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Recent Developments In the Evaluation and Optimization of Flexible Chemical Processes

I.E. Grossmann, D. A. Straub

EDRC 06-101-91

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Ignacio E. Grossmann and David A. Straub

Department of Chemical Engineering
Carnegie Mellon University
Pittsburgh, PA 15213, USA

Summary

The evaluation and optimization of flexible chemical processes remains one of the most challenging problems in Process Systems Engineering. In this paper an overview of recent methods for quantifying the property of flexibility in chemical plants will be presented. As will be shown, these methods are gradually evolving form deterministic worst-case measures for feasible operation to stochastic measures that account for the distribution functions of the uncertain parameters. Another trend is the simultaneous handling of discrete and continuous uncertainties with the aim of developing measures for flexibility and reliability that can be integrated within a common framework. It will be then shown how some of these measures can be incorporated in the optimization of chemical processes. In particular, the problems of retrofit design to improve flexibility at minimum cost will be discussed as well as the optimization of flexibility for multiproduct batch plants.

1. Introduction

The problem of accounting for uncertainty at the design stage is clearly a problem of great practical significance due to the variations that are commonly experienced in plant operation (e.g. changes in demands, fluctuations of feed compositions and equipment failure). Furthermore, at the design stage one must rely on values of technical parameters which are unlikely to be realized once a design is actually implemented (e.g. transfer coefficients and efficiencies). Finally, models that are used to predict the performance of a plant at the design stage may not even match the correct behavior trends of the process. In view of all these uncertainties, the common practice is to overdesign processes and/or perform ad-hoc case studies to try to verify the flexibility or robustness of a design. The pitfalls of such approaches, however, are well known and therefore have motivated the study and development of systematic techniques over the last 20 years (e.g. Grossmann *et al*, 1983; Grossmann and Morari, 1984).

It is the purpose of this paper to provide an overview of recent techniques that have been developed for evaluating and optimizing flexibility in the face of uncertainties of continuous parameters and discrete states. It will be assumed that the basic form of the process model is correct. In this paper we will emphasize work that has been developed by our group at Carnegie Mellon. This paper will be organized as follows. The problem statements for the evaluation and optimization problems will be given first for deterministic and stochastic approaches. An overview will then be presented for different formulations and solution methods for the evaluation problems, followed by similar items for the optimization design problems. As will be shown, the reason for the recent trend towards the stochastic approach is that it offers a more general framework, especially for integrating continuous and discrete uncertainties under a common measure (e.g. integrating flexibility and reliability). At the same time, however, the stochastic approach also involves a number of major challenges that still need to be overcome, especially for the optimization problems.

A specific application to multiproduct batch plants will be presented to illustrate how the problem structure can be exploited in specific instances to simplify the optimization.

2. Problem Statements

It will be assumed that the model of a process is described by equations and inequalities of the form:

$$\begin{aligned} h(d,z,x,q)&=0 \\ g(d,z,x,q)&\leq 0 \\ d&=Dy \end{aligned} \qquad (1)$$

where the variables are defined as follows:

d - L vector of design variables that defines the structure and equipment sizes of a process

z - n_z vector of control variables that can be adjusted during plant operation

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x - n_x vector of state variables that describe the behavior of a process

0 - n_p vector of continuous uncertain parameters

y - L vector of boolean variables that describes the unavailability (0) or availability (1) of the corresponding design variables d

D - diagonal matrix whose elements in the diagonal correspond to the design variables d

For convenience in the presentation it will be assumed that the state variables x in (1) are eliminated from the equations h(d,z,x,0)=O; the model then reduces to

$$f(d,z,6)\leq 0 \quad d=Dy \qquad (2)$$

The evaluation problems that can then be considered for a fixed design D are as follows:

A) Deterministic Problems Let y be fixed, and 0 be described by a nominal value 0^N, expected deviations in the positive and negative directions $A0^+$, A0% and a set of correlations $r(0) \leq 0$:

a) Problem Al: Determine if the design d = Dy, is feasible for every point 0 in
$T=\{0I0N -A0- \leq 0 \leq 0^N+A0^+,\ r(0)\leq O)$

b) Problem A2: Determine the maximum deviation 5 that design d = Dy can tolerate such that every point 0 in
$T(5)=\{0I0^N -5A0" \leq 0 \leq 0^N+5A0^+,\ r(0)\leq O\}$
is feasible.

Problem (Al) corresponds to the *feasibility problem* discussed in Halemane and Grossmann (1983), while problem (A2) corresponds to the *flexibility index problem* discussed in Swaney and Grossmann (1985a).

B) Stochastic Problems Let 0 be described by a joint probability distribution function j(0):

a) Problem Bl: If y is fixed, determine the probability of feasible operation.

b) Problem B2: If the discrete probability p, for the availability of each piece of equipment ^is given, determine the expected probability of feasible operation.

Problem (Bl) corresponds to evaluating the *stochastic flexibility* discussed in Pistikopoulos and Mazzuchi (1990), while problem (B2) corresponds to evaluating the *expected stochastic flexibility* discussed in Straub and Grossmann (1990).

As for the design optimization problems they will involve the selection of the matrix D so as to minimize cost and either a) satisfy the feasibility test (Al), or b) maximize the flexibility measure as given by (A2), (Bl) or (B2), where the latter problem gives rise to a multiobjective optimization problem.

