Design for Model Parameter Uncertainty Using Nonlinear Confidence Regions

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An accurate method presented accounts for uncertain model parameters in nonlinear process optimization problems. The model representation is considered in terms of algebraic equations. Uncertain quantity parameters are often discretized into a number of finite values that are then used in multiperiod optimization problems. These discrete values usually range between some lower and upper bound that can be derived from individual confidence intervals. Frequently, more than one uncertain parameter is estimated at a time from a single set of experiments. Thus, using simple lower and upper bounds to describe these parameters may not be accurate, since it assumes the parameters are uncorrelated. In 1999 Rooney and Biegler showed the importance of including parameter correlation in design problems by using elliptical joint confidence regions to describe the correlation among the uncertain model parameters. In chemical engineering systems, however, the parameter estimation problem is often highly nonlinear, and the elliptical confidence regions derived from these problems may not be accurate enough to capture the actual model parameter uncertainty. In this work, the description of model parameter uncertainty is improved by using confidence regions derived from the likelihood ratio test. It captures the nonlinearities efficiently and accurately in the parameter estimation problem. Several examples solved show the importance of accurately capturing the actual model parameter uncertainty at the design stage.

Introduction

Accounting for model uncertainty at the design stage is critical to ensure that processes are capable of operating over a range of conditions. Uncertainties arise from many sources including process disturbances (varying flow rates and unit temperatures) and external factors (product demands, feedstock changeovers). In this study, we focus on model parameters (rate constants, material properties, and so on) that are determined by regression of experimental data. Uncertainty can have a large impact on equipment decisions, plant operability, and economic analysis. Research into developing algorithms to quantitatively gauge the effects of uncertainty continues to be an active area of research in process-systems engineering.

Pistikopoulos (1995) has outlined a general formulation for design under uncertainty:

$$
\begin{aligned}
\min_{d,z,x} \quad & E[P(d,x,z,\theta)] \\
\text{s.t.} \quad & h(d,x,z,\theta)=0 \\
& g(d,x,z,\theta)\le 0 \\
& d\in D, \qquad x\in X, \qquad z\in Z \\
& \forall\theta\in\Theta.
\end{aligned}
\tag{1}
$$

The process model is defined by the equality constraints h. Further bounds (temperature limits, and so on) and performance requirements (minimum conversion, and so on) for the process are included in the inequality constraints g. The variables in Eq. 1 include design variables d, control variables z,

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and state variables x. Here, the uncertain quantities in Eq. 1 are included in the model parameter vector θ. The solution to Eq. 1 optimizes the expected (or most probable) value of a cost function $E[P]$ over the entire region of uncertainty, Θ.

Much work in design under uncertainty in the past decade has focused on techniques to evaluate stochastic flexibility, that is, the probability of feasible operation. Contributions include design under continuous and discrete uncertainty (Straub and Grossmann, 1993), design of dynamic systems with simultaneous controllability requirements (Mohideen et al., 1996; Bansal et al., 2000), algorithmic development (Pistikopoulos and Ierapetritou, 1995; Acevedo and Pistikopoulos, 1998), and design with simultaneous flexibility, reliability, and maintenance concerns (Thomaidis and Pistikopoulos, 1994; Vassiliadis and Pistikopoulos, 1998). More recently, parametric programming ideas have been developed for design and control under uncertainty (Acevedo and Pistikopoulos, 1997; Papalexandri and Dimkou, 1998; Vassiliadis and Pistikopoulos, 1998; Bansal et al., 2000). The advantage of parametric techniques is that it outlines a complete map of where process models are valid for different regions of uncertainty. This can then be used to generate all optimal solutions as the operating conditions change as a function of the parameter uncertainty. In addition, better sampling techniques have also been developed that allow for more accurate and efficient evaluation of the expectation operator in Eq. 1 (Pistikopoulos, 1997; Diwekar and Kalagnanam, 1999).

The preceding work has led to powerful numerical methods and algorithms for including uncertain information into the design process. Using these techniques, many examples have been solved where a seemingly arbitrary description of the uncertainty, Θ, has been used in Eq. 1. Yet, this description of the uncertainty can greatly affect the quality and accuracy of the solutions to Eq. 1. Moreover, solving Problem 1 accurately, with confidence regions derived from real data, has received little attention in the literature.

Instead, uncertain *model* parameters have often been discretized between a lower and upper bound in design problems. While this description for model parameters is simple and easy to implement, it may be inaccurate. Model parameter are estimated from regression analysis of experimental data that is usually associated with random measurement error.

Frequently, multiple parameters are estimated simultaneously from the same set of data. In addition, the parameter estimation problem is often highly nonlinear due to complex mathematical models associated with chemical (and other) engineering systems. This may result in the parameters being correlated. Rooney and Biegler (1999) incorporated more accurate parameter uncertainty descriptions by using elliptical-joint confidence regions. These regions are a better description of model parameter uncertainty because they capture the parameter correlation. Their results showed the importance of including these descriptions into design problems; failure to use an appropriate description of Θ in Eq. 1 can lead to poor estimates of the influence of parameter uncertainty, resulting in either suboptimal designs or infeasible operation over Θ.

The elliptical joint confidence regions are derived from asymptotic properties of the parameter estimation problem (Bard, 1974; Seber and Wild, 1989). The parameter estimation problem is frequently nonlinear, especially for models encountered in chemical engineering. Because of this, the asymptotic results may not capture the nonlinearity of the estimation problem, resulting in poor descriptions of the actual parameter uncertainty. In addition, few experimental data points may be available, making asymptotic properties (derived by assuming large sample sizes) irrelevant. For realistic chemical engineering applications, more detailed descriptions are needed for model parameter uncertainty that can accurately account for nonlinear models, and be appropriate to use for small data sets.

In this article, we apply an uncertainty description for model parameters only using confidence regions derived from the likelihood ratio test. This method translates nonlinear information from the parameter estimation problem to the design problem via more accurate confidence regions. Sample size corrections are also available to further improve the asymptotic properties of the confidence regions. We include these into design problems using a two-stage approach that combines multiperiod optimization problems and feasibility tests. As in our previous work, we focus only on the following problem (Eq. 2) that is optimized with respect to design variables only

$$\begin{aligned}
&\min_{d,z} f(d)\\
&\text{s.t.}\quad h_i(x_i, z_i, d, \theta_i) = 0\\
&g_i(x_i, z_i, d, \theta_i) \le 0\\
&\theta_i \in \Theta; \qquad i = 1, \ldots, NP.
\end{aligned} \tag{2}$$

These problems allow for direct comparison on how various uncertainty descriptions Θ affect design variables or cost estimates. Here, Problem 2 must be solved to optimality over a specified region of model parameter uncertainty (that is, optimal design at a fixed degree of flexibility). The rest of this article is organized as follows. In the second section, we present three different confidence-region descriptions for modeling the uncertainty in the parameters. Then, in the third section, we outline how we incorporate the parameter uncertainty description into a two-stage algorithm for solving design problems under uncertainty. The fourth section presents numerical examples to demonstrate the importance of using the proper uncertainty description at the design stage. Finally, the fifth section presents our conclusions and outlined several areas for future research.

