Flexibility Analysis and Design of Linear Systems by Parametric Programming

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A new, unified theory and algorithms, based on multiparametric programming techniques, for the solution of flexibility analysis and design optimization problems in linear process systems are presented. They are used for the flexibility test and index problems in systems with deterministic parameters, and for the stochastic and expected stochastic flexibility evaluation problems in systems with stochastic parameters. They are computationally efficient and give the explicit dependence of various flexibility metrics on the values of the continuous design variables. The latter feature enables the easy and efficient comparison of design alternatives. It also allows for the compact formulation of design optimization problems that can be solved parametrically to yield the exact algebraic form of the trade-off curve of economics against flexibility. Key features of the proposed approach are demonstrated through both mathematical and process examples.

Introduction

The design and operation of chemical plants are subject to considerable uncertainties. These uncertainties can be classified in the following manner (Pistikopoulos, 1995). At the design stage, values of model parameters such as heat-transfer coefficients and reaction-rate constants may not be properly established, while during operation there will commonly be fluctuations in process parameters (such as stream flow rates and qualities) and external parameters (such as product demands and prices). Moreover, there can be uncertainties in discrete states corresponding, for example, to equipment availability, while the mathematical models themselves may not accurately represent the real behavior of the process. Under these circumstances, it is clearly important to consider the ability of a system to operate feasibly in the presence of uncertainties, that is, its *flexibility*, as a process design objective.

In order for this to be achieved, it is useful to formulate problems that enable a designer to (1) evaluate the flexibility characteristics of an existing or proposed design with regard to the expected operational requirements; (2) identify the bottlenecks that limit flexibility; and (3) compare different process designs on a common basis (Swaney and Grossmann, 1985a). Over the last two decades, a substantial amount of research work has been developed for mathematically formulating and solving such flexibility analysis problems, both for *deterministic* cases, where the uncertain parameters are described through a set of lower and upper bounds, and *stochastic* cases, where the uncertain parameters are described by a joint probability density function (as reviewed in Grossmann and Straub, 1991; chap. 21 of Biegler et al., 1997). The purpose of this article is to propose a new theoretical formulation and solution approach, based on parametric programming, that provides explicit information about the dependency of a system's flexibility on the values of the uncertain parameters and the design variables. This is achieved through the solution of fewer subproblems than those required by earlier works. The focus of this article is on linear process models; this will then serve as a prelude to future work involving the flexibility of nonlinear systems and the analysis of dynamic systems under uncertainty (in the context of the interactions between process design and process control), where the use of linear(ized) models is commonplace.

The remainder of the article is organized as follows. The different types of flexibility analysis problem (flexibility test and index evaluation for deterministic systems; stochastic and expected stochastic flexibility evaluation for stochastic systems) are dealt with in separate sections. For each problem, the mathematical formulation is given and existing solution approaches are reviewed. The parametric programming

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approach is then described and novel algorithms for the solution of the respective flexibility analysis problems are outlined and illustrated with a mathematical example. Extensions of the parametric programming approach for solving design optimization problems are also discussed. Finally, three process examples are presented in order to demonstrate the applicability of the new algorithms to engineering problems.

Flexibility Test and Index

Definitions

The physical performance of a chemical process at steady state can be described by the following set of constraints

$$h_m(x, z, \boldsymbol{\theta}, d, y) = 0, \qquad m \in M, \tag{1}$$

$$g_l(x, z, \boldsymbol{\theta}, d, y) \leq 0, \qquad l \in L, \tag{2}$$

where h_m is the mth equation (such as material or energy balance); g_l is the lth inequality (such as design specification or physical operating limit) that must be satisfied for feasible operation; x is the vector of M state variables; z is the vector of control variables that can be manipulated during plant operation, depending on the values of the uncertain parameters $\boldsymbol{\theta}$; d is the vector of continuous design variables that define equipment sizes; and y is the vector of integer variables (usually 0−1) that define the structure of the process flow sheet.

Given nominal values for the uncertain parameters, $\boldsymbol{\theta}^N$, expected deviations in the positive and negative directions, $\boldsymbol{\Delta\theta}^+$ and $\boldsymbol{\Delta\theta}^-$, respectively, and a set of constraints, $r(\boldsymbol{\theta}) \leq \mathbf{0}$ (which may include equations correlating the uncertain parameters if they are not independent), the *flexibility-test* problem for a given design and structure is to determine whether there is at least one set of controls that can be chosen during plant operation such that, for every possible realization of the uncertain parameters, all of the constraints (Eq. 2) are satisfied. Mathematically, this is equivalent to evaluating a flexibility-test measure (Halemane and Grossmann, 1983)

$$\chi(d, y) = \max_{\theta \in T} \psi(\boldsymbol{\theta}, d, y), \tag{3}$$

where $T = \{\boldsymbol{\theta} | \boldsymbol{\theta}^N - \boldsymbol{\Delta\theta}^- \leq \boldsymbol{\theta} \leq \boldsymbol{\theta}^N + \boldsymbol{\Delta\theta}^+, \ r(\boldsymbol{\theta}) \leq \mathbf{0}\}$. If $\chi(d, y) \leq 0$, then the given design and structure are feasible for all $\boldsymbol{\theta} \in T$. The solution of Eq. 3 gives the "critical" parameter values, $\boldsymbol{\theta}^c$, or bottlenecks, for operation. Note also that $\psi(\boldsymbol{\theta}, d, y)$ is called the *feasibility function*, and corresponds to

$$\begin{aligned} \psi(\boldsymbol{\theta}, d, y) = &\min_{x, z, u} u, \\ \text{s.t. } &h_m(x, z, \boldsymbol{\theta}, d, y) = 0, \qquad m \in M, \\ &g_l(x, z, \boldsymbol{\theta}, d, y) \leq u, \qquad l \in L, \end{aligned} \tag{4}$$

in which u is a scalar variable.

The *flexibility-index* problem is to determine the maximum scaled deviation of the expected uncertain parameter deviations that a given design and structure can handle for feasible operation. Mathematically this is formulated as (Swaney and Grossmann, 1985a)

$$\begin{aligned} F(d, y) = &\max \ \delta, \\ \text{s.t.} \quad &0 \leq \max_{\theta \in T(\delta)} \psi(\boldsymbol{\theta}, d, y), \\ &T(\delta) = \left\{\boldsymbol{\theta} | \boldsymbol{\theta}^N - \delta\boldsymbol{\Delta\theta}^- \leq \boldsymbol{\theta} \leq \boldsymbol{\theta}^N + \delta\boldsymbol{\Delta\theta}^+, r(\boldsymbol{\theta}) \leq \mathbf{0}\right\}, \\ &\delta \geq 0. \end{aligned} \tag{5}$$

A value of $F = 1$ therefore indicates that the design has the *exact* flexibility to satisfy the system constraints [in this case, a flexibility test would give $\chi(d, y) = 0$]. A value of $F > 1$ implies that an even wider range of uncertainty than that originally expected by the designer can be handled [$\chi(d, y) < 0$]; $F < 1$ indicates that only a fraction of the expected parameter deviations can be tolerated [$\chi(d, y) > 0$].

Existing evaluation approaches

Assuming that there are no constraints, $r(\boldsymbol{\theta}) \leq \mathbf{0}$, the simplest methods for solving the flexibility test and index problems are vertex enumeration schemes (Halemane and Grossmann, 1983; Swaney and Grossmann, 1985a), which can be applied for certain classes of model (such as linear). A drawback with this kind of approach is the fact that the number of optimization problems that must be solved increases exponentially with the number of uncertain parameters, n_θ (2^{n_θ} problems). The implicit enumeration schemes developed by Swaney and Grossmann (1985b) and Kabatek and Swaney (1992) do go some way toward avoiding this.

Grossmann and Floudas (1987) developed mixed-integer formulations for the flexibility test and index problems, which utilize the fact that $\psi(\boldsymbol{\theta}, d, y)$ is a piecewise-continuous function for a particular design and structure, with segments characterized by different sets of active inequality constraints. As with the vertex enumeration schemes, this approach does not give information on the explicit dependence of the system flexibility on the values of the continuous design variables d.

For the case when the system constraints (Eqs. 1 and 2) are linear, as is the focus of this article, Pistikopoulos and Grossmann (1988) showed that the feasibility function associated with each set of active inequalities can be expressed analytically as a linear function of the uncertain parameters and design variables when the process structure is fixed. The critical uncertain parameter values can then be obtained by inspection for each active set and the flexibility readily calculated. Such an approach provides useful analytical information; the drawback, however, is that it requires the *a priori* identification of all the sets of active constraints. Although Pistikopoulos and Grossmann (1988) proposed a systematic enumeration procedure to achieve this, it can involve the solution of a large number of MILPs since the number of possible sets of active constraints is often very large.

Varvarezos et al. (1995) tried to overcome these problems with an approach that uses sensitivity information of Eq. 4 with respect to the uncertain parameters to only identify nonredundant sets of active constraints. They also indicated how, for a fixed flexibility index, the corresponding feasibility functions can be expressed linearly in terms of the design variables. In the next section, we describe an approach that generalizes this within a parametric programming framework. The parametric programming approach gives the explicit dependence of the flexibility test measure and the flexibility index on the design variables $\boldsymbol{d}$, as well as the regions in $\boldsymbol{d}$-space in which these solutions are optimal. It also provides a platform for obtaining explicit expressions for the cost of a system in terms of a target flexibility index, and for efficiently solving flexibility analysis problems in stochastic systems, as will be shown in subsequent sections.

Parametric programming approach

For linear systems, the feasibility function formulation (Eq. 4) becomes

$$\psi(\boldsymbol{\theta}, d, y) = \min_{x,z,u} u,$$
$$\text{s.t.} \quad H_x \cdot x + H_z \cdot z + H_{\boldsymbol{\theta}} \cdot \boldsymbol{\theta} + H_d \cdot d + H_y \cdot y + h_c = \mathbf{0},$$
$$G_x \cdot x + G_z \cdot z + G_{\boldsymbol{\theta}} \cdot \boldsymbol{\theta} + G_d \cdot d + G_y \cdot y + g_c \le u.e, \qquad (6)$$

where H and G are matrices of constants (or more generally, functions of the integer variables y); h_c and g_c are vectors of constants; and e is a vector whose elements are all unity. For a fixed structure, Eq. 6 can be rearranged into the following form

$$\psi(\boldsymbol{\Theta}) = \min_{w} \ (c^T \cdot w + u^L),$$
$$\text{s.t.} \quad A_1 \cdot w = b_1 + F_1 \cdot \boldsymbol{\Theta},$$
$$A_2 \cdot w \le b_2 + F_2 \cdot \boldsymbol{\Theta},$$
$$\mathbf{0} \le b_3 + F_3 \cdot \boldsymbol{\Theta},$$
$$w \ge \mathbf{0}, \qquad (7)$$

where $w = (\hat{x}^T | \hat{z}^T | \hat{u})^T$; $\boldsymbol{\Theta} = (\boldsymbol{\theta}^T | d^T)^T$; c is a column vector where the final element is 1 and all the other elements are zero; $A_1 = [H_x | H_z | \mathbf{0}]$; $b_1 = -H_x \cdot x^L - H_z \cdot z^L - H_y \cdot y - h_c$; $F_1 = [-H_\theta | -H_d]$; $A_2 = [G_x | G_z | -e]$; $b_2 = -G_x \cdot x^L - G_z \cdot z^L - G_y \cdot y - g_c + u^L e$; $F_2 = [-G_{\boldsymbol{\theta}} | -G_d]$; $\hat{x} = x - x^L$; $\hat{z} = z - z^L$; $\hat{u} = u - u^L$; x^L, z^L, u^L are lower bounds on their respective variables; and the constraints $\mathbf{0} \le b_3 + F_3 \cdot \boldsymbol{\Theta}$ incorporate the lower and upper bounds on the uncertain parameters and design variables, as well as other constraints such as relationships between dependent uncertain parameters.

The reformulated system (Eq. 7) is now in the correct form for solution as a multiparametric linear program (mp-LP) using algorithms already reported in the literature. For example, the algorithm of Gal and Nedoma (1972) (see Appendix A) can be used to give a set of expressions for ψ that are linear in $\boldsymbol{\Theta}$ (that is, in $\boldsymbol{\theta}$ and d), and a corresponding set of regions (defined by linear inequalities in $\boldsymbol{\theta}$ and d) in which these solutions are optimal.

The kth feasibility function expression given by the mp-LP algorithm for the structure under consideration is of the following form

$$\psi^k(\boldsymbol{\theta}, d) = \sum_{i=1}^{n_\theta} \alpha_i^k \cdot \theta_i + \sum_{i=1}^{n_d} \beta_i^k \cdot d_i + \gamma^k, \qquad (8)$$

where n_d is the number of design variables $\boldsymbol{d}$; and α_i^k, β_i^k, and γ^k are constants. Once these expressions have been obtained, the flexibility test measure and the flexibility index can be solved, not just for a given design as in previous works, but *as a function of the continuous design variables*. This requires the use of the properties for linear systems reported by Pistikopoulos and Grossmann (1988) and a comparison procedure similar to that proposed by Acevedo and Pistikopoulos (1997b) in the context of parametric programming. First, the critical uncertainty direction for each feasibility function is the one in which there is the largest increase in $\psi^k(\boldsymbol{\theta}, d)$. Mathematically this can be expressed as

$$\left(\frac{\partial \psi^k}{\partial \theta_i}\right) \cdot \Delta \theta_i^{c,k} > 0, \qquad i = 1, \ldots, n_\theta, \qquad (9)$$

where $\Delta \theta_i^{c,k}$ is the critical deviation of the ith uncertain parameter. From Eq. 8, the partial derivatives $\partial \psi^k / \partial \theta_i$ are α_i^k, that is, they are simply constants. It follows from Eq. 9, therefore, that

$$\text{(a) if} \ \frac{\partial \psi^k}{\partial \theta_i} < 0 \Rightarrow \Delta \theta_i^{c,k} = -\Delta \theta_i^-,$$
$$\theta_i^{c,k} = \theta_i^N - \delta^k \Delta \theta_i^-, \qquad i = 1, \ldots, n_\theta; \qquad (10)$$
$$\text{(b) if} \ \frac{\partial \psi^k}{\partial \theta_i} > 0 \Rightarrow \Delta \theta_i^{c,k} = +\Delta \theta_i^+,$$
$$\theta_i^{c,k} = \theta_i^N + \delta^k \Delta \theta_i^+, \qquad i = 1, \ldots, n_\theta, \qquad (11)$$

where δ^k is the associated flexibility index.

For the flexibility test, the critical uncertain parameter values from Eqs. 10 and 11, with $\delta^k = 1$, are substituted into Eq. 8 to give the expressions

$$\psi^k(\boldsymbol{\theta}^{c,k}, d) = \sum_{i=1}^{n_d} \beta_i^k \cdot d_i + \epsilon^k, \qquad (12)$$

where ϵ^k is a new constant term. The set of linear, parametric expressions for $\chi(d)$, and their associated regions of optimality, is then obtained by comparing the feasibility functions (Eq. 12) and retaining the *upper* bounds (see Appendix B).