3. Evaluation for Deterministic Case

3.1 Formulations

In order to address problem (Al) for determining the feasibility of a fixed design d, consider first a fixed value of the continuous parameter 0. The feasibility for fixed d at the given 9 value is then given by the following optimization problem (Halemane and Grossmann, 1983):

$$\psi(d,\theta) = \min_{u,z} u \quad \text{s.t.} \quad f_j(d, z, \theta) \leq u \quad j \in J \qquad (3)$$

where \|/ ≤. 0 indicates feasibility and \|/ > 0 infeasibility. Note that the objective in problem (3) is to find a point z* such that the maximum potential constraint violation is minimized.

In terms of the function \y(d,8), feasibility for every point 6e T, can be established by the formulation (Halemane and Grossmann, 1983):

$$\chi(d) = \max_{\theta \in T} \psi(d, \theta) \qquad (4)$$

where %(d) ≤ 0 indicates feasibility of the design d for every point in the parameter set T, and x(d) > 0 indicates infeasibility. Note that the max operator in (4) determines the point 8* for which the largest potential constraint violation can occur.

As for the flexibility index problem (A2), the formulation is given by (see Swaney and Grossmann, 1985a):

$$F = \max 5 \quad \text{s.t.} \quad \max_{0 \in T(5)} \psi(d, 6) \leq 0 \quad 5 \geq 0 \qquad (5)$$

where the objective is to inscribe the largest parameter set T(8*) in the feasible region projected in 0-space. An alternative formulation to problem (A2) is,

$$F = \min_{9 \in \tilde{T}} 5^*(\tilde{e}) \tag{6}$$

where

$$5^*(\tilde{0}) = \max_{6,z} 5$$

$$\text{s.t.} \quad fj(d, z, e) \le 0 \quad j \in J \tag{7}$$

$$9 = 0^N + 5\tilde{0}$$

$$\delta \ge 0$$

and $\tilde{T} = \{9 | -A8^- \le \tilde{6} \le A6^+\}$

The objective in (6) is to find the maximum displacement which is possible along the displacement $\tilde{0}$ from the nominal value 6^N. Note that in both (5) and (6) the solution of the critical point 9* lies at the boundary of the feasible region projected in 6-space.

3.2 Methods

Assume that no constraints r(0) ≤ 0 are present for correlating parameter variations. Then the simplest methods for solving problems (A1) and (A2) are vertex enumeration schemes which rely on the assumption that the critical points 0* lie at the vertexes of the sets T and T(5*). Such an assumption is only valid provided certain convexity conditions hold (see Swaney and Grossmann, 1985).

Let V = {k} correspond to the set of vertices in $T = \{0 | 0^N - A9^- \le 0 \le 0^N + A0^+\}$. Then, problem (4) can be reformulated as

$$X(d) = \max_{k \in V} u^k \tag{8}$$

where

$$u^k = \min_{u,z} u$$

$$\text{s.t.} \quad fj(d, z, 0^k) \le u \quad j \in J \tag{9}$$

That is, the problem reduces to solving the 2^nP optimization problems in (9).

Likewise, problem (6) can be reformulated as

$$F = \min 5^k \tag{10}$$

where

$$5^k = \max_{6,z} 5$$

$$\text{s.t.} \quad fj(d, z, e) \le 0 \quad j \in J \tag{11}$$

$$0 = 6^N + A0^k$$

$$5 \ge 0$$

and $A0^k$ is the displacement vector to vertex k. This problem again reduces to solving 2^nP optimization problems in (11).

The problem of avoiding the exhaustive enumeration of all vertices, which increase exponentially with the number of parameters, has been addressed by Swaney and Grossmann (1985b) and Kabatek and Swaney (1989) using implicit enumeration techniques. The latter author has been able to solve problems with up to 20 parameters with such an approach.

An alternative method that does not rely on the assumption that critical points correspond to vertices, is the active set strategy of Grossmann and Floudas (1987). This method relies on the fact that the feasible region projected into the space of d and 0,

$$R(d,e) = \{e | y(d,8) \le 0\} \tag{12}$$

(see Figure 1) can be expressed in terms of active sets of constraints $fj(d,z,0)=0$, $j \in J^k_A$ k=1,...NAS.

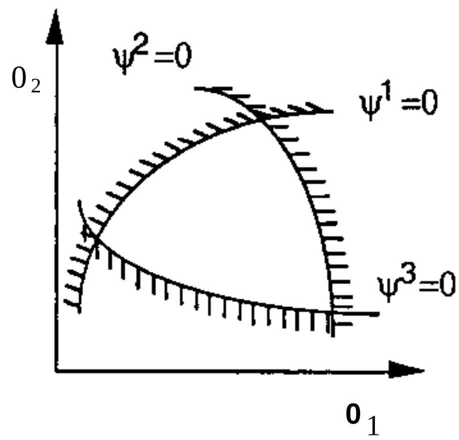

Figure 1 Constraints in the space of d and 0

These active sets are obtained from all subsets of non-zero multipliers that satisfy the Kuhn-Tucker conditions of problem (3)

$$\sum_{j \in J^k_A} \lambda^k_j = 1 \ , \ \sum_{j \in J^k_A} \lambda^k_j \frac{\partial f_j}{\partial z} = 0 \tag{13}$$

Pistikopoulos and Grossmann (1989) have proposed a systematic enumeration procedure to identify the

NAS active sets of constraints, provided that the corresponding submatrices in (13) are of full rank.

