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Open-loop and closed-loop robust optimal control of batch processes using distributional and worst-case analysis

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Abstract

The recognition that optimal control trajectories for batch processes can be highly sensitive to model uncertainties has motivated the development of methods for explicitly addressing robustness during batch processes. This study explores the incorporation of robust performance analysis into open-loop and closed-loop optimal control design. Several types of robust performance objectives are investigated that incorporate worst-case or distributional robustness metrics for improving the robustness of batch control laws, where the distributional approach computes the distribution of the performance index caused by parameter uncertainty. The techniques are demonstrated on a batch crystallization process. A comprehensive comparison of the robust performance of the open-loop and closed-loop system is provided.

Keywords: Optimal control; Batch control; Robustness analysis; Robust control; Crystallization

1. Introduction

Batch processes are common in the pharmaceutical, microelectronics, food, and fine chemical industries. Process optimization has the potential to reduce production costs, improve product quality, reduce product variability, and ease scale-up. Recent advances in the development of reliable models as well as reliable on-line measuring devices (e.g. on-line spectroscopy) have increased the use of mathematical modeling and optimization techniques for improving batch process operation. Performing off-line the open-loop optimization with nominal values of the parameters and then implementing the optimal trajectory is the approach used most frequently [1]. However, it is impossible to generate highly accurate models for most chemical processes due to the limited quality and quantity of experimental data. Thus, the practical implementation of model-based simulation results often leads to differences between reality and simulation, whether the model is used for controller design or process optimization. Consequently, taking parameter uncertainty into account during optimization and controller design is of significant importance.

A fundamental feature of batch process optimization is that the desired performance can be expressed as a function of the final states. Several approaches have been proposed for incorporating uncertainty into the end-point optimization of nonlinear batch processes [2–4]. A simplified breakdown of the approaches is presented in Fig. 1. One category of techniques deals with the determination of the best open-loop control trajectory, which ensures minimum degradation of the end-point performance under model parameter uncertainty or disturbances. Another category tries to increase robustness by using feedback control instead of open-loop control. A straightforward extension of the open-loop robust optimization techniques is based on repeating the open-loop optimization on-line based on feedback of the measured (estimated) variables [2,4]. One approach to incorporate uncertainty in the formulation of the optimal control problem is to consider the worst-case objective (this is referred to as the minmax approach). Other techniques minimize the expected value of the objective, or consider multiobjective approaches with at least one term measuring robustness. Techniques based

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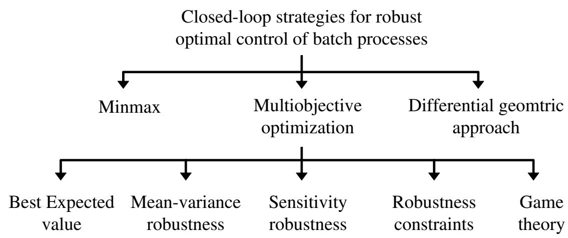

Fig. 1. Generic breakdown of robust optimal control strategies for batch processes. Most closed-loop strategies have open-loop analogues. Nearly any open-loop strategy can be formulated as a closed-loop strategy by extending the optimization vector or by using a shrinking-horizon model predictive control approach.

on the general property of using feedback to compensate for uncertainties also have been proposed that do not explicitly take parameter uncertainty into consideration in the formulation of the objective function [5]. In Alamir and Balloul [6], a robust state feedback formulation was suggested based on a receding horizon implementation of an open-loop minmax optimization problem. The problem with most minmax approaches described in the literature is that they usually handle only uncertainties in terms of independent bounds on each parameter. Although techniques that extend this approach to more general uncertainity descriptions have been proposed [7,8], since the computed profile minimizes a worst-case objective where the worst-case value has a low probability of occurring, poor results can be obtained for more representative parameter values (such as the nominal case).

Different approaches have been proposed to avoid the disadvantages of the minmax technique. Usually in these cases the objective accounts for both nominal and robust performance and the final solution is the result of the tradeoff between the two. The sensitivity robustness approach, for example, uses a deterministic framework in which the objective function is the weighted sum of the performance index computed with the nominal parameters, and a penalty term that minimizes the sensitivity of the performance index to variations of the parameters due to uncertainties [9]. The disadvantage of this approach is that usually it is unclear how to correctly weigh the effects of different parameter sensitivities.