For the flexibility index, linear parametric expressions for $\delta^k(d)$, $k = 1, \ldots, K$, are obtained by solving the linear equations $\psi^k[\boldsymbol{\theta}^{c,k}(\delta^k), d] = 0$, $k = 1, \ldots, K$. The set of linear solutions for $F(d)$ and the associated regions of optimality can then be obtained by comparing $\delta^k(d)$ and the constraints $\delta^k(d) \ge 0$, and retaining the *lower* bounds.

Based on the theory just given, the steps of the proposed parametric programming algorithm to solve the flexibility test and index problems for a linear process system with fixed structure can be summarized as follows.

Algorithm 1

Step 1. Reformulate the feasibility function problem (Eq. 6) into the form of Eq. 7.

Step 2. Solve Eq. 7 as an mp-LP using the algorithm of Gal and Nedoma (1972), described in Appendix A. This will give a set of K linear parametric solutions, $\psi^k(\boldsymbol{\Theta})$, and corresponding regions of optimality, CR^k.

Step 3. For each of the K feasibility functions, $\psi^k(\boldsymbol{\theta}, d)$, obtain the critical uncertain parameter values, $\boldsymbol{\theta}^{c,k}$ from Eqs. 10 and 11.

Step 4

- For the flexibility test:

(a) substitute $\boldsymbol{\theta}^{c,k}$ with $\delta^k = 1$ into the feasibility function expressions to obtain new expressions $\psi^k(\boldsymbol{\theta}^{c,k}, d)$, $k=1, \ldots, K$, as in Eq. 12;

(b) obtain the set of linear solutions $\chi^k(d)$, and their associated regions of optimality, $\overline{CR}^k$, $k=1, \ldots, K_\chi$, where $K_\chi \le K$, by comparing the functions $\psi^k(\boldsymbol{\theta}^{c,k}, d)$, $k=1, \ldots, K$, and retaining the upper bounds, as described in Appendix B.

- For the flexibility index:

(a) solve the linear equations, $\psi^k[\boldsymbol{\theta}^{c,k}(\delta^k), d] = 0$, $k=1, \ldots, K$, to obtain a set of linear expressions for δ^k, $k=1, \ldots, K$, in terms of d.

(b) obtain the set of linear solutions $F^k(d)$, and their associated regions of optimality, $\overline{CR}^k$, $k=1, \ldots, K_F$, by comparing the functions $\delta^k(d)$ and the constraints $\delta^k(d) \ge 0$, $k=1, \ldots, K$, and retaining the lower bounds, as described in Appendix B.

Illustrative example

The steps of Algorithm 1 are now illustrated on a small, mathematical example. The system is described by the following set of constraints

$$\begin{aligned}
h_1 &= 2x - 3z + \theta_1 - d_2 = 0,\\
g_1 &= x - \frac{1}{2}z - \frac{1}{2}\theta_1 + \frac{1}{2}\theta_2 + d_1 - \frac{7}{2}d_2 \le 0,\\
g_2 &= -2x + 2z - \frac{4}{3}\theta_1 - \theta_2 + 2d_2 + \frac{1}{3} \le 0,\\
g_3 &= -x + \frac{5}{2}z + \frac{1}{2}\theta_1 - \theta_2 - d_1 + \frac{1}{2}d_2 - 1 \le 0,\\
-50 &\le x, \quad z,\\
0 &\le \theta_1, \quad \theta_2 \le 4,\\
0 &\le d_1, \quad d_2 \le 5.
\end{aligned} \tag{13}$$

Step 1. The reformulated feasibility function problem becomes

$$\begin{aligned}
\psi &= \min \quad (\hat{u} - 50)\\
\text{s.t.}\ -2\hat{x} + 3\hat{z} &= 50 + \theta_1 - d_2\\
\hat{x} - \frac{1}{2}\hat{z} - \hat{u} &\le -25 + \frac{1}{2}\theta_1 - \frac{1}{2}\theta_2 - d_1 + \frac{7}{2}d_2,\\
-2\hat{x} + 2\hat{z} - \hat{u} &\le -50\frac{1}{3} + \frac{4}{3}\theta_1 + \theta_2 - 2d_2,\\
-\hat{x} + \frac{5}{2}\hat{z} - \hat{u} &\le 26 - \frac{1}{2}\theta_1 + \theta_2 + d_1 - \frac{1}{2}d_2,\\
0 &\le \theta_1, \quad \theta_2 \le 4,\\
0 &\le d_1, \quad d_2 \le 5,
\end{aligned} \tag{14}$$

where lower bounds of $x^L = z^L = u^L = -50$ have been used. Note that a strict lower bound u^L could have been found by solving the original feasibility function problem with x, z, $\boldsymbol{\theta}$, and d, all as free variables.

Step 2. Solving Eq. 14 as an mp-LP gives the two parametric expressions and corresponding regions of optimality, Eqs. A5 and A6, derived in Appendix A. These are repeated below

$$\psi^1(\boldsymbol{\theta}, d) = -\frac{2}{3}\theta_1 - \frac{1}{4}\theta_2 + \frac{1}{2}d_1 - d_2 + \frac{1}{6}, \tag{15}$$

$$CR^1 = \begin{cases} 2\theta_1 - \frac{3}{2}\theta_2 - 2d_1 + 3d_2 \le 1\\ 0 \le \theta_1, \quad \theta_2 \le 4\\ 0 \le d_1 \le 5. \end{cases}$$

$$\psi^2(\boldsymbol{\theta}, d) = \frac{1}{3}\theta_1 - \theta_2 - \frac{1}{2}d_1 + \frac{1}{2}d_2 - \frac{1}{3}, \tag{16}$$

$$CR^2 = \begin{cases} 2\theta_1 - \frac{3}{2}\theta_2 - 2d_1 + 3d_2 \ge 1\\ 0 \le \theta_1, \quad \theta_2 \le 4\\ 0 \le d_1, \quad d_2 \le 5. \end{cases}$$

Step 3.

$$\frac{\partial\psi^1}{\partial\theta_1} < 0 \Rightarrow \Delta\theta_1^{c,1} = -2, \quad \theta_1^{c,1} = 2 - 2\delta^1.$$

$$\frac{\partial\psi^1}{\partial\theta_2} < 0 \Rightarrow \Delta\theta_2^{c,1} = -2, \quad \theta_2^{c,1} = 2 - 2\delta^1.$$

$$\frac{\partial\psi^2}{\partial\theta_1} > 0 \Rightarrow \Delta\theta_1^{c,2} = +2, \quad \theta_1^{c,2} = 2 + 2\delta^2.$$

$$\frac{\partial\psi^2}{\partial\theta_2} < 0 \Rightarrow \Delta\theta_2^{c,2} = -2, \quad \theta_2^{c,2} = 2 - 2\delta^2.$$

Step 4.

- For the flexibility test:

(a)

$$\psi^1(\boldsymbol{\theta}^{c,1}, d) = \frac{1}{2}d_1 - d_2 + \frac{1}{6},$$

$$\psi^2(\boldsymbol{\theta}^{c,2}, d) = -\frac{1}{2}d_1 + \frac{1}{2}d_2 + 1.$$

(b)

$$\chi^1(d) = \frac{1}{2}d_1 - d_2 + \frac{1}{6}, \tag{17}$$

$$\overline{CR}^1 = \begin{cases} 2d_1 - 3d_2 \ge \frac{5}{3}\\ d_1 \le 5, \quad d_2 \ge 0. \end{cases}$$

$$\chi^2(d) = -\frac{1}{2}d_1 + \frac{1}{2}d_2 + 1, \tag{18}$$

$$\overline{CR}^2 = \begin{cases} 2d_1 - 3d_2 \le \frac{5}{3}\\ 0 \le d_1, \quad d_2 \le 5. \end{cases}$$

- For the flexibility index:

(a) $$\delta^1(d) = \frac{1}{11}(-3d_1 + 6d_2 + 10),$$

$$\delta^2(d) = \frac{1}{16}(3d_1 - 3d_2 + 10).$$

(b) $$F^1(d) = \frac{1}{16}(3d_1 - 3d_2 + 10), \tag{19}$$

$$\overline{CR}^1 = \begin{cases} -\frac{1}{2}d_1 + \frac{1}{2}d_2 \le \frac{5}{3} \\ \frac{27}{43}d_1 - d_2 \le \frac{50}{129} \\ 0 \le d_1, \quad d_2 \le 5 \\ 0 \le d_2 \le 5. \end{cases}$$

$$F^2(d) = \frac{1}{11}(-3d_1 + 6d_2 + 10), \tag{20}$$

$$\overline{CR}^2 = \begin{cases} \frac{1}{2}d_1 - d_2 \le \frac{5}{3} \\ \frac{27}{43}d_1 - d_2 \ge \frac{50}{129} \\ d_1 \le 5, \quad d_2 \ge 0. \end{cases}$$

$$F^3(d) = 0, \tag{21}$$

$$\overline{CR}^3 = \begin{cases} -\frac{1}{2}d_1 + \frac{1}{2}d_2 \ge \frac{5}{3} \\ d_1 \ge 0, \quad d_2 \le 5. \end{cases}$$

$$F^4(d) = 0, \tag{22}$$

$$\overline{CR}^4 = \begin{cases} \frac{1}{2}d_1 - d_2 \ge \frac{5}{3} \\ d_1 \le 5, \quad d_2 \ge 0. \end{cases}$$

The parametric flexibility test solutions, Eqs. 17 and 18, are illustrated graphically in d-space in Figure 1, while the flexibility index solutions, Eqs. 19 to 22, are shown in Figure 2. Note that Eqs. 21 and 22, where the flexibility index is zero, correspond to designs where the nominal uncertain parameter point, $\theta_1^N = \theta_2^N = 2$, is infeasible.

Remarks on Algorithm 1

1. In some cases, it may be computationally advantageous to first eliminate the state variables x from the equality constraints using simple matrix manipulations. If this is done, then the feasibility function formulation (Eq. 6) becomes

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

$$\text{s.t. } \hat{G}_z \cdot z + \hat{G}_{\boldsymbol{\theta}} \cdot \boldsymbol{\theta} + \hat{G}_d \cdot d + \hat{G}_y \cdot y + \hat{g}_c \le u \cdot e, \tag{23}$$

where $\hat{G}_i = G_i - G_x \cdot H_x^{-1} \cdot H_i$ for $i = z, \boldsymbol{\theta}, d,$ and y; and $\hat{g}_c = g_c - G_x \cdot H_x^{-1} \cdot h_c$.

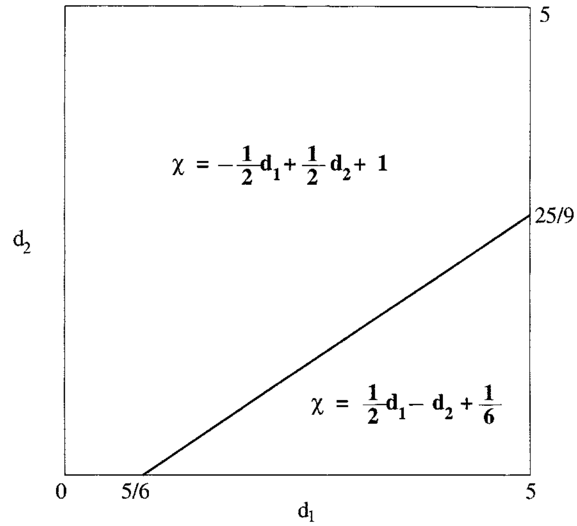

Figure 1. Parametric flexibility test solutions in *d*-space for the illustrative example.

2. The set of active constraints associated with each of the K feasibility function expressions obtained from Step 2 is automatically given by the mp-LP algorithm through the nonbasic slack variables (see Appendix A). For the illustrative example just given, ψ^1 corresponds to inequalities g_1 and g_2 being active, while ψ^2 corresponds to g_2 and g_3 being active. The process examples presented later in this article will demonstrate the advantage of this compared to finding *all potential* sets of active constraints (many of which may be redundant) using the method of Pistikopoulos and Grossmann (1988).

3. The algorithm gives the explicit (linear) dependence of the flexibility test measure and index of a system on the continuous design variables. This reduces the subsequent com-

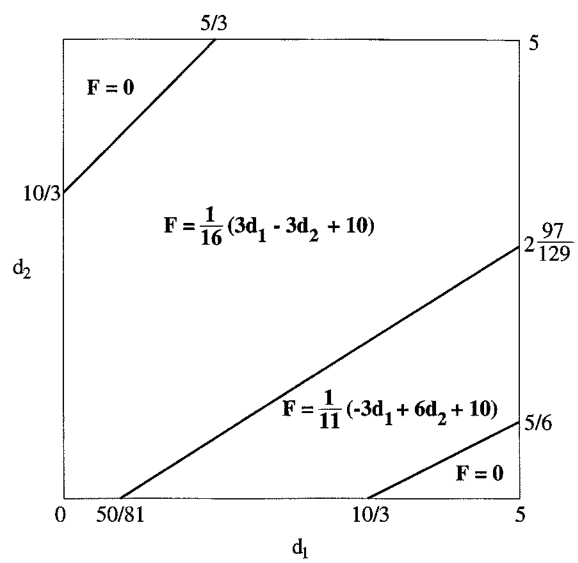

Figure 2. Parametric flexibility index solutions in *d*-space for the illustrative example.

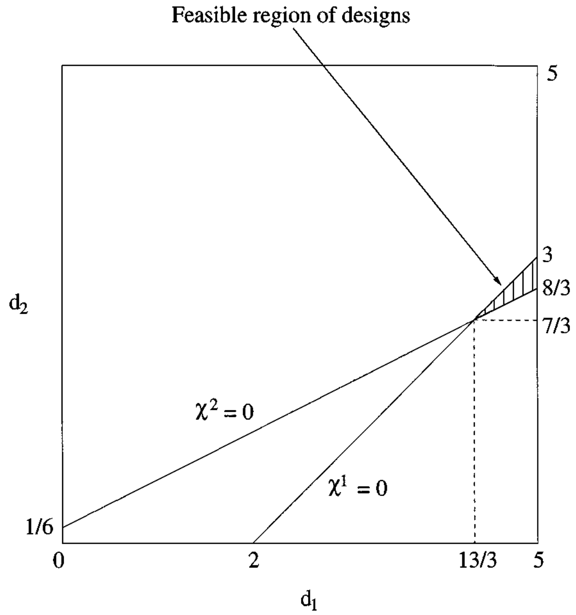

Figure 3. Feasible region in d-space for the illustrative example.

putation of these metrics for a particular design to simple function evaluations and also gives a designer insight into which design variables most strongly limit the flexibility. Moreover, for the system structure under investigation, this enables the construction of a "feasible region" in the design space through the expressions $\chi^k(d) \le 0$, $k = 1, \ldots, K_\chi$ (or, for a target flexibility index F^t, through $F^k(d) \ge F^t$, $k = 1, \ldots, K_F$). In Figure 3, the shaded area shows the "feasible region" for the illustrative example, as defined by $\chi^1(d) \le 0 \cap \chi^2(d) \le 0$. Any set of design values, $\{d_1, d_2\}$, that lies in this shaded region, leads to a system that can be operated feasibly through proper manipulation of the control variables, no matter what values the uncertain parameters take within their lower and upper bounds. This clearly demonstrates the power of this parametric programming algorithm in enabling a designer to know, *a priori*, the full range of flexible designs.

