Optimal Process Design with Model Parameter Uncertainty and Process Variability

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Optimal design under unknown information is a key task in process systems engineering. This study considers formulations that incorporate two types of unknown input parameters, uncertain model parameters, and variable process parameters. In the former case, a process must be designed that is feasible over the entire domain of uncertain parameters, while in the latter case, control variables can be adjusted during process operation to compensate for variable process parameters. To address this problem we extend the two-stage formulation for design under uncertainty and derive new formulations for the multiperiod and feasibility problems. Moreover, to simplify the feasibility problem in the two-stage algorithm, we also introduce a KS constraint aggregation function and derive a single, smooth nonlinear program that approximates the feasibility problem. Three case studies are presented to demonstrate the proposed approach.

Introduction

Design with unknown information remains an important problem in process systems engineering. While extensive surveys of the problem formulation and solution strategies are available (Biegler et al., 1997; Pistikopoulos, 1995, 1997), there is less discussion of different sources of unknown information and their impact on the design problem. In this study we deal with two types of unknown information encountered for this design problem. We consider unknown input parameters, θ, in some domain, Θ, for the process and we distinguish the following types of these parameters in the problem formulation:

Unknown parameters, $\theta^u \in \Theta^u$, are never known exactly. Although expected values and confidence regions may be known for these parameters, the value of these parameters is not well known for the design problem. Examples of these include model parameters determined from (off-line) experimental studies, as well as unmeasured and unobservable disturbances.

Variable parameters, $\theta^v \in \Theta^v$, are not known at the design stage, but are specified deterministically or measured accurately at some later operating stage. Examples of these include feed flow rates, process conditions and inputs, and product demands. Because these inputs can be specified or measured, we assume that control variables in the process can be adjusted to compensate for this variability.

Design with unknown input parameters has been treated in different ways. To deal with uncertain parameters, several researchers have formulated and considered back-off problems for the integration of design and control. For these cases, parameters include unmeasured disturbances, such as uncertain *process* parameters (flow rates, temperatures, and so on) and external unmeasured uncertainty (ambient conditions) (Walsh and Perkins, 1996; Raspanti et al., 2000; Bahri et al., 1996; Bandoni et al., 1994; Figueroa et al., 1996). In addition, we (Rooney and Biegler, 1999, 2001) considered and applied an approach similar to the back-off problem to deal with process design under *model* parameter uncertainty. Here an important concern is that the domain of uncertain parameters, Θ^u, which is typically treated as a hypercube, needs to be specified as a confidence region and incorporated into the analysis. Both elliptical and nonlinear confidence regions were considered in our previous studies.

Parameters that represent process variability include process quantities (feeds, temperatures, pressures, and so on) with reasonably well-known values during plant operation. While both sets of parameters may never be known exactly, treating the *variable* parameters separately has two advantages. First, variable parameters have far less error associated with them; treating them as exact at operation time is

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often reasonable. Second, we assume that all of the effects of these parameters can be compensated by control variables. Normally, the domain of these parameters, Θ^v, is described as a hypercube. Here manipulated or *control* variables (such as flow rates, heat inputs) can be adjusted to satisfy process constraints and also to improve the objective function directly or indirectly. A number of studies consider the incorporation of process variability to determine optimal designs or to evaluate the feasibility or flexibility of existing designs. These include the work of Grossmann and coworkers (Grossmann and Sargent, 1978; Halemane and Grossmann, 1983; Grossmann and Floudas, 1987; Pistikopoulos and Grossmann, 1988a) and others (Acevedo and Pistikopoulos, 1998; Bansal et al., 2000; Mohideen et al., 1996; Pistikopoulos, 1995, 1997; Ostrovsky et al., 1997).

Optimal design with unknown parameters is usually formulated by maximizing an objective function that represents the *expected value* of profit (or negative of cost) over Θ subject to feasibility of the process constraints over *all values* of $\theta \in \Theta$. This difficult problem is normally treated through a two-stage strategy that deals both with the objective function and with process feasibility (Halemane and Grossmann, 1983). The approach is illustrated in Figure 1 and the stages are given by:

Design Stage. Here the "expected value" problem is approximated through a quadrature scheme over Θ and transformed into a specialized multiperiod optimization problem (Eq. 2). Each period is defined by the problem constraints in (Eq. 1) at an *instance* of θ from the quadrature scheme. By solving the multiperiod problem we determine design and control variables to optimize an objective over a discrete set of points over the domain, Θ. In this approach the designer has full freedom to choose an appropriate quadrature, with the important trade-off of increasing the accuracy of the quadrature at the expense of adding more periods to (Eq. 2).

Feasibility Stage. For a fixed set of design variables, we assess the feasibility of the process constraints for all $\theta \in \Theta$. If the process constraints are infeasible for some values of $\theta \in \Theta$, then the maximum constraint violation is determined and the corresponding value of θ is called the *critical point*.

Once a critical value of θ is found in the second stage, a corresponding period is added in the design stage and the updated problem is solved again. The cycle repeats until no constraint violation is found in the feasibility stage, at which point the two-stage algorithm terminates. We note that similar strategies have also been used for the solution of semi-infinite optimization (SIO) problems [see Hettich and Kortanek (1993)]. The class of problems considered in this article is related to SIO problems, but with the added complication of control variables.

This study outlines a strategy that extends the two-stage algorithm to allow for different types of unknown information (such as process variability and model-parameter uncertainty); these are considered simultaneously in process design and synthesis problems. However, as developed below, both the multiperiod design problem and the feasibility problem require a number of modifications. Also, we note that in the last stage of this work, we were pleased to discover a similar approach by Ostrovsky et al. (2001). While they formulate the same two-stage problems, our solution strategy considers only (local) nonlinear programming solvers and an aggregated constraint function approach. In Ostrovsky et al. (2001), a branch-and-bound approach is described with upper bounds based on reversing the max and min operators in the feasibility problem.

In the next section, new problem formulations for the multiperiod and feasibility stages are presented. Next, an aggregation technique is outlined in the third section using the KS function that simplifies the feasibility problem. Three process systems are then considered in the fourth section to demonstrate the proposed formulations. Finally, conclusions are drawn and areas for future work are outlined in the fifth section.

Two-Stage Algorithm for Design Under Uncertainty and Variability

In previous work (Rooney and Biegler, 1999, 2001), we used a two-stage approach for solving problems under model-parameter uncertainty, leading to a multiperiod design problem followed by a feasibility test (Eq. 5). Extending this two-stage approach to include variability and uncertainty into the design process requires a new formulation for these problems.

Multiperiod design with process variability and uncertainty

In the previous section, we distinguished between process variability and model-parameter uncertainty, which gave rise to different multiperiod and feasibility problems that had traditionally been considered in the two-stage algorithm in Figure 1.

We now extend the problem formulation to include varying process parameters and uncertain model parameters. For generality, we write the problem of design optimization with unknown input parameters as:

$$\begin{aligned} \min_d \quad & E_{\theta \in \Theta}[P(d,u,x,\theta^v,\theta^u) \\ \text{s.t.} \quad & h(d,u,x,\theta^v,\theta^u)=0 \\ & g(d,u,x,\theta^v,\theta^u) \le 0 \\ & d \in D, x \in X, u \in U] \end{aligned}$$

$$\left.\begin{aligned} & h(d,u,x,\theta^v,\theta^u)=0 \\ & g(d,u,x,\theta^v,\theta^u) \le 0 \\ & d \in D, x \in X, u \in U \end{aligned}\right\} \forall \theta^v \in \Theta^v, \qquad \forall \theta^u \in \Theta^u \tag{1}$$

where we define $\Theta^v \cup \Theta^u = \Theta$. In addition, $d \in D \subseteq \Re^{n_d}$ are the design variables, $u \in U \subseteq \Re^{n_u}$ are the control variables, and $x \in X \subseteq \Re^{n_x}$ are the state variables. In this study, only steady-state processes are considered, and these are represented by the inequality and equality constraints, $g: \Re^{n_d+n_u+n_x} \to \Re^m$ and $h: \Re^{n_d+n_u+n_x} \to \Re^{n_x}$, respectively. We also assume that the state variables x can be implicitly eliminated by the equality constraints h.