The projected parameter feasible region in (12) can then be expressed as

$$R(d,\theta)=\{\theta \mid \psi^k(d,\theta)\le 0,\ k=1,\dots,NAS\} \qquad (14)$$

where

$$\begin{aligned} \psi^k(d,\theta) &= \min u \\ \text{s.t.} \quad f_j(d,z,\theta) &= u \quad j\in J_A^k \end{aligned} \qquad (15)$$

The above active set strategy by Grossmann and Floudas (1987) does not require, however, the *a-priori* identification of constraints ψ^k. This is accomplished by reformulating problem (4) with the Kuhn-Tucker conditions of (3) embedded in it, and expressed in terms of 0-1 variables w_j for modelling the complementarity conditions.

For the case of problem (A1), this leads to the mixed-integer optimization problem

$$\begin{aligned} &\chi(d) = \max u \\ \text{s.t.} \quad & s_j + f_j(d,z,\theta) = u \quad j\in J \\ & \sum_{j\in J} \lambda_j = 1 \\ & \sum_{j\in J} \lambda_j \frac{\partial f_j}{\partial z} = 0 \\ & \left.\begin{aligned} \lambda_j - w_j &\le 1 \\ s_j - U(1-w_j) &\le 0 \end{aligned}\right\} \ j\in J \\ & \sum_{j\in J} w_j \le n_z + 1 \\ & \theta^N - \Delta\theta^- \le \theta \le \theta^N + \Delta\theta^+ \\ & r(\theta) \le 0 \\ & w_j = 0,1 \ ; \ \lambda_j ; s_j \ge 0 \quad j\in J \end{aligned} \qquad (16)$$

where U is a valid upper bound for the violation of constraints. For the case of problem (A2), the calculation of the flexibility index can be formulated as the mixed-integer optimization problem (17).

In both cases, constraints f_j that are linear in z and θ give rise to MILP problems which can be solved with standard branch and bound methods. For nonlinear constraints models (16) and (17) give rise to MINLP problems which can be solved with Generalized Benders Decomposition (Geoffrion, 1972) or with any of the variants of the outer-approximation method (e.g. Viswanathan and Grossmann, 1989). Also, for the case when $n_z + 1$ constraints are assumed to be active and the constraints are monotone in z, Grossmann and Floudas (1987) decompose the MINLP into a sequence of NLP optimization problems, each corresponding to an active set which is identified *a-priori* from the stationary conditions of the Lagrangian.

$$\begin{aligned} &F = \min \delta \\ \text{s.t.} \quad & s_j + f_j(d,z,\theta) = 0 \quad j\in J \\ & \sum_{j\in J} \lambda_j = 1 \\ & \sum_{j\in J} \lambda_j \frac{\partial f_j}{\partial z} = 0 \\ & \left.\begin{aligned} \lambda_j - w_j &\le 1 \\ s_j - U(1-w_j) &\le 0 \end{aligned}\right\} \ j\in J \\ & \sum_{j\in J} w_j \le n_z + 1 \\ & \theta^N - \delta\Delta\theta^- \le \theta \le \theta^N + \delta\Delta\theta^+ \\ & r(\theta) \le 0 \\ & \delta \ge 0 \ ; \ w_j = 0,1 \ , \ \lambda_j , s_j \ge 0 \quad j\in J \end{aligned} \qquad (17)$$

4. Evaluation for Stochastic Case

4.1 Formulation

In order to formulate problem (B1), the probability of feasible operation given a joint distribution for θ, $j(\theta)$, this involves the evaluation of the multiple integral

$$SF(d) = \int_{\theta:\psi(d,\theta)\le 0} j(\theta)\, d\theta \qquad (18)$$

where SF(d) is the stochastic flexibility for a given design (see Pistikopoulos and Mazzuchi, 1990; Straub and Grossmann, 1990). Note that this integral must be evaluated over the feasible region projected in θ space (see eqn. (12) and Figure 2). In Figure 2 the circles represent the contours of the joint distribution function j.

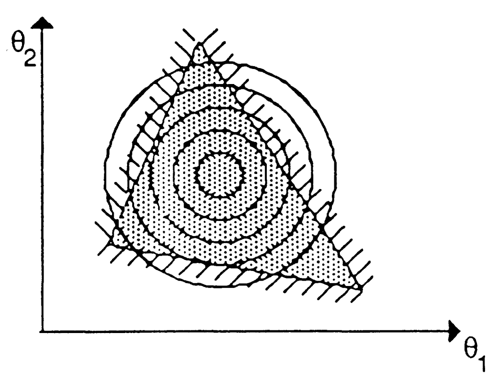

Figure 2 SF is evaluated by integration over the shaded area.