Confined Regions for Model Parameters

Parameter estimation is an important problem in process-systems engineering. The solution to the estimation problem provides point estimates of the parameters. While these estimates are important, they do not represent the complete information because these estimates rarely fit the data exactly. Rather, designers may want to know a region in which the parameters can be expected to lie, within certain probability limits. This section describes three different techniques for modeling the uncertainty associated with the parameters. Comprehensive reviews of parameter estimation and confidence interval estimation can be found in Bard (1974), Seber and Wild (1989), and Gallant (1987).

Individual confidence intervals

Confidence intervals are defined by lower and upper bounds in Eq. 3 such that the probability of selecting a random sample that will produce an interval containing the parameter θ is $1-\alpha$, or

$$P(\theta_L < \theta < \theta_U) = 1-\alpha. \quad (3)$$

The asymptotic bounds for Eq. 3 are found using Eq. 4:

$$\Theta = \left\{ \theta \mid \theta = \theta^* \pm t_{1-(\alpha/2),\, n-p}\,\sigma \right\}. \quad (4)$$

In Eq. 4, σ is the standard deviation of each parameter, and $t_{1-(\alpha/2),\, n-p}$ is the value of the Student-*t* distribution, which is a function of the desired confidence level α, the number of model parameters, p, and the number of data points used in the estimation problem, n.

Equation 4 provides bounds where each parameter can be expected to be found. Using these bounds for all parameters simultaneously leads to a hypercube (or more precisely, a hyperrectangle) mathematical description for Θ. If this method is used to model the uncertain parameters, it assumes they are independent of each other, even if multiple parameters were estimated simultaneously. Additionally, this description of the uncertain parameters assumes they vary symmetrically around θ^*. In nonlinear problems, this assumption may not hold. Moreover, this derivation considers variations of one parameter with all others held constant. As a result, it ignores interactions among parameters.

Elliptical confidence regions

Joint confidence regions arise from considering simultaneous confidence intervals for all the parameters. Considering all simultaneous *linear* combinations of the parameters ($b^T\theta$, $b \neq 0$) leads to elliptical contours in the parameter space, defined in Eq. 5:

$$(\theta-\theta^*)^T V_\theta^{-1} (\theta-\theta^*) \leq pF_{(1-\alpha,p,n-p)}. \quad (5)$$

Here, V_θ is the covariance matrix of the parameters. Equation 5 results from a Taylor series expansion around the optimal parameter estimates. It is also derived from the asymptotic results from the Wald test (Seber and Wild, 1989). Unlike the region in Eq. 4, this region treats the uncertainty in all parameters simultaneously. As with confidence intervals, the parameters vary symmetrically from the optimal estimates, θ^*. For linear regression problems, Eq. 5 is exact. However, for nonlinear problems, the region in Eq. 5 is only approximate, especially for small sample sizes. Rooney and Biegler (1999) assumed Eq. 5 was accurate for nonlinear estimation problems, noting that there were methods to check on the validity of this assumption (Bates and Watts, 1988). However, if this assumption is not appropriate for nonlinear estimation problems, a different mathematical description for the confidence region is needed.

Likelihood confidence regions

To improve the accuracy of the confidence regions derived from nonlinear inference problems, we use confidence regions derived from the likelihood ratio test, Eq. 6 (Seber and Wild, 1989; Gallant, 1987):

$$LR = 2[L(\theta^*) - L(\theta)] \leq \eta \chi^2_{1-\alpha,p}. \quad (6)$$

Here, L is the log-likelihood function. The error in setting $\eta = 1$ and using χ^2 to describe the confidence region is $O(n^{-1})$. This can be reduced to $O(n^{-2})$ by calculating the Bartlett correction, η, for nonlinearity (DiCiccio and Stern, 1993). In the absence of nuisance parameters, the Bartlett correction η can be calculated using the method described by Ghosh and Mukerjee (1991). However, computing η requires fourth derivatives of the likelihood function and sixth-order tensors.

The confidence region is mapped out in the parameter space by the contours of $L(\theta)$. An asymptotically equivalent form of Eq. 6 exists when using a nonlinear least-squares objective function in the parameter estimation problem. Using Eq. 6 for the parameters has several advantages over Eq. 5. In Eq. 5, V_θ is often estimated using the Jacobian of the response functions used for the parameter estimation problem and is usually evaluated at the optimal parameter estimates, θ^* [Donaldson and Schnabel (1987) found this method of estimating V_θ to be superior to alternative methods in their Monte Carlo computational experiments]. The Jacobian provides sensitivity near the optimal estimates, but fails to account for the nonlinearity of the response functions. On the other hand, Eq. 6 uses the response functions directly (which help form the likelihood function), and captures the nonlinear effects in the parameter estimation problem. Since Eq. 5 looks at only linear combinations of the parameters, this assumption may not hold in nonlinear problems. There are several other things to note about using Eq. 6 to map out confidence regions in nonlinear estimation problems. The confidence regions may be unbounded or disjoint (Ratkowsky, 1983; Seber and Wild, 1989; Bates and Watts, 1988). The latter can occur when multiple local minima are present in the nonlinear parameter estimation, and the same contour value of the log-likelihood function occurs around the local minima.

Motivating example

Here, we solve a nonlinear parameter estimation problem and calculate the confidence regions using Eqs. 4, 5, and 6. The model involves a single nonlinear equation where n is the number of data points:

$$y_i(\theta_1, \theta_2, t_2) = \theta_1(1 - e^{-\theta_2 t_i}) \qquad i = 1, \ldots, n. \quad (7)$$

Here, y is a function of two unknown parameters and one independent variable, time (t). Experimental data for this model are taken from Bates and Watts (1988).

