Worst-Case Performance Analysis of Optimal Batch Control Trajectories

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In open-loop optimal control, inputs to a dynamic system are computed that optimize a specified performance criterion. A novel approach is proposed that quantifies the impact of parameter and control implementation inaccuracies on the performance of open-loop control policies. Such information can be used to decide whether more laboratory experiments are needed to produce parameter estimates of higher accuracy, or to define performance objectives for lower-level control loops that implement the optimal control trajectory. The novel features of the approach include (1) computational efficiency; (2) the parametric uncertainty description, which is produced by most process identification algorithms; and (3) addressing of control implementation inaccuracies. The merits of the approach are illustrated on a batch crystallization process.

Introduction

A problem of academic and industrial interest is the computation of optimal model-based control policies for batch and semibatch processes (Barrera and Evans, 1989; Barton et al., 1998; Diwekar et al., 1989; Rippin, 1983). Recently there has been interest in the analysis of open-loop control policies that are robust to uncertainties in the model parameters (Loeblein et al., 1997; Torvi and Hertzberg, 1997). This research has been motivated by two facts. First, in practice model uncertainties are significant, including external factors such as economic cost data or feed compositions, or internal process parameters such as kinetic rate constants. Second, the optimal control policy and the resulting performance can be strongly sensitive to model uncertainties. Quantitative estimates of these effects can be used to decide whether more laboratory experiments are needed to produce parameter estimates of higher accuracy, to define performance objectives for lower-level control loops that implement the optimal control trajectory, or to design optimal control policies that are robust to a given level of model uncertainty.

While most literature studies represent model uncertainties by fixed upper and lower bounds on each parameter (Biegler et al., 1997), we will treat the parametric uncertainties as being within a hyperellipsoid. Our motivation for this is that most process identification algorithms produce uncertainty descriptions in this form (Beck and Arnold, 1977; Ljung, 1987). We will also quantify the effect of control implementation uncertainty on the performance, since open-loop control policies are usually implemented by a lower-level feedback controller whose setpoint tracking response will generally be imperfect due to actuator constraints and unmodeled time-varying behavior, nonlinearities (such as valve stiction), and disturbances. To our knowledge, this is the first time that control implementation inaccuracies are rigorously addressed in the analysis of batch or semibatch processes.

Concerning effects of the parametric and implementation uncertainties on the open-loop control policies, industrially important problems are the robustness of the optimal control trajectory to model uncertainty, the robustness of predicted optimal performance to model uncertainty, robustness of predicted performance to model uncertainty, and the robustness of predicted performance to control implementation uncertainty. For each problem, we use Taylor series to quantify the performance objective and control trajectory in a neighborhood around the optimal open-loop operation. Then matrix algebra manipulations are followed in order to estimate the worst-case performance and the associated worst-case vectors, assuming that the worst-case vectors are within the hyperellipsoid. The accuracy of the estimates are finally assessed by a nonlinear dynamic simulation using the obtained worst-case vectors.

The article is organized as follows. First the overall approach and the uncertainty description are described. This is

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followed by the mathematical formulation and solution of four analysis problems for batch and semibatch processes. The effectiveness of the analysis tools is demonstrated on a batch crystallization process.

Problem Formulation and Solution

When developing algorithms for the analysis of uncertainty in optimal batch and semibatch processing, there are several choices on how the analysis problem can be formulated. First, there is a decision as to whether the uncertainty should be represented as being stochastic (that is, the parameters described by a probability distribution) (Torvi and Hertzberg, 1997) or deterministic (that is, the parameter vector is assumed to be fixed and located within some closed set) (Biegler et al., 1997). Second, the form of the probability distribution function or the closed set must be selected. Popular choices are to use a multivariate normal distribution for representing stochastic uncertainty and independent upper and lower bounds on each parameter for representing deterministic uncertainty. Third, it must be decided how precise an analysis is desired—this decision greatly influences the computational efficiency of the algorithm that is constructed to solve the analysis problem.

In our case we assume that the parametric uncertainty is deterministic and lies within a hyperellipsoid. The hyperellipsoid can be constructed from experimental data by first computing a (stochastic) multivariate normal distribution for the parameters [such as using standard process-identification algorithms (Beck and Arnold, 1977; Ljung, 1987)], and then defining the size of the hyperellipsoid by specifying a confidence level α. In our opinion, such an uncertainty description blends the strengths of the purely stochastic and deterministic approaches. (The purely stochastic approach can be too optimistic, since some critical parameters may not have sufficient influence during the calculation of an expectation operator. The purely deterministic approach can be too pessimistic, since a highly unlikely parameter can dominate the results.) In the approach taken here, the confidence level can be selected to avoid overly pessimistic or optimistic results.

There is strong motivation to not attempt to analyze the worst-case performance of batch and semibatch processes to very high precision. First, since in practice the boundary of the parametric uncertainty set is generally estimated from experimental data with its stochastic variations, its precise location is, to some degree, uncertain. Hence, from a practical point of view, it would be a waste of effort to quantify the worst-case performance of the batch process to extremely high precision when the input data are not known to extremely high precision. Second, we are interested in the analysis of complex nonlinear systems. The approach of solving the analysis problem to very high precision (that is, to grid the parameter region, perform a time-domain simulation at each grid point, and then to tally the results) requires too much computation time to be feasible for a complex nonlinear system. For example, a grid size of 100 in each dimension leads to 100^n grid points, where n is the number of parameters. Even a batch process with only four parameters requires 10^8 grid points—if each simulation took one minute, the time to compute an analysis measure to this precision would take two centuries! In fact, the results of (Braatz, 1996) can be gener-

alized to show that the computation of either an exact or highly accurate approximate solution to the analysis problem for nonlinear systems is NP-hard.