From Figure 1 the first stage of the algorithm requires the solution of a multiperiod problem, which is constructed from discrete points from Θ. Here, we define an index set K for discrete values of the varying process parameters $\theta_k^v \in \Theta^v$, $k \in K$, and we define index set I for discrete values of the uncertain model parameters, $\theta_i^u \in \Theta^u$, $i \in I$. These points are chosen by a quadrature in Eq. 1 that approximates the expected values over Θ, as illustrated in Figure 2.

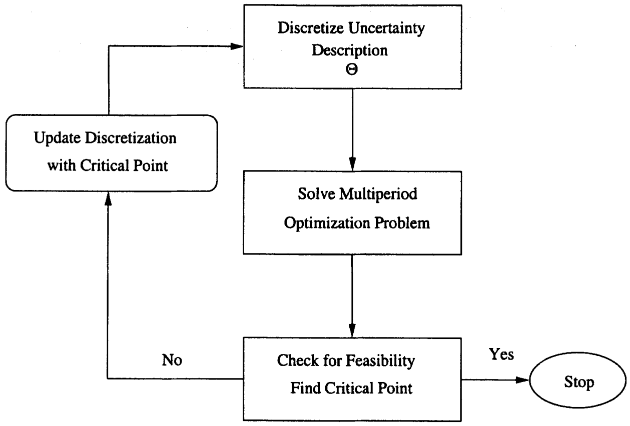

Figure 1. Two-stage algorithm for design with unknown $\boldsymbol{\theta}$.

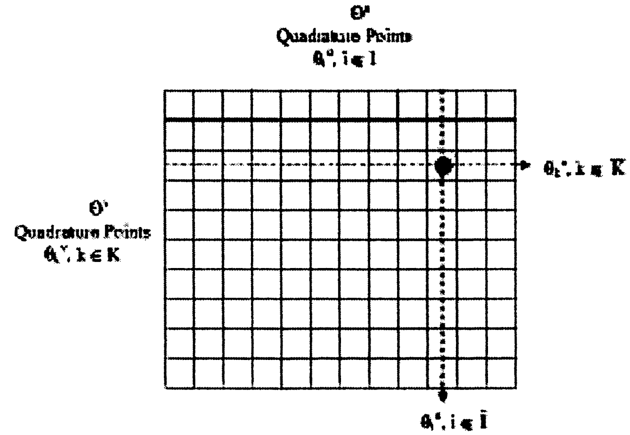

Figure 2. Grid of discretized process and model parameters.

In addition, we define additional index sets $\bar{K}$ and $\bar{I}$ that represent the critical points that are found if the constraints cannot be satisfied in the second stage (see Figure 2). If the current design from the multiperiod problem is infeasible, then the sets $\bar{K}$ and $\bar{I}$ are augmented by these critical points, corresponding periods are added in the multiperiod problem, and the problem is solved again. Note that for consistency, these critical points are *not* added to the sets K, I, that define the quadrature and the objective in Eq. 2.

We also assume that the control variable, u, can be used to compensate for the measured process variability, θ^{v}, but not the uncertainty associated with model parameters, θ^{u}. Thus, the control variables are indexed over k in the multiperiod design problem, while the state variables, x, determined by the equality constraints, are indexed over i and k. With these assumptions, the multiperiod design problem for the first stage in Figure 1 is

$$\min \quad P = f_0(d) + \sum_{k \in K} \sum_{i \in I} \omega_{ik} f_{ik}(d, u_k, x_{ik}, \theta_k^{v}, \theta_i^{u})$$

$$\text{s.t.} \quad \left.\begin{array}{l} h_{ik}(d, u_k, x_{ik}, \theta_k^{v}, \theta_i^{u}) = 0 \\ g_{ik}(d, u_k, x_{ik}, \theta_k^{v}, \theta_i^{u}) \le 0 \\ \theta_k^{v} \in \Theta^{v}; \qquad \theta_i^{u} \in \Theta^{u} \end{array}\right\} k \in K, \qquad i \in I$$

$$\left.\begin{array}{l} h_{ik}(d, u_k, x_{ik}, \theta_k^{v}, \theta_i^{u}) = 0 \\ g_{ik}(d, u_k, x_{ik}, \theta_k^{v}, \theta_i^{u}) \le 0 \\ \theta_k^{v} \in \Theta^{v}; \qquad \theta_i^{u} \in \Theta^{u} \end{array}\right\} k \in \bar{K}, \qquad i \in \bar{I} \tag{2}$$

We also note that a simpler problem results if an objective function is chosen that contains variables that are not influenced by the expected value operator (such as the objective is only a function of design variables). In this case, quadrature points are not needed and a coarser discretization is often required, only to ensure feasibility over the entire Θ domain. This problem is given by

$$\min \quad P = f_0(d)$$

$$\text{s.t.} \quad \left.\begin{array}{l} h_{ik}(d, u_k, x_{ik}, \theta_k^{v}, \theta_i^{u}) = 0 \\ g_{ik}(d, u_k, x_{ik}, \theta_k^{v}, \theta_i^{u}) \le 0 \\ \theta_k^{v} \in \Theta^{v}; \qquad \theta_i^{u} \in \Theta^{u} \end{array}\right\} k \in \bar{K}, \qquad i \in \bar{I} \tag{3}$$

Both multiperiod problems can be addressed directly as large-scale nonlinear programs. Moreover, specialized SQP-based strategies have been developed for the efficient solution of these problems (Varvarezos et al., 1994; Bhatia and Biegler, 1999). With these multiperiod formulations, we now consider the solution of the second-stage problem.

Extension of the feasibility test

Once a solution is obtained for the multiperiod problem (Eq. 2 or Eq. 3), a feasibility test is needed to ensure constraint satisfaction over values of $\theta \in \Theta$. We caution that feasibility over this entire domain may not be possible for *any* values of design and control variables. In this case there is no additional scope for optimization and the designer needs to select additional design or control variables. On the other hand, the variable and uncertain parameters considered here lead to feasibility tests with different levels of freedom in satisfying the process constraints.

Under model parameter uncertainty, the true value of θ^{u} is assumed to lie in Θ^{u}, but is never known exactly. Since we assume that no additional information will improve this estimate, we are also unable to compensate for the uncertainty with control variables. Consequently, the feasibility test can be written as (Walsh and Perkins, 1996)

$$\forall \theta^{u} \in \Theta^{u} \left(\forall j \in J \left[g_j(d, u, \theta^{u}) \le 0 \right] \right) \tag{4}$$

Equation 4 requires that for any realization of the uncertain parameters, $\theta^{u} \in \Theta^{u}$, the process constraints g_j are always satisfied for the current design and control values. (For the moment state variables and equations have been implicitly eliminated.) The equivalent optimization problem for the logical condition (Eq. 4) is

$$T(d) = \max_{\theta^u \in \Theta^u} \min_{j \in J} g_j(d,u,\theta^u) \tag{5}$$

To deal with variable parameters, θ^v, Halemane and Grossmann (1983) posed the following logical condition to determine if a given design can operate over the entire region of specified variability, Θ^v

$$\forall \theta^v \in \Theta^v \{ \exists u \in U (\forall j \in J [g_j(d,u,\theta^v) \leq 0]) \} \tag{6}$$

Equation 6 states that for any realization of the parameters, $\theta^v \in \Theta^v$, values of control variables, u, exist such that the process model equations, g_j, are always satisfied for the current design value. By using global maximum and minimum operators and inductive reasoning, Halemane and Grossmann derived an equivalent multilevel optimization problem for the logical condition (Eq. 6)

$$T(d) = \max_{\theta^v \in \Theta^v} \min_{u \in U} \max_{j \in J} g_j(d,u,\theta^v) \tag{7}$$

Equation 7 allows the control variables to be chosen to minimize the largest violation of the constraints for all the uncertain quantities in Θ. If we now separate process variability from parameter uncertainty, the control variables need to be treated differently than in Eq. 7. To accomplish this, we rewrite the feasibility problem as the following logical condition

$$\forall \theta^v \in \Theta^v [\exists u \in U \{ \forall \theta^u \in \Theta^u, \quad \forall j \in J [g_j(d,u,\theta^v,\theta^u) \leq 0] \}]. \tag{8}$$

Using the same inductive reasoning as Halemane and Grossmann (1983) and global maximum and minimum operators, Eq. 8 can be transformed into the following multilevel optimization problem

$$T(d) = \max_{\theta^v \in \Theta^v} \min_{u \in U} \max_{\theta^u \in \Theta^u} \max_{j \in J} g_j(d,u,x,\theta^v,\theta^u)$$

$$\text{s.t} \quad h(d,u,x,\theta^v,\theta^u) = 0 \tag{9}$$

Note that Eq. 9 now contains the state variables, x, and equality constraints, h. The solution to Eq. 9 determines if the current design variables can operate over $\theta^v \in \Theta^v$ and $\theta^u \in \Theta^u$. In addition, the control variables are only allowed to compensate for variability, θ^v.