The optimal parameter estimates and their standard deviations are

$$\begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix} = \begin{bmatrix} 19.1426 \\ 0.5311 \end{bmatrix}; \qquad \begin{bmatrix} \sigma_1 \\ \sigma_2 \end{bmatrix} = \begin{bmatrix} 2.4957 \\ 0.2031 \end{bmatrix},$$

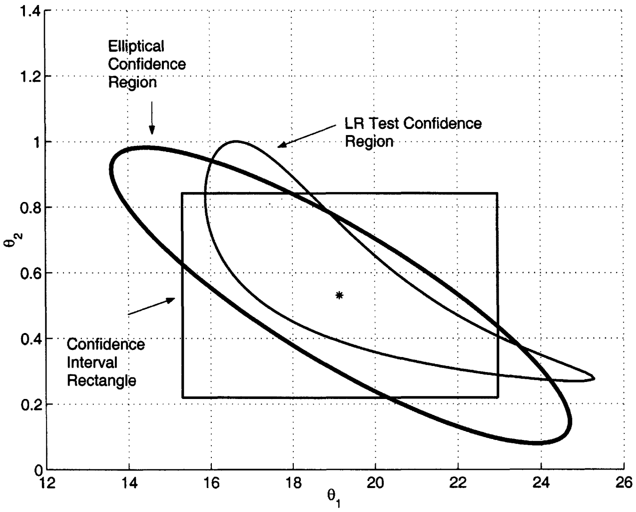

Figure 1. Comparison of the 80% confidence regions derived from Eq. 7.

and the estimated covariance matrix of the estimates is

$$V_\theta = \begin{bmatrix} 6.22864 & -0.4322 \\ -0.4322 & 0.04124 \end{bmatrix}.$$

The correlation coefficient, ρ_{12} is -0.85278. Because this estimation problem is nonlinear, we evaluate the use of Eq. 5 to calculate a confidence region for θ_1 and θ_2 and compare it with the confidence region derived from Eq. 6.

This example was chosen for a couple of reasons. First, the sample size ($n=6$) is small and the joint confidence region estimated from Eq. 5 may not be accurate. Next, as noted in Bates and Watts (1988), the response function has several properties that greatly influence the confidence regions. As $\theta_2 \to \infty$, the model reduces to $y=\theta_1$, becoming insensitive to θ_2. Thus, the actual confidence region becomes unbounded for increasing values of θ_2 at confidence levels $\geq \approx 94\%$. A similar asymptote develops as $\theta_2 \to 0$. Here, the model reduces to $y=\theta_1\theta_2 t$, leading to unbounded confidence regions for confidence levels $\geq \approx 96\%$. In addition, the joint region contains negative (physically meaningless) values of θ_2 for confidence levels $\geq 87\%$. Clearly, with these properties, the elliptical regions will likely be inaccurate.

Figure 1 shows the individual confidence intervals for the two parameters, the elliptical joint confidence region, and the confidence region calculated from the LR test at the 80% confidence level. The figure shows that the elliptical region poorly approximates the confidence region estimated using the LR test.

Design Using Nonlinear Confidence Regions

In this section, we outline how to incorporate more accurate mathematical descriptions of parameter uncertainty into a two-stage algorithm for design under uncertainty.

As in our earlier work, we are concerned about solving design problems under uncertainty more accurately, using well-established solution techniques. We use a two-stage algorithm (Figure 2) that iterates between a design stage and a feasibility stage. Usually, the uncertain parameters are discretized into a number of values from their overall uncertainty description, Θ (e.g., $\theta_i \in \Theta$). These points are then put into a multiperiod design problem, Eq. 2. The solution of the multiperiod problem results in design variables $\bar{d}$, which are optimal for only the discretized values of the parameters, θ_i, but not necessarily feasible for the entire region of uncertainty, Θ. A feasibility problem, Eq. 8, can be solved to check if the design variables operate over Θ:

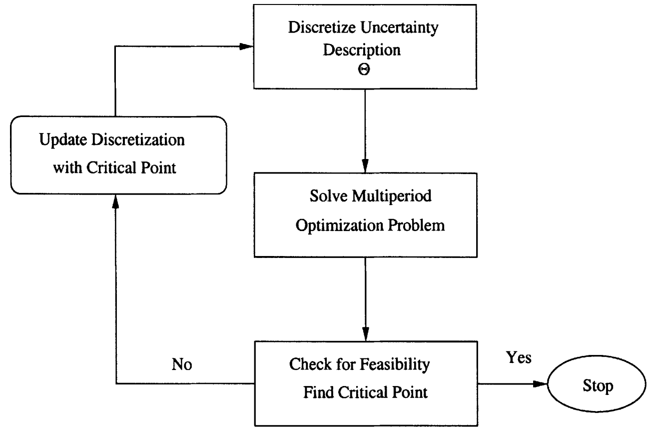

Figure 2. Two-stage algorithm for solving design problems under uncertainty.

$$T(\bar{d}) = \max_{\theta \in \Theta} \min_{z} \max_{j} g_j(\bar{d}, z, \theta). \tag{8}$$

Equation 8 assumes the state variables x have been eliminated by the equality constraints h in either Eq. 1 or Eq. 2.

If $T(\bar{d}) \leq 0 \ \forall \theta \in \Theta$, the current design is feasible. If $T(\bar{d}) > 0$ for any $\theta \in \Theta$, then $\bar{d}$ is infeasible. The solution of Eq. 8 results in critical values of the parameters, θ_c, the point in Θ where the greatest constraint violation occurs. The discretization of the uncertainty can be updated with the critical point (if $T>0$), and another multiperiod design problem is solved. This two-stage algorithm has been shown to take relatively few iterations to arrive at optimal designs (Floudas and Grossmann, 1987). In this work, we use the active-set approach of Grossmann and Floudas (1987) to solve the feasibility problems.

One challenge in using the two-stage approach is the necessity of choosing both the number of periods in Eq. 2 and the values of the uncertain parameters. In Rooney and Biegler (1999), we chose the number and values for θ_i from Eq. 5. We focused initially on the longest axis of the elliptical joint confidence region that provided two initial periods and values for the parameters, regardless of how many uncertain parameters are in the model. The extreme points of the longest axis correspond to the least well-determined (that is, farthest from the optimal estimates θ^*) points in the confidence region. While this is only a heuristic, the results showed that the two-stage algorithm converged in relatively few iterations (~ 3–4) using this approach. In addition, since we were concerned with feasibility over Θ, requiring the design variables to be initially feasible at the "worst" points in the confidence region seems reasonable.