4. An alternative to Algorithm 1 is to use the flexibility test and index formulations of Grossmann and Floudas (1987) and solve them directly as multiparametric, mixed-integer, linear programs (mp-MILPs), using, for example, the algorithm of Acevedo and Pistikopoulos (1999) or that of Dua and Pistikopoulos (2000). The latter algorithm is outlined in Appendix C, where it is illustrated for the flexibility test of the mathematical example given earlier. This method does indeed give the same parametric expressions and regions of optimality as Algorithm 1. However, such an mp-MILP method offers little advantage because (1) it involves the solution of far more subproblems (for the illustrative example: 6 MILPs, 3 mp-LPs, and a comparison of parametric solutions, compared to just 1 mp-LP and a comparison of parametric solutions with Algorithm 1); and (2) it involves the solution of much larger subproblems, since the vector of search variables, w, must be expanded to include $\boldsymbol{\theta}$, the Lagrange multipliers $\boldsymbol{\mu}$ and $\boldsymbol{\lambda}$, and extra slack variables (for the individual mp-LPs in the illustrative example, although the number of parameters is reduced from 4 to 2 compared to Algorithm 1, there are 13 search variables compared to 6).

5. For systems that are nonlinear in the continuous design variables $\boldsymbol{d}$, as well as the integer variables y, Algorithm 1 can still be applied, provided that both the design and the structure are fixed before Step 2. In this case, the complete map of solutions in the continuous design space cannot be obtained. However, linear expressions for the feasibility functions in terms of the uncertain parameters $\boldsymbol{\theta}$ will be yielded by Step 2, and the final results will be values for χ and F. To illustrate this, consider the nonlinear system described by the following set of constraints

$$
\begin{aligned}
h_1 &= 2x - d_1 \cdot z + \theta_1 - d_2 = 0,\\
g_1 &= x - \frac{1}{2}z - \frac{1}{2}\theta_1 + \frac{1}{2}\theta_2 + d_1 - \frac{7}{2}d_2 \le 0,\\
g_2 &= -2x + 2z - \frac{4\theta_1}{d_1} - \theta_2 + \frac{1}{d_1} + 2d_2 \le 0,\\
g_3 &= -x + \frac{5}{2}z + \frac{1}{2}\theta_1 - \theta_2 - d_1 + \frac{1}{2}d_2 - d_2^2 \le 0,\\
&-50 \le x, \quad z,\\
&0 \le \theta_1, \quad \theta_2 \le 4,
\end{aligned}
\tag{24}
$$

with $d_1 = 3$ and $d_2 = 1$. Applications of Algorithm 1 gives

$$\psi^1(\boldsymbol{\theta}) = -\frac{2}{3}\theta_1 - \frac{1}{4}\theta_2 + \frac{2}{3},$$

$$CR^1 = \begin{cases} 2\theta_1 - \frac{3}{2}\theta_2 \le 4 \\ 0 \le \theta_1, \quad \theta_2 \le 4. \end{cases}$$

$$\psi^2(\boldsymbol{\theta}, d) = \frac{1}{3}\theta_1 - \theta_2 - \frac{4}{3},$$

$$CR^2 = \begin{cases} 2\theta_1 - \frac{3}{2}\theta_2 \ge 4 \\ \theta_1 \le 4, \quad \theta_2 \ge 0. \end{cases}$$

$$\chi = \frac{2}{3}, \quad F = \frac{7}{11}.$$

Design optimization for target flexibility index

The most general design optimization problem for systems with deterministic uncertain parameters is to determine the design that minimizes the system cost while maximizing the flexibility index and ensuring feasibility over the associated parameter range (Grossmann and Morari, 1983). This corresponds to a bi-objective optimization problem that has no unique optimal solution, but instead an infinite number of pareto-optimal or trade-off solutions. Consider the case when the (linear) objective function only comprises investment costs, as commonly occurs in retrofit design problems. Common practice in the literature has been to obtain a finite number of these solutions by essentially formulating the problem as (Pistikopoulos and Grossmann, 1988)

$$\text{Cost} = \min_{d} \ \boldsymbol{\kappa}^T \cdot d,$$
$$\text{s.t.} \quad F^k(d) \ge F^t, \quad k = 1, \ldots, K_F, \tag{25}$$
$$d^L \le d \le d^U,$$

and then solving Eq. 25 repeatedly for different values of the target flexibility index, F^t. Pistikopoulos and Grossmann (1988) proposed an algorithm that uses range analysis in an attempt to reduce the computational effort associated with this approach. Their algorithm can be generalized, however, and the *exact, algebraic* form of the trade-off curve obtained, by using the linear expressions for $F^k(d)$, $k = 1, \ldots, K_F$, provided by Algorithm 1 and realizing that Eq. 25 actually corresponds to a single-parameter linear program (p-LP) in F^t. This can be solved (see Gal, 1995, chap. 3) to explicitly yield all the cost solutions as linear functions of F^t. For example, for the illustrative example considered previously, solving

$$\text{Cost} = \min_{d_1, d_2} \ (10 d_1 + 10 d_2),$$
$$\text{s.t.} \quad F^1 = \frac{1}{16}(3d_1 - 3d_2 + 10) \ge F^t,$$
$$F^2 = \frac{1}{11}(-3d_1 + 6d_2 + 10) \ge F^t,$$
$$0 \le d_1, \quad d_2 \le 5,$$
$$0.65 \le F^t \le 1,$$

as a p-LP gives

$$\text{Cost}^1 = 53\frac{1}{3}F^t - 33\frac{1}{3},$$
$$\overline{CR}^1 = \left\{ 0.65 \le F^t \le \frac{20}{27}, \right.$$
$$\text{Active constraint}: F^1.$$
$$\text{Cost}^2 = 233\frac{1}{3}F^t - 166\frac{2}{3},$$
$$\overline{CR}^2 = \left\{ \frac{20}{27} \le F^t \le 1, \right.$$
$$\text{Active constraint}: F^2.$$

The parametric solutions just given, illustrated in the trade-off curve of cost against target flexibility index in Figure 4, enable the cost for a desired flexibility index to be calculated through a function evaluation. They indicate the exact point at which there is a changeover from F^1 being active to F^2 being active, namely $F^t = 20/27 \simeq 0.74$. They also show that the cost is more than four times more sensitive to changes in the target flexibility index once F^2 becomes active, and as such, that there is a high economic penalty for guaranteeing feasibility over the complete space of uncertain parameters. For example, a designer may choose to design for a flexibility index of 0.80 instead of 1, since the cost of the former is less

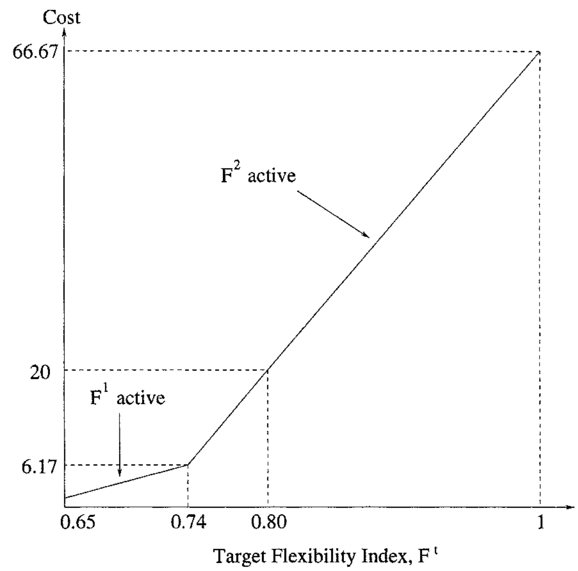

Figure 4. Cost vs. flexibility index trade-off curve for the illustrative example.

than one-third of the latter (20 compared to $66\frac{2}{3}$). Note also that the solution at $F^t = 1$ corresponds to the solution of the LP

$$\text{Cost} = \min_{d} \ \boldsymbol{\kappa}^T \cdot d,$$
$$\text{s.t.} \quad \chi^k(d) \le 0, \quad k = 1, \ldots, K_\chi,$$
$$d^L \le d \le d^U,$$

and that the optimal design for this example, $d_1 = 13/3$, $d_2 = 7/3$, lies at the intersection of $\chi^1 = 0$ and $\chi^2 = 0$, on the boundary of the "feasible region" of designs, as can be seen from Figure 3.

Stochastic Flexibility

Definition

For a system with uncertain parameters described by a joint probability density function (pdf), $j(\boldsymbol{\theta})$, the typical analysis problem is to evaluate the probability that, for a given design and structure, a system can be feasibly operated through appropriate manipulation of the control variables. This probability is referred to as the *stochastic flexibility* (SF) (Pistikopoulos and Mazzuchi, 1990; Straub and Grossmann, 1990). Mathematically, this means computing

$$SF(d, y) = Pr[\psi(\boldsymbol{\theta}, d, y) \le 0], \tag{26}$$

over all possible realizations of $\boldsymbol{\theta}$. The stochastic flexibility can also be expressed as the integral of the joint pdf over the feasible region of operation in the space of the uncertain parameters, that is,

$$SF(d, y) = \int_{\{\theta : \psi(\theta, d, y) \le 0\}} j(\boldsymbol{\theta}) \quad d\boldsymbol{\theta}. \tag{27}$$

Existing evaluation approaches

Pistikopoulos and Mazzuchi (1990) developed a procedure for evaluating the stochastic flexibility of linear systems when the uncertain parameters are all described by normal pdfs. The first step of their method is to develop linear feasibility function expressions using the active set identification algorithm of Pistikopoulos and Grossmann (1988). Since these feasibility functions are linear in the independent, normally distributed parameters $\boldsymbol{\theta}$, they themselves are normally distributed random variables with easily calculable means and variance−covariance matrix for a given design. If the variance−covariance matrix is nonsingular, the stochastic flexibility of the system can then be computed as a multivariate normal probability using existing computer codes (such as G01HBF (NAG, 1998)); for the case when this matrix is singular, Pistikopoulos and Mazzuchi (1990) have proposed an effective bounding procedure, although new methods for computing singular multivariate normal probabilities have recently been developed (Bansal et al., 2000).

The drawbacks of this approach are that it is again centered around the *a priori* identification of active sets and that it only applies to systems with normally distributed parameters. Straub and Grossmann (1990) overcame the latter limitation using an inequality reduction scheme that successively projects the functions $\psi^k(\boldsymbol{\theta}, d)$, $k = 1, \ldots, K$, into lower-dimensional spaces in $\boldsymbol{\theta}$. Lower and upper bounds for each uncertain parameter are generated and Gaussian quadrature points are placed within the feasible operating region. The integral (Eq. 27) is then numerically approximated. The major difficulty with this method, however, is that it requires identification of active sets *at each projection* of the feasibility functions.

Straub and Grossmann (1993) developed an algorithm for evaluating the stochastic flexibility in linear or nonlinear systems with generally distributed uncertain parameters that does not rely on identification of the active sets. The basic strategy is to solve an optimization problem in order to compute bounds in the feasible region for one uncertain parameter, place quadrature points for that parameter, and then for each quadrature point calculate the bounds for the next uncertain parameter, and so on. Once sufficient quadrature points have been placed, the joint pdf of the uncertain parameters can be numerically integrated over the region. A drawback of this approach is that the number of optimization subproblems that needs to be solved increases exponentially with the number of uncertain parameters, n_θ, and the number of quadrature points used for each parameter, $Q_i\{1 + Q_1\{1 + Q_2[\cdots(1 + Q_{n_\theta - 1})\}$ problems}. Straub and Grossman (1993) did propose an embedded formulation to avoid this, but, even for linear process models, this corresponds to the solution of a very large, nonlinear program (NLP). More efficient integration techniques than Gaussian quadrature also have been proposed in the context of stochastic design optimization, such as specialized quadratures and cubatures for normally distributed parameters (Bernardo et al., 1999), and Monte Carlo methods with efficient sampling techniques (Diwekar and Kalagnanam, 1997; Acevedo and Pistikopoulos, 1998). The difficulty in applying these methods to stochastic flexibility evaluation, however, is that each of the generated integration points must be checked to see if it actually lies within the feasible region of uncertain parameters. Besides the subsequent issue of integration accuracy, this will typically involve solving the feasibility function problem (Eq. 4) at each point, and so the computational burden can actually be greater than that using conventional Gaussian quadrature (as pointed out by Straub and Grossmann, 1990).

Parametric programming approach

Parametric programming can be used to overcome the computational difficulties associated with the stochastic flexibility evaluation methods outlined in the previous section. For example, instead of relying on active set identification, Algorithm 1 can be used to generate the linear feasibility function expressions required for the analysis of Pistikopoulos and Mazzuchi (1990). The method of Straub and Grossmann (1993) can also be adapted within a parametric programming framework in order to evaluate the stochastic flexibility in linear systems with continuous uncertainties described by *any* type of joint pdf. Furthermore, the use of parametric programming allows the method to be extended to give information on the dependence of the stochastic flexibility on the continuous design variables. Such an algorithm is summarized below.

Algorithm 2

Steps 1 and 2. As in Algorithm 1.

Step 3. For $i = 1$ to n_θ:

(a) Compute the upper and lower bounds of θ_i in the feasible operating region, $\theta_i^{\max}$ and $\theta_i^{\min}$, respectively, as linear functions of lower-dimensional parameters, $\theta_{p(p=1,\ldots,i-1)}$, and d (Acevedo and Pistikopoulos, 1997a), by solving the mp-LP

$$
\begin{aligned}
&\max\ \left(\theta_i^{\max q_1 \cdots q_{i-1}} - \theta_i^{\min q_1 \cdots q_{i-1}}\right),\\
&\text{s.t. } \psi^k\left(\theta_{j(j=i+1,\ldots,n_\theta)}^{a q_1 \cdots q_{i-1}}, \theta_i^{\max q_1 \cdots q_{i-1}}, \theta_{p(p=1,\ldots,i-1)}^{q_1 \cdots q_p}, d\right) \le 0, \quad k = 1, \ldots, K,\\
&\psi^k\left(\theta_{j(j=i+1,\ldots,n_\theta)}^{b q_1 \cdots q_{i-1}}, \theta_i^{\min q_1 \cdots q_{i-1}}, \theta_{p(p=1,\ldots,i-1)}^{q_1 \cdots q_p}, d\right) \le 0, \quad k = 1, \ldots, K,\\
&\theta_j^L \le \theta_j^{a q_1 \cdots q_{i-1}}, \theta_j^{b q_1 \cdots q_{i-1}} \le \theta_j^U, \quad j = i+1, \ldots, n_\theta,\\
&\theta_i^L \le \theta_i^{\min q_1 \cdots q_{i-1}} \le \theta_i^{\max q_1 \cdots q_{i-1}} \le \theta_i^U,\\
&\theta_p^L \le \theta_p^{q_1 \cdots q_p} \le \theta_p^U, \quad p = 1, \ldots, i-1,\\
&d^L \le d \le d^U.
\end{aligned}
\tag{28}
$$

Here, θ_j^a and θ_j^b reflect the fact that different values of θ_j, $j=i+1, \ldots, n_\theta$, must be chosen in order to calculate the upper and lower bounds on θ_i; while q_i is the index set for the quadrature points to be used for the ith parameter. The solution of Eq. 28 gives N_i solutions and corresponding regions of optimality in $\theta_{p(p=1,\ldots,i-1)}$ and **d**.