The first step of the approach is to use a Taylor series to quantify the performance objective and control trajectory in a neighborhood around the optimal open-loop operation. While some precision is lost when using a Taylor series, the gain will be a mathematical simplification that will allow the derivation of analytical results for quantifying the robustness of the optimal control trajectory and the performance. The second step is to perform a nonlinear simulation to improve the analysis estimates.

There are several variations on the open-loop optimal control problem, depending on the objectives of the problem being considered (such as minimum completion time, maximum profit), the generality of the constraints [such as path inequality constraints (Barton et al., 1998), tranversality conditions (Ray, 1981)], and whether lumped or distributed parameter systems are under consideration (Ray, 1981). While the approach taken here does not depend on the particulars of the optimal control problem formulation, it is assumed that there is an algorithm available that can compute the optimal control trajectory for any fixed model parameter in the hyperellipsoid uncertainty description. It is also assumed that no parameter vector in the uncertainty description results in an infeasible control problem; in other words, we assume that the process was designed properly [this flexibility issue is discussed in detail elsewhere (Biegler et al., 1997)].

Define $\hat{\theta}$ as the nominal parameter vector of dimension $n \times 1$. Since we are interested in complex systems, the corresponding control trajectory defined by the optimal control problem will be computed numerically and hence can be represented as a vector $\hat{u}$ of dimension $m \times 1$. For example, a convenient representation for $\hat{u}$ for an optimal temperature trajectory defined over a fixed range of time would be the temperatures at m discrete time instances along the trajectory.

Define $\bar{u}$ as the optimal control trajectory associated with the parameter vector θ. The model parameters are assumed to lie within the hyperellipsoid

$$\epsilon = \left\{ \theta : (\theta - \hat{\theta})^T V_\theta^{-1} (\theta - \hat{\theta}) \leq r^2(\alpha) \right\}, \qquad (1)$$

where V_θ is an $n \times n$ positive definite covariance matrix; α is the confidence level; and r is a distribution function. Uncertainty descriptions of this type are provided by algorithms that estimate the parameters from experimental data (Beck and Arnold, 1977; Ljung, 1987). For example, assume that
- There are no errors in the independent variables;
- This is no prior information regarding the parameters;
- The measurement errors are additive, zero mean, normal, and have known positive definite covariance matrix; and,
- Maximum likelihood estimation is used.

Then V_θ is given by

$$V_\theta = \left(X^T \text{cov}(e) X \right)^{-1}, \qquad (2)$$

where e is the measurement noise vector; $\text{cov}(e)$ is the covariance of e; X is the input data matrix; and $r^2(\alpha) = \chi_n^2(\alpha)$, the chi-squared distribution (Beck and Arnold, 1977). Other

assumptions, such as taking into account a prior parameter distribution (that is, Bayesian estimation) and making other statistical assumptions on the measurement noise (such as unknown error covariance), lead to different expressions for V_θ and $r(\alpha)$, which can be looked up in standard identification texts (Beck and Arnold, 1977). Taylor series expansions can be used to estimate parameter hyperellipsoids for nonlinear systems (Beck and Arnold, 1977).

In what follows we address four worst-case analysis problems:

1. Robustness of the optimal control trajectory to model uncertainty

2. Robustness of predicted optimal performance to model uncertainty

3. Robustness of predicted performance to model uncertainty

4. Robustness of predicted performance to control implementation uncertainty.

In each case the worst-case change in process operation and the associated worst-case parameter vector within the uncertainty set are estimated.

Step 1: analysis estimates based on Taylor series

Problem 1: Robustness of the Optimal Control Trajectory. The dependence of the optimal control policy on a fixed-parameter vector θ is represented by a nonlinear operator N that maps the parameter space into the space of optimal control trajectories:

$$\bar{u} = N(\theta) \tag{3}$$

$$\delta\bar{u} \equiv \bar{u} - \hat{u} = N(\theta) - N(\hat{\theta}). \tag{4}$$

Assume N is locally differentiable. Linearize N about the nominal parameter vector $\hat{\theta}$

$$L_{ij} = \left.\frac{\partial \bar{u}_i}{\partial \theta_j}\right|_{\theta = \hat{\theta}} \qquad m \times n \text{ matrix} \tag{5}$$

$$\delta\bar{u} = N(\theta) - N(\hat{\theta}) \approx L(\theta - \hat{\theta}) \equiv L\delta\theta. \tag{6}$$

The computation of L, as well as all other derivatives discussed in this article, is described in the Appendix.