Techniques based on the minimization of the expectation of the end-point performance can cope with general stochastic formulations of the uncertainty [10]. However, this leads to a high dimensional augmented dynamic system due to the discretization of the parameter space or to multiple simulations using Monte Carlo sampling. These approaches are computationally expensive, but on the other hand the structure of the problem is well suited for efficient implementation via parallelization. Although this approach takes into account the variation of parameters due to uncertainty, it can provide inadequate robustness since there is no explicit penalty of the variation in the performance objective due to parameter variations. As an example, it is straightforward to show that minimizing the expected value will provide *no* improvement in robustness when the performance objective is linear in the parameters. The mean–variance approach uses the same general stochastic framework as the expected performance minimization but explicitly takes into account the effects of parameter uncertainties by minimizing the weighted sum of the expected value of the performance index and the variance of the performance index to the effects of uncertainty [11].

The problem with the weighted-sum approaches is that the weighting coefficient does not directly correspond to the relative importance of the objectives, so that obtaining a proper trade-off requires trial-and-error. An approach that addresses this issue is to add robustness constraints to the formulation of the optimization problem rather then using the penalty robustness term in the objective function. Valappil and Georgakis [12,13] proposed an extended Kalman filter (EKF)-based model predictive control approach to control the end-use properties in batch reactors. The approach handles model uncertainty by determining the uncertainty in the predicted final values of the properties, in the form of elliptical confidence regions, and ensures that the complete confidence region is within the target region by adding some hard constraints to the on-line optimization problem. Mohideen et al. [14] proposed the introduction of robust stability constraints in the formulation of the optimization problem, based on the measure of a matrix. Although the approach provides the optimal design of a dynamic system under robust stability consideration, the conceptual mathematical formulation of the approach leads to a computationally expensive infinite-dimensional stochastic mixed-integer optimal control problem. Visser et al. [15] proposed a cascade optimization framework in which the feasibility of the open-loop optimization under uncertainty is guaranteed by adding a back-off term to the constraints and the robust performance is enhanced by repeating the optimization on-line.

An elegant generalization of the aforementioned multiobjective approaches can be formulated in the differential game framework. This approach simulates a game of "engineer" versus "nature" where the engineer represents the nominal performance and nature represents the uncertainty [16]. Although this technique can be considered a unifying framework for all other approaches, it involves highly complex numerical problems and large computing effort, with very few applications in chemical engineering.

Robust feedback control laws have been developed for the end-point optimization of nonlinear batch processes, using a differential geometric approach [17,18].

This approach requires the analytical computation of Lie brackets and has many restrictions including that the process must be minimum phase. In Terwiesch and Astolfi [16], robust state-feedback and output-feedback control laws are proposed based on the nonlinear H_∞ formulation. In this approach a positive definite function that solves the Hamilton–Jacobi partial differential equation needs to be computed. The solution is then obtained by performing a high order series expansion of the partial differential equation, leading to a set of ordinary differential equations. The main drawback of the approach is that the nonlinear system has to be written in a form that is affine in the model parameters and control inputs, which is seldom possible. Additionally, the series expansion for complex systems results in a prohibitively large number of differential equations (e.g. for the crystallization system considered in this paper a fourth-order expansion would lead to almost one thousand equations).

A conceptually different approach to account for parameter uncertainties is to use the measurements to estimate the uncertain parameters on-line and recompute the optimal trajectories using the estimated values [3,19–23]. In this approach the on-line optimization problem is split into two subproblems. First measurements are used to estimate the parameters and states, and next this information is used to determine the control input by solving an optimization problem with respect to some performance criteria. The advantages of this approach are that the on-line parameter estimation allows for model prediction in the optimization which can produce small end-point deviations even in the presence of unmeasured disturbances and model-plant mismatch, and that the approach can successfully handle time-varying parameters. In this approach the states and model parameters usually have to be estimated simultaneously. This can be done in a unifying framework in which the parameters appear as a subset of the state variables in the combined process and parameter models and using an estimator (e.g., an Extended Kalman filter) for the simultaneous state and parameter estimation. However, this technique requires that the observability condition is satisfied for the augmented system. This condition is often not satisfied even if the initial model is observable. Also, a sufficiently exciting input is required for successful parameter estimation. Unfortunately, the optimal inputs usually do not provide sufficient excitation of the system, causing a conflict between the objectives of optimization and parameter identification.