For the case when uncertainties are also involved in the equipment, discrete states result from all the combinations of the vector y. It is convenient to define for each state s the index sets

$$Y^s i = \{/ | y \wedge = l\} \ , \ Y5 \ll (/ | y J = 0\} \quad (19)$$

to denote the identity of available and unavailable equipment. Note that state s is defined by a particular choice of y^s which in turn determines the design variables for that state, $d^s=Dy^s$. Also, denoting by p/ the probability that equipment /be available, the probability of each state P(s) is given by:

$$P(s) = \prod_{\ell \in Y_1^s} p_\ell \prod_{\ell \in Y_0^s} (1 - p_\ell) \quad s=1,...2^L \quad (20)$$

In this way the probability of feasible operation over both the discrete and continuous uncertainties (i.e. problem (B2)) is given by

$$E(SF) = f_{s=1} SF(s)P(s) \quad (21)$$

where E(SF) is the expected stochastic flexibility as proposed by Straub and Grossmann (1990).

4.2 Methods

The solution of problems (18) and (21) poses great computational challenges. Firstly, because (18) involves a multiple integral over an implicitly defined domain. Secondly, (19) involves the evaluation of these integrals for 2^L states. For this reason solution methods for these problems have been only reported for the case of linear constraints:

$$f_j(d, z, \theta) = a_j^T d + b_j^T z + c_j^T \theta + c_j^0 \quad (22)$$

Pistikopoulos and Mazzuchi (1990) have proposed the computation of bounds for the stochastic flexibility, SF(d) by assuming that j(9) is a normal distribution. Firstly, expressing the feasibility function $v^k(d,6)$ as given in (15) through the Lagrangian, this yields for (22) the linear equation

$$v^k(d,e) = S_{j \in J_\lambda^k} \lambda_j^k [c_j^T \theta + c_j'] \quad (23)$$

where $c' \wedge c \wedge + a/\dot{d}$. Since (23) is linear in 9 and these are normally distributed NQIQJZQ), then the distribution function <)>(Y^k) is also normally distributed with mean and variance,

$$H_{\psi^k} = \sum_{j \in J_\lambda^k} \lambda_j^k [c_j^T \mu_\theta + c_j'] \quad (24)$$

$$\sigma_{\psi^k}^2 = \left[\sum_{j \in J_\lambda^k} \lambda_j^k c_j^T\right] l e \left[\sum_{j \in J_\lambda^k} \lambda_j^k c_j^T\right]^T \quad (25)$$

where £Q is the variance-convariance matrix for the parameters 0.

The probability of feasible operation for the above set k is then given by the one-dimensional integral

$$SF^* = \int_{-\infty} \phi(\psi^k) d\psi^k \quad (26)$$

which can be readily evaluated.

Lower and upper bounds of the stochastic flexibility SF(d) are then given by

$$SF^L(d) = \sum_{k-I}^{NAS} SF^k - \pounds_{k<\ell} SF^k SF' +]T_{k<\ell<m} SF'' SF' SF^m ... \quad (27)$$

$$SF^u(d) = \min \left\{ \prod_{k \in JA(q)} SF^k \right\} \quad (28)$$

where JA(q) ⊆ JA, q=l,...Q, are all possible subsets of the inequalities $y^k(d,0) < O$, k=l,...NAS. It should be noted that the bounds in (27) and (28) are often quite tight providing good estimates for the stochastic flexibility.

Straub and Grossmann (1990) have proposed a numerical approximation scheme for arbitrary distribution functions using Gaussian quadrature within the feasible region of the projected region R(d,6) (see Fig. 1).

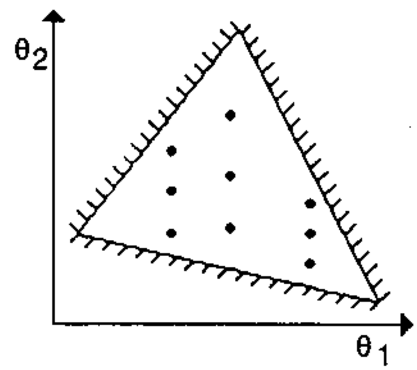

Figure 3 Location of Quadrature Points.

The location of the quadrature periods is performed by first projecting the functions \j/^{k}(d,8), k=l...NAS into successively lower dimensional spaces in 0 ; i.e. :$[e_{1f}e_2,...e_M]$ -> $[e_{1>}e_2,...e_{M-1}]$...-*$[e_1]$ This is accomplished by analytically solving the problems $r=1,2,..M-1$:

$$\psi^{r+1,k}(d,\theta_1,\theta_2,...\theta_{M-r}) = \min u \quad \text{s.t.} \quad \psi^{r,k}(d,\theta_1,\theta_2,...) \leq u \quad k=1...NAS(r) \tag{29}$$

where $V^{1Jc} = \psi^k(d,\theta) = \sum_{j \in J_k^k} f_j(d,z,\theta)$, and NAS(r) is the number of active sets at the rth state of the projection.

