Robustness Metrics for Dynamic Optimization Models under Parameter Uncertainty

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Recent research in process systems engineering has focused mostly on the issue of making decisions under uncertainty. Various approaches used over the years include optimizing the expected and worst cases, maximizing the feasibility of operation, and constraining variances of performance measures. The consideration of robustness, that is, guaranteeing a reasonable performance over a wide range of uncertainty, is either implicit or explicit in these approaches, and is certainly receiving more attention. In this article, we argue that mathematical techniques for robust optimization must be capable of capturing different perspectives on risk of different users. We define some general robustness metrics that can represent significantly different robustness objectives simply by modifying functions and parameters. We also describe a solution procedure along with two illustrative examples.

Introduction

It has long been accepted that the effects of various sources of uncertainty should be considered during both process design and operation. To this end, considerable effort has been expended by researchers to develop approaches to solve this problem in a systematic manner. Various techniques introduced differ in handling sources of uncertainty or in solving resulting problems. Rather than give an exhaustive literature review here, we refer the reader to the comprehensive reviews of Grossmann et al. (1983), Pistikopoulos (1995), and Wets (1996) and then highlight some of the more recent articles in this area. First, we give an overview of the approaches applied to the problem.

The following mathematical model is germane to dynamic optimization under uncertainty:

$$\max_{u,\nu,\tau} E_\theta\{\Phi(\dot{x},x,y,u,\nu,\tau;\,\theta)\} = \max_{u,\nu,\tau}\int_{\theta\in\Theta}\Psi(\theta)\Phi(\dot{x},x,y,u,\nu,\tau;\theta)\,d\theta$$

subject to

$$J_0(\dot{x}(0),x(0),y,u(0),\nu,\tau;\theta)=0,$$
$$h(\dot{x},x,y,u,\nu,t;\theta)=0,$$
$$g(\dot{x},x,y,u,\nu,t;\theta)\le 0, \qquad \text{(M1)}$$

where x are the differential state variables, $\dot{x}$ their derivatives with respect to time, y the algebraic state variables, u the time-dependent optimization parameters (controls), ν the time-invariant optimization parameters, t time, τ the final time, θ the uncertain model parameters over the domain Θ, $\Psi(\theta)$ the joint probability density function (PDF), Φ a performance metric to be optimized, and $E_\theta\{\Phi\}$ the expected value of Φ. The equations J_0 represent the initial conditions of the system. The equality constraints h generally represent the process model equations but also could equally include constraints on the process or performance requirements. The inequality constraints g, however, are more commonly associated with performance requirements (e.g., product purity specifications), equipment limitations, and safety regulations.

In general, the direct solution of model (M1) can be problematic due to the difficulty in both evaluating the integral over the uncertain parameter space and ensuring feasibility of the inequalities for all parameter realizations. However, one method to solve model (M1) directly is to apply sampled optimization algorithms, such as Monte Carlo or Latin Hypercube (Diwekar and Kalagnanam, 1996; Liu and Sahinidis, 1996). Here, one uses a pseudorandom number generator and samples from it the probability distributions of the uncertain parameters. If enough samples are taken, accurate measures of the objective function and constraints (and their sensitivities with respect to the degrees of freedom) can be obtained. The advantage of this approach is that it can handle very large models, as the model size does not explode by increas-

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ing the number of uncertain parameters, but numerous samples may be required for accurate prediction of the objective function and constraints. The latter, together with the likely poor gradient information provided to the optimization algorithm, may result in undesirably high computation times.

An alternative way to tackle model (M1) is first to reformulate it to an equivalent deterministic problem and then to solve it by using standard techniques. Common approaches to reformulate model (M1) that have been reported in the literature can crudely be categorized into two main approaches: chance-constrained programming and explicit/implicit scenario-based approaches.

Chance-constrained programming (Charnes and Cooper, 1959, 1963), sometimes described as the probabilistic approach, is useful when dealing with "soft" inequality constraints (i.e., their satisfaction is not required for all realizations of the uncertain parameters). If the uncertain parameters are independent, follow stable probability density functions (i.e., normal, Poisson), and appear linearly in the constraints and objective function, the stochastic problem can then be reformulated to a deterministic one, where the *probability* that the constraint is satisfied can then be constrained. This approach has been successfully applied to chemical engineering problems by, for instance, Maranas (1997) for molecular design and Petkov and Maranas (1997) for planning and scheduling of multiproduct batch plants.

The scenario-based approach is perhaps the most commonly applied method for approximating model (M1). This requires the discretization of the uncertain parameter space (hence, generating scenarios) and results in a multiscenario deterministic optimization problem. The scenarios may be determined *explicitly* if one knows *a priori* which combinations of parameter realizations and associated probabilities are important (Shah and Pantelides, 1992; Subrahmanyam et al., 1994). Otherwise, the scenarios may be generated *implicitly* by assuming probability density functions for the parameters and using an approximation to the integral expression. One example of this would be Gaussian quadrature, which has been applied by, among others, Straub and Grossmann (1992) and Pistikopoulos and Ierapetritou (1995). However the scenarios are generated, the approximate deterministic model can be described by:

$$\max_{u,\nu,\tau} E_\theta\{\Phi(\dot{x},x,y,u,\nu,\tau;\theta)\} = \max_{u,\nu,\tau} \sum_{k=1}^{N_k} \psi_k \Phi_k(\dot{x}_k,x_k,y_k,u,\nu,\tau;\theta_k)$$

subject to

$$J_{0k}(\dot{x}_k(0),\, x_k(0),\, y_k,\, u(0),\, \nu;\, \theta_k) = 0 \qquad \forall k = 1..N_k,$$
$$h_k(\dot{x}_k,x_k,y_k,u,\nu,t;\theta_k) = 0 \qquad \forall k = 1..N_k,$$
$$g_k(\dot{x}_k,x_k,y_k,u,\nu,t;\theta_k) \le 0, \qquad \forall k = 1..N_k, \qquad \text{(M2)}$$

where N_k is the number of scenarios and ψ_k is the associated probability of occurrence of scenario k. Note that in (M2), u is independent of the scenarios ("here and now") but that dependence on the scenarios could be included to represent the "wait and see" case (u_k rather than u) where controls are optimally adjusted for the values of the uncertain parameters realized in the scenario ("recourse"). More recently, adaptive approaches have been developed to combine the better performance that one would expect to gain from using a "wait and see" approach with the simplicity of the "here and now" approach (Terwiesch and Agarwal, 1994; Bhatia and Biegler, 1997).

One final issue that must be considered, before introducing the concept of robustness, is the effect that the uncertainty has on the inequality constraints ($g \le 0$). These constraints can be classified into two general areas depending on whether or not violations caused by the uncertainty are acceptable (Wellons and Reklaitis, 1989). Constraints that must not be violated under any circumstances are classified as "hard" constraints. One example of a hard constraint would be safety limitations. When some violation can be tolerated, as in the case of product specifications, the constraints are described as "soft." The methods employed to deal with these two types of constraints depend on how the overall problem is tackled. In the chance-constrained programming approach, the stochastic problem is reduced to a deterministic one involving constraints of the form $Pr[Ax < b] \le \gamma$. The distinction between hard and soft constraints can be made simply by selecting an *appropriate* value for γ by taking into account the desired region of the probability distribution ($\pm 2\sigma$, $\pm 3\sigma$, etc. for normal distributions). In the scenario-based approach, one can directly enforce the hard constraints for each scenario, while soft constraints are often dealt with using constraints on the expectation and variance. However, it is important to select the scenarios appropriately, to ensure that satisfaction of the approximate model equates to full feasibility with respect to hard constraints in the exact model. One method of ensuring that hard constraints are enforced fully is to solve a feasibility subproblem, where the objective is to find some combination of uncertain parameters (now treated as bounded continuous variables) that maximizes the constraint violations. These critical values are then appended to the main multiscenario problem as an additional scenario (Swaney and Grossmann, 1985a, b). This method has also been applied by Mohideen et al. (1996), who consider parametric uncertainty and process disturbances in an integrated process and control systems design procedure for dynamic processes. Although the treatment of hard constraints is an important issue, in this paper we are concerned with soft constraints and appropriate measures of their satisfaction. The extent of soft constraint satisfaction is a measure of the robustness of a process. This is discussed in the next paragraph.