If we replace Eq. 5 with Eq. 6, several modifications to the algorithm we originally proposed are needed. First, both the initial number of periods and values for the parameters are not readily available, as they were using the elliptical confidence regions. Here, we solve an off-line problem Eq. 9 to find the initial values of θ_i to use in the multiperiod design problem:

$$\max \quad \sum_{i=1}^{p} (\theta_i - \theta_i^*)^2$$
$$\text{s.t.} \quad 2[L(\theta^*) - L(\theta)] \le \eta \chi^2_{1-\alpha,p}. \tag{9}$$

Here, we simply find the point in the confidence region that lies furthest away (in Euclidean space) from the optimal estimates. This mimics our previous approach. Since we are concerned with feasibility, we use a heuristic requiring the designs to operate at the "worst" point in the confidence region. Sensitivity analysis could also be used to help choose the number and values of parameters (Grossmann and Sargent, 1978), but this analysis may be expensive for solving large problems. After an initial design is obtained, the feasibility test can be solved where Θ is modeled by Eq. 6. A disadvantage of using the LR test in the feasibility test instead of Eq. 5 is that Eq. 6 is not always convex in θ, and the properties for convex flexibility analysis (Swaney and Grossmann, 1985a,b) no longer are guaranteed to hold, since the LR test may result in nonconvex confidence regions.

While we consider only the LR test to derive parameter confidence regions, other methods, such as the Wald and LM tests, profiling techniques [based upon the square root of the LR region (Eq. 6)] (Bates and Watts, 1988; Watts, 1994), or even Monte Carlo simulations could also be used to derive confidence regions from nonlinear inference problems. Also, exact methods are available (Hartley, 1964; Ratkowsky, 1990) that do not use a large sample-size assumption in their derivation. However, the accuracy of this test depends greatly on the choice of a projection matrix needed for its computation (Seber and Wild, 1989). In addition, profiling uses a series of constrained regression problems that must be solved repeatedly for each parameter. While this method is easy to implement and gives good results (Watts, 1994), it has two disadvantages over using the LR test. First, it only looks at interactions among parameter pairs, not all parameters simultaneously, Second, the confidence regions using this technique cannot be written in a closed form, which is necessary for inclusion into the feasibility problem. On the other hand, the extensive computational experience of Donaldson and Schnabel (1987) confirms that confidence regions derived from the LR test were accurate for many nonlinear parameter estimation problems.

Finally, we use the results of the parameter estimation problem to generate the confidence regions described in Eqs. 4, 5, and 6. We assume that the parameter estimation problem has been solved to a satisfactory answer and that appropriate assumptions regarding the data were used (Bates and Watts, 1988; Bard, 1974):

- The expectation function is correct.
- Responses are functions of the expectation function (deterministic part) plus the disturbances (random part).
- The disturbance is independent of the expectation function.
- Each disturbance has a normal distribution with a zero mean.
- The disturbances have equal variances.
- The disturbances are independently distributed.

We also assume that issues such as using appropriate response models, outliers in the data, bias concerns, and so forth, have been addressed in the solution to the parameter estimation problem. Thus, they do not appear in our analysis.

Example Problems

In this section, we compare the results of using Eqs. 4, 5, and 6 to describe the model parameters in several design problems. The problems include a linear retrofit problem, design of a pressure relief valve, and a reactor−separator flow sheet. All problems were modeled in GAMS (Brooke et al., 1988) and solved using a DEC Alpha 400 MHz workstation. When faced with model uncertainty, the true values of the parameters are unknown. The only information known about the parameters θ is that they reside somewhere in Θ for a particular confidence level. Because the parameters are unknown, we assume that control variables cannot be used to compensate for model parameter uncertainty in each period. Thus, we use robust formulations where the control variables are the same across all periods.

Example 1: linear retrofit under uncertainty

We solve the linear retrofit problem from our previous article. This problem, (Eq. 10), involves two design variables, d_1 and d_2, one control variable, z, and two uncertain parameters, θ_1 and θ_2. Because we don't use control variables to improve operation under model parameter uncertainty, z takes on the role of a no-cost design variable in this problem:

$$\begin{aligned}
\min C = \quad & \Delta d_1 + \Delta d_2 \\
\text{s.t.} \quad & (1) \quad z + d_1 - 3d_2 \le \theta_{1,i} - 0.5\theta_{2,i} \\
& (2) \quad -z + d_2 \le -\frac{1}{3} + \frac{\theta_{1,i}}{3} + \theta_{2,i} \\
& (3) \quad z - d_1 \le 1 - \theta_{1,i} + \theta_{2,i} \\
& \Delta d_1 = d_1 - d_{1c} \\
& \Delta d_2 = d_2 - d_{2c} \\
& \Delta d_1, \Delta d_2 \ge 0 \\
& -3 \le z \le 3 \\
& d_{1c} = 3.0, \ d_{2c} = 1.0 \\
& \theta_{1,i}, \theta_{2,i} \in \Theta \\
& i = 1, NP.
\end{aligned} \tag{10}$$

The results from Eq. 7 are used for modeling the uncertain parameters at the 80% confidence level. Using the method described in Ghosh and Mukerjee (1991), the Bartlett correction factor η is estimated to be 0.9332. The nominal contour value (assuming $\eta = 1$) for the LR test is 44.4428, and includ-

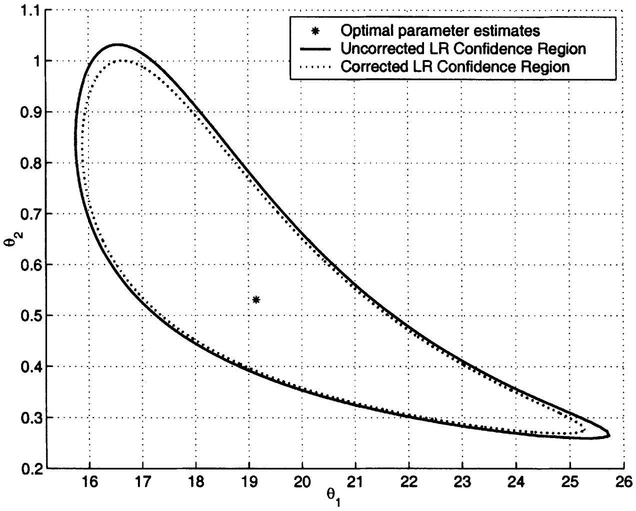

Figure 3. Comparison of Bartlett corrected and uncorrected LR confidence regions.

ing the Bartlett correction reduces the contour level to 42.8802. The corrected and uncorrected LR confidence regions are plotted in Figure 3.