Here the problem of interest is to estimate how close the optimal control trajectory computed for the model is to the optimal control trajectory for the real system (assumed to lie within the hyperellipsoid ϵ). With the closeness measured using a weighted Euclidean norm, this problem is stated mathematically as

$$\max_{\theta \in \epsilon} (\delta\bar{u})^T W_u (\delta\bar{u}), \tag{7}$$

where W_u is a specified positive semidefinite matrix (usually identity) and

$$\delta\bar{u}^T W_u \delta\bar{u} = (L\delta\theta)^T W_u(L\delta\theta) = \delta\theta^T L^T W_u L\delta\theta. \tag{8}$$

To simplify the algebra, define

$$x = r^{-1}(\alpha) V_\theta^{-1/2} \delta\theta. \tag{9}$$

Substituting Eqs. 8 and 9 into Eq. 7 results in

$$\max_{x^T x \leq 1} r^2(\alpha) x^T \left(V_\theta^{1/2}\right)^T L^T W_u L V_\theta^{1/2} x. \tag{10}$$

Recognizing that the maximization is a Raleigh quotient (Golub and van Loan, 1983) implies that a solution to the optimization problem is

$$x_{\max} = \pm v_1 \qquad (\text{either} + \text{or} - \text{will do}), \tag{11}$$

where

$$W_u^{1/2} L V_\theta^{1/2} = U\Sigma V^T \tag{12}$$

is the singular-value decomposition, and v_1 is the leftmost column of V. A worst-case parameter is

$$\delta\theta_{\max} = \pm r(\alpha) V_\theta^{1/2} v_1, \tag{13}$$

giving a worst-case deviation in control trajectory

$$\delta\bar{u}_{\max} = \pm r(\alpha) L V_\theta^{1/2} v_1 \tag{14}$$

with the objective value

$$\max_{\theta \in \epsilon} (\delta\bar{u})^T W_u(\delta\bar{u}) = r^2(\alpha)\sigma_{\max}^2, \tag{15}$$

where $\sigma_{\max}$ is the maximum singular value of $W_u^{1/2} L V_\theta^{1/2}$. This is an estimate of how far the optimal control trajectory based on the model can be from the optimal trajectory for the real system, and gives the corresponding worst-case parameter vector within the hyperellipsoid.

Some engineers may prefer to compute the worst-case optimal control move for each u_j, rather than to measure the worst-case change in u in terms of the weighted Euclidean norm (Eq. 7). In this case, the optimization problem is

$$\max_{x^T x \leq 1} |\delta\bar{u}_j|, \tag{16}$$

where

$$\delta\bar{u}_j = L_j\delta\theta = r(\alpha) L_j V_\theta^{1/2} x \tag{17}$$

and L_j is the jth row of L. A solution to this optimization problem is

$$x_{\max} = \pm \frac{1}{\|L_j V_\theta^{1/2}\|} V_\theta^{1/2} L_j^T, \tag{18}$$

where $\|\cdot\|$ is the Euclidean norm (Golub and van Loan, 1983). A worst-case parameter vector is

$$\delta\theta_{j,\max} = \pm \frac{r(\alpha)}{\|L_j V_\theta^{1/2}\|} V_\theta L_j^T, \tag{19}$$

with the worst-case jth control move being

$$\delta\bar{u}_{j,\max} \equiv \max_{x^T x \leq 1} |\delta\bar{u}_j| = r(\alpha)\|L_j V_\theta^{1/2}\|. \tag{20}$$

Problem 2: Robustness of Predicted Optimal Performance.
Here the problem of interest is to estimate how close the optimal performance objective computed from the model is to the optimal performance objective for the real system.

Define $\hat{y}$ as the (scalar) performance objective when the control trajectory has been optimized for the nominal parameter vector $\hat{\theta}$; $\bar{y}$ as the optimal performance objective for θ; and $\delta\bar{y} = \bar{y} - \hat{y}$. Then the problem of interest is to compute

$$\max_{\theta \in \epsilon} |\delta\bar{y}|. \qquad (21)$$

The approach to estimating the solution to this nonlinear program is similar as for Problem 1. Assume that $\bar{y}$ is locally differentiable in θ. Linearize $\bar{y}$ about the nominal parameter $\hat{\theta}$

$$\delta\bar{y} = \bar{y} - \hat{y} = \check{L}\delta\theta, \qquad (22)$$

where

$$\check{L}_j = \left.\frac{\partial \bar{y}}{\partial \theta_j}\right|_{\theta = \hat{\theta}} \qquad \text{(a row vector).} \qquad (23)$$

Following similar mathematics as in Problem 1 gives

$$\delta\theta_{\max} = \pm \frac{r(\alpha)}{\|\check{L}V_\theta^{1/2}\|} V_\theta \check{L}^T \qquad (24)$$

(one sign gives the worst case, and the other gives the best case), and

$$\delta\bar{y}_{\max} \equiv \max_{\delta\theta \in \epsilon} |\delta\bar{y}| = r(\alpha)\|\check{L}V_\theta^{1/2}\|. \qquad (25)$$

Problem 3: Robustness of Predicted Performance to Model Uncertainty. For this problem, we estimate how much performance objective y can be degraded by model uncertainty when the optimal control trajectory for the nominal process is implemented perfectly. Assume that y is locally differentiable in θ. Linearize y about the nominal parameter $\hat{\theta}$, *with the control trajectory fixed to its optimal value for $\hat{\theta}$*:

$$\tilde{L}_j = \left.\frac{\partial y}{\partial \theta_j}\right|_{\theta = \hat{\theta}} \qquad \text{(a row vector).} \qquad (26)$$

The optimization problem is posed and solved exactly as in Problem 2, with $\check{L}$ replaced with $\tilde{L}$.