Note that lower and upper bounds on the uncertain parameters can be obtained by truncating the probability distributions at points beyond which there is a negligible change in probability. For example, for a normally distributed parameter with mean μ and standard deviation σ, bounds of $\theta^L = \mu - 4\sigma$ and $\theta^U = \mu + 4\sigma$ can be used.

(b) Express the quadrature points, $\theta_i^{q_1 \cdots q_i}$, in terms of the locations of Gauss-Legendre quadrature points in the $[-1, 1]$ interval (Carnahan et al., 1969), $\nu_i^{q_i}$, from

$$\theta_i^{q_1 \cdots q_i}(d) = \frac{1}{2}\left[\theta_i^{\max q_1 \cdots q_{i-1}}(1+\nu_i^{q_i}) + \theta_i^{\min q_1 \cdots q_{i-1}}(1-\nu_i^{q_i})\right], \quad q_i = 1, \ldots, Q_i. \quad (29)$$

Step 4.

$$SF(d) = \frac{\theta_1^{\max} - \theta_1^{\min}}{2} \sum_{q_1=1}^{Q_1} w_1^{q_1} \frac{\theta_2^{\max q_1} - \theta_2^{\min q_1}}{2} \cdots \sum_{q_{n_\theta}=1}^{Q_{n_\theta}} w_{n_\theta}^{q_{n_\theta}} j(\theta_1^{q_1}, \ldots, \theta_{n_\theta}^{q_1 \cdots q_{n_\theta}}), \quad (30)$$

where $w_i^{q_i}$, $q_i = 1, \ldots, Q_i$, are the weights of the Gauss-Legendre quadrature points (Carnahan et al., 1969) for the ith parameter.

Illustrative example

Consider the problem of evaluating the stochastic flexibility of the system described by Eq. 13, for uncertain parameters that are independently, normally distributed, according to $\theta_1, \theta_2 \sim N(2, 1/4)$.

Steps 1 and 2. These give the feasibility functions (Eqs. 15 and 16).

Step 3.

(a)

$$\theta_1^{\max} = 4, \quad \theta_1^{\min} = 0, \quad CR^{1,1} = \left\{ d_1 - 2d_2 \le \frac{5}{3}. \right.$$

$$\theta_1^{\max} = 4, \quad \theta_1^{\min} = \frac{3}{4}d_1 - \frac{3}{2}d_2 - \frac{5}{4}, \quad CR^{1,2} = \left\{ d_1 - 2d_2 \ge \frac{5}{3}. \right.$$

$$\theta_2^{\max q_1} = 4, \quad \theta_2^{\min q_1} = -\frac{8}{3}\theta_1^{q_1} + 2d_1 - 4d_2 + \frac{2}{3},$$

$$CR^{2,1} = \begin{cases} -\dfrac{8}{3}\theta_1^{q_1} + 2d_1 - 4d_2 \le \dfrac{10}{3} \\ -\dfrac{8}{3}\theta_1^{q_1} + 2d_1 - 4d_2 \ge -\dfrac{2}{3}. \end{cases}$$

$$\theta_2^{\max q_1} = 4, \quad \theta_2^{\min q_1} = 0,$$

$$CR^{2,2} = \begin{cases} \dfrac{8}{3}\theta_1^{q_1} - 4d_1 + 4d_2 \le \dfrac{8}{3} \\ -\dfrac{8}{3}\theta_1^{q_1} + 2d_1 - 4d_2 \le -\dfrac{2}{3}. \end{cases}$$

$$\theta_2^{\max q_1} = 4, \quad \theta_2^{\min q_1} = \frac{1}{3}\theta_1^{q_1} - \frac{1}{2}d_1 + \frac{1}{2}d_2 - \frac{1}{3},$$

$$CR^{2,3} = \left\{ \frac{8}{3}\theta_1^{q_1} - 4d_1 + 4d_2 \ge \frac{8}{3}. \right.$$

(b)

In $CR^{1,1}$: $\theta_1^{q_1} = 2(1+\nu_1^{q_1}), \quad \forall q_1.$

In $CR^{1,2}$: $\theta_1^{q_1} = \frac{1}{8}(11 + 21\nu_1^{q_1}) + \frac{3}{8}(1-\nu_1^{q_1})(d_1 - 2d_2), \quad \forall q_1.$

In $CR^{2,1}$: $\theta_2^{q_1 q_2} = \frac{1}{3}(7 + 5\nu_2^{q_1}) - (1-\nu_2^{q_2})\left(\frac{4}{3}\theta_1^{q_1} - d_1 + 2d_2\right), \quad \forall q_1, \quad \forall q_2.$

In $CR^{2,2}$: $\theta_2^{q_1 q_2} = 2(1+\nu_2^{q_2}), \quad \forall q_1, \quad \forall q_2.$

In $CR^{2,3}$: $\theta_2^{q_1 q_2} = \frac{1}{6}(11 + 13\nu_2^{q_1}) + \frac{1}{12}(1-\nu_2^{q_2})(2\theta_1^{q_1} - 3d_1 + 3d_2), \quad \forall q_1, \quad \forall q_2.$

Step 4. The stochastic flexibility for a given set of design variables and quadrature points can be calculated by substituting the relevant values in the expressions obtained in Steps 3(a) and 3(b) and then substituting these values in Eq. 30. Note that the bivariate pdf defined by θ_1 and θ_2 is given by (Lapin, 1990):

$$j(\theta_1^{q_1}, \theta_2^{q_1 q_2}) = \frac{2}{\pi} \cdot \exp\left\{-2\left[(\theta_1^{q_1} - 2)^2 + (\theta_2^{q_1 q_2} - 2)^2\right]\right\}.$$

Table 1 shows the stochastic flexibility results for the three different designs.

Table 1. Stochastic Flexibility of Illustrative Example: Parametric vs. Sequential Approach

			No. of Subproblems		CPU (s)	
d	$Q_1 = Q_2$	SF	Algorithm 2	Sequential	Algorithm 2	Sequential
$(4, 1/2)^T$	8	0.6691	↑	9 LPs	↑	0.1
	12	0.6806	3 mp-LPs	13 LPs	0.2	0.2
	16	0.6801		17 LPs		0.2
	32	0.6801	↓	33 LPs	↓	0.4
$(5, 1.4)^T$	8	0.9393	↑	9 LPs	↑	0.1
	12	0.9440	No	13 LPs	neg.	0.2
	16	0.9442	extra	17 LPs		0.2
	32	0.9442	↓	33 LPs	↓	0.4
$(3.2, 0.4)^T$	8	0.8981	↑	9 LPs	↑	0.1
	12	0.9050	No	13 LPs	neg.	0.2
	16	0.9050	extra	17 LPs		0.2
	32	0.9050	↓	33 LPs	↓	0.4
Total			3 mp-LPs	216 LPs	0.2	2.7

Remarks on Algorithm 2

1. Algorithm 2 clearly demonstrates the power of a parametric programming approach to flexibility analysis in terms of the solution information it gives. The algorithm provides the explicit dependence of the uncertain parameter bounds (and hence, ultimately, the stochastic flexibility) on the values of d and the parameters of the quadrature method being used. This means that by applying the algorithm just once, a designer can then calculate the stochastic flexibility of any design, for any given number of quadrature points, by simply performing a sequence of function evaluations. This feature makes the application of Algorithm 2 particularly amenable as a tool for comparing design alternatives on the basis of their stochastic flexibility. For the illustrative example just presented, Table 1 demonstrates this, where it can be seen that no further optimization subproblems need to be solved in order to obtain the stochastic flexibilities of the second and third designs. In this case, the second design, $d = (5, 1.4)^T$, has the highest flexibility of the three designs considered.

2. The parametric programming approach leads to a reduction in the *size* of the individual optimization subproblems. This is achieved through the use of the feasibility functions rather than the complete system equations and inequalities, as, for example, in the "sequential" approaches of Straub and Grossmann (1993) and Pistikopoulos and Ierapetritou (1995). In Algorithm 2, the number of constraints in Step 3(a), excluding the parameter bounds, is 2 K. Using the complete model of the system leads to 2 $(\dim\{h\} + \dim\{g\})$ constraints. The former number is, in general, considerably smaller, since there are usually far fewer sets of active constraints than equations and inequalities in the process model. Furthermore, the number of optimization search variables is reduced in Algorithm 2 since the states x and controls z are eliminated. All this comes at the expense of the solution of only one mp-LP in Steps 1 and 2. For the illustrative example just given, the use of Algorithm 2 essentially *halves* the size of the problems in Step 3(a) compared to using the full set of system equations. For example, there are only 4 constraints instead of 8, while for $i = 2$, the number of search variables is reduced from 4 to 2.

3. Algorithm 2 leads to a significant reduction in the *number* of optimization subproblems that need to be solved and hence in the computation time compared to a sequential approach. As stated earlier, the latter requires the solution of $1 + Q_1\{1 + Q_2[\cdots(1 + Q_{n_\theta - 1})]\}$ LPs. Algorithm 2, on the other hand, only requires the solution of $(1 + n_\theta)$ mp-LPs. The benefit of this can be seen in Table 1 for the illustrative example. In order to generate the stochastic flexibilities shown requires the solution of a total of 216 LPs using the sequential approach compared to just three mp-LPs with Algorithm 2. This translates to a total of 2.7 s CPU on a Sun ULTRA 1 work station for the former approach using GAMS/CPLEX (Brooke et al., 1992), compared to 0.2 s for the latter approach using the prototype Fortran code of Acevedo and Pistikopoulos (1997b). Thus, even for such a tiny problem, a more than tenfold computational saving is achieved. This saving will increase as the number of uncertain parameters increases, as will be demonstrated with the process examples later in this article.

Note that the computational effort associated with both the sequential and parametric programming approaches can be diminished through parallelization. For the former, this is achieved by solving the first LP, then solving the next Q_1 LPs in parallel, then the next $Q_1 \cdot Q_2$ LPs in parallel, and so on. For the latter, the benefit is even greater, since *all* of the mp-LPs in Step 3(a) can be solved in parallel.

(4) For systems that are nonlinear in d, such as Eq. 24, the design is fixed before Step 2, and Algorithm 2 then proceeds in a similar fashion.

(5) In principle, the information from Algorithm 2 can be used to formulate a design optimization problem for target stochastic flexibility

$$\begin{aligned} \text{Cost} &= \min_d \ \boldsymbol{\kappa}^T \cdot d, \\ \text{s.t.} \quad SF^k(d) &\geq SF^t, \qquad \forall k, \\ d^L &\leq d \leq d^U, \end{aligned} \tag{31}$$

where SF^t is the target stochastic flexibility. However, since $SF^k(d)$, $\forall k$, are, in general, nonlinear and nonconvex, Eq. 31 corresponds to a nonconvex, single-parameter, nonlinear program (p-NLP). Global optimization methods for the solution of such problems are currently under development (Dua et al., 1999b).

Expected Stochastic Flexibility

Definition

If the discrete probability for the availability of each piece of equipment in a process with stochastic parameters is given, then the appropriate analysis problem is to determine the expected probability of feasible operation. This is known as the combined *flexibility-availability* index (Pistikopoulos et al., 1990), or *expected stochastic flexibility* (ESF) (Straub and Grossmann, 1990). Mathematically, it is defined as

$$ESF(d) = \sum_{s = S_1}^{2^{eq}} SF(d, y^s) \cdot P(y^s), \tag{32}$$

where s is the index set for the system states; $P(y^s)$ is the (discrete) probability that the system is in state s; and eq is the number of pieces of equipment in the system. Each state of the system is defined by different combinations of available and unavailable equipment. Thus, if y_i^s is a binary variable that takes a value of 1 if equipment i is available, and is zero otherwise; and p_i is the probability that equipment i is available, then

$$P(y^s) = \prod_{\{i | y_i^s = 1\}} p_i \prod_{\{i | y_i^s = 0\}} (1 - p_i). \tag{33}$$

Existing evaluation approaches

The obvious way to evaluate the expected stochastic flexibility for a particular set of continuous design variables is to calculate the stochastic flexibility for each state s using the method of Pistikopoulos and Mazzuchi (1990), Straub and Grossmann (1990), or Straub and Grossmann (1993), and then apply Eqs. 32 and 33. A drawback with this approach is the

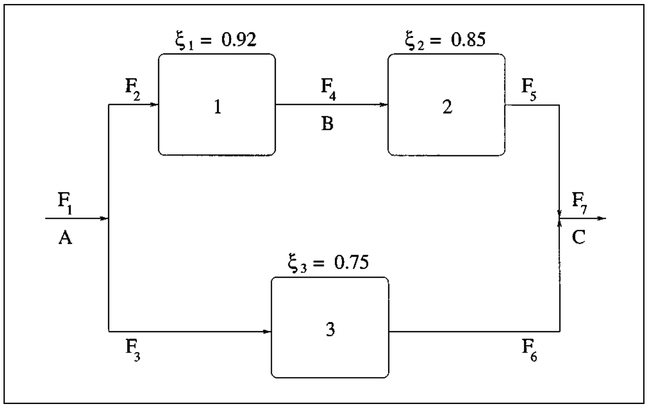

Figure 5. Process example 1: chemical complex.

potentially large number of system states, 2^{eq}, and hence summation terms in Eq. 32. For such cases, Straub and Grossmann (1990) have proposed an effective bounding scheme that requires the examination of much fewer states.

Parametric programming approach

By using Algorithm 2, the evaluation of the expected stochastic flexibility for any given design can be reduced to a series of function evaluations, thus enabling the very efficient comparison of design alternatives. This approach is illustrated in the first process example below.