The models described above attempt to account for uncertainty by optimizing the expected value of the most important performance measure (we denote this as the key metric, $\Phi(\dot{x},x,y,u,\nu,\tau;\theta)$), usually based on economics. In one sense, the designs obtained in this fashion could be deemed more robust than deterministic designs based on nominal parameter values, but there is no guarantee that the process will perform to a certain level over all of the uncertain parameter space; the only guarantee is that the *average* is optimized. A more appropriate approach to robustness also needs to consider some measure of the *variability*, and to include all of the performance metrics in the analysis (in this paper, the performance metrics are denoted by z and are usually associated with differential or algebraic variables, x or y, or simple functions of them). The most common approach found in the literature is to define robustness in terms of the *variance* of one of the performance metrics, and to constrain or minimize this or some combination of mean and variance. Some of these approaches are as follows, where $E_\theta\{\Phi\}$ is the expectation of the key metric and $V_\theta\{\Phi\}$ is its corresponding variance.

Expectation only—max $E_\theta\{\Phi\}$ (see Bhatia and Biegler (1997), Mohideen et al. (1996)).

Worst-case scenario-max$\{\min_\theta \Phi\}$ (see Nishida et al. (1974), Ruppen et al. 1995)).

Weighted mean-variance form—max$\{\lambda E_\theta\{\Phi\} + (\lambda - 1) V_\theta\{\Phi\}\}$ (See Darlington et al. (1997)).

Guaranteed variance form—max $E_\theta\{\Phi\}$ subject to $V_\theta\{\Phi\} \leq V_{\max}$ (see Terwiesch et al. (1994), Ruppen et al. (1995)).

Guaranteed expectation form—min $V_\theta\{\Phi\}$ subject to $E_\theta\{\Phi\} \geq E_{\min}$ (see Terwiesch et al. (1994)).

Some of the more relevant articles that consider various aspects of robustness are as follows:

The results of a survey among industrial companies were presented by Terwiesch et al. (1994). The primary objective was typically found to be reproducibility of final product properties, rather than maximization of yield. The remainder of their article reviews various approaches to modeling uncertainty, possible optimization objectives as described above, and methods used to solve the problems. They also summarize an approach for calculating the probability of feasible operation, based on determining the feasible region and applying Gaussian quadrature to evaluate the integral of the joint probability density function.

This general approach was earlier described by Pistikopoulos and Mazzuchi (1990) and Straub and Grossmann (1990, 1993). In these articles, the "stochastic flexibility" of a process is defined as the probability of feasible operation. This is determined by solving a subproblem that first locates and then places quadrature points efficiently within the feasible region. The advantage of this approach is that the integral will be more accurate than simply integrating over the whole uncertain parameter space. The stochastic flexibility can then be evaluated as the integral of the joint probability density function over the feasible region. The stochastic flexibility concept has been extended to incorporate robustness aspects in terms of product quality in the design and operation of continuous processes by Georgiadis and Pistikopoulos (1997), who constrain variability using the signal-to-noise ratio of a key quality indicator. In addition, they propose a novel objective function containing both expectation of profit and cost of quality loss—the latter being the product of the variance and a quality loss coefficient.

More recently, Terwiesch et al. (1998) applied the approach of Straub and Grossmann (1993) to a number of examples of batch reaction systems. They modified the approach by including a binary variable (representing feasible or infeasible operation) in the integrand in order to overcome problems that may arise with nonconvex feasible regions. This approach may also be applied to an economic objective function so that revenue is only generated from scenarios that result in feasible operation.

In summary, most of the published work on design under uncertainty does not consider robustness explicitly. Where robustness is considered, the variance (or a function of it such as signal-to-noise ratio) of one of the performance metrics is used to measure it. Various approaches have been applied to soft and hard inequality constraints, but appropriate definitions of robustness with respect to soft inequalities are rarely considered. The work of Straub and Grossmann (1993) is one example where robustness with respect to hard and soft inequality constraints has been considered directly, but only in terms of the probability that all constraints are met.

Although it may appear that constraining or minimizing the variance of a performance metric is a reasonable approach to robustness, it is unsuitable for many cases and results in designs that overcompensate for uncertainty. While chance-constrained programming techniques allow one to define robustness in terms of probability of constraint violation, and the approach of Straub and Grossmann (1993) may be applied in a similar manner, it is clear that a *general* approach to robustness that can be applied in a number of circumstances has not yet been described. In this paper, we present a general approach to robustness that can be tailored for various types of constraint that might be imposed on the system and, in particular, on the performance metrics. It is widely acknowledged that any techniques applied to optimization under uncertainty must take account of the user's perspective on risk. We argue that the techniques described here easily take this into account via adjustable parameters.

The remainder of the article is structured as follows. We introduce a general robustness metric in the next section and derive from it two specific forms for use in a number of example problems. Then we describe a procedure used to solve the resulting problems. In the subsequent two sections, we consider a typical batch reaction system and a simple fermentation example, both of which exhibit significant uncertainty in the model parameters. Finally, some concluding remarks are given.

Robustness Metrics

As discussed earlier, the resilience of a process to variations in various uncertain parameters (robustness) is usually determined through the variance of one or more critical performance metrics. Robust designs are then obtained by minimizing the variance of one metric or by optimizing the expected performance while keeping the variability below an acceptable level. However, for many performance metrics, variability itself is not necessarily a problem. In many cases, a performance metric will only be constrained by an inequality where only the variability that results in violation of the constraint is detrimental to the process. This one-sided property is not usually captured by the typical approach of using the variance as a robustness metric. This is illustrated in the following example constraints, where it is required that $z \geq z^*$:

$$E_\theta\{z\} \geq z^*, \tag{1}$$

$$V_\theta\{z\} \leq \gamma, \tag{2}$$

where z in the case is a symmetrically-distributed performance metric and z^* is its lower bound.