Solution Strategy for Feasibility Problem

Equations 7 and 9 are difficult to solve because they are described by nested optimization problems. In Grossmann and Floudas (1987) and Pistikopoulos and Grossmann (1988a), Eq. 7 is formulated as a mixed-integer programming problem with constraints derived from the optimality conditions of the inner $\min_u$, $\max_j$ problems. Integer variables are then included to determine the active set of these constraints. However, the solution of Eq. 9 includes an additional nested optimization, which we found difficult to handle with a mixed-integer formulation. Instead, we develop a solution strategy based on nonlinear aggregation of the inequality constraints, based on the KS function. This aggregation allows us to eliminate the innermost max_j operator in Eq. 9. Our approach can be viewed as an extension of the one in Raspanti et al. (2000) that was applied to Eq. 7. The approach for Eq. 9 requires the derivation of first-order conditions for each nested problem and modification to a set of smooth equations. This then allows for the approximate formulation of Eq. 9 as a nonlinear program.

Constraint aggregation using the KS function

The innermost max_j operator in Eq. 9 introduces nondifferentiable elements into the optimization problem. To deal with this, we replace the innermost optimization problem in Eq. 9 with an approximation function that aggregates all of the inequality constraints. This is known as the KS function, and is defined by the following equivalent expressions (Kreisselmeier and Steinhauser, 1983; Raspanti et al., 2000):

$$KS(z,\rho) = \frac{1}{\rho} \ln \left\{ \sum_{j=1}^{m} \exp[\rho g_j(z)] \right\} \qquad \rho > 0 \tag{10}$$

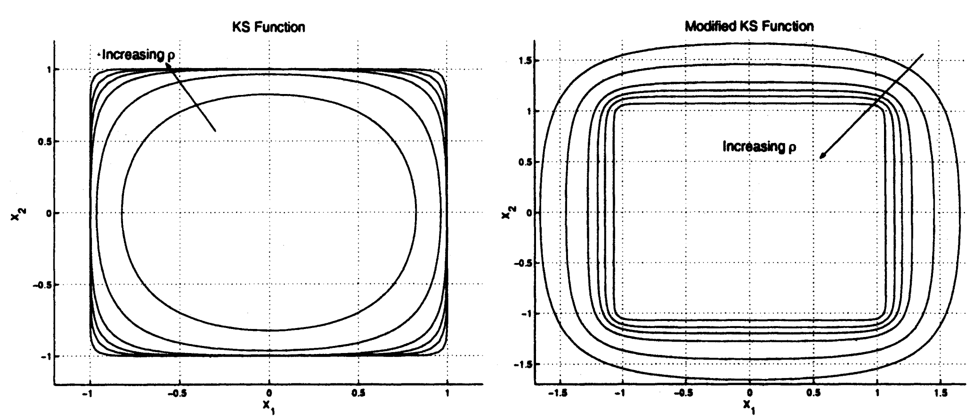

Figure 3. Relationship between $g(z)$, $KS(z)$, and $\widehat{KS}(z)$ for the feasible region $-1 \leq z \leq 1$.

or, equivalently

$$KS(z,\rho) = M + \frac{1}{\rho}\ \ln\left\{\sum_{j=1}^{m} \exp\left[\rho\left(g_j(z) - M\right)\right]\right\} \qquad \rho > 0 \tag{11}$$

where $z^T = [d^T,\ u^T,\ x^T,\ (\theta^v)^T,\ (\theta^u)^T]$, $m = |J|$ for $j \in J$ and M in Eq. 11 is defined as $M \approx \max_j g_j(z)$. Note that Eq. 11 is used for scaling purposes to minimize overflow and underflow errors in the exponential function. Some relevant properties of the KS function are (Raspanti et al., 2000):

- The KS function overapproximates the constraint values at any given point z

$$KS(z,\rho) \geq \max_j g_j(z), \qquad \rho > 0$$

Therefore, the constraint $KS(z,\rho) \leq 0$ underapproximates the feasible region $g(z) \leq 0$.

- As $\rho \to \infty$, $KS(z,\rho) \to \max_j g_j(z)$.
- If the feasible region $g(z) \leq 0$ is convex, then the constraint $KS(z,\rho) \leq 0$ also corresponds to a convex region.
- The KS function can be bounded above and below using $\max_j g_j(z)$. The largest value obtained by the summation of the exponential terms in Eq. 10 or Eq. 11 occurs when $g_j(z)$ is equal to $\max_j g_j(z)$ for all $j \in J$. This gives rise to

$$\max_j g_j(z) \leq KS(z,\rho) \leq \max_j g_j(z) + \ln(m)/\rho \tag{12}$$

As seen in Figure 3, the KS function, Eq. 10 or Eq. 11, underestimates the feasible region of the constraints $g_j(z) \leq 0$. On the other hand, an overestimate of the feasible region is obtained by subtracting the constant, $\ln(m)/\rho$, from the KS function to yield the modified KS function

$$\widehat{KS}(z,\rho) = KS(z,\rho) - \frac{\ln(m)}{\rho} = \frac{1}{\rho}\ \ln\left\{\frac{\sum_j^m \exp\left[\rho g_j(z)\right]}{m}\right\} \tag{13}$$

Bounds on $\max_j g_j(z)$ in terms of $KS(z,\rho)$ can be written by combining Eqs. 10 and 13 to yield

$$\max_j g_j(z) - \frac{\ln(m)}{\rho} \leq \widehat{KS}(z,\rho) \leq \max_j g_j(z) \leq KS(z,\rho) \tag{14}$$

Figure 3 illustrates these ideas in two dimensions for a feasible region defined by the square $-1 \leq z \leq 1$.

As a result of the properties of the KS function, we replace the innermost optimization problem in Eq. 9 to yield:

$$\begin{aligned} \max_{\theta^u} \quad & \widehat{KS}(d,u,x,\theta^v,\theta^u,\rho) \\ \text{s.t.} \quad & h(d,u,x,\theta^v,\theta^u) = 0 \\ & \phi(\theta^u) \leq 0 \end{aligned} \tag{15}$$

where the constraints $\phi(\theta^u) \leq 0$ are used to define the domain, $\theta^u \in \Theta^u$ and $\rho > 0$ is a fixed parameter. We now examine the KKT conditions of Eq. 15, which are

$$\begin{aligned} & -\nabla_{\theta^u}\widehat{KS}(d,u,x,\theta^v,\theta^u,\rho) + \nabla_{\theta^u}\phi(\theta^u)\lambda + \nabla_{\theta^u}h(d,u,x,\theta^v,\theta^u)\nu = 0 \\ & -\nabla_x\widehat{KS}(d,u,x,\theta^v,\theta^u,\rho) + \nabla_x h(d,u,x,\theta^v,\theta^u,\rho)\nu = 0 \\ & h(d,u,x,\theta^v,\theta^u) = 0 \\ & \phi(\theta^u) + s = 0 \\ & \lambda^T s = 0 \\ & \lambda \geq 0 \qquad s \geq 0 \end{aligned} \tag{16}$$