Problem 4: Robustness of Predicted Performance to Control Implementation Uncertainties. Here we would like to estimate how much performance can be degraded by control implementation uncertainties, which is represented mathematically by

$$a \leq \delta u \leq b, \qquad (27)$$

where u is the control vector; $\delta u = u - \hat{u}$; a and b are vectors, and the inequalities are element by element. Approximate δy by the second-order Taylor series expansion about the optimal control trajectory:

$$\delta y = M\delta u + \delta u^T H_u \delta u, \qquad (28)$$

where

$$M_j = \left.\frac{\partial y}{\partial u_j}\right|_{u = \hat{u}} \qquad \text{(a row vector)} \qquad (29)$$

and

$$(H_u)_{ij} = \left.\frac{\partial^2 y}{\partial u_i \partial u_j}\right|_{u = \hat{u}} \qquad \text{(an } m \times m \text{ matrix).} \qquad (30)$$

In contrast to Problems 1, 2 and 3, the second-order terms may be required to obtain a good approximation in Eq. 28. Since the linearization is about the optimal control trajectory, elements of M that do not lie on an active constraint are zero (Luenberger, 1984), and the dependence of y on the corresponding elements of u are captured only in the second-order terms.

Mathematically, the analysis problem is to compute

$$\max_{a \leq \delta u \leq b} |\delta y| = \max_{a \leq \delta u \leq b} |M\delta u + \delta u^T H_u \delta u|. \qquad (31)$$

This problem, which is nonconvex in general, cannot be solved analytically, but can be written in terms of the mixed structured singular value μ, which is a matrix function commonly used in robustness analysis (Doyle, 1982; Fan et al., 1991). Define

$$w = \frac{1}{2}(b - a) \qquad (32)$$

and

$$z = \frac{1}{2}(b + a). \qquad (33)$$

Then for any real number k [this follows from similar algebraic manipulations as in (Braatz et al., 1994)]:

$$\max_{a \leq \delta u \leq b} |M\delta u + \delta u^T H_u \delta u| \geq k \Leftrightarrow \mu_\Delta(N) \geq k, \qquad (34)$$

where

$$N = \begin{bmatrix} 0 & 0 & kw \\ kH_u & 0 & kH_u z \\ z^T H_u + M & w^T & z^T H_u z + Mz \end{bmatrix}, \qquad (35)$$

and the perturbation block $\Delta = \text{diag}\{\Delta_r, \Delta_r, \delta_c\}$, where Δ_r consists of independent real scalars and δ_c is a complex scalar. Thus the optimization problem (Eq. 31) is equivalent to

$$\max_{\mu_\Delta(N) \geq k} k. \qquad (36)$$

Upper and lower bounds for this problem can be computed by iterative μ-computations, but a more efficient way is to use skewed-μ, which requires no more effort than that required for a single μ calculation (Fan and Tits, 1992; Ferreres and Fromion, 1997; Smith, 1990). These polynomial-time computations can be performed within a few minutes on a workstation for a problem with $m = 100$, with the upper and lower bounds usually quite tight (Young et al., 1991).

Step 2: improvement of estimates

In Step 1, Taylor series approximations were used to compute the worst-case analysis estimates. The accuracy of the estimates can be assessed by comparing their values with those obtained by a nonlinear dynamic simulation using the estimated worst-case parameter vector (Problems 1, 2 and 3) or control vector (Problem 4). In Step 2, the values obtained by the nonlinear dynamic simulation are used as the final analysis estimates. This procedure is illustrated in the following crystallization simulation.

Application: Crystallization Process

A crystallization process was selected for testing the effectiveness of the robustness analysis tools because: (1) it is industrially important, and (2) it is highly nonlinear, which should push the limits of the Taylor series approach.

The population-balance equation (PBE) approach accounts for the crystal distribution in size, location, and other state variables (Hulburt and Katz, 1964; Randolph and Larson, 1988). Let $f(L, t)$ be the population density distribution function for crystals such that

$f(L, t) dL =$ the number of particles in the system in the

range $L \pm dL$ at time t

where L is the characteristic length of the crystal and t is time. Assume that the crystals are characterized by one characteristic length L and have symmetrical shape so that the volumetric shape factor k_v, defined as

$$k_v = \frac{\text{Volume}}{L^3} \qquad (37)$$

is constant. Also, assume that the crystallizer is well-mixed, and growth dispersion, agglomeration, fracture, and attrition are negligible.

For a batch crystallizer, the population balance equation is given by

$$\frac{\partial f(L, t)}{\partial t} + \frac{\partial \{G(S, \boldsymbol{\theta}_g, L) f\}}{\partial L} = B(S, \boldsymbol{\theta}_b), \qquad (38)$$

where $G(S, \boldsymbol{\theta}_g, L)$ is the rate of crystal growth in units of length per time; $B(S, \boldsymbol{\theta}_b)$ is the nucleation rate (number of particles per unit time); $S = (C - C_{\text{sat}})/C_{\text{sat}}$ is the relative supersaturation; C_{sat} is the saturation concentration; C is the solute concentration; and $\boldsymbol{\theta}_g$ and $\boldsymbol{\theta}_b$ are the growth and nucleation parameters, respectively.