Process Example 1: Chemical Complex

Figure 5, adapted from Straub and Grossmann (1990), shows a system where a species A is converted to a species C via two different process routes. In the first, plant 1 is used to convert A to an intermediate B, with a conversion factor $\xi_1 = 0.92$, and then plant 2 converts B to C with a conversion factor $\xi_2 = 0.85$. In the second process, plant 3 converts A directly into C with a conversion factor $\xi_3 = 0.75$. The linear-process model, comprising molar balances and specifications, is shown in Table 2. Note that F refers to molar flow rate; d_i is the processing capacity of plant i; and y_i is a binary variable that takes a value of 1 when plant i is available and a value of zero when it is unavailable. It is assumed that the supply of raw material, S, is uncertain, with a nominal value of 12 and range $8 \leq S \leq 16$; as is the product demand, D, which has a nominal value of 7 and range $3 \leq D \leq 11$. The process model thus consists of five state variables, $x = [F_3, F_4, F_5, F_6, F_7]^T$; two control variables, $z = [F_1, F_2]^T$; two uncertain parameters, $\boldsymbol{\theta} = [S, D]^T$; and three design variables, $\boldsymbol{d} = [d_1, d_2, d_3]^T$. The ranges of interest for the latter are $3 \leq d_1 \leq 7$, $7 \leq d_2 \leq 9$, and $7 \leq d_3 \leq 9$.

Table 2. Model for Process Example 1

Equalities	Inequalities
$F_1 = F_2 + F_3$	$g_1 = F_1 - S \leq 0$
$F_4 = 0.92 F_2$	$g_2 = F_2 - d_1 \cdot y_1 \leq 0$
$F_5 = 0.85 F_4$	$g_3 = F_4 - d_2 \cdot y_2 \leq 0$
$F_6 = 0.75 F_3$	$g_4 = F_5 - d_3 \cdot y_3 \leq 0$
$F_7 = F_5 + F_6$	$g_5 = D - F_7 \leq 0$

Flexibility test and index

Consider the case when all three plants are available, denoted as system state $S1$ (that is, $y^{S1} = [1, 1, 1]^T$). Algorithm 1 gives two feasibility function expressions (as opposed to the four given by the method of Pistikopoulos and Grossmann, 1988), one expression for the flexibility test measure, valid over the whole range of d, and two flexibility index expressions

$$\psi^1(\boldsymbol{\theta}, d, y^{S1}) = -0.421\theta_1 + 0.561\theta_2 - 0.018 d_1,$$

$$CR^1 = \{1.421\theta_1 - 0.561\theta_2 - 0.982 d_1 - d_3 \leq 0,$$

Active constraints: g_1, g_2 and g_5.

$$\psi^2(\boldsymbol{\theta}, d, y^{S1}) = 0.395\theta_2 - 0.309 d_1 - 0.296 d_3,$$

$$CR^2 = \{1.421\theta_1 - 0.561\theta_2 - 0.982 d_1 - d_3 \geq 0,$$

Active constraints g_2, g_4 and g_5.

$$\chi(d, y^{S1}) = \psi^1(\boldsymbol{\theta}^{c,1}, d, y^{S1}) = 2.806 - 0.018 d_1.$$

$$F^1(d, y^{S1}) = 0.046 d_1 + 0.286, \quad \text{if } \{1.018 d_1 + d_3 \geq 10.857.$$

$$F^2(d, y^{S1}) = 0.196 d_1 + 0.188 d_3 - 1.750, \quad \text{if } \{1.018 d_1 + d_3 \leq 10.857.$$

Notice how the two feasibility functions are independent of the capacity of plant 2, d_2. Also, the flexibility test measure is only dependent on the capacity of plant 1, d_1. The smallest value of $\chi(d, y^{S1})$ occurs for $d_1 = 7$, which gives $\chi(y^{S1}) = 2.680$. Thus, for the given processing capacity ranges, the chemical complex cannot be operated feasibly over the whole ranges of supply and demand, even if all three processing plants are available.

The parametric flexibility index solutions are illustrated graphically in $d_1 d_3$-space in Figure 6. The maximum value of the flexibility index occurs for $d_1 = 7$, which gives $F = 0.318$. This means that the maximum supply and demand ranges that can be simultaneously tolerated are $10.73 \leq S \leq 13.27$ and $5.73 \leq D \leq 8.27$, respectively.

Design optimization for target flexibility index

Consider an economic objective function, $\text{Cost} = 10 d_1 + 3 d_2 + 10 d_3$. Solving the p-LP (Eq. 25) over the range of possible target flexibility indices given by F^1 and F^2, $0.149 \leq F^t \leq 0.318$, leads to

$$\text{Cost}^1 = 51.15 F^t + 113.38, \quad \text{if } \{0.149 \leq F^t \leq 0.303.$$

$$\text{Cost}^2 = 2{,}187.50 F^t - 534, \quad \text{if } \{0.303 \leq F^t \leq 0.318.$$

The trade-off curve of cost against target flexibility index is shown in Figure 7. It can be seen that the slope of the curve is forty times steeper than when F^1 is active compared to when F^2 is active. The result of this is that a target flexibility index, $F^t = 0.303$, which is 95% of the maximum possible index, $F^t = 0.318$, has an associated cost that is only 80% of the latter (128.9 units vs. 161 units).

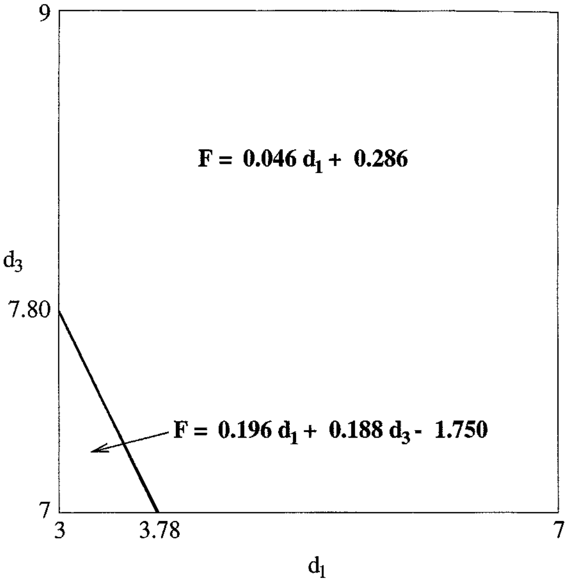

Figure 6. Parametric flexibility index solutions for process example 1.

Expected stochastic flexibility

Let the probability of operation of plants 1, 2, and 3 be $p_1 = 0.95$, $p_2 = 0.92$, and $p_3 = 0.87$, respectively. Since there are three plants, there are $2^3 = 8$ different system states, which are listed in Table 3 along with their respective probabilities of occurrence (calculated using Eq. 33). In order to evaluate the expected stochastic flexibility from Eq. 32, the stochastic flexibility of each state must be calculated. It is clear that states $S5$, $S6$, and $S8$ all have associated stochastic flexibilities of zero, since there is no way of producing species C in these cases. It is also clear that the stochastic flexibilities of states $S3$ and $S4$ will be identical to that of state $S7$, since if either plant 1 or plant 2 is unavailable, the only way to produce species C is by directing all the inlet flow to plant 3. Thus, for this example, the *expected stochastic flexibility* (ESF) can be expressed as

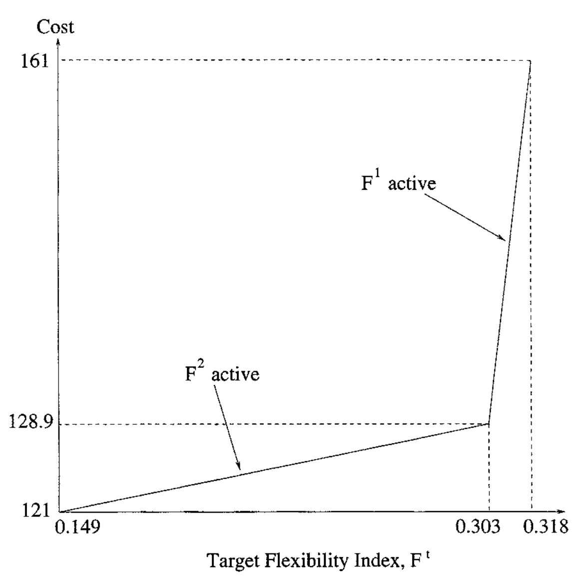

Figure 7. Cost vs. flexibility index trade-off curve for process example 1.

Table 3. System States and Associated Probabilities for Process Example 1

State, s	y_1^s	y_2^s	y_3^s	$P(y^s)$
$S1$	1	1	1	0.760
$S2$	1	1	0	0.114
$S3$	1	0	1	0.066
$S4$	0	1	1	0.040
$S5$	1	0	0	0.010
$S6$	0	1	0	0.006
$S7$	0	0	1	0.003
$S8$	0	0	0	0.001

$$ESF(d) = 0.760\,SF(d, y^{S1}) + 0.114\,SF(d, y^{S2}) + 0.110\,SF(d, y^{S7}). \quad (34)$$

Consider the case where (1) the supply is log-normally distributed with parameters $m = 1$, $\sigma = 0.6$ (Hastings and Peacock, 1975); and (2) the demand is normally distributed according to $D \sim N(7,1)$. The joint pdf is then given by

$$j(\theta_1^{q_1}, \theta_2^{q_1 q_2}) = \frac{1}{1.2\pi(\theta_1^{q_1} - 8)} \exp\left\{ -1.39\left[\ln(\theta_1^{q_1} - 8)\right]^2 - \frac{1}{2}(\theta_2^{q_1 q_2} - 7)^2 \right\}. \quad (35)$$

Applying Algorithm 2 for each of the three states, $S1$, $S2$, and $S7$, requires the solution of three mp-LPs, with a total CPU time of 0.42 s in each case. The following expressions are obtained:

- For state $S1$:

$$\theta_1^{\max} = 16, \quad \theta_1^{\min} = 8.$$
$$\theta_2^{\max q_1} = 0.782\,d_1 + 0.750\,d_3, \quad \theta_2^{\min q_1} = 3, \quad \text{if } \{d_1 + d_3 \le \theta_1^{q_1}.$$
$$\theta_2^{\max q_1} = 0.750\,\theta_1^{q_1} + 0.032\,d_1, \quad \theta_2^{\min q_1} = 3, \quad \text{if } \{d_1 + d_3 \ge \theta_1^{q_1}.$$

- For state $S2$, if $3.836 \le d_1 \le 7$ (otherwise, $SF = 0$):

$$\theta_1^{\max} = 16, \quad \theta_1^{\min} = 8.$$
$$\theta_2^{\max q_1} = 0.782\,d_1, \quad \theta_2^{\min q_1} = 3.$$

- For state $S7$:

$$\theta_1^{\max} = 16, \quad \theta_1^{\min} = 8.$$
$$\theta_2^{\max q_1} = 0.750\,d_3, \quad \theta_2^{\min q_1} = 3, \quad \text{if } \{d_3 \le \theta_1^{q_1}.$$
$$\theta_2^{\max q_1} = 0.750\,\theta_1^{q_1}, \quad \theta_2^{\min q_1} = 3, \quad \text{if } \{d_3 \ge \theta_1^{q_1}.$$

The preceding expressions obtained using the parametric programming approach, together with Eqs. 29, 30, 34, and 35,

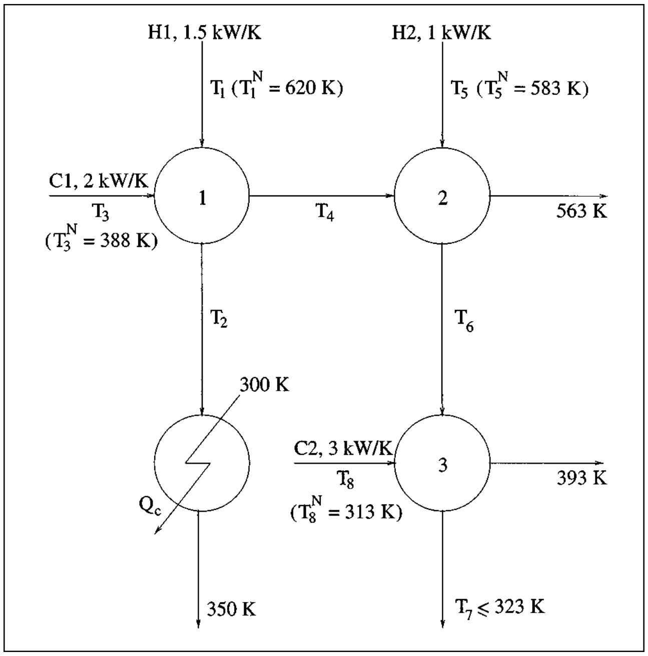

Figure 8. Process example 2: HEN with 2 hot, 2 cold streams.

give information on the dependence of the expected stochastic flexibility of the system on the continuous design variables that could not have been obtained using earlier evaluation approaches. For instance, in this example, the analysis indicates that if the capacity of plant 1 is less than 3.836, then state $S2$ is incapable of meeting the constraints and does not contribute to the expected probability of feasible operation of the system. Furthermore, the calculation of the expected stochastic flexibility for different values of the design variables (and different numbers of quadrature points) is reduced to sequences of function evaluations, thus facilitating a computationally efficient comparison of design alternatives. For example, using 10 quadrature points for both uncertain parameters, plant capacities $d^1 = [5,7,9]^T$ give $SF(y^{S1}) = 0.510$, $SF(y^{S2}) = 0.001$, $SF(y^{S7}) = 0.353$, and $ESF = 0.427$. Alternatively, plant capacities $d^2 = [7,7,7]^T$ give $SF(y^{S1}) = 0.533$, $SF(y^{S2}) = 0.064$, $SF(y^{S7}) = 0.041$, and $ESF = 0.417$. Hence, although d^2 is more attractive in state $S1$, that is, when all the plants are operational, d^1 has a marginally higher probability of feasible operation when all the possible system states are considered.

Process Example 2: HEN with 2 Hot, 2 Cold Streams

Consider the heat-exchanger network (HEN) structure shown in Figure 8, which is taken from Grossmann and Floudas (1987), and was subsequently studied by Pistikopoulos and Mazzuchi (1990), Straub and Grossmann (1990), and Varvarezos et al. (1995). The process model comprises energy balances around each exchanger and temperature feasibility constraints, as shown in Table 4 for a minimum temperature approach, $\Delta T_{\min} = 0$ K. This system has four state variables, $x = [T_2, T_4, T_6, T_7]^T$; one control variable, $z = Q_c$; four uncertain parameters, $\boldsymbol{\theta} = [T_1, T_3, T_5, T_8]^T$; and no design variables. The expected deviations in the uncertain parameters are all ± 10 K.