In the next step, lower and upper bounds are generated together with the quadrature points for each 0i component in the order 0_1-»0_2...->0_M. This is accomplished by using the analytical expressions \(/^{r}>^{k}(d,0_1,02,...,0M+r-l) in the order r=M> M-l,..., to determine the bounds. For instance, the bounds $0!^L$ and $0i^u$ are determined from the linear inequalities V^{M}>^{k}(d,0!)<(), k=l,...NAS(M). The quadrature points *Qft* then are given by:

$$\theta_1^{q_1} = \frac{v_{q_1}(\theta_1^u - \theta_1^L) + \theta_1^u + \theta_1^L}{2} \quad q_1=1,..QP_1 \tag{30}$$

where $v_{q}i$, ql=l,..., QPj represent the location of QPl quadrature points in [-1,1]. In the next step, bounds for 02 are computed for each e^^{1} from \K^M-^{1}»^{k}(d,0_1,0_2)<O, k=l,...NAS(M-l). These bounds are denoted as 0_2^L(^^{1}) since they depend on the value of 0^^{1}. Quadrature points are then computed as in (30) and the procedure continues until the the bounds 8 M[0 I ,62 -SM-I]» 9 MIQI ,82 ...9M-I] and quadrature points ©jj^^{2}'"^ are determined.

The numerical approximation to (18) is then given by

$$SF(d) = \frac{\theta_1^U-\theta_1^L}{2}\sum_{q_1=1}^{QP_1} w_{q_1}\frac{[\theta_2^U(\theta_1^{q_1})-\theta_2^L(\theta_1^{q_1})]}{2}\sum_{q_2=1}^{QP_2} w_{q_2}\frac{[\theta_3^U(\theta_1^{q_1},\theta_2^{q_1q_2})}{2} - \frac{\theta_3^L(\theta_1^{q_1},\theta_2^{q_1q_2})]}{2} \cdots \frac{\theta_M^U(\theta_1^{q_1},...\theta_{M-1}^{q_1q_2..q_{M-1}}) - \theta_M^L(\theta_1^{q_1},...\theta_{M-1}^{q_1q_2..q_{M-1}})}{2} \times \sum^{QP_M} w_{q_M} f(\theta_1^{q_1},\theta_2^{q_1q_2},...\theta_M^{q_1q_2..q_M}) \tag{31}$$

where w_q, are the weights corresponding to each quadrature point.

It should be noted that equation (31) becomes computationally more expensive as the number of parameters 0 increases which is not the case with the bounds in (27) and (28). However, as pointed out before, (31) can be applied to any distribution function (e.g. normal, beta, log) while the bounds can only be applied to normal distribution. Also, both methods require the identification of active sets which may become large if the number of constraints is large.

As for the solution of equation (21) for the expected flexibility, Straub and Grossmann (1990) have developed a bounding scheme that requires the examination of relatively few states which can become quite large. They represent the states through a network as shown in Fig. 4.

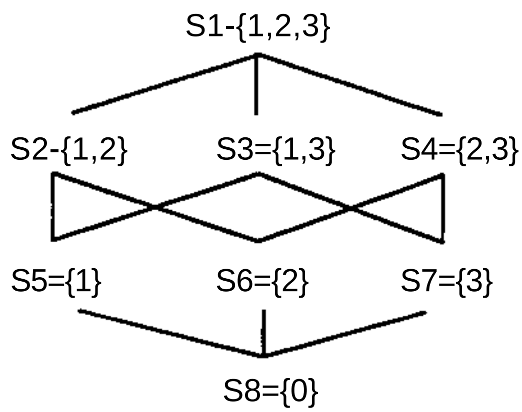

Figure 4 State Network showing different possible sets of active units.

Here the top state has all the units active (i.e. y/ = 1), while the bottom state has all units inactive. Since the states with active units will usually have the higher probability, the evaluation starts with the top state.

At any point of the search the following index sets are defined:

$$E=\{s|SF(s) \text{ is evaluated}\} \qquad U=\{s|SF(s) \text{ is not evaluated}\} \tag{32}$$

The lower and upper bounds are then given as follows:

$$E(SF)^L = \sum_{s\in E} SF(s)\ P(s)$$

$$E(SF)^U = \sum_{s\in E} SF(s)\ P(s) + \sum_{s\in U} BSF(s)\ P(s) \tag{33}$$

where BSF(s) are valid upper bounds that are propagated through the subnetwork from higher states that have **been** evaluated. Convergence with this scheme for a small tolerance is normally achieved within 5 to 6 state evaluations (see Figure 5) provided the discrete probabilities p/>0.5. The significance of this method is that it allows the evaluation of flexibility and reliability within a single measure accounting for the interactions of the two.

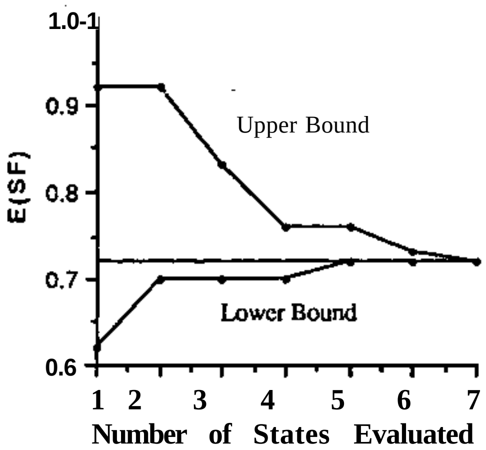

Figure 5 Example of the progression of the bounds.