The equations in Eq. 16 define $x^* = x(d,u,\theta^v)$ and $\theta^{u*} = \theta^u(d,u,\theta^v)$ implicitly. However, the complementarity conditions involving the slack variables s are degenerate; hence, we replace them by a smoothing approximation, where ϵ is a small, positive number (Balakrishna and Biegler, 1996; Chen and Mangasarian, 1996)

$$\begin{aligned} & 0 = \lambda^T s,\ \lambda \geq 0,\ s \geq 0 \\ & \Updownarrow \\ & 0 = \lambda_j - \max\left(0, \lambda_j - s_j\right) \\ & \approx \frac{\lambda_j + s_j}{2} - \frac{1}{2}\sqrt{\left(\lambda_j - s_j\right)^2 + \epsilon^2} \end{aligned} \tag{17}$$

We denote the modified first-order KKT conditions of Eq. 15 as $h_1(d,\ u,\ x^*,\ \theta^v,\ \theta^{u*},\ s^*,\ \lambda^*,\ \nu^*) = 0$:

$$h_1 = \begin{cases} -\nabla_{\theta^u}\widehat{KS}(d,u,x,\theta^v,\theta^u,\rho) + \nabla_{\theta^u}\phi(\theta^u)\lambda + \\ \nabla_{\theta^u}h(d,u,x,\theta^v,\theta^u)\nu \\ -\nabla_x\widehat{KS}(d,u,x,\theta^v,\theta^u,\rho) + \nabla_x h(d,u,x,\theta^v,\theta^u,\rho)\nu \\ h(d,u,x,\theta^v,\theta^u) \\ \phi(\theta^u) + s \\ \dfrac{\lambda_j + s_j}{2} - \dfrac{1}{2}\sqrt{\left(\lambda_j - s_j\right)^2 + \epsilon^2}\, s \end{cases} \tag{18}$$

Equations 18 are used as constraints in the next optimization problem in Eq. 9

$$
\begin{aligned}
\min_{u} \quad & \widehat{KS}(d,u,x^*,\theta^v,\theta^{u*},\rho) \\
\text{s.t.} \quad & h_1(d,u,x^*,\theta^v,\theta^{u*},s^*,\lambda^*,\nu^*)=0 \\
& \phi_U(u)+s_u=0
\end{aligned} \tag{19}
$$

where the domain $u \in U$ is defined by $\phi_U(u) \le 0$. Writing the first-order KKT conditions for Eq. 19 leads to the following constraints

$$
\begin{aligned}
&\nabla_u \widehat{KS}(d,u,x^*,\theta^v,\theta^{u*},\rho)+\nabla_u h_1(d,u,x^*,\theta^v,\theta^{u*},s^*,\lambda^*,\nu^*)\sigma + \nabla_u \phi_U \gamma = 0 \\
&\nabla_{x^*} \widehat{KS}(d,u,x^*,\theta^v,\theta^{u*},\rho)+\nabla_{x^*} h_1(d,u,x^*,\theta^v,\theta^{u*},s^*,\lambda^*,\nu^*)\sigma = 0 \\
&\nabla_{\theta^{p*}} \widehat{KS}(d,u,x^*,\theta^v,\theta^{u*},\rho)+\nabla_{\theta^{p*}} h_1(d,u,x^*,\theta^v,\theta^{u*},s^*,\lambda^*,\nu^*)\sigma = 0 \\
&\nabla_s h_1(d,u,x^*,\theta^v,\theta^{u*},s^*,\lambda^*,\nu^*)\sigma = 0 \\
&\nabla_{\nu^*} h_1(d,u,x^*,\theta^v,\theta^{u*},s^*,\lambda^*,\nu^*)\sigma = 0 \\
&\nabla_{\lambda^*} h_1(d,u,x^*,\theta^v,\theta^{u*},s^*,\lambda^*,\nu^*)\sigma = 0 \\
&h_1(d,u,x^*,\theta^v,\theta^{u*},s^*,\lambda^*,\nu^*) = 0 \\
&\phi_U(u)+s_u=0 \\
&\gamma^T s_u = 0 \\
&\gamma \ge 0 \\
&s_u \ge 0
\end{aligned} \tag{20}
$$

Smoothing approximations are again used to replace the dependent complementarity conditions that involve slack variables s_u for the control variable bounds. We denote this set of KKT conditions as $h_2(d,\ u^*,\ x^*,\ \theta^v,\ \theta^{u*},\ s^*,\ \lambda^*,\ \nu^*,\ s_u^*)=0$

$$
h_2 = \begin{cases}
\nabla_u \widehat{KS}(d,u,x^*,\theta^v,\theta^{u*},\rho) + \\
\nabla_u h_1(d,u,x^*,\theta^v,\theta^{u*},s^*,\lambda^*,\nu^*)\sigma + \nabla_u \phi_U \gamma \\
\nabla_{x^*} \widehat{KS}(d,u,x^*,\theta^v,\theta^{u*},\rho) + \\
\nabla_{x^*} h_1(d,u,x^*,\theta^v,\theta^{u*},s^*,\lambda^*,\nu^*)\sigma \\
\nabla_\theta^{u*} \widehat{KS}(d,u,x^*,\theta^v,\theta^{u*},\rho) + \\
\nabla_\theta^{u*} h_1(d,u,x^*,\theta^v,\theta^{u*},s^*,\lambda^*,\nu^*)\sigma \\
\nabla_s h_1(d,u,x^*,\theta^v,\theta^{u*},s^*,\lambda^*,\nu^*)\sigma \\
\nabla_{\nu^*} h_1(d,u,x^*,\theta^v,\theta^{u*},s^*,\lambda^*,\nu^*)\sigma \\
\nabla_{\lambda^*} h_1(d,u,x^*,\theta^v,\theta^{u*},s^*,\lambda^*,\nu^*)\sigma \\
h_1(d,u,x^*,\theta^v,\theta^{u*},s^*,\lambda^*,\nu^*) \\
\dfrac{\gamma_j + s_{u_j}}{2} - \dfrac{1}{2}\sqrt{(\gamma_j - s_{u_j})^2 + \epsilon^2}
\end{cases} \tag{21}
$$

The KKT conditions for the first two problems in Eqs. 9, 18, and 21 are inserted into the remaining optimization problem in Eq. 9 to obtain

$$
\begin{aligned}
\max_{\theta^v} \quad & \widehat{KS}(d,u^*,x^*,\theta^v,\theta^{u*},\rho) \\
\text{s.t.} \quad & h_2(d,u^*,x^*,\theta^v,\theta^{u*},s^*,\lambda^*,\nu^*,s_u^*)=0 \\
& \theta^v \in \Theta^v
\end{aligned} \tag{22}
$$

Several points are worth noting. First, the constraints h_1 and h_2 represent first-order KKT conditions of the two innermost problems in Eq. 9. Since global operators were assumed in Eq. 9, the constraints in Eq. 22 represent only the necessary optimality conditions of these operators. We, therefore, admit there may be local solutions to Eq. 22 and, compared to global (Ostrovsky et al., 2001; Floudas et al., 2001) and mixed-integer approaches (Grossmann and Floudas, 1987; Floudas et al., 2001), this is a limitation of the current approach. Nevertheless, Raspanti et al. (2000) showed that quite good solutions of Eq. 7 could be obtained, especially if the variables are initialized carefully. This can be done by first solving these problems with a small value of ρ and then using their solutions to resolve these problems with increasingly larger values of ρ. A suitably large value of ρ (as well as a suitably accurate solution to Eq. 9) can be validated from the bounds of Eq. 14.