Table 4. Model for Process Example 2

Equalities	Inequalities
$1.5(T_1 - T_2) = 2(T_4 - T_3)$	$g_1 = T_3 - T_2 \le 0$
$(T_5 - T_6) = 2(563 - T_4)$	$g_2 = T_4 - T_6 \le 0$
$(T_6 - T_7) = 3(393 - T_8)$	$g_3 = T_8 - T_7 \le 0$
$Q_c = 1.5(T_2 - 350)$	$g_4 = 393 - T_6 \le 0$
	$g_5 = T_7 - 323 \le 0$

Flexibility test and index

The application of Algorithm 1 gives four feasibility function expressions, contrasting with the six (two redundant) using the method of Pistikopoulos and Grossmann (1988)

$$\psi^1(\boldsymbol{\theta}) = -\frac{3}{5}\theta_1 - \frac{1}{5}\theta_2 - \frac{2}{5}\theta_3 - \frac{4}{5}\theta_4 + 922,$$

$$CR^1 = \begin{cases} \frac{6}{5}\theta_1 + \frac{2}{5}\theta_2 + \frac{4}{5}\theta_3 + \frac{13}{5}\theta_4 \le 2{,}167 \\ \frac{3}{10}\theta_1 + \frac{1}{10}\theta_2 - \frac{3}{10}\theta_3 + \frac{7}{5}\theta_4 \le 487\frac{1}{2}, \end{cases}$$

Active constraints: g_1 and g_4,

$$\psi^1(\boldsymbol{\theta}^{c,1}) = 8\frac{4}{5}, \quad \delta^1 = \frac{14}{25}.$$

$$\psi^2(\boldsymbol{\theta}) = \frac{1}{2}\theta_4 - 161\frac{1}{2},$$

$$CR^2 = \begin{cases} \frac{6}{5}\theta_1 + \frac{2}{5}\theta_2 + \frac{4}{5}\theta_3 + \frac{13}{5}\theta_4 \ge 2{,}167 \\ \frac{1}{2}\theta_3 - \frac{3}{4}\theta_4 \ge 54\frac{1}{4}, \end{cases}$$

Active constraints: g_4 and g_5,

$$\psi^2(\boldsymbol{\theta}^{c,2}) = 0, \quad \delta^2 = 1.$$

$$\psi^3(\boldsymbol{\theta}) = -\frac{3}{7}\theta_1 - \frac{1}{7}\theta_2 - \frac{4}{7}\theta_3 + 643\frac{3}{7},$$

$$CR^3 = \begin{cases} \frac{3}{10}\theta_1 + \frac{1}{10}\theta_2 - \frac{3}{10}\theta_3 + \frac{7}{5}\theta_4 \ge 487\frac{1}{2} \\ \frac{9}{7}\theta_1 + \frac{3}{7}\theta_2 + \frac{5}{7}\theta_3 + 3\theta_4 \le 2{,}306\frac{2}{7}, \end{cases}$$

Active constraints: g_1 and g_2,

$$\psi^3(\boldsymbol{\theta}^{c,3}) = \frac{4}{7}, \quad \delta^3 = \frac{19}{20}.$$

$$\psi^4(\boldsymbol{\theta}) = -\frac{1}{3}\theta_3 + \theta_4 - 125\frac{1}{3},$$

$$CR^4 = \begin{cases} \frac{1}{2}\theta_3 - \frac{3}{4}\theta_4 \le 54\frac{1}{4} \\ \frac{9}{7}\theta_1 + \frac{3}{7}\theta_2 + \frac{5}{7}\theta_3 + 3\theta_4 \ge 2{,}306\frac{2}{7}, \end{cases}$$

Active constraints: g_2 and g_5,

$$\psi^4(\boldsymbol{\theta}^{c,4}) = 6\frac{2}{3}, \quad \delta^4 = \frac{1}{2}.$$

Thus, the flexibility test measure, $\chi = 8^4\!/\!_5$, indicating that the network cannot be operated feasibly over the whole range of uncertain parameters. This is confirmed by the flexibility index, $F = 1/2$, which shows that the network can tolerate simultaneous variations in the inlet temperatures of the process streams of up to ± 5 K.

Stochastic flexibility

Consider the case where T_1 and T_3 are normally distributed, while T_5 and T_8 are uniformly distributed, according to $T_1 \sim N$ (620, 6.25), $T_3 \sim N$ (388, 6.25), $T_5 \sim U$ [573, 593], and $T_8 \sim U$ [303, 323], respectively. Applying Algorithm 2 gives the following expressions

$$\theta_1^{\max} = 630, \quad \theta_1^{\min} = 610.$$

$$\theta_2^{\max q_1} = 398, \quad \theta_2^{\min q_1} = 378.$$

$$\theta_3^{\max q_1 q_2} = 593.$$

$$\theta_3^{\min q_1 q_2} = -\frac{3}{4}\theta_1^{q_1} - \frac{1}{4}\theta^{q_1 q_2} + 1126,$$

$$\text{if } \left\{ \frac{3}{4}\theta_1^{q_1} + \frac{1}{4}\theta_2^{q_1 q_2} \leq 553. \right.$$

$$\theta_3^{\min q_1 q_2} = 573, \quad \text{if } \left\{ \frac{3}{4}\theta_1^{q_1} + \frac{1}{4}\theta_2^{q_1 q_2} \geq 553. \right.$$

$$\theta_4^{\max q_1 q_2 q_3} = \frac{1}{3}\theta_3^{q_1 q_2 q_3} + 125\frac{1}{3}.$$

$$\text{If } \left\{ \frac{3}{4}\theta_1^{q_1} + \frac{1}{4}\theta_2^{q_1 q_2} + \frac{1}{2}\theta_3^{q_1 q_2 q_3} \leq 849\frac{1}{2} \right.$$

$$\text{and} \quad \frac{3}{4}\theta_1^{q_1} + \frac{1}{4}\theta_2^{q_1 q_2} + \theta_3^{q_1 q_2 q_3} \geq 1{,}126:$$

$$\theta_4^{\min q_1 q_2 q_3} = -\frac{3}{4}\theta_1^{q_1} - \frac{1}{4}\theta_2^{q_1 q_2} - \frac{1}{2}\theta_3^{q_1 q_2 q_3} + 1{,}152\frac{1}{2}.$$

$$\text{If } \left\{ \frac{3}{4}\theta_1^{q_1} + \frac{1}{4}\theta_2^{q_1 q_2} + \frac{1}{2}\theta_3^{q_1 q_2 q_3} \geq 849\frac{1}{2}: \right.$$

$$\theta_4^{\min q_1 q_2 q_3} = 303.$$

$$\text{If } \left\{ \frac{3}{4}\theta_1^{q_1} + \frac{1}{4}\theta_2^{q_1 q_2} + \frac{1}{2}\theta_3^{q_1 q_2 q_3} \leq 1{,}126: \right.$$

$$\theta_4^{\min q_1 q_2 q_3} = \text{N/A (infeasible problem)}.$$

Using the preceding expressions, together with Eqs. 29, 30, and the joint pdf, given by

$$j(\theta_1^{q_1}, \theta_2^{q_1 q_2}, \theta_3^{q_1 q_2 q_3}, \theta_4^{q_1 q_2 q_3 q_4})$$

$$= \frac{1}{5{,}000\pi}\exp\left\{ -0.08\left[(\theta_1^{q_1} - 620)^2 + (\theta_2^{q_1 q_2} - 388)^2 \right] \right\},$$

the stochastic flexibility of the system can be calculated for different numbers of quadrature points through a simple sequence of function evaluations. The results are shown in Table 5, which indicates that, although the heat-exchanger network can only tolerate ± 5 K deviations in the uncertain inlet temperatures, there is actually an 82.3% probability that it can be operated feasibly through proper manipulation of the cooling duty. Table 5 also compares the number of subproblems that have to be solved using Algorithm 2, and the associated computation times, with those required by the sequential approach of Straub and Grossmann (1993) and Pistikopoulos and Ierapetritou (1995). It can be seen that the computational savings given by the parametric programming approach are very large. In order to generate the three stochastic flexibility values in Table 5 using Algorithm 2 requires the solution of a total of four mp-LPs and one LP, with a total CPU time of 0.9 s. This contrasts sharply with the sequential approach, where a total of 6,839 LPs must be solved, taking 84.3 s CPU.

Table 5. Stochastic Flexibility of Process Example 2: Parametric vs. Sequential Approach

Q_i		No. of Subproblems		CPU (s)	
$i = 1, 2, 3, 4$	*SF*	Algorithm 2	Sequential	Algorithm 2	Sequential
8	0.8209	4 mp-LPs	585 LPs	↑	7.1
12	0.8230	and	1885 LPs	0.9	24.2
16	0.8230	1 LP	4369 LPs	↓	53.0
Total		4 mp-LPs + 1 LP	6839 LPs	0.9	84.3

Process Example 3: HEN with 4 Hot, 3 Cold Streams

Figure 9 shows another HEN structure taken from Grossmann and Floudas (1987), and also studied by Pistikopoulos and Mazzuchi (1990). This system has seven uncertain pa-

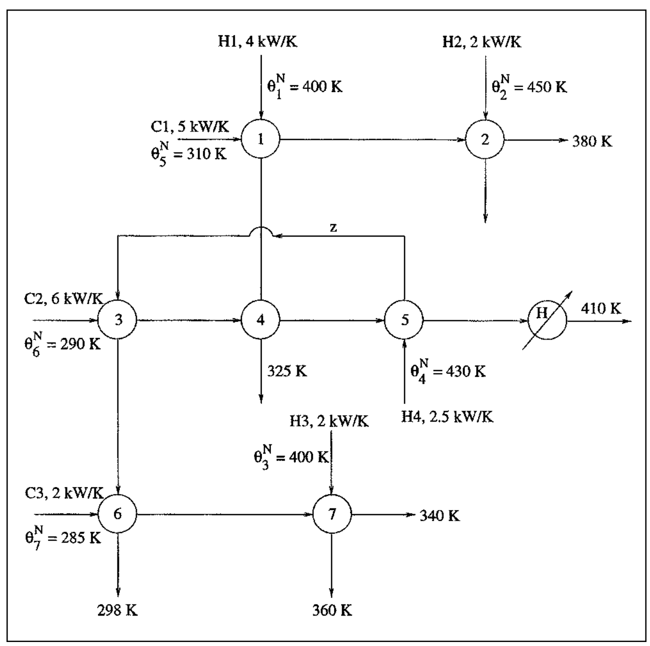

Figure 9. Process example 3: HEN with 4 hot, 3 cold streams.

Table 6. Reduced Inequality Set for Process Example 3

$f_1 = \frac{5}{12}z + \frac{1}{3}\theta_3 + \theta_6 + \frac{1}{3}\theta_7 - 682\frac{1}{2} \le 0$
$f_2 = \frac{5}{12}z - \frac{1}{3}\theta_1 - \frac{1}{6}\theta_2 + \frac{1}{3}\theta_3 - \frac{5}{12}\theta_5 + \theta_6 + \frac{1}{3}\theta_7 - 357\frac{1}{2} \le 0$
$f_3 = -\frac{7}{12}z + \frac{2}{3}\theta_1 + \frac{1}{3}\theta_2 + \frac{1}{3}\theta_3 + \frac{5}{6}\theta_5 + \theta_6 + \frac{1}{3}\theta_7 - 1{,}007\frac{1}{2} \le 0$
$f_4 = -\frac{5}{12}z - \frac{1}{3}\theta_3 - \frac{1}{3}\theta_7 + 357\frac{1}{2} \le 0$
$f_5 = z - \theta_4 \le 0$
$f_6 = \frac{4}{5}\theta_3 + \theta_6 + \frac{4}{5}\theta_7 - 858 \le 0$
$f_7 = \theta_3 + \theta_7 - 700 \le 0$

rameters (with nominal values as shown, and expected deviations of ± 10 K), and one control variable, z, which is the temperature of the hot stream flowing from exchanger 5 to exchanger 3. The full model of the system consists of eight energy balances and a number of inequalities describing feasible heat exchange ($\Delta T_{\min} = 0$ K). In this case, it is advantageous to eliminate the state variables according to Eq. 23 because this reduces the model to the seven nonredundant constraints shown in Table 6 (c.f. nineteen reported by Grossmann and Floudas, 1987).

Flexibility test and index

Algorithm 1 gives four feasibility function expressions:

$$\psi^1(\boldsymbol{\theta}) = \frac{5}{18}\theta_1 + \frac{5}{36}\theta_2 + \frac{1}{3}\theta_3 + \frac{25}{72}\theta_5 + \theta_6 + \frac{1}{3}\theta_7 - 817\frac{11}{12},$$

$$CR^1 = \begin{cases} -\frac{5}{18}\theta_1 - \frac{5}{36}\theta_2 + \frac{7}{15}\theta_3 - \frac{25}{72}\theta_5 + \frac{7}{15}\theta_7 \le 40\frac{1}{12} \\ \frac{5}{18}\theta_1 + \frac{5}{36}\theta_2 - \frac{2}{3}\theta_3 + \frac{25}{72}\theta_5 + \theta_6 - \frac{2}{3}\theta_7 \ge 117\frac{11}{12} \\ \frac{5}{18}\theta_1 + \frac{5}{36}\theta_2 + \frac{1}{3}\theta_3 + \frac{25}{72}\theta_5 + \frac{1}{2}\theta_6 + \frac{1}{3}\theta_7 \ge 655\frac{5}{12}. \end{cases}$$

$$\text{Active constraints: } f_1 \text{ and } f_3,$$

$$\psi^1(\boldsymbol{\theta}^{c,1}) = 5\frac{35}{36}, \quad \delta^1 = \frac{132}{175}.$$

$$\psi^2(\boldsymbol{\theta}) = \frac{4}{5}\theta_3 + \theta_6 + \frac{4}{5}\theta_7 - 858,$$

$$CR^2 = \begin{cases} -\frac{5}{18}\theta_1 - \frac{5}{36}\theta_2 + \frac{7}{15}\theta_3 - \frac{25}{72}\theta_5 + \frac{7}{15}\theta_7 \ge 40\frac{1}{12} \\ -\frac{1}{5}\theta_3 + \theta_6 - \frac{1}{5}\theta_7 \ge 158 \\ \frac{4}{5}\theta_3 + \frac{1}{2}\theta_6 + \frac{4}{5}\theta_7 \ge 695\frac{1}{2}. \end{cases}$$

$$\text{Active contraints: } f_6,$$

$$\psi^2(\boldsymbol{\theta}^{c,2}) = 6, \quad \delta^2 = \frac{10}{13}.$$

$$\psi^3(\boldsymbol{\theta}) = \theta_3 + \theta_7 - 700,$$

$$CR^3 = \begin{cases} \frac{5}{18}\theta_1 + \frac{5}{36}\theta_2 - \frac{2}{3}\theta_3 + \frac{25}{72}\theta_5 + \theta_6 - \frac{2}{3}\theta_7 \le 117\frac{11}{12} \\ -\frac{1}{5}\theta_3 + \theta_6 - \frac{1}{5}\theta_7 \le 158 \\ \theta_3 - \frac{1}{2}\theta_6 + \theta_7 \ge 537\frac{1}{2}, \end{cases}$$

$$\text{Active constraints: } f_7,$$

$$\psi^3(\boldsymbol{\theta}^{c,3}) = 5, \quad \delta^3 = \frac{3}{4}.$$

$$\psi^4(\boldsymbol{\theta}) = \frac{1}{2}\theta_6 - 161\frac{1}{2},$$

$$CR^4 = \begin{cases} \frac{5}{18}\theta_1 + \frac{5}{36}\theta_2 + \frac{1}{3}\theta_3 + \frac{25}{72}\theta_5 + \frac{1}{2}\theta_6 + \frac{1}{3}\theta_7 \le 655\frac{5}{12} \\ \frac{4}{5}\theta_3 + \frac{1}{2}\theta_6 + \frac{4}{5}\theta_7 \le 695\frac{1}{2} \\ \theta_3 - \frac{1}{2}\theta_6 + \theta_7 \le 537\frac{1}{2}, \end{cases}$$

$$\text{Active constraints: } f_1 \text{ and } f_4,$$

$$\psi^4(\boldsymbol{\theta}^{c,4}) = -12\frac{1}{2}, \quad \delta^4 = 3\frac{1}{2}.$$

These lead to $\chi = 6$ and $F = 3/4$, indicating that the network can only tolerate simultaneous variations in the inlet temperatures of up to ± 7.5 K.