5. Design Optimization

Most of the previous work (Johns *et al,* 1976; Malik and Hughes, **1979)** has **only** considered the effect of the continuous uncertain parameters 0 for the design optimization, and for which the minimization of the expected value of the cost function has been considered using a two-stage strategy:

$$\min_{d} E_{\theta} \left[\min_{z} C(d, z, \theta) \mid f(d, z, \theta) \le 0 \right] \qquad (34)$$

In order to handle infeasibilities in the inner minimization, one approach is to assign penalties for the violation of constraints (e.g. $C(d,z,q)=\bar{C}$ if $f(d,z,q) > 0$. This however can lead to discontinuities. The other approach is to enforce feasibility for a specified flexibility index F (e.g. Halemane and Grossmann, 1983) through the parameter set $T(F)=\{\theta \mid \theta^L - F\Delta\theta^- \le \theta \le \theta^U + F\Delta\theta^+, r(\theta)\le 0\}$ In this case (34) is formulated as

$$\begin{aligned} &\min_{d} E_{\theta \in T(F)} \left[\min_{z} c(d, z, \theta) \mid f(d, z, \theta) \le 0 \right] \\ &\text{s.t.} \quad \max_{\theta \in T(F)} \psi(d, \theta) \le 0 \end{aligned} \qquad (35)$$

A particular case of (35) is when only a discrete set of points θ^k, k=1..K are specified which then gives rise to the problem

$$\begin{aligned} &\min_{d, z^1, \ldots, z^k} \sum_{k=1}^{K} w_k \\ &\text{s.t.} \quad f(d, z^k, \theta^k) \le 0 \qquad k=1..K \end{aligned} \qquad (36)$$

where w_k are weights that are assigned to each point θ^k, and $\sum_{k=1}^{K} w_k = 1$.

Problem (36) can be interpreted as a multiperiod design problem which is an important problem in its own right for the design of flexible chemical plants. However, as shown by Halemane and Grossmann (1983) this problem can also be used to approximate the solution of (35), This is accomplished by selecting an initial set of points θ^k, solving problem (36) and verifying its feasibility over T(F) by solving problem (A1) as given by (4). If the design is feasible the procedure terminates. Otherwise the critical point from (4) is included to the set of K 0 points and the solution of (36) is repeated. Computational experience **has shown** that commonly one or two major iterations must be performed to achieve feasibility with this method (e.g. see Floudas and Grossmann, 1987).

While the above procedure can be applied to general linear and nonlinear problems, one can exploit the structure for specialized cases. For instance, consider the case of constraints that are linear in d, z, and 0, and where the objective function only involves the design variables d. This case commonly arises in retrofit design problems.

As shown by Pistikopoulos and Grossmann (1988), equation (23) holds for linear constraints. Therefore, the constraint in (35) can be simplified into NAS inequalities as shown in the following model:

$$\begin{aligned} &\min_{d} C(d) \\ &\text{s.t.} \quad \sum_{j \in J_A^k} \lambda_j^k \left[c_j^T \theta^{ck} + c_j^o + a_j^T d \right] \le 0 \qquad k=1..NAS \\ &d^L \le d \le d^u \end{aligned} \qquad (37)$$

where

$$\theta_i^{ck} = \begin{cases} \theta^N + F\Delta\theta^+ & \text{if } \dfrac{\partial \psi^k}{\partial \theta_i} > 0 \\ \theta^N - F\Delta\theta^- & \text{if } \dfrac{\partial \psi^k}{\partial \theta_i} < 0 \end{cases}$$

The significance of problem (37) is that the optimal design can be obtained through one single optimization which however requires prior identification of the NAS active sets.

Pistikopoulos and Grossmann (1988) have presented an alternative formulation to (37) in which one can easily derive the trade-off curve of cost versus the flexibility index. The formulation is given by

$$\min_{\Delta d} \; C\left(d^E + \Delta d\right)$$

$$\text{s.t.} \quad \left.\begin{array}{l} \delta^k \ge F \\ \delta^k = \delta_E^k + \sum_{\ell=1}^{L} \sigma_\ell^k \, \Delta d_\ell \end{array}\right\} k=1,..NAS \qquad (38)$$

$$\Delta d^u \le \Delta d \le \Delta d^U \;, \quad \delta^k \ge 0$$

where δ_E^k is the flexibility index for active set k at the

base design d_E and $\sigma_\ell^k = \frac{\partial \delta^k}{\partial \psi^k} \frac{\partial \psi^k}{\partial d_\ell}$ are sensitivity coefficients that can be determined explicitly; Δd are design changes with respect to the existing design d_E.

Also, these authors extended the formulation in (37) to the case of nonlinear constraints. Here, the inequalities in (37) are augmented within an iterative procedure similar to the scheme based on the use of the multiperiod design problem, except that problem (15) is solved for each active set to determine the critical points and multipliers.

Finally, the determination of the optimal degree of flexibility can be formulated for the case of linear constraints as

$$\max Z = \underset{\theta \in T(F)}{E} \left\{ \max_z p(z, \theta) \,|\, f(d, z, \theta) \le 0 \right\} - C(\Delta d)$$

$$\text{st.} \quad \left.\begin{array}{l} \delta^k \ge F \\ \delta^k = \delta_E^k + \sum_{\ell=1}^{L} \sigma_\ell^k \Delta d_\ell \end{array}\right\} k=1,..NAS \qquad (39)$$

$$d = d_E + \Delta d \;, \quad \delta^k \ge 0$$

where $p(z,\theta)$ is a profit function.

