1^L}^{\tau_1^U} G(\tau_1)\, d\tau_1 \qquad (C4)$$

The guassian quadrature formula can be applied to this resulting in the following.

$$SF(S_i) = \frac{\tau_1^U - \tau_1^L}{2} \sum_{q1=1}^{QP1} G(\tau_1^{q1})\, w_{q1} \quad \text{where} \quad \tau_1^{q1} = \frac{\gamma_{q1}(\tau_1^U - \tau_1^L) + \tau_1^U + \tau_1^L}{2} \qquad (C5)$$

Next the quadrature formula is applied to the second integral.

$$G(\tau_1^{q1}) = \int_{\tau_2^L(\tau_1^{q1})}^{\tau_2^U(\tau_1^{q1})} H(\tau_2)\, d\tau_2$$

$$= \frac{\tau_2^U(\tau_1^{q1}) - \tau_2^L(\tau_1^{q1})}{2} \sum_{q2=1}^{QP2} H(\tau_2^{q1,q2})\, w_{q2} \qquad (C6)$$

This procedure can be repeated until the last integral is put into quadrature formula.

$$I(\tau_1^{q1},\tau_2^{q1,q2},\ldots,\tau_{M-1}^{q1,q2,\ldots,qM-1}) = \int_{\tau_M^L(\tau_1^{q1},\tau_2^{q1,q2},\ldots,\tau_{M-1}^{q1,q2,\ldots,qM-1})}^{\tau_M^U(\tau_1^{q1},\tau_2^{q1,q2},\ldots,\tau_{M-1}^{q1,q2,\ldots,qM-1})} j(\tau)\, d\tau_M$$

$$= \frac{\tau_M^U(\tau_1^{q1},\tau_2^{q1,q2},\ldots,\tau_{M-1}^{q1,q2,\ldots,qM-1}) - \tau_M^L(\tau_1^{q1},\tau_2^{q1,q2},\ldots,\tau_{M-1}^{q1,q2,\ldots,qM-1})}{2} \sum_{qM=1}^{QPM} j(\tau_1^{q1},\tau_2^{q1,q2},\ldots,\tau_M^{q1,q2,\ldots,qM-1})\, w_{qM} \tag{C7}$$

Thus the stochastic flexibility can be written in the following form.

$$SF(S_i) = \frac{\tau_1^U - \tau_1^L}{2} \sum_{q1=1}^{QP1} w_{q1} \left[\frac{\tau_2^U(\tau_1^{q1}) - \tau_2^L(\tau_1^{q1})}{2}\right] \sum_{q2=1}^{QP2} w_{q2} \frac{\tau_3^U(\tau_1^{q1},\tau_2^{q1,q2}) - \tau_3^L(\tau_1^{q1},\tau_2^{q1,q2})}{2} \cdots$$

$$\cdots \left[\frac{\tau_M^U(\tau_1^{q1},\tau_2^{q1,q2},\ldots,\tau_{M-1}^{q1,q2,\ldots,qM-1}) - \tau_M^L(\tau_1^{q1},\tau_2^{q1,q2},\ldots,\tau_{M-1}^{q1,q2,\ldots,qM-1})}{2}\right] \sum_{qM=1}^{QPM} w_{qM}\, j(\tau_1^{q1},\tau_2^{q1,q2},\ldots,\tau_M^{q1,q2,\ldots,qM}) \tag{C8}$$

Appendix D Modification of Upper Bound

The bounding procedure described in the paper can be modified to improve the convergence of the upper bound. Specifically, there are two modifications to the truncated term that can significantly improve the upper bound. The first modification is most easily motivated with Figure D1.