Stochastic flexibility

Consider the case where θ_3, θ_6, and θ_7 are uniformly distributed between their lower and upper bounds, while the other inlet temperatures are described by beta distributions between their bounds with pdf parameters $a = b = 1.2$ (Ross, 1988). Applying Algorithm 2 gives

$$\theta_1^{\max} = 410, \quad \theta_1^{\min} = 390.$$

$$\theta_2^{\max q_1} = 460, \quad \theta_2^{\min q_1} = 378.$$

$$\theta_3^{\max q_1 q_2} = 410, \quad \theta_3^{\min q_1 q_2} = 390.$$

$$\theta_5^{\max q_1 q_2 q_3} = 320, \quad \theta_5^{\min q_1 q_2 q_3} = 300.$$

$$\theta_6^{\max q_1 q_2 q_3 q_5} = 300, \quad \theta_6^{\min q_1 q_2 q_3 q_5} = 280.$$

$$\theta_7^{\min q_1 q_2 q_3 q_5 q_6} = 275.$$

$$\theta_7^{\max q_1 q_2 q_3 q_5 q_6} = 295,$$

$$CR^{7,1} = \begin{cases} \frac{4}{5}\theta_3^{q_1 q_2 q_3} + \theta_6^{q_1 q_2 q_3 q_5 q_6} \le 622 \\ \theta_3^{q_1 q_2 q_3} \le 405 \\ \frac{5}{18}\theta_1^{q_1} + \frac{5}{36}\theta_2^{q_1 q_2} + \frac{1}{3}\theta_3^{q_1 q_2 q_3} + \frac{25}{72}\theta_5^{q_1 q_2 q_3 q_5} \\ \qquad + \theta_6^{q_1 q_2 q_3 q_5 q_6} \le 719\frac{7}{12}. \end{cases}$$

$$\theta_7^{\max q_1 q_2 q_3 q_5 q_6} = -\theta_3^{q_1 q_2 q_3} - \frac{5}{4}\theta_6^{q_1 q_2 q_3 q_5 q_6} + 1{,}072\frac{1}{2},$$

$$CR^{7,2} = \begin{cases} \frac{4}{5}\theta_3^{q_1 q_2 q_3} + \theta_6^{q_1 q_2 q_3 q_5 q_6} \ge 622 \\ \theta_6^{q_1 q_2 q_3 q_5 q_6} \ge 298 \\ \frac{5}{18}\theta_1^{q_1} + \frac{5}{36}\theta_2^{q_1 q_2} + \frac{25}{72}\theta_5^{q_1 q_2 q_3 q_5} + \frac{7}{12}\theta_6^{q_1 q_2 q_3 q_5 q_6} \\ \qquad \le 460\frac{5}{12}. \end{cases}$$

$$\theta_7^{\max\, q_1 q_2 q_3 q_5 q_6} = -\theta_3^{q_1 q_2 q_3} + 700,$$

$$CR^{7,3} = \begin{cases} \theta_3^{q_1 q_2 q_3} \ge 405 \\ \theta_6^{q_1 q_2 q_3 q_5 q_6} \le 298 \\ \frac{5}{18}\theta_1^{q_1} + \frac{5}{36}\theta_2^{q_1 q_2} + \frac{25}{72}\theta_5^{q_1 q_2 q_3 q_5} + \theta_6^{q_1 q_2 q_3 q_5 q_6} \\ \qquad \le 584\frac{7}{12}. \end{cases}$$

$$\theta_7^{\max\, q_1 q_2 q_3 q_5 q_6} = -\frac{5}{6}\theta_1^{q_1} - \frac{5}{12}\theta_2^{q_1 q_2} - \theta_3^{q_1 q_2 q_3} - \frac{25}{24}\theta_5^{q_1 q_2 q_3 q_5} - 3\theta_6^{q_1 q_2 q_3 q_5 q_6} + 2{,}453\frac{3}{4},$$

$$CR^{7,4} = \begin{cases} \frac{5}{18}\theta_1^{q_1} + \frac{5}{36}\theta_2^{q_1 q_2} + \frac{1}{3}\theta_3^{q_1 q_2 q_3} + \frac{25}{72}\theta_5^{q_1 q_2 q_3 q_5} \\ \qquad + \theta_6^{q_1 q_2 q_3 q_5 q_6} \ge 719\frac{7}{12} \\ \frac{5}{18}\theta_1^{q_1} + \frac{5}{36}\theta_2^{q_1 q_2} + \frac{25}{72}\theta_5^{q_1 q_2 q_3 q_5} + \frac{7}{12}\theta_6^{q_1 q_2 q_3 q_5 q_6} \\ \qquad \ge 460\frac{5}{12} \\ \frac{5}{18}\theta_1 + \frac{5}{36}\theta_2 + \frac{25}{72}\theta_5 + \theta_6 \ge 584\frac{7}{12}. \end{cases}$$

Notice how the use of the parametric feasibility function expressions, which are independent of θ_4, allows us to eliminate this parameter from consideration (and so reduce the dimensionality of the subproblems) in the evaluation of the stochastic flexibility. Using the preceding expressions, together with Eqs. 29, 30, and the joint pdf, given by

$$j = (5.00e-8)\cdot(\omega_1^{q_1})^{0.2}(1-\omega_1^{q_1})^{0.2}(\omega_2^{q_1 q_2})^{0.2} \times (1-\omega_2^{q_1 q_2})^{0.2}(\omega_5^{q_1 q_2 q_3 q_5})^{0.2}(1-\omega_5^{q_1 q_2 q_3 q_5})^{0.2},$$

where $\omega_1^{q_1} = 0.05\ (\theta_1^{q_1} - 390)$, $\omega_2^{q_1 q_2} = 0.05\ (\theta_1^{q_1 q_2} - 440)$, and $\omega_5^{q_1 q_2 q_3 q_5} = 0.05\ (\theta_5^{q_1 q_2 q_3 q_5} - 300)$, leads to the stochastic flexibility values shown in Table 7. It can be seen that the probability of feasible operation of the network is 96.8%. The table also compares the number of optimization subproblems and associated computation times with those required by a sequential approach. In order to generate the four values in Table 7 using the latter approach may be impractical, since it does require the solution of almost 89 million LPs, with a projected total CPU time of approximately 350 h. The parametric programming approach, on the other hand, only requires the solution of six mp-LPs and one LP, with a total CPU time of just 2.3s. This clearly demonstrates the enormous computational savings that can be obtained by using a parametric programming approach, especially when the system has a large number of uncertain parameters.

Table 7. Stochastic Flexibility of Process Example 3: Parametric vs. Sequential Approach

Q_i $i = 1, \ldots, 7$	SF	No. of Subproblems: Algorithm 2	No. of Subproblems: Sequential	CPU (s): Algorithm 2	CPU (s): Sequential
8	0.9732	↑	3.00e5 LPs	↑	≃ 4.0e3
12	0.9689	6 mp-LPs	3.26e6 LPs	2.3	≃ 4.4e4
16	0.9684	+ 1 LP	1.79e7 LPs		≃ 2.5e5
20	0.9682	↓	6.74e7 LPs	↓	≃ 9.6e5
Total		6 mp-LPs + 1 LP	8.88e7 LPs	2.3	≃ 1.3e6

Concluding Remarks

This article has presented a new theory and novel algorithms that use multiparametric programming techniques for the solution of flexibility analysis problems in linear process systems. For systems with deterministic uncertain parameters, an algorithm has been presented for the flexibility test problem and for flexibility-index evaluation. This algorithm identifies all the critical directions and values of the uncertain parameters that limit flexibility. It also provides explicit expressions for the flexibility test measure and the flexibility index of the system as linear functions of the continuous design variables. This feature reduces the flexibility test and index problems to simple function evaluations for a given design and enables a designer to know *a priori* which designs have the desired level of flexibility. It also enables the compact formulation of design optimization problems, which can be solved using parametric programming to readily obtain the exact algebraic form of the trade-off curve of cost against target flexibility index for a system.

For systems with stochastic parameters of any kind of probability distribution, an algorithm has been presented for stochastic flexibility and expected stochastic flexibility evaluation. This algorithm reduces the evaluation of these metrics for a given design and a given number of integration points to a series of function evaluations. This makes the algorithm particularly useful for the efficient comparison of design alternatives. The computational efficiency of the algorithm and enormous reduction in the number of subproblems that need to be solved, compared to earlier methods, has been clearly demonstrated through the illustrative and the process examples (Tables 1, 5, and 7). It is evident that the benefits offered by the parametric programming approach increase markedly as the number of uncertain parameters increases.

It is envisaged that the work presented in this article can also serve as a foundation for the development of new approaches for the flexibility analysis of nonlinear process systems that utilize recently developed algorithms for the solution of single-parameter and multiparametric, (mixed-integer) nonlinear programs (Pertsinidis et al., 1998; Acevedo and Pistikopoulos, 1996; Papalexandri and Dimkou, 1998; Dua and Pistikopoulos, 1999a). This will be the subject of a future article.

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Appendix A: An Algorithm for mp-LP Problems

An algorithm for the solution of nondegenerate mp-LPs is given by Gal and Nedoma (1972), and is fully described in chap. 4 of Gal (1995), and summarized by Acevedo and Pistikopoulos (1997b). Here, the fundamental steps of the algorithm are outlined and then illustrated with a mathematical example.

Phase 1: Finding an initial optimal basis

1. Solve the LP (Eq. 7) with $\mathbf{\Theta}$ as a variable in order to obtain a feasible point (w_1, $\mathbf{\Theta}_1$). If no feasible point is found, then the algorithm is terminated.

2. Fix $\mathbf{\Theta} = \mathbf{\Theta}_1$ and solve Eq. 7 as an LP using the Simplex algorithm. As part of the Simplex algorithm, slack variables are added to the inequalities. This converts the system into the following form:

$$\psi(\mathbf{\Theta}) = \min_{\tilde{w}} (c^T \cdot \tilde{w} + u^L),$$

$$\text{s.t.} \quad A \cdot \tilde{w} = b + F \cdot \mathbf{\Theta},$$

$$\mathbf{0} \le b_3 + F_3 \cdot \mathbf{\Theta},$$

$$\tilde{w} \ge \mathbf{0}, \tag{A1}$$

where the vector $\tilde{w}$ now incorporates the original vector w and slack variables, and the constraints are usually rearranged such that b is a vector of positive constants. The Simplex tableau will give the optimal basis B_1 associated with the solution. For the region in $\boldsymbol{\Theta}$-space that this basis is optimal,

$$\tilde{w}^1(\boldsymbol{\Theta}) = B_1^{-1} \cdot (b + F \cdot \boldsymbol{\Theta}), \tag{A2}$$

and hence the associated objective function is $\psi^1(\boldsymbol{\Theta}) = c^T \cdot \tilde{w}^1(\boldsymbol{\Theta}) + u^L$.

The region in which the basis is optimal, CR^1, is uniquely defined by the conditions $\tilde{w}^1(\boldsymbol{\Theta}) \geq \mathbf{0}$ and $\mathbf{0} \leq b_3 + F_3 \cdot \boldsymbol{\Theta}$, that is, from

$$- B_1^{-1} \cdot F \cdot \boldsymbol{\Theta} \leq B_1^{-1} \cdot b, \tag{A3}$$

and

$$- F_3 \cdot \boldsymbol{\Theta} \leq b_3. \tag{A4}$$

Note that some of the constraints in Eqs. A3 and A4 may be redundant. These can be identified by adding a positive slack variable to each constraint and then minimizing the value of each slack variable subject to the constraints in Eqs. 38 and 39. If the minimum value of a slack variable is positive, then the associated constraint is strongly redundant and can be dropped from the definition of CR^1. Conversely, if the minimum value is zero, then the associated constraint is either binding or weakly redundant and is kept in the definition.

Note also that in the parametric programming literature, the region of optimality of a basis is commonly referred to as the "critical region" of optimality. This term is not used in this work in order to avoid confusion with the "critical" uncertain parameter values in flexibility analysis.

Phase 2: Finding all other optimal bases

CR^1 is a closed, convex, polyhedral set, and each of the constraints in Eqs. A3 and A4 defines a "face" of this region. Another optimal basis is said to be a neighbor of B_1 along its ith face, if and only if the associated ith constraint from Eqs. A3 and A4 is nonredundant *and* it is possible to pass from B_1 to this other basis by one dual (pivot) step (and vice versa). For the latter condition to be possible, the corresponding ith row of the matrix $B_1^{-1} \cdot A$, which appears in the Simplex tableau from Phase 1, Step 2, must have at least one negative element. Phase 2 thus consists of identifying which nonredundant rows of $B_1^{-1} \cdot A$ have negative elements; pivoting; finding the next optimal basis, its associated objective function, region of optimality, and neighbors; and then repeating until the whole $\boldsymbol{\Theta}$-space, for which finite optimal solutions to Eq. 7 exist, has been covered.

Illustrative example

Consider the system described by the set of constraints (Eq. 13).

Phase 1. 1. Solving the feasibility function problem (Eq. 18) gives an initial solution $\boldsymbol{\Theta}_1 = [4, 4, 5, 3]^T$, where $\boldsymbol{\Theta} = [\theta_1, \theta_2, d_1, d_2]^T$.