The main problem here is that, if the first constraint is active (i.e., $E_\theta\{z\} = z^*$), the probability of z being less than z^* will be 50% despite the presence of the variance con-

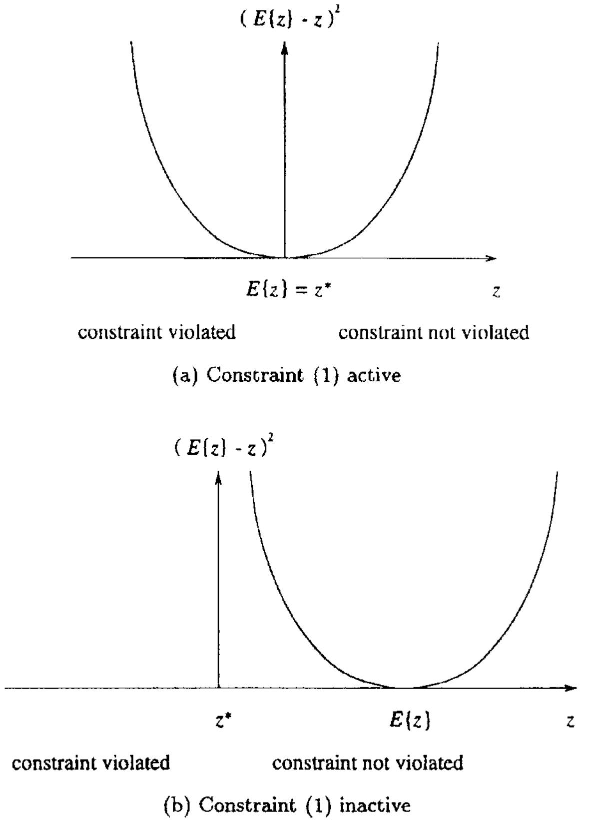

Figure 1. Variance constraint unsuitable for an inequality constraint on z.

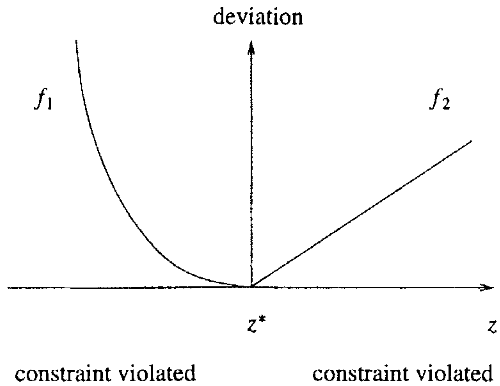

Figure 2. Example of general deviation function for constraint (3).

straint (as illustrated in Figure 1a). Moreover, constraining the variance takes *no* specific account of the value of z^*; the variance only gives a measure of the derivation from the mean. This is shown in Figure 1b, which shows that deviations from the mean contribute to the variance *regardless* of whether or not the constraint $z \geq z^*$ is violated.

Clearly, a number of robustness metrics are required so that different requirements on the performance metrics can be treated in an appropriate manner. In this section, we describe a general robustness metric, based on constraint violations only, that can be applied to any type of constraint to be imposed on the performance metrics. The robustness metric may be reduced to more common measures of robustness, such as the variance.

The general robustness metric is based on the violation of the following soft constraint:

$$z(x, y, u, v, \tau; \theta) - z^* = 0, \tag{3}$$

where z is the vector of performance metrics (which may include the key metric Φ) and z^* the vector of corresponding target values. To define the robustness metric, we introduce the concept of a *general deviation function*, $q(z, z^*)$, defined in terms of two general functions, f_1 and f_2 (see Figure 2), the violation as follows:

$$q(z, z^*) = \begin{cases} f_1(\Delta z) & \text{if } \Delta z < 0, \\ f_2(\Delta z) & \text{if } \Delta z \geq 0, \end{cases} \tag{4}$$

where $\Delta z \equiv z - z^*$ is the violation, which takes negative and positive values below and above the target value (z^*) respectively. This general deviation function may take many forms depending on f_1 and f_2, thus reflecting different contexts, including those that appear in the literature such as variance, quality loss, inequality constraint penalties, and so forth.

By setting either f_1 or f_2 to zero, the original equality constraint (Eq. 3) reduces to an inequality and the robustness metric has the desired one-sided property (see Figure 3).

Finally, the robustness metric is defined to account for violations of the constraint over all of the uncertain parameter space by taking the expectation of the general deviation function, q, and can be bounded by:

$$E_\theta\{q(z, z^*)\} \leq \gamma, \tag{5}$$

where γ is the maximum allowable expected deviation.

While the implementation of the robustness metric, as defined above, in a simulation (or a sampling-based optimization) is a simple matter, there are certain difficulties that arise in the case of optimization due to the discontinuous and nondifferentiable nature of the functions, for instance, if a *max* formulation is used to represent Eq. 4, that is, $q(z, z^*) = \max(f_1(\Delta z), f_2(\Delta z))$. In addition, the latter representation is restricted to monotonic functions, and therefore is not suitable for our approach, which can accommodate general deviation functions.

The optimization algorithm used here (see section on solution approach) requires functions that are continuous and at least twice differentiable as it applies an analytical gradient approach. Therefore, the discontinuous definition of q in Eq. 4 can be replaced by the following smooth function:

$$q = w f_1 + (1 - w) f_2, \tag{6}$$

by defining the binary variables $w(\Delta z)$, such that:

$$w(\Delta z) = \begin{cases} 1 & \text{if } \Delta z < 0, \\ 0 & \text{if } \Delta z \geq 0. \end{cases} \tag{7}$$

In the section on the solution approach, we describe some methods for approximating the binary variables using continuous smooth functions, so that a mixed-integer programming problem need not be solved.

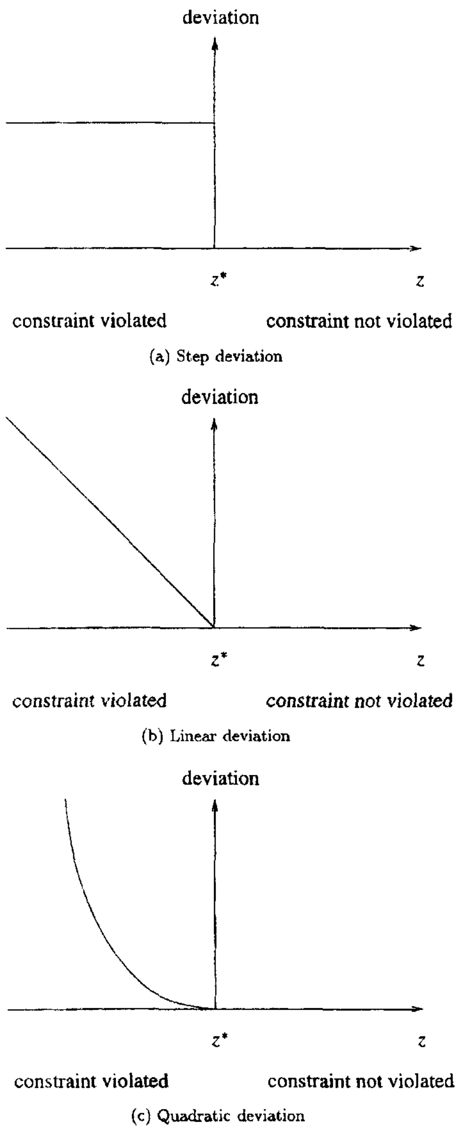

Figure 3. Examples of one-sided deviation functions.

For the general case, the mixed-integer stochastic programming problem can be stated as follows:

$$\max_{u,\nu,\tau} E_\theta\{\Phi(\dot{x},x,y,u,\nu,\tau;\theta)\}$$

$$= \max_{u,\nu,\tau} \int_{\theta\in\Theta} \Psi(\theta)\Phi(\dot{x},x,y,u,\nu,\tau;\theta)\,d\theta$$

subject to

$$J_0[\dot{x}(0),x(0),\,y,\,u(0),\,\nu;\theta]=0,$$

$$h(\dot{x},x,y,u,\nu,t;\theta)=0,$$

$$g(\dot{x},x,y,u,\nu,t;\theta)\le 0,$$

$$q(z,z^*)=wf_1+(1-w)f_2,$$

$$E_\theta\{q(z,z^*)\}\le\gamma. \qquad \text{(M3)}$$

where the dimensionality of the constraints h and g is reduced to encompass only the hard constraints; soft constraints are handled only through the robustness metrics.