A feature of most of the aforementioned robust optimization papers is the lack of a systematic analysis of the robust performance of the proposed approach. Usually simulations are presented by selecting several values for the uncertain parameters. Monte Carlo simulations can be used for more detailed stochastic analysis. However these methods are often prohibitively expensive. To reduce computational burden the parametric uncertainty analysis can be performed based on series expansion of the detailed model [7,8,24] or using a polynomial chaos expansion-based probabilistic collocation method [25]. Despite the abundant robust control literature there is a lack of robust performance comparison studies between open-loop and closed-loop control strategies. The main objective of this paper is to provide a comprehensive analysis of the robust performance of the end-point optimal control of nonlinear batch processes. The effects of using feedback are compared to open-loop optimal control in the case of nominal and robust optimization approaches applied to both the open-loop and closed-loop systems. This paper utilizes a technique that computes the entire distribution of the process outputs along the whole batch run. The approach is based on an analysis tool [7,8,26] that computes the worst-case deviation of the output due to uncertainties described by general Hölder norms. This analysis tool provides a quantifiable link between parameter uncertainty and its effect on all process variables, and it can be incorporated in the optimization process (in both the open-loop and closed-loop cases) to enhance robust performance. Two robust optimization approaches that incorporate this analysis tool are presented and used to obtain both the open-loop and closed-loop robust control laws. The advantages and disadvantages of various methods are emphasized through application to the batch crystallization of an inorganic chemical subject to uncertainties in the nucleation and growth kinetics.

2. Worst-case and distributional robustness analysis

This section briefly summarizes the worst-case robustness analysis technique [7,8,26] and its extension to distributional analysis. Define the perturbed model parameter vector of dimension n_θ,

$$\theta = \hat{\theta} + \delta\theta, \tag{1}$$

where $\hat{\theta}$ is the nominal model parameter vector of dimension n_θ and $\delta\theta$ is the perturbation about $\hat{\theta}$. Due to stochastic measurement noise, parameter estimates fit to data are stochastic variables. Define $\hat{\psi}$ as the performance for the nominal model parameters $\hat{\theta}$, ψ as its value for the perturbed model parameter vector θ, and the difference $\delta\psi = \psi - \hat{\psi}$. The worst-case robustness approach writes $\delta\psi$ as a power series in $\delta\theta$ and then uses analytical expressions (for the first-order case [27]) or the skewed structured singular value [28,29] to compute worst-case values for $\delta\psi$ and $\delta\theta$. Accurate analysis can be obtained with very few terms in the series expansion (typically one or two) because for robustness analysis purposes the expansion only needs to be accurate for the trajectories (each trajectory being associated with one perturbed model parameter vector) about the nominal trajectory. The terms in the series expansion can be computed by finite differences or by integrating the original differential-algebraic equations augmented with an additional set of differential equations known as sensitivity equations [30].

Although the methods of [7,8,26] apply to general p-norm uncertainty descriptions including independent bounds on each parameter, this presentation will focus on the hyperellipsoidal uncertainty description since it is produced by more than 90% of the available algorithms to estimate parameters from experimental data [31,32]. Under the most common assumptions, this description is

$$E_\theta = \{\theta : (\theta - \hat{\theta})^{\mathrm{T}} \mathbf{V}_\theta^{-1} (\theta - \hat{\theta}) \leqslant \chi^2_{n_\theta}(\alpha)\}, \tag{2}$$

where $\mathbf{V}_\theta$ is the $(n_\theta \times n_\theta)$ positive definite covariance matrix, α is the confidence level, and $\chi^2_{n_\theta}(\alpha)$ is the chi-squared distribution function with n_θ degrees of freedom. A "hard" or worst-case model uncertainty description is obtained by fixing the confidence level.