Moreover, the KS function eliminates problems with nondifferentiability from Eq. 9 and solutions are obtained quickly, as only a single, smooth NLP problem needs to be solved. Finally, to improve the likelihood of obtaining a global solution, we add a "safeguard" constraint to Eq. 22; this helps to avoid undesirable local solutions. From the solution of a multiperiod design problem (Eq. 2 or Eq. 3), we find the maximum inequality constraint, g_{max}, and use this to form a lower bound, $\widehat{KS}_0(\rho)$, given by

$$
\widehat{KS}_0(\rho) = \max_{i,k} \widehat{KS}(d,u_k,x_{ik},\theta_k^v,\theta_i^u) \tag{23}
$$

where $\widehat{KS}_0(\rho)$ is a valid lower bound to Eq. 22, since we know $g(d,u_k,x_{ik},\theta_k^v,\theta_i^u) \le 0$ are satisfied by the solution of the multiperiod problem (Eq. 2 or Eq. 3), and that any violation in the feasibility problem must be greater than any inequality constraint in the multiperiod problem. Adding this lower bound to Eq. 22 leads to an approximate single-level optimization problem for the feasibility problem (Eq. 9)

$$
\begin{aligned}
\max_{\theta^v} \quad & \widehat{KS}(d,u^*,x^*,\theta^v,\theta^{u*},\rho) \\
\text{s.t.} \quad & h_2(d,u^*,x^*,\theta^v,\theta^{u*},s^*,\lambda^*,\nu^*,s_u^*)=0 \\
& \widehat{KS}(d,u^*,x^*,\theta^v,\theta^{u*},\rho) \ge \widehat{KS}_0(\rho) \\
& \theta^v \in \Theta^v
\end{aligned} \tag{24}
$$

The properties of the *KS* function can also be used to enclose a solution to Eq. 9. If we obtain a solution to Eq. 24, then for $z^T=[d^T,\ u^T,\ x^T,\ (\theta^v)^T,\ (\theta^u)^T]$, we know that

$$
\widehat{KS}(z^*,\rho) \le \max_{j \in J} g(z^*) \le KS(z^*,\rho) \tag{25}
$$

and these bounds can be made tight by increasing ρ. Also, it is interesting to note that both KS and $\widehat{KS}$ share the *same* extreme points, z^*, for Eq. 24. Therefore, by using either of these aggregating functions, we can obtain an arbitrarily close solution to Eq. 9 from $\widehat{KS}$ and KS. In practice, a tolerance, $\bar{\epsilon}$, is specified so the difference between $\widehat{KS}$ and $\max_j g_j(d,u,\theta^v,\theta^u)$ is reduced to desired levels by increasing ρ to satisfy

$$\frac{\ln(m)}{\rho} \le \bar{\epsilon} \tag{26}$$

Thus, we now use the multiperiod problem (Eq. 2 or Eq. 3) and the feasibility problem (Eq. 24) in the two-stage algorithm in Figure 1 to solve design problems that include both process variability and model-parameter uncertainty, and control variables compensate only for process variability. The next section demonstrates this approach with a number of examples.

Case Studies

We consider three process examples containing model-parameter uncertainty and process variability.

Linear retrofit problem

We first consider the following linear program adapted from Pistikopoulos and Ierapetritou (1995)

$$\begin{aligned}
\min \quad & 10(d_1+d_2)+u_{\max} \\
\text{s.t.} \quad & u+d_1-3d_2 \le \theta_1-0.5\theta_2-2\theta_3+8 && \text{(a)} \\
& -u+d_2 \le \frac{\theta_1}{3}+\theta_2+\frac{\theta_3}{3}+\frac{8}{3} && \text{(b)} \\
& u-d_1 \le \theta_2-\theta_1-\theta_3+4 && \text{(c)} \\
& u_{\max} \ge u \\
& d_1,d_2,u \ge 0 \\
& \theta_1,\theta_2 \in \Theta^u, \quad \theta_3 \in \Theta^v.
\end{aligned} \tag{27}$$

The goal is to minimize the cost as a function of two design variables d_1 and d_2, and the largest control variable, $u_{\max}$, such that the inequalities are always satisfied over Θ^v and Θ^u. Because the variables in the objective are not affected by θ, a quadrature approximation of Eq. 1 is not necessary and the resulting multiperiod problem takes the form of Eq. 3

$$\begin{aligned}
\min \quad & 10(d_1+d_2)+u_{\max} \\
\text{s.t.} \quad & u_k+d_1-3d_2 \le \theta_{1,i}-0.5\theta_{2,i}-2\theta_{3,k}+8 \\
& -u_k+d_2 \le \frac{\theta_{1,i}}{3}+\theta_{2,i}+\frac{\theta_{3,k}}{3}+\frac{8}{3} \\
& u_k-d_1 \le \theta_{2,i}-\theta_{1,i}-\theta_{3,k}+4 \\
& u_{\max} \ge u_k \\
& d_1,d_2,u_k \ge 0 \\
& \theta_{1,i},\theta_{2,i} \in \Theta^u, \\
& \theta_{3,k} \in \Theta^v, \qquad i \in \bar{I},\ k \in \bar{K}
\end{aligned} \tag{28}$$

Moreover, we consider two ways to describe the domain of uncertain parameters, θ_1, $\theta_2 \in \Theta^u$. First, an elliptical domain is given by the following confidence region

$$\begin{bmatrix} \theta_1-15 \\ \theta_2-10 \end{bmatrix}^T \begin{bmatrix} 0.4004 & 0.5105 \\ 0.5105 & 0.9009 \end{bmatrix} \begin{bmatrix} \theta_1-15 \\ \theta_2-10 \end{bmatrix} \le 2.4078 \tag{29}$$

Second, we consider a hypercube domain with confidence intervals for θ_1 and θ_2 given by

$$\begin{aligned} 11.8907 \le \theta_1 \le 18.1093 \\ 7.92714 \le \theta_2 \le 12.0729 \end{aligned} \tag{30}$$

Moreover, we assume θ_3 varies uniformly between lower and upper bounds

$$\Theta^v(\theta_3) = 10 \le \theta_3 \le 20 \tag{31}$$

The control variable, u, is used to compensate only for the variability in θ_3.

Using the elliptical domain for Θ^u, initial points for the set $\bar{I}$ are the extreme points for θ_1 and θ_2 of the longest axis of the ellipse in Eq. 29. Two initial points were used for the set $\bar{K}$, corresponding to its lower and upper bounds of θ_3. Following the algorithm in Figure 1, Eq. 28 is solved for these initial periods and leads to the following variable values: $d_1 = 31.9498$, $d_2 = 21.1557$, and $u_{\max} = 6.8224$.

We then solve Eq. 24 to test the feasibility of the preceding design and control variables with ρ for the KS functions initialized to 0.10. Equation 24 is then solved repeatedly with increasingly doubled values of ρ. The solution to Eq. 24 with $\rho = 48$ finds the following critical points: $\theta_1 = 17.5762$, $\theta_2 = 7.1784$, $\theta_3 = 10.00$, with $\widehat{KS} = 0.606524$ and $KS = 0.629423$.

The values of the three inequality constraints in Eq. 27 at this critical point are

$$\begin{bmatrix} \text{Ineq. (a)} \\ \text{Ineq. (b)} \\ \text{Ineq. (c)} \end{bmatrix} = \begin{bmatrix} -26.68176 \\ 0.629423 \\ -8.72962 \end{bmatrix} \tag{32}$$

Equation 32 shows that inequality (b) in Eq. 27 is violated by the amount bounded by $\widehat{KS}$ and KS, with θ_3 at its lower bound. The solution to Eq. 24 sets the control variable u to its upper bound, as this setting minimizes the violation in the second inequality constraint. Finally, the values for θ_1 and θ_2 correspond to the smallest that $(\theta_1/3 - \theta_2)$ (in constraint (b)) can achieve in the joint confidence region (Eq. 29). Two more iterations through the algorithm in Figure 1 are required to find the optimal design in Table 1.

Using the two-stage algorithm, we also solved Eq. 27 with $\Theta = \Theta^v$ and the control variable u_{ik} indexed for all periods in the problem. In this formulation θ_1 and θ_2 are now treated as variable parameters and u is now used to compensate for all three unknown parameters. Finally, we solved Eq. 27 using a conservative approach where $\Theta = \Theta^u$ and the control variable is the same for all periods in Eq. 27. In this case, the control variable, u, acts as a design variable. Table 1 shows the optimal designs using the elliptical and hypercube descriptions for Θ^u and for the different control-variable formulations.