It is important to note that the solution method for the above model has not been postulated in defining the robustness metrics; most approaches may be used.

Commonly applied metrics

As discussed in the Introduction, previous work has addressed robustness in optimization using other metrics. Model (M3) is sufficiently general that it can accommodate most of these metrics with little or no modification. Below, we demonstrate how such metrics can be derived from the above formulation.

A one-sided linear penalty for the inequality $z - z^* \ge 0$ can be captured. By defining $f_1 = z^* - z$ and $f_2 = 0$ we obtain:

$$q = w(z^* - z). \qquad (8)$$

Taguchi's quality loss function (Taguchi, 1986; Phadke, 1989) can be directly implemented by setting $f_1 = f_2 = k(z - z^*)^2$, giving:

$$q = k(z - z^*)^2, \qquad (9)$$

where k is the quality loss coefficient and z^* the target quality.

A classical variance constraint can be modeled by setting $f_1 = f_2 = (z - z^*)^2$, thus giving:

$$q = (z - z^*)^2. \qquad (10)$$

The following equality constraint should also be added to the model:

$$E_\theta\{z\} = z^*, \qquad (11)$$

where, for this specific case, z^* may either be determined by the algorithm or assigned a value (thus constraining the expectation of z to a target value).

Other measures to indicate quality loss can also be derived. For example, by applying the standard variance constraints (Eqs. 10 and 11), the signal-to-noise ratio can be defined as follows:

$$r_{S/N} = 10\log_{10}\left(\frac{z^{*2}}{E_\theta\{q\}}\right) \ge \alpha, \qquad (12)$$

where α is a lower bound on $r_{S/N}$ (see Georgiadis and Pistikopoulos (1997)).

In fact, model (M3) can be generalized further by modifying Eq. 5 as follows:

$$\mathfrak{F}(E_\theta\{q(z,z^*)\}) \le \gamma, \qquad (13)$$

where $\mathfrak{F}$ is a general function. It is possible to derive any of the above metrics directly from this formulation.

Of course, any of these metrics may be used in constraints or included in the objective function. However, it is difficult to determine appropriate values for the additional parameters introduced, such as k, α, and γ. Therefore more intuitive measures of robustness should be derived. In the next subsection, we describe two such one-sided metrics for inequality constraints.

One-sided robustness metrics for inequality constraints

We have described a general approach to robustness, such that metrics quantifying the robustness of a process with respect to equality and inequality constraints can be defined in terms of any asymmetric two-sided or one-sided deviation function. In many cases, performance metrics will be constrained by inequalities, e.g., product purity/quality constraints, productivity constraints, and constraints on the economic performance of the plant. For these cases, not only is it more suitable to use a one-sided robustness metric than, for instance, a variance-based constraint, but it may also be important to define the robustness in terms of a meaningful quantity, probability. To this end, we describe two simple one-sided robustness metrics: one based on the probability of a constraint being violated, and the other related to the extent of constraint violation that one can expect.

Probability of constraint violation. An important measure of robustness is the probability that a constraint will be violated. In the chance-constrained programming method, one can directly constrain the probability of constraint violation provided that certain conditions are met (see the Introduction). In the general case, this will not be possible and a different approach is needed to evaluate the probability, such as the approach of Straub and Grossmann (1993).

The enforcement of a maximum probability of violation can easily be accommodated in our approach. The probability of the constraint being violated, P_{viol}, must not be more than a specified value, γ, which can be written mathematically as:

$$P_{\text{viol}} = Pr[z < z^*] \le \gamma. \tag{14}$$

In the definition of the general robustness metric, the binary variables, w, were defined to represent whether the performance metric z was greater or less than a desired value z^*. The above constraint can therefore be rewritten in terms of the binary variables:

$$Pr[w = 1] \le \gamma, \tag{15}$$

which can be evaluated by

$$Pr[w=1] = \int_{\theta \in \Theta} \Psi(\theta) w \, d\theta \le \gamma, \tag{16}$$

which is the equivalent of constraining the expected value of w. This is achieved directly in model (M3) by setting $f_1 = 1$ and $f_2 = 0$, to give:

$$q = w, \tag{17}$$

$$P_{\text{viol}} = E_\theta\{q\} \le \gamma. \tag{18}$$

Expected constraint violation. Although the above metric, defined as the probability of a constraint violation, is a useful and important measure of the robustness of a process, it gives no indication of the extent of the violation. Such a measure would be useful to distinguish between process designs resulting in similar probabilities of constraint violation. The expected violation may also be useful when the scenario-based approach is employed to solve the design problem, and it is necessary to limit the number of scenarios for computational reasons. As fewer scenarios are used, and the accuracy of the multiscenario model reduces, the accuracy of the probability metric is more likely to be affected than the expected violation metric. This is because the expected violation metric depends on two properties: (i) whether or not the constraint is violated and (ii) by how much, whereas the probability of a constraint violation depends only on the first property; more information is provided to the optimizer for the same number of scenarios.

The expected constraint violation, E_{viol}, is defined as follows:

$$E_{\text{viol}} = \int_{\theta \in \Theta} \Psi(\theta) q \, d\theta \le \gamma, \tag{19}$$

where in this case γ may be thought of as the maximum expected violation, and q is defined by:

$$q = \begin{cases} z^* - z & \text{if } z < z^*, \\ 0 & \text{if } z \ge z^*. \end{cases} \tag{20}$$

This is the equivalent of specifying $f_1 = z^* - z$ and $f_2 = 0$ for the general robustness metric, that is, the one-sided linear deviation function shown in Figure 3b:

$$q = w(z^* - z). \tag{21}$$

Constraint 19 therefore reduces to:

$$E_{\text{viol}} = E_\theta\{q\} \le \gamma. \tag{22}$$

A slight limitation with this metric (and with many others) is that it allows all scenarios to violate the constraint by a small amount while constraint on the metric is satisfied. To remedy this problem, one can easily combine the above metric with the probability of constraint violation.

Solution Approach

As discussed earlier, a number of approaches can be used to solve models (M1) to (M3). For the example problems presented in this article, we use a scenario-based approach to model the problem of design and operation under uncertainty, as this approach can capture general distribution functions, uncertain parameters that appear nonlinearly in the model, and more importantly can take advantage of current optimization algorithms which require good gradient information.

The scenario-based approach adopted involves discretizing the uncertain parameter space, which means that even modestly sized process models rapidly become computationally intensive as the number of uncertain parameters increases. Furthermore, due to the binary variables introduced in the previous section, the resulting mixed-integer optimal control problem is likely to be intractable if all uncertain parameters are considered and if, for each of the scenarios, binary variables are used in the definition of the robustness metrics. We therefore propose a solution method based on a hierarchical procedure with smooth approximating functions for the binary variables.

A second method for reducing the problem complexity is to include only the uncertain parameters that have the greatest influence on the process, both in terms of the magnitude and the type of response. Based on a perturbation analysis of the system, some of the less important parameters may be excluded from the multiscenario model, thus reducing its size. Here, we apply a simple rule where each uncertain parameter is perturbed in turn from its mean value by plus or minus one standard deviation.