Pistikopoulos and Grossmann (1988b) simplified this problem as maximizing the revenue subject to minimizing the investment cost; that is (see Fig. 6):

$$\max_F \quad Z = R(F) - C(F)$$

$$\text{s.t.} \quad C(F) = \min C(\Delta d)$$

$$\delta^k \ge F \qquad (40)$$

$$\delta^k = \delta_E^k + \sum_{\ell=1}^{L} \sigma_\ell^k \Delta d_\ell$$

and where

$$R(F) = \underset{\theta \in T}{E} \left\{ \max_z p(z, \theta) \,|\, f(d, z, \theta) \le 0 \right\}$$

$$\Delta d = \arg\left[C(F)\right] \qquad (41)$$

which is solved by a modified Cartesian integration method. Since problem (40) is expressed in terms of only the flexibility index F, its optimal value is found by a direct search method.

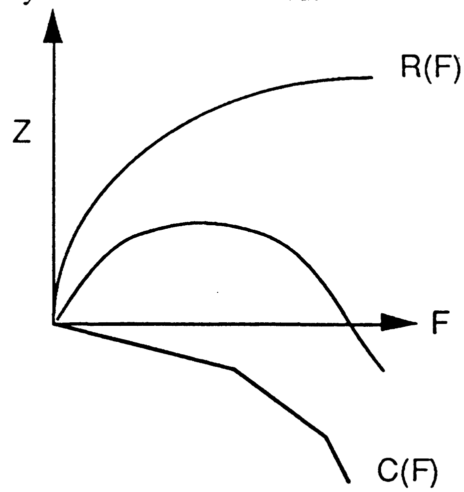

Figure 6 Curves for Determination of Optimal Flexibility

6. Application to Multiproduct Batch Design

The methods presented in the previous section have been only applied to continuous processes. On the other hand batch processes offer also an interesting application since these plants are built because of their flexibility for manufacturing several products. Reinhardt and Rippin (1985, 1986) have reported a design method when demand uncertainties are described by distribution functions. Wellons and Reklaitis (1989) have developed a design method for staged expansions for the same type of uncertainties. In this section we will summarize the recent work by Straub and Grossmann (1990) which accounts for uncertainties in the demands (continuous parameter) and equipment failure (states). This will serve to illustrate some of the concepts of Section 4 and show how the structure of the problem can be exploited to simplify the calculations; particularly the optimization of the stochastic flexibility. Consider the model for the design of multiproduct batch plants with single product campaigns (see Grossmann and Sargent, 1978):

$$\min_{N\,V} \sum_{j=1}^{M} \alpha_j N_j V_j^{\beta_j}$$

$$\text{s.t.}\quad \left.\begin{array}{l} V_j \geq S_{ij}B_i \\ T_{Li} \geq t_{ij}/N_j \end{array}\right\} i=1,NP,\ j=1,M$$

$$\sum_{i=1}^{N} \frac{Q_i}{B_i} T_{Li} \leq H \qquad (42)$$

$$V_j^L \leq V_j \leq V_j^U, \quad Nj=1,2.. \quad j=1..M$$

$$B_i\ ,\ T_{Li} \geq 0 \qquad i=1,NP$$

Although problem (42) is nonlinear, for fixed design variables Vj (sizes), Nj (number of parallel units), the feasible region can be described by the linear inequality

$$\sum_{i=1}^{NP} Q_i \gamma_i \leq H \qquad (43)$$

where $\gamma_i = \max_j \{t_{ij}/N_j\}/\min_j \{V_j/S_{ij}\}$.

If we define

$$H_A = \sum_{i=1}^{NP} Q_i \gamma_i \qquad (44)$$

then the problem of calculating the probability of feasible operation for uncertain demands Qi, i=l,N, can be expressed through the one-dimensional integral

$$SF = \int_0^H \phi(H_A)dH_A \qquad (45)$$

which avoids the direct solution of the multiple integral in (18). Furthermore, the distribution $\phi(H_A)$ can be easily determined if normal distributions are assumed for the product demands with mean μ_Q and variance σ_Q.. Then proceeding in a similar way as in (24) and (25) the mean and the variance of $\phi(H_A)$ are given by

$$\mu_{H_A} = \sum_{i=1}^{NP} \gamma_i \mu_{Q_i}$$

$$\sigma_{H_A}^2 = \sum_{i=1}^{NP} \gamma_i^2 \sigma_{Q_i}^2 \qquad (46)$$

with which the integral in (45) can be readily evaluated for the stochastic flexibility.

As for the expected stochastic flexibility, let pj be the probability that a unit in stage j is available. Also let n_j^s, j=1,M be the number of units that are available for any given state s. Then it can be shown that the number of feasible states where at least some production can be obtained is given by

$TFS = \prod_{j=1}^{M} (N_j)$, and that the probability of each state is given by

$$P(s) = \prod_{j=1}^{M} \frac{N_j!}{(n_j^s)!\,(N_j - n_j^s)!} p_j^{n_j^s} (1-p_j)^{(N_j - n_j^s)} \qquad (47)$$

In this way the expected stochastic flexibility can be expressed as

$$E(SF) = \sum_{s=1}^{TFS} SF(s)\, P(s) \qquad (48)$$

where SF(s) and P(s) are given by (45) and (47), respectively. The value of E(SF) can then be obtained by applying the bounding procedure at the end of Section 4 (eqns. (32) and (33)).