Problem 10 is solved to find the optimal designs that operate over each of the uncertainty descriptions, Eqs. 4, 5 and 6. The results are seen in Table 1.

Table 1 shows that using simple lower and upper bounds from Eq. 4 for each of the parameters leads to the cheapest design. However, these design variables do not operate over the actual confidence region found via the LR test. A similar result holds if the elliptical joint confidence region (Eq. 5) is used to model the parameters. Even though the cost in using Eq. 5 for Θ is similar to the LR-based designs, the design is infeasible over the actual region of uncertainty. Using Eq. 5, design variable d_2 is approximately 42% larger than on the uncorrected LR region. Table 2 shows the righthand sides (RHS) of the inequalities in Problem 10 at the solution. Here, the elliptical confidence region shows that the inequalities (1)–(2) in Problem 10 are more restrictive than the LR region would indicate. Thus, variable d_2 requires a large change for optimality, since it only appears on the left side of these two inequalities. On the other hand, inequality (3) in Eq. 10 is more restrictive according to the LR confidence region than the elliptical or hypercube regions. This explains the larger change in d_1 needed for optimality. Also in this example, the Bartlett correction makes the confidence regions smaller, which leads to a slightly cheaper design.

Table 1. Comparison of Θ on the Retrofit Problem

Uncertainty Description Θ	Cost	d_1	d_2
Nominal	11.6115	14.6115	1.0000
Eq. 4	15.7490	18.7493	1.0000
Eq. 5	18.0230	20.5507	1.4722
Eq. 6 ($\eta = 1.0$)	18.5181	21.4706	1.0475
Eq. 6 ($\eta = 0.9332$)	18.0060	21.0060	1.0000

Table 2. RHS of the Inequality Constraints (1–3) in Problem 10 for Various Θ

Uncertainty Description Θ	Inequality in Problem 10	Value of RHS
Eq. 4	1	14.895
	2	4.992
	3	−21.749
Eq. 5	1	13.134
	2	5.119
	3	−23.551
Eq. 6 $\eta = 1.0$	1	15.328
	2	5.793
	3	−24.471
Eq. 6 $\eta = 0.9332$	1	15.4591
	2	5.7246
	3	−24.0060

Example 2: Design of a flexible relief valve

Here we consider the design of a relief valve for a flash tank. We want to size the relief valve based upon the maximum pressure at various vapor compositions w at a specified maximum operating temperature. The uncertain parameters are the interaction parameters, Λ_{12} and Λ_{21}, in the Wilson equation for a binary mixture of heptane and ethanol. The experimental data were taken from Hirata and Ohe (1975). The data consist of sets of equilibrium data at 70°C. Here, we use a 99% confidence level since an improperly sized relief valve could overly stress the tank.

The parameters were estimated using maximum-likelihood estimation, assuming general, unknown covariance. The optimal parameter estimates and their standard deviations are

$$\begin{bmatrix}\theta_1\\ \theta_2\end{bmatrix} = \begin{bmatrix}0.1838\\ 0.1989\end{bmatrix}; \qquad \begin{bmatrix}\sigma_1\\ \sigma_2\end{bmatrix} = 10^{-3}\begin{bmatrix}7.249\\ 8.143\end{bmatrix}.$$

The correction coefficient $\rho_{12} = -0.8003$. The Bartlett correction to the LR test is estimated to be 0.993 using the method in Ghosh and Mukerjee (1991) and was unimportant in this example.

Following the two-stage algorithm in Figure 2, the design problem is

$$\begin{aligned}
&\max \quad P \\
&\text{s.t.} \quad P - P_i && \le 0 \\
&w_{ij} - \frac{P_{ij}^0}{P_i} x_{ij}\gamma_j && = 0 \\
&\log_{10}\left(P_j^0\right) - A_j + \frac{B_j}{C_j + T(C)} && = 0 \\
&\sum_j x_{ij} - 1 && = 0
\end{aligned}$$

$$\gamma_1 = \exp\Bigg[-\ln\left(x_{i1} + \Lambda_{12_i} x_{i2}\right) + x_{i2}\left(\frac{\Lambda_{12_i}}{x_{i1} + \Lambda_{12_i} x_{i2}} - \frac{\Lambda_{21_i}}{x_{i2} + \Lambda_{21_i} x_{i1}}\right)\Bigg] = 0$$

$$\gamma_2 - \exp\left[-\ln\left(x_{i2} + \Lambda_{21_i} x_{i1} \right) - x_{i1}\left(\frac{\Lambda_{12_i}}{x_{i1} + \Lambda_{12_i} x_{i2}} - \frac{\Lambda_{21_i}}{x_{i2} + \Lambda_{21_i} x_{i1}} \right) \right] = 0$$

$$T - 70 \leq 0$$

$$\Lambda_{12}, \Lambda_{21_i}, \in \Theta; \qquad j = 1, 2; \qquad i = 1, \ldots, NP. \tag{11}$$

In the absence of control variables and with only one inequality constraint, the feasibility test (Eq. 8) can be written as a NLP:

$$\max \quad T$$

$$\text{s.t.} \quad w_j - \frac{P_j^0}{\overline{P}} x_j \gamma_j = 0$$

$$\log_{10}\left(P_j^0 \right) - A_j + \frac{B_j}{C_j + T(C)} = 0$$

$$\sum_j x_j = 1$$

$$\gamma_1 - \exp\left[-\ln(x_1 + \Lambda_{12} x_2) + x_2\left(\frac{\Lambda_{12}}{x_1 + \Lambda_{12} x_2} - \frac{\Lambda_{21}}{x_2 + \Lambda_{21} x_1} \right) \right] = 0$$

$$\gamma_2 - \exp\left[-\ln(x_2 + \Lambda_{21} x_1) - x_1\left(\frac{\Lambda_{12}}{x_1 + \Lambda_{12} x_2} - \frac{\Lambda_{21}}{x_2 + \Lambda_{21} x_1} \right) \right] = 0$$

$$\Lambda_{12}, \Lambda_{21} \in \Theta; \qquad j = 1, 2. \tag{12}$$

Any $\Lambda \in \Theta$ that results in $T - 70°\text{C} > 0$ is a critical point. In the feasibility problem, the design pressure, $\overline{P}$, is fixed to the value from Problem 11.