The method of moments replaces the partial differential equation (Eq. 38) by a set of ordinary differential equations, which simplifies the simulation and optimization of the batch crystallizer. Assume that the growth rate is independent of characteristic size L. The moment equations are derived by multiplying Eq. 38 by L^j, integrating over L, and placing on a per-mass-of-solvent basis (Hulburt and Katz, 1964):

$$\frac{d\hat{\mu}_0}{dt} = B$$

$$\frac{d\hat{\mu}_j}{dt} = jG\hat{\mu}_{j-1} + Br_0^j, \qquad j = 1, 2, \ldots, \qquad (39)$$

where r_0 is crystal size at nucleation and is assumed to be a constant, and the jth moment is defined by

$$\hat{\mu}_j \equiv \int_0^\infty L^j \hat{f}(L, t) \, dL, \qquad (40)$$

where $\hat{f}(L, T)$ is the population density distribution function on a per-mass-of-solvent basis.

The final crystals can be characterized in terms of the final amount of nucleated crystal mass relative to seed crystal mass (Jones, 1974). Quantifying this requires determining the final state of the crystals grown from seed. Writing a mass balance only over the seed crystals, and applying the method of moments gives

$$\frac{d\hat{\mu}_0'}{dt} = 0$$

$$\frac{d\hat{\mu}_j'}{dt} = jG\hat{\mu}_{j-1}', \qquad j = 1, 2, \ldots, \qquad (41)$$

where the prime indicates seed.

Assume constant volume. The amount of solute leaving the solution must be accounted for by crystal growth and nucleation:

$$\frac{d\hat{C}}{dt} = -3\rho_c k_v G\hat{\mu}_2 - \rho_c k_v Br_0^3, \qquad (42)$$

where ρ_c is the density of the crystal, and the solute concentration $\hat{C}$ is on a per-mass-of-solvent basis.

Several models for growth kinetics have been developed depending on the crystal growth mechanisms (Garside, 1984; O'Hara and Reid, 1973; Burton et al., 1951). The most popular model is given by (Randolph and Larson, 1988):

$$G = k_g S^g, \qquad (43)$$

where k_g and g are the growth parameters.

There are several different types of nucleation mechanisms (Randolph and Larson, 1988). This article considers secondary nucleation from crystal surfaces, since it is the predominant mechanism taking place in most seeded batch crystallizers. The nucleation rate is assumed proportional to the collision energy, with the rest of the kinetics being in standard power-law form (Nyvlt et al., 1985):

$$B = k_b S^b \hat{\mu}_3, \qquad (44)$$

where k_b and b are the nucleation parameters.

For specificity we consider the case where the supersaturation is created by reducing the temperature $T(t)$, although other methods of achieving supersaturation, such as antisolvent addition (Charmolue and Rousseau, 1991), can be formulated in a similar manner.

The optimal control formulation is a generalization of (Miller and Rawlings, 1994):

$$\text{optimize} \quad \Phi$$
$$T(t)$$

$$\text{subject to} \quad g_1(t) = T_{\min} - T(t) \le 0$$
$$g_2(t) = T(t) - T_{\max} \le 0 \qquad (45)$$
$$g_3(t) = \frac{dT(t)}{dt} - R_{\max} \le 0$$
$$g_4(t) = R_{\min} - \frac{dT(t)}{dt} \le 0$$
$$g_5 = \hat{C}_{\text{final}} - \hat{C}_{\max} \le 0,$$

where Φ is some desired characteristic of the crystals at the end of the batch (details below). The temperature constraints $g_1(t)$ to $g_4(t)$ ensure that the temperature profile stays within the operating range of the crystallizer. The constraint g_5 is the minimum yield constraint, as the final solute concentration specifies the amount of crystals produced.

Several objectives have been recommended to favor downstream operations or product quality. Ajinkya and Ray (1974) maximized the mean crystal size and suggested minimizing the second moment of the CSD. Jones (1974) maximized the final size of the seed crystals. Chang and Epstein (1982) maximized the number average size, maximized the total volume, and jointly (using a weighted factor) minimized the variance and maximized the number average size of the product CSD. Eaton and Rawlings (1990) minimized the ratio of the nucleated-crystal mass to seed-crystal mass.

In this article, three properties of the final CSD are investigated: weight mean size, coefficient of variation, and ratio of nucleated-crystal mass to seed-crystal mass. The three properties can be calculated directly from the moments (Randolph and Larson, 1988) (whether the goal is to maximize or minimize the property is also listed):

$$\text{Weight mean size} = \frac{\hat{\mu}_4}{\hat{\mu}_3} \quad \text{(maximize)} \qquad (46)$$

$$\text{Coefficient of variation} = \sqrt{\frac{\hat{\mu}_2 \hat{\mu}_0}{(\hat{\mu}_1)^2} - 1} \quad \text{(minimize)} \quad (47)$$

$$\frac{\text{Nucleated-crystal mass}}{\text{Seed-crystal mass}} = \frac{\hat{\mu}_3 - \hat{\mu}_3'}{\hat{\mu}_3'} \quad \text{(minimize)}. \qquad (48)$$