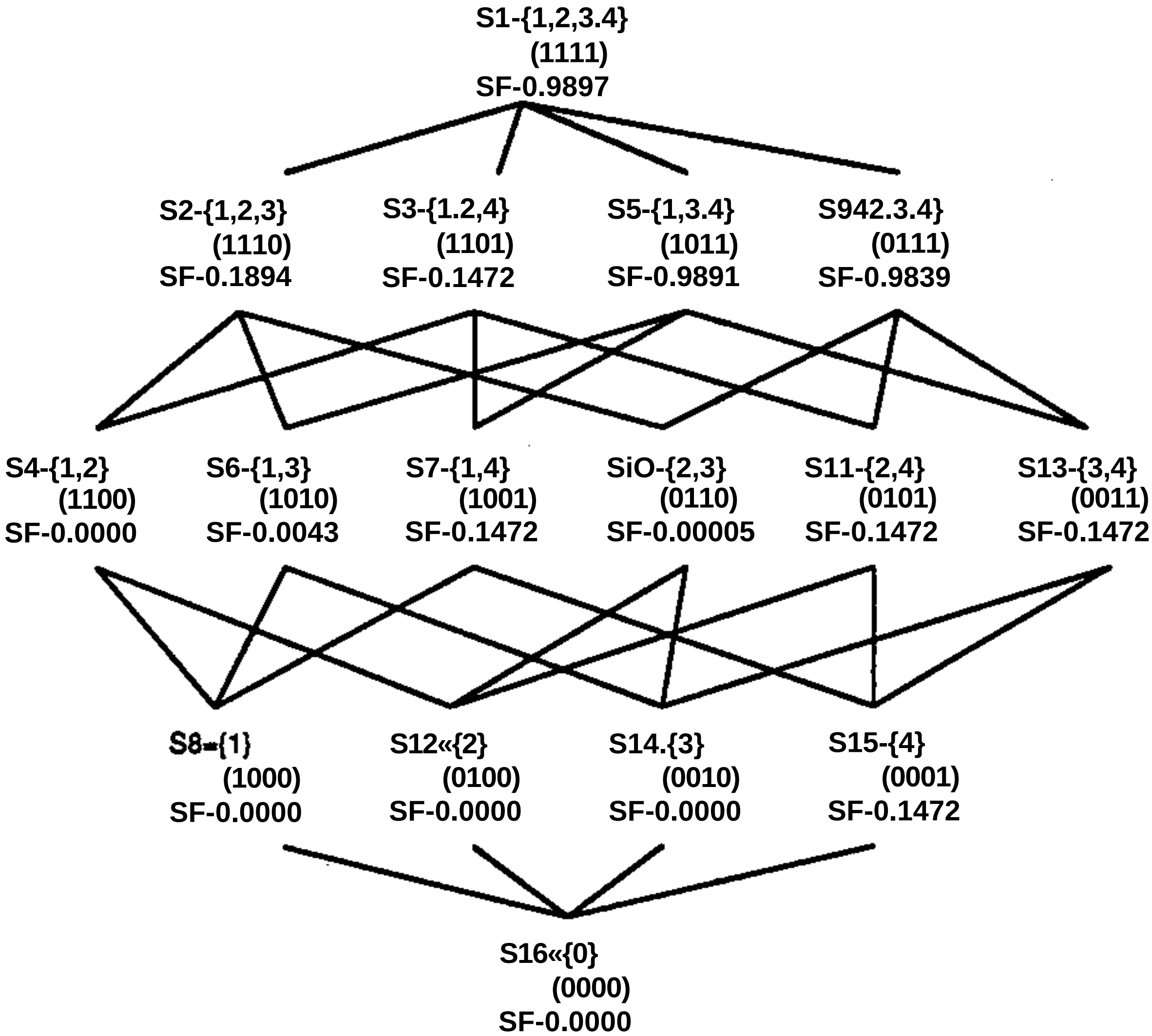

Figure D1 States and SF from Example 2.