Problems 11 and 12 are solved using Eqs. 4, 5 and 6 for Θ for various vapor compositions w. The results are plotted in Figure 4. The pressure for each uncertainty description Θ was normalized by the nominal pressure in Figure 4. Figure 4 shows that using the individual confidence limits for the parameters results in an overly conservative design for most of the vapor composition. In other words, this description of the parameter uncertainty overconstrains the valve pressure. On the other hand, the design based upon the elliptical confidence region underestimates the effect of uncertainty. Here, the pressure is too high compared to the design based upon the LR region. For most of the vapor compositions, the LR-based design lies between the designs from the hypercube and elliptical regions. However, at compositions greater than approximately 78%, the LR-based design results in slightly lower operating pressures than according to the hypercube-based design. In this region, both elliptical and hypercube approach lead to designs that underestimate the effect of uncertainty.

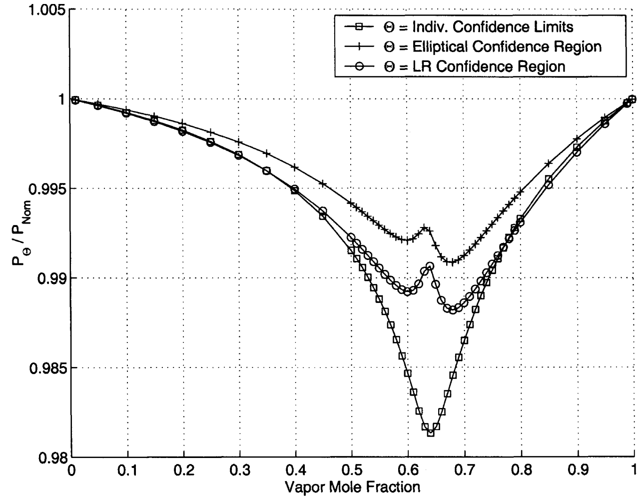

Figure 4. Pressure-ratio comparisons for Problem 11.

Figure 5 shows the confidence regions used in this example. Analysis of the multiperiod problem using Eq. 4 for Θ shows that the design is feasible everywhere over the hypercube if it is feasible when both Λ_{12} and Λ_{21} are at their upper bounds. As Figure 5 shows, this point is not relevant if you consider the joint information, via either the elliptical or LR region. Thus, the hypercube approach for describing the model parameters has constrained the design to consider a region that will lie outside the 99% confidence region. Finally, the small "bumps" seen in Figure 4 using Eqs. 5 and 6 for Θ are due to the nonmonotonic behavior of the design pressure as a function of the vapor composition.

Design of a reactor–separator system

In this example, we design a reactor−separator system considered by Grossmann and Sargent (1978), but with a different reaction mechanism. We assume that an isothermal, constant density, liquid-phase reaction takes place following

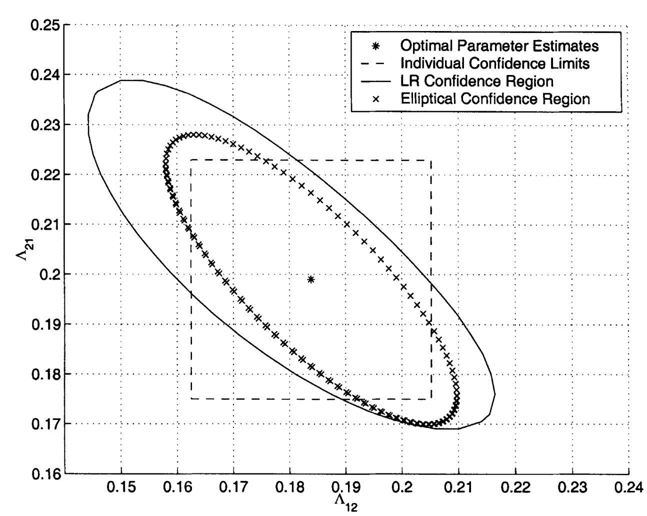

Figure 5. Confidence regions used in Problem 11.

Denbigh kinetics, Eq. 13:

$$\begin{array}{ccc} A & \xrightarrow{k_1} B & \xrightarrow{k_2} C \\ k_3 \downarrow & k_4 \downarrow & \\ D & E. & \end{array} \tag{13}$$

To find the confidence region for the kinetic parameters, experimental data for the reactions in Eq. 13 were simulated by taking the analytical solution to a CSTR model using Eq. 13, adding normally distributed noise to the analytical solution, and then solving the parameter estimation problem using the simulated data. The simulated experimental data appear in the Appendix. Even though the kinetics are first order, the analytical solution using a CSTR model is nonlinear in the kinetic parameters. The Bartlett correction factor in this problem was set to 1.0, as the computation time to calculate it was excessive.

The optimal parameter estimates (in units of time^{-1}) and their standard deviations are

$$\begin{bmatrix} k_1 \\ k_2 \\ k_3 \\ k_4 \end{bmatrix} = \begin{bmatrix} 0.9945 \\ 0.5047 \\ 0.3866 \\ 0.3120 \end{bmatrix}; \qquad \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \end{bmatrix} = \begin{bmatrix} 0.02075 \\ 0.01340 \\ 0.01176 \\ 0.01099 \end{bmatrix}.$$

The estimated correlation matrix (normalized covariance matrix) of the parameters is

$$C_\theta = \begin{bmatrix} 1.0 & -0.00107 & 0.2249 & 0.3614 \\ -0.00107 & 1.0 & 0.1791 & 0.5789 \\ 0.2249 & 0.1791 & 1.0 & 0.3530 \\ 0.3614 & 0.5789 & 0.3530 & 1.0 \end{bmatrix}.$$

Example 3

In this example, it is desired to produce at least 40 mol/time to component C in the separator overhead (Figure 6) while the rest of the components are either recycled or sent downstream. The objective here is to minimize the cost, C, of the flowsheet over the region of uncertainty at the 95% confidence level. The multiperiod design problem for this example is

$$\begin{aligned} \min \quad & C = 10V^2 + 5F \\ \text{s.t.} \quad & F_{a0} - x_{a,i}F_i(1-\delta) - Vc_{a_0}(-k_{1,i} - k_{3,i})x_{a,i} = 0 \\ & -F_i x_{b,i}(1-\delta) + Vc_{a0}(k_{1,i}x_{a,i} - k_{2,i}x_{b,i} - k_{4,i}x_{b,i}) = 0 \\ & -F_i x_{c,i} - Vc_{a0}(k_{2,i}, x_{b,i}) = 0 \\ & -F_i x_{d,i}(1-\beta) + Vc_{a0}k_{3,i}x_{a,i} = 0 \\ & -F_i x_{e,i}(1-\beta) + Vc_{a0}(k_{4,i}x_{b,i}) = 0 \\ & x_{a,i} + x_{b,i} + x_{c,i} + x_{d,i} + x_{e,i} - 1 = 0 \\ & F_i x_{c,i} \geq 40 \\ & F \geq F_i \\ & 0 \leq \delta \leq 1 \qquad 0 \leq \beta \leq 1 \\ & c_{a0} = 10 \text{ mol/m}^3 \qquad F_{a0} = 100 \text{ mol/time} \\ & i = 1, \ldots, NP \qquad k_1, k_2, k_3, k_4 \in \Theta. \end{aligned} \tag{14}$$