Finally, since the scenario-based approach is an approximation to the true nature of the uncertainty, it is necessary to validate the results of the optimizations using stochastic simulation. In this case, we use a Monte Carlo method.

Overall, the solution procedure comprises the following steps:

Step 1. A deterministic optimal control problem is solved based on the nominal values of the uncertain parameters.

Step 2. Based on this deterministic operating policy, a perturbation analysis is carried out to determine the critical uncertain parameters.

Step 3. A stochastic simulation is then performed to determine the true effect of these critical parameters on the performance metrics.

Step 4. A multiscenario robust optimal control problem is solved, taking account of the critical parameters and applying various robustness metrics.

Step 5. A second stochastic simulation is performed on the robust operating policy, to evaluate the effectiveness of the procedure (comparison with Step 3).

Here, we use the *gPROMS* (Barton and Pantelides, 1994) modeling system to describe the model equations and the *gOPT* (*gPROMS* Project Team, 1995) extension, which is based on the control vector parameterization approach of Vassiliadis et al. (1994a,b), to solve the resulting dynamic optimization problems (Steps 2 and 4).

Approximations for binary variables

The combinatorial nature of the problem can be reduced by approximating the binary variables, w, by continuous ones. In this subsection, we discuss two alternatives; switching parameters and smooth approximation functions.

In the first case, the binary variables can be treated as additional degrees of freedom taking discrete values in different regions which are determined by the following inequalities (Bhatia and Biegler, 1997):

$$w(z^* - z) \geq 0, \tag{23a}$$

$$w(z^* - z) \geq z^* - z, \tag{23b}$$

$$0 \leq w \leq 1. \tag{23c}$$

However, a number of practical issues reduce the effectiveness of this approach. First, the constraints do not guarantee that the w variables will be assigned correctly when $z = z^*$. In addition, the resulting model size may be quite large since one degree of freedom and four constraints are required for each combination of scenarios and constraints on the metrics.

In the second case, the w variables can be defined explicitly by using the following smooth approximation function:

$$w = \frac{1}{2}[\tanh\{\xi(z^* - z)\} + 1], \tag{24}$$

where ξ is a suitably large number. With this approach, the w variables are defined correctly unless the value of z is within about 1% of z^* (depending on the value of ξ). Although possibly prone to numerical difficulties at certain points, in practice this smooth approximation function performs as well as the previous approach, with a much smaller model size.

Of course, a number of other smooth approximation functions (Duran and Grossmann (1986), Balakrishna and Biegler (1992)) may also be used.

Applying Eq. 24, the final optimization model (Step 4) is:

$$\max_{u,v,\tau} \sum_{k=1}^{N_k} \psi_k \Phi_k(\dot{x}_k, x_k, y_k, u, v, \tau; \theta_k)$$

subject to

$$J_{0k}(\dot{x}_k(0), x_k(0), y_k, u(0), v; \theta_k) = 0, \qquad \forall k = 1..N_k$$

$$h_k(\dot{x}_k, x_k, y_k, u, v, t; \theta_k) = 0, \qquad \forall\, k = 1..N_k$$

$$g_k(\dot{x}_k, x_k, y_k, u, v, t; \theta_k) \leq 0, \qquad \forall\, k = 1..N_k$$

$$w_k(z_k, z^*) = \frac{1}{2}[\tanh\{\xi(z^* - z_k)\} + 1], \qquad \forall\, k = 1..N_k$$

$$q_k(z_k, z^*) = w_k(\Delta z_k) f_1(\Delta z_k) + (1 - w_k(\Delta z_k)) f_2(\Delta z_k), \qquad \forall\, k = 1..N_k$$

$$\sum_{k=1}^{N_k} \psi_k q_k(z_k, z^*) \leq \gamma. \tag{M4}$$

It is evident that model M4 refers to a "here and now" approach, since the degrees of freedom, u, v, and τ, do not depend on the scenario. However, the approach can easily be extended to cover the "wait and see" case, or even a hybrid scheme, simply by making all or some of the degrees of freedom scenario dependent.

It should also be noted that the smoothing functions (Eq. 24) are not convex. However, most dynamic process optimization models of industrial relevance are highly nonconvex anyway and even deterministic approaches can only guarantee local optima.

In the next two sections, we apply the above optimization strategy to two illustrative examples.

Example 1: A Two-Stage Reactor System

The first example problem is based on the two-stage reactor system used by Vassiliadis et al. (1994a). The first reactor, operated within temperature limits of 298 and 398 K, contains a solid catalyst to promote the following reactions.

$$2A \rightarrow B \rightarrow C$$

Table 1. Model Equations for the Two-Stage Reactor System

Model Eqs. for Stage 1; $t \in [0, \tau_1]$	Initial Conditions	Rate Equations
$\frac{dC_A}{dt} = -2k_1(T)C_A^2$	$C_A(0) = 2{,}000$	$k_1(T) = 0.0444e^{2{,}500/T}$
$\frac{dC_B}{dt} = k_1(T)C_A^2 - k_2(T)C_B$	$C_B(0) = 0$	$k_2(T) = 6{,}889e^{5{,}000/T}$
$\frac{dC_C}{dt} = k_2(T)C_B$	$C_C(0) = 0$	
Model Eqs. for Stage 2; $t \in [0, \tau_2]$	**Initial Conditions**	
$\frac{dC_A}{dt} = 0$	$C_A(0) = 0.1C_A(\tau_1)/(S+0.1)$	
$\frac{dC_B}{dt} = -0.02C_C - 0.05C_B - 4.0\times 10^{-5}C_B^2$	$C_B(0) = (0.1C_B(\tau_1) + 600S)/(S+0.1)$	
$\frac{dC_C}{dt} = 0$	$C_C(0) = 0.1C_C(\tau_1)/(S+0.1)$	
$\frac{dC_D}{dt} = 0.02C_C$	$C_D(0) = 0$	
$\frac{dC_E}{dt} = 0.05C_C$	$C_E(0) = 0$	
$\frac{dC_F}{dt} = 4.0\times 10^{-5}C_B^2$	$C_F(0) = 0$	

The initial charge is 0.1 m^3 of an aqueous solution of A, at a concentration of 2,000 mol/m^3.

At the end of the first reaction stage, the contents are transferred to the second reactor. Then, an amount of B (to be optimized) is added at a concentration of 600 mol/m^3. The second stage, operated at a fixed temperature, involves the following three reactions: $B \rightarrow D$, $B \rightarrow E$, and $2B \rightarrow F$. The objective is to maximize the amount of D produced, subject to a minimum final product concentration of 145 mol/m^3 and a maximum combined processing time of 180 min. The degrees of freedom are the processing time for each reaction, τ_1 and τ_2, the temperature profile for the first reaction, $T(t)$, and the volume of aqueous B added to the second stage, S.

The above two-stage reactor system is described by the differential and algebraic equations shown in Table 1.

The deterministic optimization problem can then be posed as:

$$\max_{S,\tau_1,\tau_2,T(t)} \quad \Phi = (0.1 + S)C_D(\tau_2)$$

subject to

model equations (Table 1),

$$298 \leq T(t) \leq 398 \qquad \forall t \in [0, \tau_1],$$

$$0 \leq S \leq 0.1,$$

$$\tau_1 + \tau_2 \leq 180,$$

$$C_D(\tau_2) \geq 145. \tag{D1}$$

Table 2. Two-Stage Reaction Operating Policy for Nominal Optimization

Controls		
Interval	Duration (min)	T (K)
1	16.3	320.4
2	15.5	316.0
3	23.6	313.5
4	50.9	308.0
Time-Invariant Parameters		
S (m^3)	τ_1 (min)	τ_2 (min)
0.1	106.3	73.7

Nominal optimization

The system described above is optimized based on the nominal values of the parameters. A piecewise-constant control is used for the temperature of the first reactor with four time intervals over the range $[0, \tau_1]$ and one time interval for the second reactor. The results are summarized in Table 2, and the computational statistics (for all optimization problems presented in this paper) are shown in Table 15.