In this figure the lines connect a superstate to its substates. A substate is a state S& that is a subset of the superstate S_a, St>cS_a . For example S_{13}-{3,4} is a subset of S_5-{1,3.4} and S_9-{2,3,4}. Because S_{13} is a subset of S_5 and S_9 its associated SF is subject to SF(S_{13})sSF(S_5) and SF(S_{13})SSF(S_9). The first modification involves noting that each state in level n_A-2 has 2 superstates in level n_A«3. Thus, the largest possible SF for any state in n_A-2 has to be smaller than the 2nd largest SF in n_A-3. The idea being that the SF of a subset is less than or equal to the smallest SF of its supersates. In general a state in level n_A is a subset of L-n_A states in level n_A+1. Thus, the largest possible SF for level n_A is the (L-n_A)'th largest SF in level n_A+1. In example 3 the 2nd (L-n_A«4-2) largest SF in level 3 (n_A+1) is 0.9839, equation (47b) can be modified as follows:

$$UB\ .0.8196+0.9839(1-0.9692)$$

$$-0.8499 \qquad (D1)$$

This is not a significant improvement since the values of the first two SF are similar, but by exploiting the structure further the upper bound can be improved.

Consider the following two levels of states, which do not correspond to Figure D1.

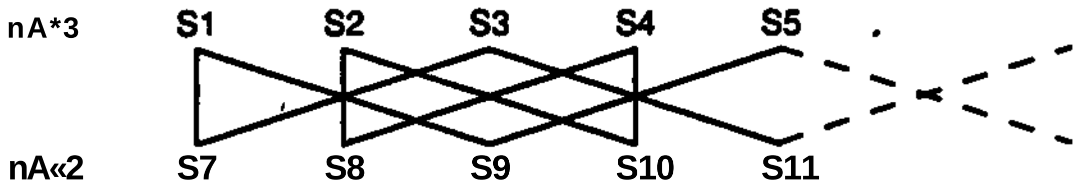

Figure D2 Example states showing how the relation between the states can be used to improve the UB.

Assume that the states in level n_A«3 are arranged in order from the largest, S_1, to the smallest, *S$.* The states in level n_A«3 are also connected to their substates in level n_A«2. Note that S_1 has S_7 and Sg as substates, and S_2 has S_8 and S_{10} as substates. According to the previous section, if the states in level n_A-3 were the last to be included in the lower bound then SF(S_2) (2nd largest) would be used to approximate the SF of the unevaluated level n_A«2. But note that S_1 and S_2 do not compose a family since they have no common substates. Thus the largest SF in level n_A-2 must be less than or equal to SF(S_3), since a substate is always bounded by its smallest superstate. Therefore S_1 and S2 do not represent tight bounds on the states in level n_A«2 since each of the states is also bounded by S_3 to S_5, which are smaller than S_1 and S_2. This suggests the following scheme, arrange the states in the last level that has been evaluated from the one with the largest SF to that with the smallest SF. Proceeding from the largest to the smallest, stop when any (L-n_A) states , n_A referring to the unevaluated level, have a common substate. The last state examined would be used in the remainder term of the upper bound. Unfortunately for example 3, both S_5 and Sg (the two largest states in level n_A-3 in Figure D1) have a common subset S_{13}, thus the upper bound can not be improved.

But Figure D2 also suggests further improvements in the order in which the states in level n_A-2 are evaluated if the bounds obtained from level n_A-3 are not sufficiently tight. The next state evaluated should be the substate In level n_A«2 that limited the progress of the examination of the states in level n_A«3 just described. In the case of Figure D2 this state is S_7. If SF(S_7) is evaluated both new upper and lower bounds can be evaluated, but more importantly the SF in the upper bound remainder term can be modified. Referring back to Figure D2, the states $SF(S_1)$, $SF(S_2)$ and $SF(S_3)$ can be ignored and "replaced" with the $SF(S_7)$.

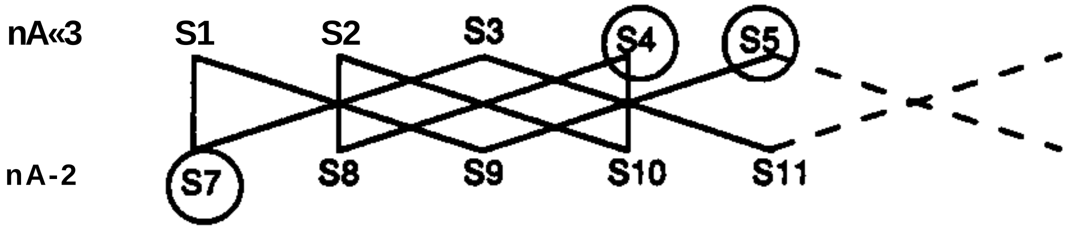

Figure D3 Showing the states that bound the SF in the truncated part of the summation.