For brevity, the parameters (with units) for an industrial-scale crystallizer for potassium nitrate are reported elsewhere (Chung and Braatz, 1998). The nominal nucleation and growth parameters estimated from simulation data were

$$g = 1.31, \quad b = 1.84, \quad k_g = e^{8.79} \frac{\mu m}{\min},$$

$$k_b = e^{17.38} \frac{\text{particles}}{\text{cm}^3 \cdot \min}, \qquad (49)$$

Table 1. Optimal Nominal Performance Objectives

Performance Objective	$\hat{y}$
Weight mean size	455 μm
Coefficient of variation	1.11
Nucleation to seed mass ratio	0.23

with covariance matrix

$$V_\theta^{-1} = \begin{bmatrix} 102,873 & -21,960 & -7,509 & 1,445 \\ -21,960 & 4,714 & 1,809 & -354 \\ -7,509 & 1,809 & 24,225 & -5,198 \\ 1,445 & -354 & -5,198 & 1,116 \end{bmatrix} \qquad (50)$$

$\alpha = 0.05$, and $r^2(\alpha) = \chi^2(\alpha) = 9.49$. The covariance matrix indicates significant correlations among the parameter uncertainties.

The optimal nominal performance objectives are reported in Table 1.

Problem 1. For Step 1, the estimated worst-case changes in the 2-norm of the control trajectory (Eq. 15) with respect to weight mean size, coefficient of variation, and nucleation to seed mass ratio are summarized in Table 2. Table 3 gives the corresponding parameter vectors.

Table 2 indicates an insensitivity of the optimal temperature trajectory to the parameter variations with respect to the first and the third objectives. All of the worst-case $|\delta \bar{u}_j|$ in Eq. 20, for these two objectives, were less than 0.01°C for the entire length of the batch, also indicating this insensitivity. For the coefficient-of-variation objective, the optimal temperature trajectory for the real system differs significantly from that computed for the model. The importance of a temperature deviation greater than 0.1°C is demonstrated in the Problem 4 analysis given later.

The computed values of worst-case $|\delta \bar{u}_j|$ are given in Table 4. It shows that the parameter variations have a small effect on the optimal temperature trajectory at the beginning and the end of the batch, but has a large effect on the temperature trajectory during the middle of the batch run.

For Step 2, nonlinear dynamic simulation performed using $\delta\theta_{\max}$ as the model parameters suggests that the Taylor series expansion is sufficiently accurate for analysis purposes (see Table 2).

Table 2. Worst-Case Changes in the 2-Norm of the Control Trajectory

	Step 1 $\|\delta\bar{u}\|$	Step 2 $\|\delta\bar{u}\|$
Weight mean size	0.013°C	0.011°C
Coefficient of variation	0.37°C	0.30°C
Nucleation to seed mass ratio	0.0066°C	0.0075°C

Table 3. Worst-Case Parameter Vectors for Each Objective

	$\delta\theta_{\max}^T$			
Weight mean size	[−0.015	−0.045	−0.87	−4.05]
Coefficient of variation	[0.0076	0.0053	0.86	4.01]
Nucleation to seed mass ratio	[−0.042	−0.16	−0.87	−4.01]

Table 4. Worst-Case Optimal Control Move for Each $\bar{u}_j$, for the Coefficient of Variation Performance Objective

j	$|\delta \bar{u}_j|$	j	$|\delta \bar{u}_j|$
1	0	9	0.13
2	0	10	0.12
3	0	11	0.10
4	0	12	0.081
5	0.13	13	0.062
6	0.15	14	0.042
7	0.15	15	0.021
8	0.14	16	0.001

Problem 2. The worst-case changes in optimal weight mean size, coefficient of variation, nucleation to seed ratio, and their corresponding parameter vectors, are summarized in the Tables 5 and 6.

Table 5 indicates that the effects of uncertainty on the weight mean size and the coefficient of variation are relatively small, whereas the nucleation to seed mass ratio is highly sensitive to parametric uncertainty. For the weight mean size and coefficient of variation objectives, the nonlinear simulation values agree quite well with the values obtained by the Taylor series expansion. The larger difference between the performance objectives for the nucleation to seed mass ratio indicates the usefulness of Step 2 in improving the accuracy of the worst-case performance estimate.

Problem 3. The results for Problem 3 are nearly identical to those of Problem 2, both for the performance estimates from the Taylor series expansion, and for the nonlinear dynamic simulations. While this will not be true in general, the first author's MS Thesis contains a theoretical explanation why this occurs for some optimal control problems (Ma, 1999).

Problem 4. The worst-case performance degradations due to control implementation uncertainties are reported in Table 7. All of the performance objectives are relatively insensitive to 0.01°C variations in temperature, while being sensitive to 0.1°C variations in temperature. Among three objectives, we see that the nucleation to seed mass ratio objective is the most sensitive to control implementation uncertainties. The ratio is not affected significantly by 0.01°C temperature variations, but increases 143% when the temperature differs from the optimal trajectory by only 0.1°C. Note that controlling the temperature within 0.1°C is challenging for an industrial crystallizer, and that a perfectly implemented optimal cooling policy reduces the nucleation to seed mass ratio by 30% compared to natural cooling (Miller and Rawlings, 1994). This implies that the potential benefits from using an optimal control policy can be completely wiped out by variations in temperature of the magnitude expected in the operation of an industrial crystallizer. This agrees with the main conclusion