Perturbation analysis on this operating policy shows that the two most important parameters are the activation energy constants in the Arrhenius expressions. Considering these two parameters to be the only sources of uncertainty, and assuming them to be distributed normally with a standard deviation of 5% of the mean value, Monte Carlo simulations are performed to determine the effect of uncertainty on various performance and robustness metrics. The results are summarized in Table 3, and the distribution of the product concentration is shown in Figure 4.

Table 3. Monte Carlo Simulations for the Nominal Two-Stage Reaction Operating Policy

Performance/Robustness Metric	Monte Carlo Simulation
$E_\theta\{\Phi\}$ (mol)	29.1
$E_\theta\{C_D(\tau_2)\}$ (mol/m^3)	145.3
E_{viol} (mol/m^3)	2.12
P_{viol}	0.446

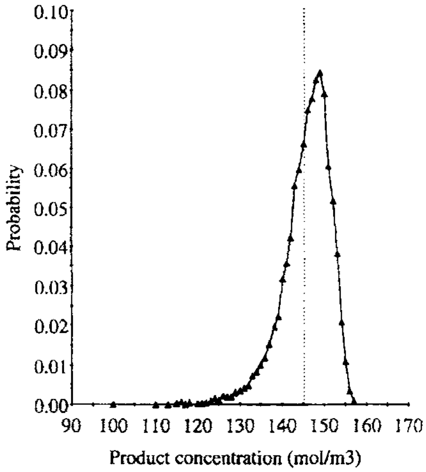

Figure 4. Product concentration distribution for the deterministic two-stage reaction operating policy.

The results show that although the *expected* values of the product concentration and objective are satisfactory, there is significant variability in these metrics, resulting in a high probability (44.6%) that the product quality constraint ($C_D(\tau_2) \geq 145$) will be violated. Also of interest is that the product concentration distribution (Figure 4) is asymmetric, where the vertical dotted line represents the minimum required concentration. Next, we apply a robust optimization procedure considering in sequence the two *one-sided* metrics of expected violation and probability of a constraint violation.

Robust optimization

In the previous subsection, we demonstrated that an optimal design based on nominal parameter values can result in poor overall performance when subjected to typical levels of uncertainty in only two of the model parameters. Here, we apply a robust design procedure using appropriate metrics to derive an operating policy that is more resilient to the uncertainty.

Case I: Expected Violation. We first consider improving the performance by limiting the expected violation to no more than 1.5 mol/m^3. By applying 7th order Gaussian quadrature to evaluate the integral expressions, the following 49-scenario model is generated.

$$\max_{S,\tau_1,\tau_2,T(t)} E_\theta\{\Phi\} = \sum_{k=1}^{49} \psi_k (0.1+S) C_{D,k}(\tau_2)$$

subject to

$$\text{model equations}, \quad \forall\, k = 1..49$$

$$298 \leq T(t) \leq 398 \quad \forall\, t \in [0,\tau_1],$$

$$0 \leq S \leq 0.1,$$

$$\tau_1 + \tau_2 \leq 180,$$

$$w_k = \frac{1}{2}\{\tanh[\xi(145 - C_{D,k})] + 1\}, \quad \forall\, k = 1..49$$

$$q_k = w_k(145 - C_{D,k}), \quad \forall k = 1..49$$

$$E_{\text{viol}} = \sum_{k=1}^{49} \psi_k q_k \leq 1.5. \tag{R1}$$

With only modest computational requirements (see Table 15), the above formulation determines the robust operating policy summarized in Table 4. The values of the relevant performance and robustness metrics, predicted by Monte Carlo simulation, are listed in Table 5.

The results in Table 5 show that the robust formulation is quite accurate, and that the robust operating policy has significantly reduced both the expected constraint violation and the probability of the constraint being violated. Compared with the nominal case, the probability has been reduced from 44.6% to 30.7%, and the expected violation has been reduced from 2.12 mol/m^3 to 1.48 mol/m^3. Comparison of the product concentration distributions for the deterministic and robust operating policies (Figure 5) shows that the reductions come mainly from a shift in the distribution rather than the distribution becoming narrower. The most important feature of these results is that robustness can be increased without reducing the variance; the algorithm has not prevented variability that results in higher product concentrations.

Although the distribution has been shifted noticeably to the right, there is still a 30% chance that the product concentration will fail to meet the specification. In order to reduce this further, and increase the robustness of the operating policy, an alternative optimization can be performed with a constraint on the probability of a constraint violation.

Case II: Probability of Constraint Violation. By redefining the general deviation function, q_k, the robust optimization model (R1) can be modified to constrain the probability of a constraint violation:

Table 4. Robust Operating Policy for the Two-Stage Reaction Example

Controls		
Interval	Duration (min)	T (K)
1	5.0	337.0
2	18.2	314.4
3	23.3	307.3
4	61.2	303.5
Time-Invariant Parameters		
S (m^3)	τ_1 (min)	τ_2 (min)
0.08	107.7	72.3

$E_{\text{viol}} \leq 1.5$.

Table 5. Monte Carlo Simulations for the Robust Two-Stage Reaction Operating Policy

Performance/Robustness Metric	Robust Model	Monte Carlo Simulation
$E_\theta\{\Phi\}$ (mol)	26.3	26.5
$E_\theta\{C_D(\tau_2)\}$ (mol/m^3)	146.3	147.1
E_{viol} (mol/m^3)	1.50	1.48
P_{viol}	0.353	0.307

$E_{\text{viol}} \leq 1.5$.

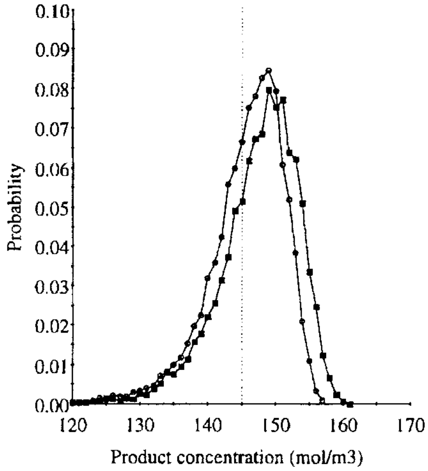

Figure 5. Product concentration distributions for deterministic (circles) and Case I (squares) two-stage reaction operating policies.

$$\max_{S,\tau_1,\tau_2,T(t)} E_\theta\{\Phi\} = \sum_{k=1}^{49} \psi_k (0.1+S) C_{D,k}(\tau_2)$$

subject to

$$\text{model equations}, \quad \forall\, k = 1..49$$

$$298 \le T(t) \le 398 \quad \forall\, t \in [0, \tau_1],$$

$$0 \le S \le 0.1,$$

$$\tau_1 + \tau_2 \le 180,$$

$$w_k = \frac{1}{2}\{\tanh[\xi(145 - C_{D,k})] + 1\}, \quad \forall\, k = 1..49$$

$$q_k = w_k, \quad \forall\, k = 1..49$$

$$P_{\text{viol}} = \sum_{k=1}^{49} \psi_k q_k \le 0.25. \tag{R2}$$

Once more, the above model can be solved relatively easily to simultaneously obtain the robust operating policy shown in Table 6 and the associated performance and robustness metrics shown in Table 7. The distribution of the product concentration for this case compared with that of the deterministic operating policy is shown in Figure 6.