These states are ignored since they no longer represent the "tight" bound on any unevaluated states. The tight bound is determined by the state with the smallest SF in a substates family. In this case S_8, S_9,... all have tight bounds determined by S_4, S_5,... all of which are smaller than S_1, S_2 and S_3. Now the SF in the remainder term is the largest SF of the set of tight bounds and S_7 since it replaced a tight bound. From this point on the reduction of the upper bound becomes complicated. It is suggested that the remaining set of tight bounds simply be used to evaluate additional terms in the next level rather than doing so in order to find a smaller SF to use in the remainder term.

If this idea is applied to Figure D1 of Example 3, we would evaluate S_{13} and replace S_5 and S_9. The largest SF from the remaining group (S_2, S_3, S_{13}) is S_2 with a SF of 0.1894. The new upper and lower bounds having evaluated S_{13} are as follows:

$$LB=(0.7224*0.9897)+(0.1079*0.1894)+(0.0628*0.1472)+(0.0380*0.9891)+(0.0380*0.9839)+(0.0020*0.1472) = 0.8199 \quad (D2)$$

$$UB=0.8199+(0.1894*(1-0.9692-0.0020)) = 0.8254 \quad (D3)$$

These bounds are very tight and for this example it is not necessary to go further, but there is a second modification which can tighten the upper bound even more without the evaluation of any more states. The second modification also involves the remainder term. Recall that the probability portion of the term takes on the following form.

$$\sum_{i=N+1} P(S_i) = 1 - \sum_{i=1}^{N} P(S_i) \quad (D4)$$

Note that the left hand side represents the total probability of the states that were not used in the evaluation of the lower bound; some of which are infeasible. The right side simple subtracts the probability of the states that were evaluated from 1. The probability of the infeasible states are included despite the fact that they have SF=0, and thus do not contribute to the E(SF). It is beneficial to remove the probability of the infeasible states. The sum can be divided up into two portions, a sum over feasible states and a sum over infeasible states.

$$\sum_{i=N+1}^{2^L} P(S_i) = \sum_{i=feasible} P(S_i) + \sum_{i=infeasible} P(S_i) = 1 - \sum_{i=1}^{N} P(S_i) \qquad \text{(D5)}$$

By subtracting the infeasible states form both sides the desired sum over only the the feasible states is obtained. The important point to note is that one minus the sum over the infeasible states is simply the total probability of feasible states, which is simply the reliability of the system. This assumes that none of the states that have already been evaluated (i=1,..,N) are infeasible.

$$\sum_{i=feasible} P(S_i) = 1 - \sum_{i=infeasible} P(S_i) - \sum_{i=1}^{N} P(S_i) = \text{Reliability} - \sum_{i=1}^{N} P(S_i) \qquad \text{(D6)}$$

Thus by calculating the reliability of the system the upper bound can be reduced further. The upper bound can be written as follows:

$$UB = LB + SF_{max} * (REL - \sum_{i=N}^{N} P(S_i)) \qquad \text{(D7)}$$

For example 3 the following upper bounds are obtained, the first uses the largest SF from $n_A=3$, similar to equation (47b).

UB=0.8196+(0.9891*(0.9893-0.9692))

=0.8395

The second uses the modified SF, equation (D3), in the remainder term

UB=0.8199+(0.1894*(0.9893-0.9712))

=0.8233

Recall that the actual value for the E(SF)=0.8209. Using these modifications the bounds have been changed from 0.8196≤E(SF)≤0.8501 to 0.8199≤E(SF)≤0.8233 by simply evaluating one more state.