The state variables are the mole fractions x for each component and the flow rate F_i (mol/time) in each period, V is the volume of the CSTR in m^3, c_{a0} is the inlet concentration, and F is the largest of the period flow rates used for costing purposes. The control variables in this problem are δ and β, Here, δ refers to the amounts of A and B recycled, while β refers to the amounts of components D and E recycled. We solve Problem 14 twice. In the first formulation, we use a robust formulation where the control variables are not indexed across the periods. In the second formulation, we consider the unlikely case that we know the uncertain parameters exactly at run time. As a result, we now allow the control variables to be free in each period to improve the solution. After using the algorithm in Figure 2, the results for this problem are seen in Table 3.

For the robust control-variable case, the results show that the hypercube approach overestimates the uncertainty in this example, leading to a design that is almost $76,000 more expensive than the design based upon the LR confidence regions. The design based upon Eq. 5 is also more expensive than the LR design by $21,700, although the difference in the volumes and the flow rates is approximately 2%. The cost differences become smaller as expected with the addition of

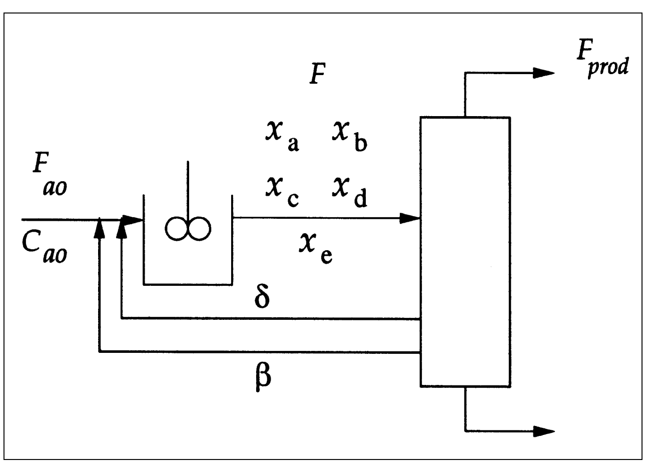

Figure 6. Simple reactor–separator flow sheet.

Table 3. Results for Example 3

Uncertainty Description Θ	Indexed Controls V m^3	F mol/time	C $\times 10^3$ \$	Robust Controls V m^3	F mol/time	C $\times 10^3$ \$
Nominal	19.07	413.8	570.7	—	—	—
Eq. 4	20.06	441.2	623.4	20.88	468.32	670.5
Eq. 5	19.57	431.9	599.2	19.98	434.26	616.5
Eq. 6	19.54	424.9	594.3	19.55	425.2	594.8

Table 4. Results for Example 4

Uncertainty Description Θ	Indexed Control V m^3	F $\frac{mol}{time}$	C $\times 10^3$ \$	Robust Controls V m^3	F $\frac{mol}{time}$	C $\times 10^3$ \$
Nominal	8.93	443.8	301.7	—	—	—
Eq. 4	9.23	504.1	337.4	9.32	520.0	346.9
Eq. 5	9.24	494.5	332.6	9.35	504.6	339.9
Eq. 6	9.11	458.7	312.4	9.13	458.2	312.4

indexed control variables in each period. In this example, the impact of the nonlinearities in the parameter estimation problem are seemingly small, and the elliptical and LR confidence regions lead to similar designs, while using Eq. 4 led to a more conservative and expensive design.

Example 4

In this example, the product demands are changed. It is now required that at least 50 units of component B and 20 units of component D be produced in the separator overhead. The amount of recycle for components A and C is now controlled by δ. The recycle of component E is controlled by β. Problem 13 was modified to reflect these changes and the results are seen in Table 4.

For this example, the results indicate that the influence of uncertainty on the design is only moderate, regardless of which uncertainty description is used for Θ. The difference in the reactor volumes in all three cases is less than 2.5%. However, the flow rate using Eq. 4 is 13.5% larger than with LR information. The combined effect is a design that is 11% more expensive. The elliptical confidence region leads to a design that is approximately 8.8% more expensive than the LR design. As in the last example, the differences are even less pronounced when including control variables in each period in Problem 14.

To further understand the results in this problem, consider the lower and upper bounds for each of the uncertain parameters calculated using Eqs. 4, 5 and 6 at the 95% confidence level. What is interesting here is that except for k_3, the range of the parameters is smallest in the LR confidence region, indicating that both the individual confidence limits and the elliptical confidence region overestimate the uncertainty.

Table 5. Lower and Upper Bounds for Various Θ in Problem 14

Uncertainty Description Θ	Parameter	Lower Bound	Upper Bound
Eq. 4	k_1	0.9541	1.0373
	k_2	0.4792	0.5329
	k_3	0.3638	0.4109
	k_4	0.2908	0.3348
Eq. 5	k_1	0.9284	1.0606
	k_2	0.4620	0.5474
	k_3	0.3492	0.4241
	k_4	0.2770	0.3470
Eq. 6 $(\gamma = 1)$	k_1	0.9672	1.0225
	k_2	0.4843	0.5256
	k_3	0.3636	0.4102
	k_4	0.2989	0.3258

Example 5

In this example, we now maximize an estimate of the average value of a profit function instead of simply minimizing the design costs as was done in the previous two examples. This requires the solution of a different multiperiod optimization problem seen in Eq. 15

$$\begin{aligned} &\max_{x_{ci}, d, z} \frac{1}{2{,}400} \sum_{i=1}^{2{,}400} P_i(x_{c_i}, z, d, \theta_i) \\ &\text{s.t.} \quad h(x_i, z, d, \theta_i) = 0 \\ &\qquad g(x_i, z, d, \theta_i) \le 0 \\ &\qquad \theta_i \in \Theta; \qquad i = 1, \ldots, 2{,}400. \end{aligned} \tag{15}$$

The cost function from Example 4 is replaced with the following profit function, P_i for each period [adapted from Georgiadis and Pistikopoulos (1999)]

$$P_i = 400 f_{c,i} - 12{,}500 - 10V^2 - 5 f_{c,i}\big(\delta(x_{a,i} + x_{b,i}) + \beta(x_{d,i} + x_{e,i})\big). \tag{16}$$

Twenty-four hundred points in each confidence region were used to estimate the average profit. Additional sample sizes ranging from 600 points to 4800 points were used, with no significant change noted in the estimated average profit. We also assumed that each period in Eq. 15 should be equally weighted. This again reflects the fact that the true values of the model parameters are unknown and that they may reside anywhere in Θ. The control variables were not indexed for these profit estimates.