2. With the addition of slack variables to each of the inequality constraints, s_l, $l = 1, 2, 3$, Eq. 14 can be written in the form of Eq. A1 where

$$\tilde{w} = \left[\hat{x}, \hat{z}, \hat{u}, s_1, s_2, s_3 \right]^T,$$

$$A = \begin{bmatrix} -2 & 3 & 0 & 0 & 0 & 0 \\ -1 & \frac{1}{2} & 1 & -1 & 0 & 0 \\ 2 & -2 & 1 & 0 & -1 & 0 \\ -1 & \frac{5}{2} & -1 & 0 & 0 & 1 \end{bmatrix},$$

$$b = \left[50, 25, 50\frac{1}{3}, 26 \right]^T,$$

$$c^T = [0, 0, 1, 0, 0, 0],$$

$$F = \begin{bmatrix} 1 & 0 & 0 & -1 \\ -\frac{1}{2} & \frac{1}{2} & 1 & -\frac{7}{2} \\ -\frac{4}{3} & -1 & 0 & 2 \\ -\frac{1}{2} & 1 & 1 & -\frac{1}{2} \end{bmatrix}.$$

Solving this at $\boldsymbol{\Theta}_1$ using the Simplex algorithm shows that the optimal basic variables are $\{\hat{x}, \hat{z}, \hat{u}, s_3\}$, thus indicating that $s_1 = s_2 = 0$, and so inequalities g_1 and g_2 are active. The optimal basis B_1 is formed from the first, second, third, and sixth columns of A. From Eq. A2, the following expressions are then obtained

$$\tilde{w}^1 = \begin{bmatrix} 50\frac{1}{4} \\ 50\frac{1}{6} \\ 50\frac{1}{6} \\ 1 \end{bmatrix} + \begin{bmatrix} 0 \\ \frac{1}{3} \\ -\frac{2}{3} \\ -2 \end{bmatrix} \theta_1 + \begin{bmatrix} -\frac{9}{8} \\ -\frac{3}{4} \\ -\frac{1}{4} \\ \frac{3}{2} \end{bmatrix} \theta_2 + \begin{bmatrix} -\frac{3}{4} \\ -\frac{1}{2} \\ \frac{1}{2} \\ 2 \end{bmatrix} d_1 + \begin{bmatrix} \frac{7}{2} \\ 2 \\ -1 \\ -3 \end{bmatrix} d_2.$$

The objective function ψ^1 is simply given by the third row of the vector $\tilde{w}^1$ plus $u^L = -50$, while the region of optimality for B_1 is defined by $\tilde{w}^1 \geq 0$ and the lower and upper bounds on θ_1, θ_2, d_1, and d_2. After removal of the redundant constraints, the following solution is obtained

$$\psi^1(\boldsymbol{\theta},d) = -\frac{2}{3}\theta_1 - \frac{1}{4}\theta_2 + \frac{1}{2}d_1 - d_2 + \frac{1}{6}, \qquad \text{(A5)}$$

$$CR^1 = \begin{cases} 2\theta_1 - \frac{3}{2}\theta_2 - 2d_1 + 3d_2 \le 1 \\ 0 \le \theta_1,\ \theta_2 \le 4 \\ 0 \le d_1 \le 5. \end{cases}$$

Phase 2. Since the only nonredundant constraint describing CR^1 comes from the fourth row of $\tilde{w}^1$, only the fourth row of the matrix $B_1^{-1}A$ (corresponding to the basic variable s_3) needs to be examined for negative elements. This row contains a negative element (equal to -1) in its fourth column, indicating that s_3 is replaced by s_1 in the neighboring optimal basic solution. Repeating the calculations from Phase 1, Step 2, for the new set of optimal basic variables, gives the following solution

$$\psi^2(\boldsymbol{\theta},d) = \frac{1}{3}\theta_1 - \theta_2 - \frac{1}{2}d_1 + \frac{1}{2}d_2 - \frac{1}{3}, \qquad \text{(A6)}$$

$$CR^2 = \begin{cases} 2\theta_1 - \frac{3}{2}\theta_2 - 2d_1 + 3d_2 \ge 1 \\ 0 \le \theta_1,\ \theta_2 \le 4 \\ 0 \le d_1,\ d_2 \le 5. \end{cases}$$

It can be seen that the regions CR^1 and CR^2 cover the whole of $\boldsymbol{\Theta}$-space. It can also be confirmed that the only neighboring optimal basis to the new basis B_2 is the basis B_1 investigated in Phase 1. Hence the algorithm is terminated. Note that the solution of this problem, as implemented in the prototype Fortran code of Acevedo and Pistikopoulos (1997b), takes only 0.08s CPU on a Sun ULTRA 1 workstation.

Appendix B: A Procedure for Comparing Parametric Solutions

For the flexibility test and index problems in this article, the procedure of Acevedo and Pistikopoulos (1997b) can be adapted for comparing the resulting parametric solutions.

Flexibility test

Step 4(a) of Algorithm 1 gives K linear expressions $\psi^k(d)$, $k = 1, \ldots, K$. In order to find the set of linear solutions $\chi^k(d)$, $k = 1, \ldots, K_\chi$, where $K_\chi \le K$:

1. Set $\psi^1(d)$ as the "upper bound" for all $d \in D$, where $D = \{d | d^L \le d \le d^U\}$.

2. Compare $\psi^1(d)$ with $\psi^2(d)$ by defining a constraint $\psi^2(d) - \psi^1(d) \ge 0$ and performing a redundancy test (as described in Appendix A) in d-space. There are three possibilities:

(a) $\psi^2(d) \ge \psi^1(d)$, $\forall d \in D$: $\psi^2(d)$ becomes the upper bound in the whole space.

(b) $\psi^2(d) \le \psi^1(d)$, $\forall d \in D$: $\psi^1(d)$ remains the upper bound in the whole space.

(c) $\psi^2(D) \ge \psi^1(d)$ for some $d \in D$. In this case, the space is partitioned into two smaller spaces with $\psi^2(d)$ the upper bound in one and $\psi^1(d)$ the upper bound in the other.

3. Within each of the subspaces resulting from Step 2, compare $\psi^3(d)$ with the respective upper-bound solutions. Repeat until $\psi^K(d)$ has been compared.

Flexibility index

The procedure for comparing the K linear expressions $\delta^k(d)$, $k = 1, \ldots, K$, resulting from Step 4(a) of Algorithm 1, is similar to that presented earlier. In this case, however, the *lower* bounds must be retained, and the additional constraints $\delta^k(d) \ge 0$, $k = 1, \ldots, K$, must be enforced.

Appendix C: An Algorithm for mp-MILPs

Dua and Pistikopoulos (2000) have proposed an algorithm for the solution of general mp-MILPs for the form

$$\begin{aligned} \text{Obj}(\boldsymbol{\Theta}) = \min_{w,y}\ & c_w^T \cdot w + c_y^T \cdot y \\ \text{s.t.}\quad & A_1 \cdot w + E_1 \cdot y = b_1 + F_1 \cdot \boldsymbol{\Theta}, \\ & A_2 \cdot w + E_2 \cdot y \le b_2 + F_2 \cdot \boldsymbol{\Theta}, \\ & \mathbf{0} \le b_3 + F_3 \cdot \boldsymbol{\Theta}, \\ & w \ge \mathbf{0}, \end{aligned} \qquad \text{(C1)}$$

where y is the vector of $0-1$ binary variables. The steps of the algorithm are outlined below:

1. Solve Eq. C1 as an MILP with $\boldsymbol{\Theta}$ treated as a search variable. This will give an initial integer solution $y = \bar{y}$. If the problem is infeasible, stop.

2. Fix $y = \bar{y}$ and solve Eq. C1 as an mp-LP. This will give a set of K linear expressions, $\text{Obj}^k(\boldsymbol{\Theta})$, and associated regions of optimality, CR^k. The former represent upper bounds to the final optimal solution within each of the regions CR^k. Note that if any regions in $\boldsymbol{\Theta}$-space are infeasible, then the upper bound is $+\infty$.

3. Within each of the regions CR^k, solve an MILP similar to that in step 1, but with the addition of constraints defining $CR^k(\Theta)$, an integer cut to exclude the previous integer solution, and a constraint to ensure that the objective function is less than $\text{Obj}^k(\boldsymbol{\Theta})$. This will give a new candidate integer solution for each CR^k. If any of the MILPs are infeasible, then the algorithm is terminated for that region. The current upper bound represents the final solution in that region.

4. Within each of the regions CR^k, solve an mp-LP as in Step 2, but this time at the new integer solution from Step 3. This will give new parametric expressions and a set of corresponding regions of optimality that are subspaces of CR^k.

5. Compare the parametric solutions from Step 4 with the current upper bounds. Retain the lower solutions and define the regions in $\boldsymbol{\Theta}$-space in which they are optimal.

6. Go back to Step 3 within each of the new (smaller) regions from Step 5, and so on, until there are infeasible MILPs in all of the regions.

Note that in Step 5, a similar comparison procedure to that described in Appendix B is used. The difference here is that, when comparing two parametric solutions with regions of optimality CR^1 and CR^2, the intersection of these regions, CR^{int}, must first be defined by removal of the redundant constraints from the total set defining CR^1 and CR^2. The comparison procedure for the parametric solutions can then be applied within CR^{int}.

Illustrative example

Consider the flexibility test formulation of Grossmann and Floudas (1987) applied to the system described by Eq. 13. After defining $\hat{x} = x + 50$; $\hat{z} = z + 50$; $\hat{u} = u + 50$; $\hat{\mu} = \mu + 50$; and $\hat{\chi} = -\chi$, the formulation becomes

$$
\begin{aligned}
&\hat{\chi}(d) = \min\ (-\hat{u} + 50),\\
\text{s.t.}\quad & -2\hat{x} + 3\hat{z} - \theta_1 = 50 - d_2,\\
& -s_1 - \hat{x} + \frac{1}{2}\hat{z} + \frac{1}{2}\theta_1 - \frac{1}{2}\theta_2 + \hat{u} = 25 + d_1 - \frac{7}{2}d_2,\\
& -s_2 + 2\hat{x} - 2\hat{z} + \frac{4}{3}\theta_1 + \theta_2 + \hat{u} = 50\frac{1}{3} + 2d_2,\\
& s_3 - \hat{x} + \frac{5}{2}\hat{z} + \frac{1}{2}\theta_1 - \theta_2 - \hat{u} = 26 + d_1 - \frac{1}{2}d_2,\\
& \lambda_1 + \lambda_2 + \lambda_3 = 1,\\
& 2\hat{\mu} + \lambda_1 - 2\lambda_2 - \lambda_3 = 100,\\
& 3\hat{\mu} + \frac{1}{2}\lambda_1 - 2\lambda_2 - \frac{5}{2}\lambda_3 = 150,\\
& \lambda_l - p_l \le 0, \quad l = 1, 2, 3,\\
& s_l + 1{,}000\, p_l \le 1{,}000, \quad l = 1, 2, 3,\\
& p_1 + p_2 + p_3 \le 2,\\
& 0 \le \theta_1, \quad \theta_2 \le 4,\\
& 0 \le d_1, d_2 \le 5,\\
& \hat{x}, \hat{z}, \hat{u}, \hat{\mu} \ge 0,\\
& p_l = 0, 1; \quad \lambda_1, s_1 \ge 0, \quad l = 1, 2, 3.
\end{aligned}
\tag{C2}
$$

The mp-MILP algorithm of Dua and Pistikopoulos (2000) can now be applied. Note that in this case, $w = [\hat{x}, \hat{z}, \theta_1, \theta_2, \hat{u}, \hat{\mu}, \lambda_l, l = 1, 2, 3]^T$, $y = [p_1, p_2, p_3]^T$, and $\Theta = [d_1, d_2]^T$.

1. Solving Eq. C2 as an MILP with d_1 and d_2 as search variables gives an initial integer solution $p_1 = 0$, $p_2 = 1$, and $p_3 = 1$.

2. Substituting the preceding solution in Eq. C2 and solving as an mp-LP gives

$$
\text{s.t.}\quad \hat{\chi}_1(d) = +\infty,
$$

$$
CR^1 = \begin{cases} 2d_1 - 3d_2 \ge 7 \\ d_1 \le 5, \quad d_2 \ge 0. \end{cases}
$$

$$
\hat{\chi}^2(d) = \frac{1}{2}d_1 - \frac{1}{2}d_2 - 1,
$$

$$
CR^2 = \begin{cases} 2d_1 - 3d_2 \le 7 \\ 0 \le d_1, \quad d_2 \le 5. \end{cases}
$$

$\hat{\chi}^i(d)$, $i = 1, 2$, represent current upper bounds in CR^i, $i = 1, 2$.

3. For each of CR^1 and CR^2, Eq. C2 is transformed into an MILP by again treating d_1 and d_2 as search variables; adding an integer cut, $p_2 + p_3 - p_1 \le 1$, to exclude the integer solution from Step 1, and adding constraints for the objective function and region (for example, for CR^2, the constraints, $\hat{\chi} \le (1/2)d_1 - (1/2)d_2 - 1$ and $2d_1 - 3d_2 \le 7$, are added). The MILPs in CR^1 and CR^2 both give $p_1 = 1$, $p_2 = 1$, and $p_3 = 0$ as the new candidate integer solution.

4. Fixing $p_1 = 1$, $p_2 = 1$, and $p_3 = 0$ in Eq. C2 and solving two mp-LPs, one in CR^1 and one in CR^2, gives

$$
\hat{\chi}^{1a}(d) = -\frac{1}{2}d_1 + d_2 - \frac{1}{6},
$$

$$
CR^1 = \begin{cases} 2d_1 - 3d_2 \ge 7 \\ d_1 \le 5,\ d_2 \ge 0. \end{cases}
$$

$$
\hat{\chi}^{2a}(d) = +\infty,
$$

$$
CR^{2a} = \begin{cases} 2d_1 - 3d_2 \le -1 \\ 0 \le d_1 \le 5,\ d_2 \le 5. \end{cases}
$$

$$
\hat{\chi}^{2b}(d) = -\frac{1}{2}d_1 + d_2 - \frac{1}{6},
$$

$$
CR^{2b} = \begin{cases} -1 \le 2d_1 - 3d_2 \le 7 \\ 0 \le d_1 \le 5,\ d_2 \ge 0. \end{cases}
$$

5. • Within CR^1, the current upper bound becomes $\hat{\chi}^{1a}(d)$.

• Within CR^{2a}, the algorithm is terminated since there is an infeasible solution. The final solution in this region corresponds to $\hat{\chi}^2(d)$.

• Within CR^{2b}, the parametric solutions $\hat{\chi}^2(d)$ and $\hat{\chi}^{2b}(d) = \hat{\chi}^{1a}(d)$ are compared in order to retain the lower of the solutions. This results in two new subregions

$$
\hat{\chi}^{1a}(d) = -\frac{1}{2}d_1 + d_2 - \frac{1}{6}
$$

$$
CR^{2c} = \begin{cases} \frac{5}{3} \le 2d_1 - 3d_2 \le 7 \\ d_1 \le 5,\ d_2 \ge 0. \end{cases}
$$

$$
\hat{\chi}^2(d) = \frac{1}{2}d_1 - \frac{1}{2}d_2 - 1
$$

$$
CR^{2d} = \begin{cases} -1 \le 2d_1 - 3d_2 \le \frac{5}{3} \\ 0 \le d_1 \le 5,\ d_2 \ge 0. \end{cases}
$$

6. MILPs are solved within CR^1, CR^{2c}, and CR^{2d}, as in Step 3, with another integer cut $(p_1 + p_2 - p_3 \le 1)$, and objective function constraints. All three MILPs are infeasible and hence the current upper bounds are the final solutions. Substituting $\hat{\chi} = -\chi$ and amalgamating the regions of optimality leads to Eqs. 17 and 18.

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