As expected, the formulation where the control variable is the same in all periods leads to the most expensive design. Allowing control variables to compensate for the variability in θ_3 leads to smaller design variables and a lower cost. Finally, the formulation with the control variable indexed over all periods leads to the cheapest design. Moreover, the difference between using u_k and $u_{i,k}$ can be used to estimate the expected value of perfect information for θ_1 and θ_2 (such as knowing θ_1 and θ_2 exactly at run time) (Infanger, 1994). This cost difference could motivate process improvements to obtain better values for unmeasured disturbances, or additional experimental studies to obtain more accurate model parameters. Finally, we see in this example that the designs based on the hypercube confidence intervals (Eq. 30) are more expensive than the ones based on the elliptical confidence region, (Eq. 29).

Design of a reactor-cooler system

We consider the following reactor-cooler model in Figure 4 consisting of a CSTR connected to a heat exchanger, as considered in Halemane and Grossmann (1983), Pistikopoulos and Grossmann (1988b), Varvarezos et al. (1994), and Georgiadis and Pistikopoulos (1999). The nominal design problem is given by

$$
\begin{aligned}
\min\ P = \quad & 0.3(2304V^{0.7}+2912A^{0.6})+2.2\times10^{-4}W_{\max} \\
& +8.82\times10^{-4}F_{1,\max} \\
\text{s.t.} \quad & F_0\frac{c_{A0}-c_A}{c_{A0}} = Vk_0e^{-E/RT_1}c_A \\
& (-\Delta H)_{rxn}F_0\frac{c_{A0}-c_A}{c_{A0}} = F_0c_p(T_1-T_0)+Q \\
& Q = F_1c_p(T_1-T_2) \\
& Q = Wc_w(T_{w2}-T_{w1}) \\
& Q = UA\left(\frac{T_1-T_{w2}-T_2+T_{w1}}{\ln\left(\dfrac{T_1-T_{w2}}{T_2-T_{w1}}\right)}\right) \\
& 0.9-\frac{c_{A0}-c_A}{c_{A0}} \le 0 \\
& \frac{c_{A0}-c_A}{c_{A0}}-1 \le 0 \\
& \Delta T_{\min}-T_1+T_{w2} \le 0 \\
& \Delta T_{\min}-T_2+T_{w1} \le 0 \\
& T_1-T_{1\max} \le 0 \\
& T_{w1}-T_{w2} \le 0 \\
& T_{w2}-356 \le 0 \\
& T_2-T_1 \le 0 \qquad (33)
\end{aligned}
$$

with constants given in Table 2. The goal is to minimize equipment and utility costs such that the process always operates within specifications over the region of variability and model-parameter uncertainty. The design variables, d, are the CSTR volume V (m^3) and the area A (m^2) of the heat exchanger. The state variables x are T_1, T_2, T_{w2} (all in K), c_A (kmol/m^3), and Q (kJ), which are calculated from the five equality constraints. The two control variables u are F_1 (kmol/h) and W (kmol/h). To estimate costs in the multiperiod version of Eq. 33, the largest values of W and F_1, $W_{\max}$ and $F_{1,\max}$, are used in the objective function. Two variable disturbances, θ^v, inlet temperature ($T_0 \in [328, 338\ \text{K}]$) and inlet flow rate ($F_0 \in [40, 50\ \text{kmol/h}]$), are considered. The uncertain model parameters, k_0 and $-E_i/R$ lie in the domain ($\theta^u \in \Theta^u$)

$$
\begin{bmatrix} k_0-1.25 \\ \dfrac{-E}{R}-15.56 \end{bmatrix}^T
\begin{bmatrix} 79.0123 & -7.61687 \\ -7.61687 & 1.1473 \end{bmatrix}
\begin{bmatrix} k_0-1.25 \\ \dfrac{-E}{R}-15.56 \end{bmatrix}
\le 4.83324 \qquad (34)
$$

These model parameters were initially discretized into eight periods, corresponding to the four points on the principal axes of the joint elliptical confidence region. The same values are used for T_0 and F_0. Thus, Eq. 33 is now solved with 240 periods and its solution yielded the following results: $V = 16.638$ m^3, $A = 4.402$ m^2, $W_{\max} = 70{,}846$ kmol/h, and $F_{1,\max} = 5561.11$ kmol/h.

Iteration 1. Solving the feasibility problem (Eq. 24) for these parameters shows that T_1 violates its upper bound by 2.10012 K. The control variables are both at their upper bounds, as this provides maximum cooling for the reactor. The critical values of the parameters are $\theta_1 = 1.6621$, $\theta_2 = 18.25141$, $F_0 = 50.00$, and $T_0 = 338$. The objective function, $\widehat{KS}$, in Eq. 24, is 1.95522 and $KS = 2.10012$. The feasibility problem (Eq. 24) was initialized with $\rho = 0.1$. A final value of $\rho = 14.5$ is sufficient for bounding the infeasibilities.

Iteration 2. The periods in Eq. 33 are updated with these critical parameters and its solution results in new design and

Table 1. Optimal Designs for Example

Uncertainty Description Θ^u	Control Variable Formulation	d_1	d_2	$u_{\max}$	Cost
Elliptical Θ^u	u	40.837	27.213	14.655	695.166
	u_k	30.837	20.546	7.989	521.833
	$u_{i,k}$	24.619	16.400	4.885	414.044
Hypercube Θ^u	u	51.169	33.964	22.695	874.041
	u_k	33.866	22.429	8.725	571.693
	$u_{i,k}$	32.343	21.451	10.182	548.134

Table 2. Constants Used in Equation 33

Parameter in Eq. 33	Value	Units
$(-\Delta H_{rxn})$	23,260	kJ/mol
c_{a0}	32.04	kmol/m^3
c_p	167.4	kJ/(kmol·K)
c_w	4.18	kJ/(kmol·K)
$T_{1\max}$	389.00	K
u	1,635.34	kJ/(m^2·h·K)
$\Delta T_{\min}$	11.1	K
T_{w1}	300.00	K

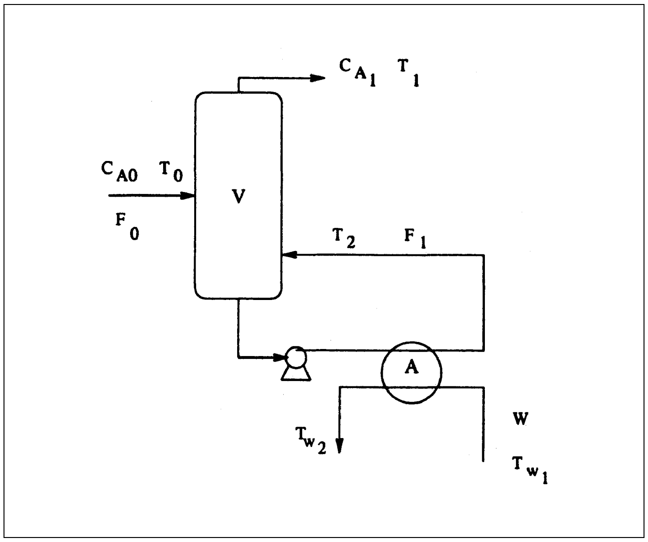

Figure 4. Reactor-cooler flow sheet.

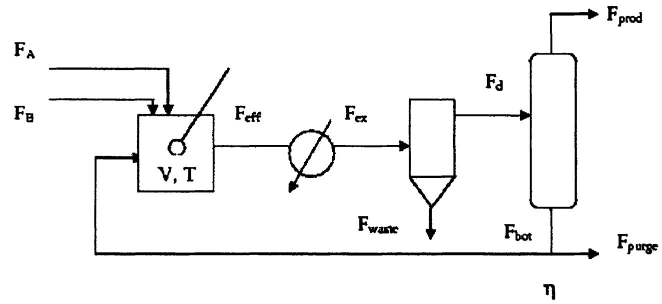

Figure 5. Williams–Otto flow sheet.