Table 6. Robust Operating Policy for the Two-Stage Reaction Example

Controls		
Interval	Duration (min)	T (K)
1	8.6	334.3
2	43.2	313.7
3	24.4	309.1
4	32.0	308.4
Time-Invariant Parameters		
S (m^3)	τ_1 (min)	τ_2 (min)
0.06	108.2	71.8

$P_{\text{viol}} \le 0.25$.

Table 7. Monte Carlo Simulations for the Robust Two-Stage Reaction Operating Policy*

Performance/Robustness Metric	Robust Model	Monte Carlo Simulation
$E_\theta\{\Phi\}$ (mol)	23.9	23.9
$E_\theta\{C_D(\tau_2)\}$ (mol/m^3)	148.0	148.4
E_{viol} (mol/m^3)	1.34	1.48
P_{viol}	0.250	0.238

*$P_{\text{viol}} \le 0.25$.

In this second case, the product concentration distribution has been shifted substantially to the right, while the variance has actually increased. This highlights the importance of selecting the appropriate robustness metric for the process: a variance constraint would have produced a narrower distribution, with fewer scenarios producing high concentrations.

The results in Table 7 show that the probability of the quality constraint not being met has been reduced from 30.7% to 23.8%, while the expected violation remains relatively unaffected. This seems to indicate that the optimization has modified the operating policy so that scenarios that were just failing to meet the required concentration are now able to meet this constraint, whereas those scenarios in which a substantial violation exists remain relatively unaffected.

Example 2: A Fermentation Process

Fermentation processes are particularly difficult to model accurately. There are two general approaches to modeling these processes. One approach is to model as many as possible of the chemical and enzyme reactions, which make up the metabolic pathways within the cells, in order to describe the behavior of the cell culture accurately. The second approach is to use lumped models based on empirical relations to give approximate predictions of the system behavior using limited data. For either approach, there is significant difficulty associated with obtaining values for the model parameters. In the

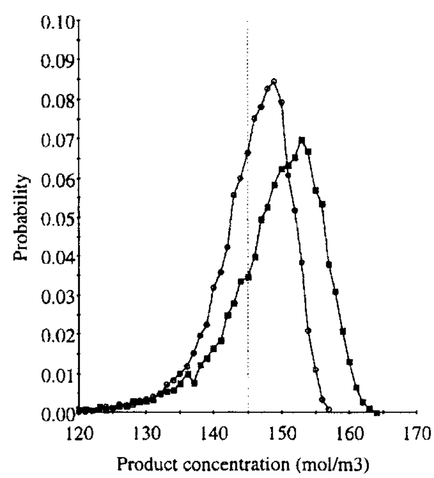

Figure 6. Product concentration distributions for deterministic (circles) and Case II (squares) two-stage reaction operating policies.

Table 8. Model Equations for the Fermentation System

Overall material balance:

$$\frac{dV}{dt} = F_{in}$$

Material balance for the biomass:

$$\frac{d(VX)}{dt} = F_{in} X_{in} + \mu VX$$

Specific growth rate of biomass:

$$\mu = \left(1 - \frac{P_{by}}{P_{by,max}}\right) \frac{\mu_{max} S}{K_S + S + S^2/K_I}$$

Material balance for the byproduct:

$$\frac{d(VP_{by})}{dt} = VX(\alpha\mu + \beta)$$

Material balance for the intracellular product:

$$\frac{d(VP)}{dt} = \mu VXY_{P/X}$$

Material balance for the limiting substrate:

$$\frac{d(VS)}{dt} = F_{in} S_{in} - VX\left(\frac{\mu}{Y_{X/S}} + K_{Sm} + \frac{\alpha\mu + \beta}{Y_{P_{by}/S}}\right)$$

Revenue function:

$$\mathfrak{R} = C_P P(\tau)V(\tau) + C_{P_{by}} V(\tau) P_{by}(\tau)$$

Operating cost function:

$$\mathfrak{C} = C_X V_0 X_0 + C_S\left(V_0 S_0 + \int_0^{\tau} F_{in} S_{in} dt\right)$$

Profit rate function (relative monetary units per hour (rmu/h)):

$$\Phi = \frac{\mathfrak{R} - \mathfrak{C}}{\tau + \tau_{clean}}$$

first case, there are many parameters whose values are difficult to determine. In the second case, there are usually too few parameters to describe the system fully; their values must be obtained by regression based on experimental data to provide the best approximation of the system behavior. In both cases there is a significant level of uncertainty associated with the modeling of the process that is either due to structural uncertainty, parametric uncertainty, or both. Consequently, fermentation processes are ideal examples for the application of robust optimization. In this example, we take the approach that a typical lumped model will be satisfactory to describe the process behavior, and that all of the above sources of uncertainty can be modeled by a high level of uncertainty in the model parameters.

The model used for this example has been described in more detail by Uesbeck et al. (1998), where the effect of using the expected constraint violation was considered. The system is summarized as follows.

Table 9. Mean Values for the Uncertain Parameters

Parameter	Mean Value
K_I	22
K_S	1.2
K_{Sm}	0.001
$P_{by,max}$	50
$Y_{P_{by}/S}$	0.51
$Y_{P/X}$	0.05
$Y_{X/S}$	0.4
μ_{max}	0.48

Table 10. Optimal Fermentation Operating Policy for the Nominal Case

Control Variables			
Interval	Duration (h)	F_{in} (L/h)	S_{in} (g/L)
1	0.41	0	200
2	2.20	292	200
3	2.96	400	200
4	0.32	0	0
Time-Invariant Parameters			
V_0 (L)	S_0 (g/L)	τ (h)	
3,171	9.6	5.89	

The product is an intracellular enzyme, while an extracellular byproduct is also formed and has a small economic value. For simplicity, we only consider batch or fed-batch operation, which will be determined by the optimization algorithm. We also assume isothermal operation of the fermenter, and that the feed consists only of substrate. The set of differential and algebraic equations that describes the fermentation process is outlined in Table 8 and the model parameter values are outlined in Table 9.

For the nominal optimization, the profile rate Φ is to be maximized subject to a minimum product concentration requirement of at least 0.4 g/L. The operating policy determined by the nominal optimization is summarized in Table 10. By adopting this operating policy, a profit rate of 80.46 rmu/h and a product concentration of 0.454 g/L are obtained.

It is assumed that all uncertain parameters are normally distributed with a standard deviation of 20% of the mean value. As described by Uesbeck et al. (1998), a perturbation analysis on this system shows that two critical parameters are μ_{max} and $Y_{P_{by}/S}$. Negative deviations in μ_{max} are shown to have a much greater effect on the performance metrics than positive deviations. For $Y_{P_{by}/S}$, however, deviations from the mean in both directions cause a decrease in both of the performance metrics.