Table 5. Worst-Case Optimal Performance Objectives for Problem 2

	Step 1 $\delta \bar{y}_{max}$	Step 1 $\bar{y}_{max}$	Step 2 $\bar{y}_{max}$
Weight mean size	34	421	417
Coefficient of variation	0.04	1.15	1.14
Nucleation to seed mass ratio	0.14	0.37	0.46

Table 6. Worst-Case Parameter Vectors for Problem 2

	$\delta \theta_{max}^T$
Weight mean size	[−0.025 −0.15 0.76 3.55]
Coefficient of variation	[−0.07 −0.35 0.59 2.7]
Nucleation to seed mass ratio	[0.093 0.42 0.76 3.6]

Table 7. Worst-Case Performance Degradation Due to Different Levels of Control Implementation Uncertainty (Eq. 31)*

	Wt. Mean Size	Coeff. of Variation	Nucl. to Seed Mass Ratio
$b_j = − a_j = 0.1°C$	411 (408)	1.18 (1.26)	0.76 (0.56)
$b_j = − a_j = 0.01°C$	453 (450)	1.12 (1.15)	0.27 (0.24)

*The results of a nonlinear dynamic simulation using the estimated worst-case control implementation uncertainty are reported in parentheses. In all cases the upper and lower bounds for μ were nearly identical.

of a detailed parametric study by Bohlin and Rasmuson (1992)—that the benefits of controlled cooling could be lost without extremely accurate temperature control.

Miller and Rawlings (1994) showed that optimal control increased the weight mean size by 20% compared to using natural cooling. With Table 7 this indicates that, while 0.1°C variations in the implemented temperature trajectory may significantly reduce the weight mean size, attempting to implement the optimal control trajectory will still give better results than natural cooling. Approximately 50% of the expected benefits of optimal control could be lost due to control implementation uncertainties up to 0.1°C.

Problem 4 was repeated with H_u set to zero to see the importance of including second-order terms in the Taylor series expansion in Problem 4. The results were given in Table 8. From Table 8, it can be observed that if the temperature variations are $\leq 0.01°C$, the same results were obtained. However, if the temperature variations are up to 0.1°C, the results are significantly different. In particular, the estimate of the worst-case change in the weight mean size is significantly improved by including second-order terms in the Taylor series expansion.

Conclusions

Algorithms were developed for estimating the effects of parametric uncertainty and control implementation inaccuracy on the optimal open-loop control policy. The first step of the approach computes a worst-case parameter vector and an initial estimate of performance degradation based on a Taylor series expansion that describes the local behavior about the nominal trajectory. The second step uses a nonlin-

Table 8. Worst-Case Performance Degradation Due to Different Level of Control Implementation Uncertainty (Eq. 31) Without Using H_u

	Wt. Mean Size	Coeff. of Variation	Nucl. to Seed Mass Ratio
$b_j = − a_j = 0.1°C$	435	1.18	0.64
$b_j = − a_j = 0.01°C$	453	1.12	0.27

ear dynamic simulation to compute improved estimates. The difference between the initial and final estimates provides an indication as to the accuracy of the Taylor series expansion in capturing the process dynamics in the vicinity of the optimal control trajectory. These quantitative estimates can be used to decide whether more laboratory experiments are needed to produce parameter estimates of higher accuracy, or to define performance objectives for lower-level control loops that implement the optimal control trajectory.

The analysis tools were applied to a batch cooling crystallizer simulation. The nucleation to seed mass ratio was determined to be highly sensitive to both parametric uncertainty and control implementation inaccuracy. With all of the performance objectives, the benefits of controlled cooling could be lost without very accurate temperature control. Nonlinear dynamic simulations indicated that the Taylor series estimates were accurate enough for process engineering purposes.

Literature Cited

Ajinkya, M. B., and W. H. Ray, "On the Optimal Operation of Crystallization Processes," *Chem. Eng. Commun.*, **1**, 181 (1974).

Barrera, M. D., and L. B. Evans, "Optimal Design and Operation of Batch Processes," *Chem. Eng. Commun.*, **82**, 45 (1989).

Barton, P. I., R. J. Allgor, W. F. Feehery, and S. Galan, "Dynamic Optimization in a Discontinuous World," *Ind. Eng. Chem. Res.*, **37**, 966 (1998).

Beck, J. V., and K. J. Arnold, *Parameter Estimation in Engineering and Science*, Wiley, New York (1977).

Biegler, L. T., I. E. Grossmann, and A. W. Westerberg, *Systematic Methods of Chemical Process Design*, Prentice Hall, Upper Saddle River, NJ (1997).

Bohlin, M., and A. C. Rasmuson, "Application of Controlled Cooling and Seeding in Batch Crystallization," *Can. J. Chem. Eng.*, **70**, 120 (1992).

Braatz, R. D., "Robustness Margin Computation for Large Scale Systems," AIChE Meeting, Chicago, IL (1996).

Braatz, R. D., P. M. Young, J. C. Doyle, and M. Morari, "Computational Complexity of μ Calculation," *IEEE Trans. Automat. Cont.*, **AC-39**, 1000 (1994).

Burton, W., N. Cabrera, and F. Frank, "The Growth of Crystals and the Equilibrium Structure of Their Surfaces," *Philos. Trans. Roy. Soc. London, Ser. B— Biol. Sci.*, **243**, 299 (1951).