Figure 7 shows the average profits for each uncertainty description considered in this article and how the profit estimates change with the confidence level. The plot shows that using either Eq. 4 or Eq. 5 for Θ in Eq. 15 results in lower profit estimates than when Eq. 6 is used to model the parameter uncertainty. This is consistent with the results from Example 3, where using Eqs. 4 and 5 led to a slightly more expensive design when compared to the design based upon the LR confidence region. Additionally, the slopes of lines in

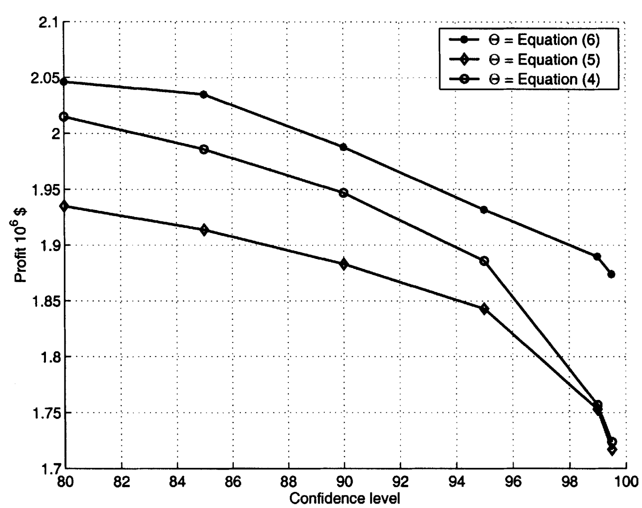

Figure 7. Profit estimates for different uncertainty descriptions and varying confidence levels.

Figure 7 are expected. Because the confidence level tends to 100%, the confidence region tries to enclose all parameter values. Consequently, the design variables are constrained to operate over this large region of uncertainty and the profit decreases. Similarly, as the confidence level decreases, the region of uncertainty shrinks toward the nominal parameter estimates, θ^*. All three curves in Figure 7 converge to the nominal profit of 2.231×10^6\$ as the confidence level goes to zero.

Conclusions

This article presents an approach for design under uncertainty that accurately incorporates uncertain model parameters derived from nonlinear estimation problems. A two-stage algorithm, consisting of multiperiod optimization problems and a feasibility test, was used to arrive at optimal designs under uncertainty. The periods in the optimization problem correspond to discretized values of the uncertain parameters. In this work, we focused on choosing discrete values for uncertain model parameters. Previously, these discretized points were often set to lower and upper bounds based on their confidence intervals. Other work has focused on choosing the discretized points from elliptical joint confidence regions. However, in this work, we chose points for the multiperiod design problems using the LR test. This represents the actual parameter uncertainty more accurately, because it directly includes the effects from nonlinear parameter estimation models. Our results show that the nonlinear behavior of the estimation problem can greatly affect the confidence regions derived for the parameters, and this translates into designs that can better handle the actual model parameter uncertainty.

In this work, we mainly considered optimization problems that were optimized with respect to design variables only. By doing so, we are able to clearly see the effect of using the different methods to describe the region of parameter uncertainty. While this approach may seem restrictive, our work can be readily adapted to problems that optimize expected cost or revenues by sampling points from each of the respective confidence regions and then calculating the expectation operator (or some approximation to it) in Eq. 1. This was demonstrated by changing the objective function in one example to estimate profits instead of design costs.

Also, we have assumed that the designs must operate over the entire region of uncertainty. Here we solved problems for a fixed degree of flexibility, while in the stochastic optimization literature, the degree of flexibility can also be traded with an economic objective (Ierapetritou et al., 1996). However, in the face of model parameters estimated from experimental data, the confidence regions are completely determined by the data. What we have argued implicitly in this work is that the only degree of freedom in the face of uncertain parameters should be the confidence level. Once the confidence level is fixed, trading off feasibility vs. optimality (via the size of the feasible region, as done in stochastic optimization formulations) may not be appropriate, as the true model parameters are unknown and may lie anywhere within the confidence region. Except in the third example, we do not consider control variables that compensate for uncertainty in the model parameters. When faced with other sources of uncertainty (such as process disturbances, varying flow rates, and so on), control variables play a key role in helping to minimize the effect of these disturbances. If multiple sources of uncertainty are to be included at the design level, techniques need to be developed that allow for control variables to mitigate the effects of the process disturbances without compensating for the uncertainty in the model parameters. Future research will involve developing systematic methods for dealing with these various uncertainty sources at the design stage.

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Table A1. Simulated Experimental Data

CSTR Res. Time	x_a	x_b	x_c	x_d	x_e
0.1000	0.8710	0.0877	0.0041	0.0344	0.0028
0.5000	0.6158	0.1919	0.0469	0.1212	0.0241
0.9000	0.4373	0.2245	0.1078	0.1699	0.0606
1.3000	0.3376	0.2485	0.1657	0.1544	0.0937
1.7000	0.2823	0.2261	0.1875	0.1805	0.0999
2.1000	0.2788	0.1907	0.2112	0.2041	0.1021
2.5000	0.2326	0.1866	0.2494	0.2209	0.1273
2.9000	0.1898	0.1612	0.2574	0.2371	0.1544
3.3000	0.1726	0.1648	0.2429	0.2292	0.1627
3.7000	0.1747	0.1330	0.2494	0.2123	0.1880
4.1000	0.1510	0.1462	0.2929	0.2245	0.1903
4.5000	0.1332	0.1388	0.3131	0.2384	0.1906
4.9000	0.1310	0.1143	0.3213	0.2403	0.1977
5.3000	0.1152	0.1176	0.2954	0.2554	0.1990
5.7000	0.1181	0.1041	0.3404	0.2649	0.2070

Appendix

The simulated experimental data used in Examples 3, 4, and 5 appear in Table A1.

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