Performing a Monte Carlo simulation using this operating policy provides the values of the following performance and robustness metrics: expected profit rate of 42.5 rmu/h, expected product concentration of 0.374 g/L, expected constraint violation of 0.052 g/L, and a 53% probability that the constraint is violated. We note that the underlying model pa-

Table 11. Optimal Robust Fermentation Operating Policy

Control Variables			
Interval	Duration (h)	F_{in} (L/h)	S_{in} (g/L)
1	3.45	194	200
2	3.91	326	200
3	0.00	319	200
4	0.28	135	200
Time-Invariant Parameters			
V_0 (L)	S_0 (g/L)	τ (h)	
3,015	3.34	7.64	

$P_{viol} \leq 0.3$.

Table 12. Performance of the Robust Fermentation Operating Policy

Performance/Robustness Metric	Robust Model	Monte Carlo Simulation
$E_\theta\{\Phi\}$ (rmu/h)	50.6	48.4
P_{viol}	0.300	0.382

$P_{\text{viol}} \leq 0.3$.

rameter uncertainty has a dramatic effect on the process performance. More significantly, the probability of the product concentration constraint being violated is greater than 50%. Next, we perform a robust optimization to maximize the expected profit while keeping the probability of a constraint violation within tighter bounds.

For the robust optimization, we use 5th-order Gaussian quadrature to generate the scenarios implicitly, and apply the probability of a constraint violation to enforce robustness. The resulting 25-scenario model, shown below as model (R3), is solved for two cases: (i) $P_{\text{viol}} \leq 0.3$ and (ii) $P_{\text{viol}} \leq 0.2$.

$$\max_{V_0, S_0, \tau, F_{\text{in}}(t), S_{\text{in}}(t)} E_\theta\{\Phi\} = \sum_{k=1}^{25} \psi_k \frac{\mathcal{R}_k - C}{\tau + \tau_{\text{clean}}}$$

subject to

$$\text{model equations (Table 8)}, \qquad \forall\, k = 1..25$$

$$w_k = \frac{1}{2}\{\tanh[\xi(0.4 - P_k(\tau))] + 1\}, \qquad \forall\, k = 1..25$$

$$q_k = w_k, \qquad \forall\, k = 1..25$$

$$P_{\text{viol}} = \sum_{k=1}^{25} \psi_k q_k \leq \gamma. \tag{R3}$$

The results of these optimizations, along with the corresponding Monte Carlo simulations, are shown in Tables 12 and 13. The robust operating policy is contrasted with the deterministic policy, shown in Figure 7, which illustrates the product concentration distributions. As can be seen in Tables 12 and 14, both of the robust operating policies result in greater expected profit rates than the deterministic design while increasing the robustness of the process. The trend

Table 13. Optimal Robust Fermentation Operating Policy

Control Variables			
Interval	Duration (h)	F_{in} (L/h)	S_{in} (g/L)
1	3.47	202	200
2	4.32	345	200
3	0.00	204	200
4	0.28	144	200

Time-Invariant Parameters		
V_0 (L)	S_0 (g/L)	τ (h)
2,770	3.02	8.07

$P_{\text{viol}} \leq 0.2$.

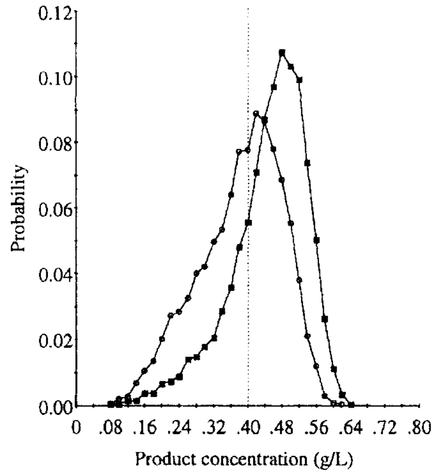

Figure 7. Product concentration distributions for deterministic (circles) and robust (squares) fermentation operating policies.

$P_{\text{viol}} \leq 0.2$.

seems to be that lower initial volumes and substrate concentrations help to increase the robustness, and, as can be expected, longer processing times also improve robustness.

It should be noted that the 5th-order Gaussian quadrature does not provide a very close approximation to the desired targets, especially due to the strong nonlinearity appearing in the model. However, the optimal robust solutions significantly improve the performance obtained by the nominal case. In order to remedy the above deficiency, one can either increase the order of the Gaussian quadrature approximation or repeat the robust optimization with a stricter constraint.

As in the first example problem, Figure 7 shows that the product concentration distribution has shifted to the right, while in this case the variance has also been reduced.

Conclusion

Many approaches to design under process uncertainty do not consider robustness directly or impose robustness by using variance-based constraints. In this paper, we have reiterated the fact that many performance measures only require one-sided constraints, and in general the undesirability of variation in the measures about a nominal value is not symmetric. We have therefore defined appropriate robustness metrics to accommodate this property. For example, any realization of the uncertain parameters that results in a purity constraint being comfortably satisfied will not be penalized,

Table 14. Performance of the Robust Fermentation Operating Policy

Performance/Robustness Metric	Robust Model	Monte Carlo Simulation
$E_\theta\{\Phi\}$ (rmu/h)	50.1	47.3
P_{viol}	0.201	0.267

$P_{\text{viol}} \leq 0.2$.

Table 15. Computational Statistics for the Optimization Problems

Example	Problem	Iter.*	CPU**
1	Nominal	11	15
1	Case I	22	1,680
1	Case II	17	1,424
2	Nominal	8	19
2	$P_{viol} \leq 0.3$	12	362
2	$P_{viol} \leq 0.2$	9	408

*Number of optimization iterations.
**CPU time (s) on a Sun Ultra 1 workstation.

as would be the case with a variance constraint. Overall, the general deviation functions can capture widely varying robustness objectives.

For single- and multistep dynamic processes, the design problem results in a mixed-integer stochastic optimal control problem. For the examples presented here, it was possible to approximate the problem by a continuous multiple scenario optimal control problem. The solutions obtained to the examples are assessed using stochastic simulation, and the effectiveness of the robust design techniques is apparent. Although the uncertainty in the examples was only due to the model parameters, the approach may be applied to other cases (such as market uncertainty).

An issue that will require further consideration is the efficient solution of larger scale problems, arising either out of more complex processes or a more accurate representation of the joint distribution functions of the uncertain parameters.

Acknowledgment

This research was partially supported by EPSRC grant ref. GR/L63020.

Notation

C = operating cost
C_i = concentration of component $i \in \{A, B, C, D, E, F\}$
C_P = price factor for main product
$C_{P_{by}}$ = price factor for extracellular byproduct
C_S = cost of substrate
C_X = cost of inoculum
F_{in} = volumetric flowrate into the fermenter
k_i = rate constants for the reactions in the first stage $i \in \{1, 2\}$
K_I = substrate inhibition coefficient
K_S = substrate saturation constant
K_{Sm} = cell maintenance coefficient
P_{by} = extracellular product concentration
$P_{by,max}$ = extracellular product inhibition constant
P = product concentration
$\mathcal{R}$ = revenue
S = substrate concentration
S_0 = initial substrate concentration
S_{in} = inlet substrate concentration
V = broth volume
V_0 = initial broth volume
X = biomass concentration
X_0 = initial biomass concentration
X_{in} = inlet biomass concentration
$Y_{P/X}$ = product yield coefficient
$Y_{P_b/S}$ = byproduct yield coefficient
$Y_{X/S}$ = cell yield coefficient
α = growth-associated byproduct formation constant
β = nongrowth-associated byproduct formation constant
μ = specific growth rate of cells
μ_{max} = maximum specific growth rate of cells
τ_{clean} = cleaning time between successive batches

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Manuscript received Feb. 25, 1998, and revision received June 5, 1998.