Caracotsios, M., and W. E. Stewart, "Sensitivity Analysis of Initial Value Problems with Mixed ODEs and Algebraic Equations," *Comput. Chem. Eng.*, **9**, 359 (1985).

Chang, C., and M. A. Epstein, "Identification of Batch Crystallization Control Strategies Using Characteristic Curves," *Nucleation, Growth, and Impurity Effects in Crystallization Process Engineering*, Vol. 78, AIChE Symposium Series No. 215, AIChE, New York, p. 68 (1982).

Charmolue, H., and R. W. Rousseau, "L-Serine Obtained by Methanol Addition in Batch Crystallization," *AIChE J.*, **37**, 1121 (1991).

Chung, S. H., and R. D. Braatz, "Modeling and Simulation of Crystallization," LSSRL Tech. Memo UIUC-LSSRL 98-004, Univ. of Illinois, Urbana, IL (1998).

Diwekar, U. M., K. P. Madhavan, and R. E. Swaney, "Optimization of Multicomponent Batch Distillation Columns," *Ind. Eng. Chem. Res.*, **28**, 1011 (1989).

Doyle, J. C., "Analysis of Feedback Systems with Structured Uncertainties," *IEE Proc., Pt. D*, **129**, 242 (1982).

Eaton, J. W., and J. B. Rawlings, "Feedback Control of Chemical Processes Using On-Line Optimization Techniques," *Comput. Chem. Eng.*, **14**, 469 (1990).

Fan, M. K. H., and A. L. Tits, "A Measure of Worst-Case H_∞ Performance and of Largest Acceptable Uncertainty," *Syst. Control Lett.*, **18**, 409 (1992).

Fan, M. K. H., A. L. Tits, and J. C. Doyle, "Robustness in the Presence of Mixed Parametric Uncertainty and Unmodeled Dynamics," *IEEE Trans. Automat. Cont.*, **AC-36**, 25 (1991).

Ferreres, G., and V. Fromion, "Computation of the Robustness Margin with the Skewed μ Tool," *Syst. Control Lett.*, **32**, 193 (1997).

Garside, J., "Advances in Characterisation of Crystal Growth," *Advances in Crystallization from Solutions*, Vol. 80, AIChE Symp. Ser. No. 240, AIChE, New York, p. 23 (1984).

Golub, G. H,, and C. F. van Loan, *Matrix Computations*, Johns Hopkins Univ. Press, Baltimore, MD (1983).

Hulburt, H. M., and S. Katz, "Some Problems in Particle Technology," *Chem. Eng. Sci.*, **19**, 555 (1964).

Jones, A. G., "Optimal Operation of a Batch Cooling Crystallizer," *Chem. Eng. Sci.*, **29**, 1075 (1974).

Ljung, L., *System Identification: Theory for the User*, Prentice Hall, Englewood Cliffs, NJ (1987).

Loeblein, C., J. D. Perkins, B. Srinivasan, and D. Bonvin, "Performance Analysis of On-Line Batch Optimization Systems," *Comput. Chem. Eng.*, **21**, S867 (1997).

Leunberger, D. G., *Linear and Nonlinear Programming*, 2nd ed., Addison-Wesley, Reading, MA (1984).

Ma, D. L., "Worst-Case Performance Analysis of Optimal Control Trajectories in Batch Crystallization," MS Thesis, Univ. of Illinois, Urbana, IL (1999).

Miller, S. M., and J. B. Rawlings, "Model Identification and Control Strategies for Batch Cooling Crystallizers," *AIChE J.*, **40**, 1312 (1994).

Nyvlt, J., O. Sohnel, M. Matuchova, and M. Broul, *The Kinetics of Industrial Crystallization*, Vol. 19, Chem. Eng. Monographs, Elsevier, Amsterdam (1985).

O'Hara, M., and R. C. Reid, *Modelling Crystal Growth Rates from Solution*, Prentice Hall, Englewood Cliffs, NJ (1973).

Randolph, A., and M. A. Larson, *Theory of Particulate Processes*, 2nd ed. Academic Press, San Diego (1988).

Ray, W. H., *Advanced Process Control*, McGraw-Hill, New York (1981).

Rippin, D. W. T., "Simulation of Single and Multiproduct Batch Chemical Plants for Optimal Design and Optimization," *Comput. Chem. Eng.*, **7**, 137 (1983).

Smith, R. S. R., "Model Validation for Uncertain Systems," PhD Thesis, California Institute of Technology, Pasadena (1990).

Torvi, H., and T. Hertzberg, "Estimation of Uncertainty in Dynamic Simulation Results," *Comput. Chem. Eng.*, **21**, S181 (1997).

Young, P. M., M. P. Newlin, and J. C. Doyle, "μ Analysis with Real Parametric Uncertainty," *Proc. IEEE Conf. on Decision and Control*, IEEE Press, Piscataway, NJ, p. 1251 (1991).

Appendix: Derivative Computation

An easy-to-implement method to compute the derivatives is by divided differences. Criteria for selecting the size of the perturbations are provided in textbooks (Beck and Arnold, 1977). An alternative approach, which augments the original differential equations with sensitivity equations (Beck and Arnold, 1977; Caracotsios and Stewart, 1985), can be applied directly to compute $\tilde{L}$, M, and H_u.