Table 3. Optimal Design Values for Example 2

Θ^u	Control Index	V m^3	A m^2	W_{max} kmol/h	$F_{1,max}$ kmol/h	Cost M$
Hypercube	u	15.746	4.641	73,911	5,800.435	6.975
	u_k	15.736	4.640	73,905	5,800.130	6.974
	$u_{k,i}$	15.730	4.639	73,905	5,799.509	6.972
Ellipse	u	17.339	4.705	74,716	5,863.811	7.326
	u_k	17.332	4.704	74,712	5,863.468	7.324
	$u_{k,i}$	17.331	4.703	74,702	5,863.468	7.323

control variables: $V = 17.331$ m^3, $A = 4.703$ m^2, $W_{max} =$ 74,712, and $F_{1,max} = 5863.405$. The next critical point is found by solving Eq. 24 for these parameters. The feasibility problem finds that the minimum conversion inequality constraint is violated by 0.000019. The values of the uncertain parameters are $\theta_1 = 0.837808$, $\theta_2 = 12.846138$, $T_0 = 328$, and $F_0 =$ 50.00. The feasibility problem (Eq. 24) was initialized with $\rho = 0.10$ and was solved repeatedly with increasing values of ρ. For $\rho = 1{,}900$, $\widehat{KS} = -0.001075$, and $KS = 0.000019$. This infeasibility is small, but evaluation of the model constraints at the critical point confirms that the minimum conversion constraint is slightly violated.

Iteration 3. Another multiperiod problem (Eq. 3) is solved with these updated critical parameters. The feasibility of the design variables is then tested by solving Eq. 24. No further critical points were found from repeated solutions of the feasibility problem.

Table 3 shows the optimal designs for this problem using the elliptical domain for Θ^u. In addition, we solved this problem using confidence intervals for Θ^u that ignore interactions between k_0 and E/R. The hypercube description of these confidence intervals is $k_0 \in [0.9355,\ 1.5645\}$ and $E/R \in$ [12.9502, 18.1698], and the corresponding optimal design is presented in Table 3. Also shown in this table are the solutions when the control variables are indexed across all periods (u_{ik}) and when they are treated as additional design variables (u). The cost difference between using hypercube confidence intervals and the elliptical confidence region (Eq. 34) for Θ^u in this problem is only 5.04%. While the cost difference is not very large, the elliptical region is needed to treat model parameters that are correlated. Also, there is little difference between the three formulations used for the control variables in this problem.

Design of Williams–Otto process

As the third case study we consider design under uncertainty for the Williams–Otto flow sheet (Williams and Otto, 1960), shown in Figure 5. Two feed streams containing pure components A and B are fed to a CSTR with the three reactions

$$\begin{aligned} A + B &\overset{k_1}{\rightarrow} C \\ C + B &\overset{k_2}{\rightarrow} P + E \\ P + C &\overset{k_3}{\rightarrow} G \end{aligned} \tag{35}$$

where C is an intermediate component, P is the main product, E is a byproduct, and G is a waste product. The effluent is cooled in a heat exchanger and is sent to a centrifuge to separate G from the process. The remaining components are then separated to remove product P overhead. Due to the presence of an azeotrope, some of the product (equal to 10 wt. % of component E) is retained in the bottoms. The bottoms is then split into a purge and recycle stream, which is mixed with the feed and sent back to the reactor. More details of this well-known process optimization example can be found in Ray and Szekely (1973) and Biegler et al. (1997). The objective of the optimization problem is to maximize the return on investment (ROI), and the nominal design problem is given by:

$$\max \text{ROI} = -\Big(2{,}207F^P_{\text{prod}} + 50\Sigma_j F^j_{\text{purge}} - 168F_A - 252F_B - 2.22\Sigma_j F^j_R - 84\Sigma_j F^j_{\text{waste}} - 60V\rho\Big)/(600V\rho)$$

$$
\begin{aligned}
\text{s.t.}\quad & \log(k_1) - \log(a_1) + 12{,}000/T = 0 \\
& \log(k_2) - \log(a_2) + 15{,}000/T = 0 \\
& \log(k_3) - \log(a_3) + 20{,}000/T = 0 \\
& F_{\text{eff}}^{A} - \left(F_A + F_R^A - k_1 x_r^A x_r^B V\rho\right) = 0 \\
& F_{\text{eff}}^{B} - \left(F_B + F_R^B - \left(k_1 x_r^A + k_2 x_r^C\right) x_r^B V\rho\right) = 0 \\
& F_{\text{eff}}^{C} - \left(F_R^C + \left(2k_1 x_r^A x_r^B - 2k_2 x_r^B x_r^C - k_3 x_r^P x_r^C\right) V\rho\right) = 0 \\
& F_{\text{eff}}^{E} - \left(F_R^E + \left(2k_2 x_r^C x_r^B\right) V\rho\right) = 0 \\
& F_{\text{eff}}^{P} - \left(F_R^P + \left(k_2 x_r^C x_r^B - 0.5 k_3 x_r^P x_r^C\right) V\rho\right) = 0 \\
& F_{\text{eff}}^{G} - \left(F_R^G + \left(1.5 k_3 x_r^C x_r^P\right) V\rho\right) = 0 \\
& F_{\text{eff}}^{j} - \left(\textstyle\sum_j F_{\text{eff}}^{j}\right) x^j = 0 \quad j = A,B,C,E,P,G \\
& F_{\text{ex}}^{j} - F_{\text{eff}}^{j} = 0 \quad j = A,B,C,E,P,G \\
& F_d^{j} - F_{\text{ex}}^{j} = 0 \quad j = A,B,C,E,P \\
& F_d^{G} = 0 \\
& F_{\text{waste}}^{j} = 0 \quad j = A,B,C,E,P \\
& F_{\text{waste}}^{G} - F_{\text{ex}}^{G} = 0 \\
& F_{\text{prod}}^{j} = 0 \quad j = A,B,C,E,G \\
& F_{\text{prod}}^{P} - F_d^{P} - 0.1 F_d^{E} = 0 \\
& F_d^{A} - F_{\text{bot}}^{A} = 0 \quad j = A,B,C,E,G \\
& F_{\text{bot}}^{P} - 0.1 F_d^{E} = 0 \\
& F_{\text{purge}}^{j} - \eta F_{\text{bot}}^{j} = 0 \quad j = A,B,C,E,P,G \\
& F_R^{j} - (1-\eta) F_{\text{bot}}^{j} = 0 \quad j = A,B,C,E,P,G \\
& F_{\text{prod}}^{P} \geq 4763.0
\end{aligned}
\qquad (36)
$$

Here the design variable, d, is the CSTR volume, V, and the density is fixed at $\rho = 50$. The two control variables are purge fraction $\eta \in (0,1]$ and reactor temperature $T \in [580, 680]$. The two variable parameters θ^{v}, F_A and F_B, are assumed to vary uniformly within a fraction, δ, of their normal values, so that the region Θ^{v} is defined by: $F_A = 10{,}000(1 \pm \delta)$ and $F_B = 40{,}000(1 \pm \delta)$. The uncertain model parameters θ^{u} for this problem are the three preexponential factors for the rate constants. Here we consider two cases with either a hypercube and an ellipse for the region Θ^{u}. The hypercube for Θ^{u} is defined by

$$a_1 = 5.9755 \times 10^9 (1 \pm \delta)$$

$$a_2 = 2.5962 \times 10^{12} (1 \pm \delta)$$

$$a_3 = 9.6283 \times 10^{15} (1 \pm \delta)$$

while the elliptical region Θ^{u} is given by

$$\left(\frac{a_1 - 5.9755 \times 10^9}{5.9755 \times 10^9}\right)^2 + \left(\frac{a_2 - 2.5962 \times 10^{12}}{2.5962 \times 10^{12}}\right)^2 + \left(\frac{a_3 - 9.6283 \times 10^{15}}{9.6283 \times 10^{15}}\right)^2 \leq \delta^2 \quad (37)$$

The remaining state variables are all nonnegative and represent the flows, rate constants k_1, k_2, k_3, and weight fractions $x_r \in [0, 1]$. Otherwise, the only inequality constraint is a lower limit on the product flow rate ($F_{\text{prod}}^{P} \geq 4{,}763.0$), as dictated by customer demand. The goal of this case study is to maximize an expected ROI so that the flow sheet always operates within specifications over the region of variability and model parameter uncertainty, $\Theta^{v} \cup \Theta^{u}$.