In order to determine the sizes Vj and number of parallel units Nj that maximize the stochastic flexibility (i.e. only uncertainties in the demands) given a limit for the capital investment, $\bar{C}$, one would have to optimize in principle the integral in (45) over the constraint set in (42). However, this can be avoided in view of the fact that maximizing the normal deviate $z = (H-\mu_{H_A})/\sigma_{H_A}$ is equivalent to maximizing the integral. Thus by applying appropriate exponential transformations to (42) to convexity the problem, the optimal design that maximizes the stochastic flexibility for a limit in the investment cost, can be formulated as the MINLP (see Straub and Grossmann, 1990):

$$\max\ z = (H-\mu_{H_A})/\sigma_{H_A}$$

$$\text{s.t.}\quad \left.\begin{array}{l} b_i \leq V_j - \log(S_{ij}) \\ t_{Li} \geq \log(t_{ij}) - T_{lj} \end{array}\right\} \begin{array}{l} i=1,\ldots,NP \\ j=1,\ldots,M \end{array}$$

$$\left.\begin{array}{l} n_j = \sum_r w_{jr} \log(r) \\ \sum_r w_{jr} = 1 \end{array}\right\} j=1,\ldots,M$$

$$\sum_j \alpha_j \exp(\eta_j + \beta_j v_j) \leq C$$

$$\xi_i = t_{Li} - b_i \qquad i=1,\ldots,NP$$

$$\mu_{H_A} = \sum_i \exp(\xi_i)\, \mu_{Q_i} \qquad (49)$$

$$\sigma^2_{H_A} = \sum_i \exp(2\xi_i)\,\sigma^2_{Q_i}$$
$$\ln(B_i^L) \le b_i \le \ln(B_i^U) \quad i=1,\dots,NP$$
$$\ln(V_j^L) \le v_j \le \ln(V_j^U) \quad j=1,\dots,M$$
$$\ln(T_{Li}^L) \le t_{Li} \le \ln(T_{Li}^U)$$
$$-\infty \le \xi_i \le \infty \quad i=1,\dots,NP$$
$$H, \mu_{H_A}, \sigma^2_{H_A} \ge 0$$
$$\ln(V_j^L) \le V_j \le \ln(V_j^U) \quad j=1,\dots,M$$
$$w_{jr}=0,1 \quad j=1,\dots,M \quad r=1,\dots,N_j^U$$

By solving this MINLP for different values of $\overline{C}$ one can then determine trade-off curves of the expected stochastic flexibility versus cost (see Figure 7). Also, note that if the number of parallel units is fixed (49) reduces to an NLP problem.

As for the optimization of expected flexibility, problem (49) can be extended as a multiperiod design problem if Nj is fixed, where each period corresponds to a given state s. There is no need to solve, however, for all the states since a preanalysis can easily establish the relative magnitudes of (47) and valid upper bounds for SF(s). The optimization of Nj and Vj is in principle considerably more complicated. However, here Straub and Grossmann (1990) have developed an enumeration procedure that relies on the state network representation and which minimizes the number of multiperiod optimization problems that need to be examined. The details of this method can be found in their paper.

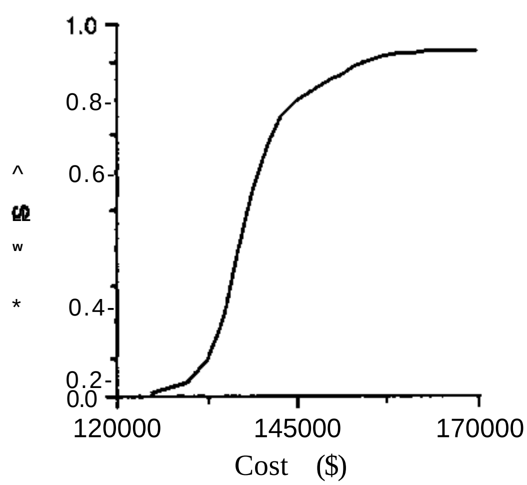

Figure 7 Trade-off Curve

7. Conclusions

This paper has given an overview of methods and formulations for evaluating and optimizing flexibility in chemical processes. As has been shown, deterministic methods have reached a stage of maturity whereby their wider application, like in process simulators, should be technically feasible, although not necessarily trivial (e.g. computation of flexibility index and multiperiod design problems). Stochastic methods on the other hand are in principle computationally more expensive, except for few specific cases (e.g. bounds for linear models, optimization of multiproduct batch plants). However, the major advantage with the stochastic approach is that it offers the possibility of integrating flexibility and reliability under a common measure as has been discussed in this paper. It is clear that major advances are required to make computationally feasible the optimization with the stochastic approach.

Acknowledgments

The authors would like to acknowledge financial support from the Department of Energy under Grant DOE: DE-FG-02-85ER13396

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