For this problem, we apply a coarse quadrature and construct the initial multiperiod design problem (Eq. 2). Referring to Eq. 2, we define the index set, K, by choosing the four extreme points for F_A and F_B as θ_k^{v}, $k \in K$. For the hypercube description of Θ^{u} we define the index set I through the eight extreme points for a_1, a_2, and a_3 as θ_i^{u}, $i \in I$. Otherwise, for the elliptical description (Eq. 37), we define the index set I and θ_i^{u}, $i \in I$ by the six points of a_1, a_2, and a_3 on the principal axes of this ellipse. Also note that the sizes of both Θ^{u} and Θ^{v} are controlled by the factor δ.

In the solution of the feasibility problems for the two-stage algorithm, a number of simplifications can be made based on the structure of the Williams–Otto model.

- Because the bounds for the state variables are generally inactive, the KS function for the feasibility problem becomes ($4{,}763.0 - F_{\text{prod}}^{P}$), and the maximization over $j \in J$ in Eqs. 5, 6, and 9 disappears.
- From this lower-bound constraint for F_{prod}^{P} one would expect that critical values of θ_v would be the lower bounds on F_A and F_B. This follows if all of the decision variables (u

Table 4. Summary of Example 3, Williams–Otto Results Using I, $\bar{I}$ (Eq. 5), K, $\bar{K}$ (Eq. 7), and I, $\bar{I}$ and K, $\bar{K}$ (Eq. 9)

Θ^{u}	δ Nominal (0)	$V(I)$ 70	ROI(I), % 41.154	$V(K)$ 70	ROI(K), % 41.154	$V(I,K)$ 70	ROI(I,K), % 41.154
Hypercube	0.01	70	41.084	70	41.154	70	41.092
	0.05	71	39.424	73	39.873	72	39.778
	0.07	73	37.802	75	39.727	74	38.553
	0.10	108	31.925	83	35.961	94	34.346
Ellipse	0.01	70	41.092	70	41.101	70	41.100
	0.05	71	39.621	72	40.003	72	39.972
	0.07	73	38.176	74	38.967	74	38.904
	0.10	84/90	34.983/34.481	78	36.843	80	36.627

and d) are *intensive*, as production rate would be a linear scaling of the feed flows. Although in this case $d = V$ is an extensive variable, we still observe that the lowest value of F^P_{prod} occurs when F_A and F_B are at their lower bounds in all of our calculations. This fact can be used to simplify the solutions of Eqs. 5, 7 and 9.

For this case study we again consider three approaches to dealing with design under uncertainty: one where all unknown parameters are treated as θ^u, another where all unknown parameters are treated as θ^v, and the third were uncertain and variable parameters are partitioned as θ^u and θ^v.

For the first approach we define $\theta^u = [F_A, F_B, a_1, a_2, a_3]^T$, and we solve Eq. 2 with sets K and $\bar{K}$ empty. Initially, Eq. 2 contains 32 periods when a hypercube description is used. Otherwise, it contains 24 periods when using Eq. 37. Also, as the control variables η and T are fixed for all periods, this approach leads to the most conservative design. The two-stage algorithm is executed for increasing values of δ from 1% to 10% of the parameter values. The optimal ROIs for this approach are given in Table 4 along with corresponding reactor volumes. As expected, the ROIs decrease and reactor volumes increase with increases in δ. Also, since the elliptical description contains a smaller region for unknown parameters, the corresponding values of ROI are better than for the hypercube. The feasibility test (Eq. 5) requires only a single maximization and was executed as part of the two-stage algorithm. This test was satisfied by the solution of the initial multiperiod problem (Eq. 2), with $\bar{I}$ empty, in all but one case. The only case that required an additional iteration of the two-stage algorithm was for an elliptical Θ^u and $\delta = 0.1$. As seen in Table 4, adding an additional period to Eq. 2 decreases the ROI from 34.983% to 34.481%.

For the second approach we define $\theta^v = [F_A, F_B, a_1, a_2, a_3]^T$ and we solve Eq. 2 with sets I and $\bar{I}$ empty. Initially Eq. 2 contains 32 periods when a hypercube description is used. Otherwise, it contains 24 periods when using Eq. 37. Also, as the control variables η and T are now independent in all periods, this approach leads to the most optimistic design. Again, the two-stage algorithm is executed for increasing values of δ from 1% to 10% of the parameter values. The optimal ROIs for this approach are also given in Table 4 along with corresponding reactor volumes. As expected, the ROIs decrease and reactor volumes increase with increases in δ. Also, since the elliptical description contains a smaller region for unknown parameters, the corresponding values of ROI are better than for the hypercube. The feasibility test (Eq. 7) is now more complicated than in Eq. 5, and the two-level optimization is solved in a nested manner, with an inner minimization for η and T and an outer grid search for θ_v. This test was satisfied by the solution of the initial multiperiod problem (Eq. 2), with $\bar{K}$ empty in all cases. As expected, the worst-case point for θ^v occurs when F_A and F_B are at their lower bounds.

Finally, for the third approach we define $\theta^v = [F_A,\ F_B]^T$ and $\theta^u = [a_1, a_2, a_3]^T$, and we solve Eq. 2 for sets I and K. Initially Eq. 2 contains 32 periods when a hypercube description is used. Otherwise, it contains 24 periods when using Eq. 37. Also, as the control variables η and T are independent only for periods $k \in K$, this approach leads to intermediate designs when compared to the first two strategies. Again, the two-stage algorithm is executed for increasing values of δ from 1% to 10 % of the parameter values. The optimal ROIs for this approach are also given in Table 4 along with corresponding reactor volumes. Again, since the elliptical description contains a smaller region for unknown parameters, the corresponding values of ROI are better than for the hypercube description. The feasibility test (Eq. 9) is executed in a similar manner as with Eq. 7. Here the three-level optimization is solved in a nested manner, with an inner maximization for a_1, a_2, and a_3, a grid search over η and T, and an outer grid search for θ_v. This feasibility test was satisfied by the solution of the initial multiperiod problem (Eq. 2), with $\bar{K}$ and $\bar{I}$ empty in all cases. Again, the worst-case point for θ^v occurs when F_A and F_B are at their lower bounds. Moreover, since η and T can only be adjusted in response to variable feed rates and not for unknown rate constants, we believe that these designs represent more realistic approaches.

Conclusions

We present a formulation that treats different types of unknown input parameters separately in a two-stage approach for solving design problems under uncertainty. We assume that exact values for model parameters are rarely available, although they are known to have a range of values described by their confidence regions. Because exact values are unavailable, we further assume control variables cannot be used to compensate for model-parameter uncertainty. On the other hand, control variables are available to compensate for process variability. With the exception of Ostrovsky et al. (2001), we do not believe this distinction has been made in the process-engineering literature. To accomplish this, we first assume that the process model must be feasible over the entire region of model-parameter uncertainty, Θ^u. We then allow for control variables to be adjusted to ensure the process is also feasible for all $\theta^v \in \Theta^v$. The feasibility problem that assesses these designs is formulated as a four-level optimization problem using global maximum and minimum operators.

The feasibility problem was simplified through an aggregation of the inequality constraints through the use of the modified KS function. The KKT conditions of the two innermost optimization problems were then used as constraints in the outermost problem, allowing the feasibility problem to be approximated as a single NLP. Three example problems were solved to demonstrate the proposed approach. As expected, this treatment of uncertainty and variability gives intermediate designs between formulations that treat variability (and compensate through control variables) and uncertainty (which offer no compensation). As a result, we believe that this approach allows a more realistic treatment of unknown information at the design stage. Moreover, it also provides an expected value of perfect information and motivates additional analysis to quantify uncertain parameters more accurately.

Future work will deal with larger and more complex systems, and will explore strategies to improve the solution of multiperiod and feasibility problems. In particular, global optimization strategies, including those of Ostrovsky et al. (2001) and Floudas et al. (2001) need to be considered and extended for the solution of the large-scale feasibility problem.

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