A probability density function (PDF) for the model parameters is needed to compute the PDF of the performance index. More than 90% of the available algorithms to estimate parameters from experimental data [31,32] produce a multivariate normal distribution:

$$f_{\mathrm{p.d.}}(\theta) = \frac{1}{(2\pi)^{n_\theta/2} \det(\mathbf{V}_\theta)^{1/2}} \exp\left(-\frac{1}{2}[(\theta - \hat{\theta})^{\mathrm{T}} \mathbf{V}_\theta^{-1} (\theta - \hat{\theta})]\right). \tag{3}$$

When a first-order series expansion is used to relate $\delta\psi$ and $\delta\theta$, then the estimated PDF of ψ is

$$f_{\mathrm{p.d.}}(\psi) = \frac{1}{V_\psi^{1/2}\sqrt{2\pi}} \exp(-(\psi - \hat{\psi})^2/(2V_\psi)), \tag{4}$$

where the variance of ψ is

$$V_\psi = L\mathbf{V}_\theta L^{\mathrm{T}} \tag{5}$$

with

$$L_i(t) = \left.\frac{\partial \psi(t)}{\partial \theta_i}\right|_{\theta=\hat{\theta}} \quad \forall i = 1, \ldots, n_\theta, \tag{6}$$

where t is time. The distribution is a function of time since the nominal value for ψ and the vector of sensitivities L are functions of time.

Analytical expressions for the distribution cannot be obtained for higher order series expansions. In this case the relationship between θ and ψ is nonlinear and the probability distribution function must be computed numerically. The PDF could be obtained by performing Monte Carlo simulation by sampling the parameter space given by the uncertainty description. The drawback of this approach is that it requires a large number of samples to accurately describe the distribution especially for values with low probability, which is computationally expensive. A more computationally efficient approach is to map only the contours of the uncertainty hyperellipsoids obtained for different α levels. The mapping is performed via the worst-case analysis techniques by computing the worst-case $\delta\psi$ for different α-levels, which are used to construct its PDF. In other words, the hard bound defined by the confidence region on the parameter uncertainties is mapped to hard bounds on ψ, with each set of hard bounds parameterized by a confidence level α. The α-level sets on ψ produced by repeating this calculation for different confidence levels is used to construct its probability distribution function.

This mapping requires taking the different dimensionalities of the model parameter vector and performance objective into account. For specificity this accounting is illustrated with the uncertainty description (2). The mapping of the α levels is performed from the n_θ dimensional space characterized by a χ^2 distribution of n_θ degrees of freedom $(\chi^2_{n_\theta}(\alpha))$ to an n_ψ dimensional space in which the same α-levels are characterized by a chi-squared distribution but with n_ψ degrees of freedom $(\chi^2_{n_\psi}(\alpha))$. To capture the probability mapping between the two spaces characterized by different degrees of freedom, the worst-case deviations $(\delta\psi_{\mathrm{w.c.}})$ is multiplied by the ratio $\sqrt{\chi^2_{n_\psi}(\alpha)}/\sqrt{\chi^2_{n_\theta}(\alpha)}$. Hence, an estimate of the mapped confidence interval for a certain α is

$$\Psi(\alpha) = [\hat{\psi} - (\chi^2_{n_\psi}/\chi^2_{n_\theta})^{1/2}\delta\psi_{\mathrm{w.c.}}(\alpha), \hat{\psi} + (\chi^2_{n_\psi}/\chi^2_{n_\theta})^{1/2}\delta\psi_{\mathrm{w.c.}}(\alpha)]. \tag{7}$$

When the series expansion is linear it can be shown analytically that this approach gives the PDF (4). The accuracy of this approach for higher order series expansions has been tested numerically using Monte Carlo simulations [24].

These robustness analysis approaches can be applied to any state or function of the states. Also note that the approach can be applied to unmodeled dynamics by inserting additional differential equations with uncertain parameters (for example, an additional first-order response with uncertain gain and time constant) or by inserting phase using an uncertain time delay [33]. The approaches also can be applied to analyze the effects of measurement noise and disturbances, since their mathematical representation is similar to model uncertainties.

3. Robust end-point optimization of batch processes

3.1. Robust open-loop optimal control

In batch optimization the objective corresponds to some specifications at the end of the batch:

$$\min_{u(t)\in\mathscr{U}} \quad \psi(x(t_\mathrm{f}),\theta), \tag{8}$$

$$\text{s.t.} \quad \dot{x}(t) = f(x(t),u(t),\theta), \quad x(0)=x_0, \tag{9}$$

$$h(x(t),u(t),\theta) \leqslant 0, \tag{10}$$

where t_f is the final time, $x(t)\in\mathbb{R}^{n_x}$ is the n_x vector of states, $u(t)\in\mathscr{U}$ is the n_u set of all possible trajectories, $\theta\in\mathscr{P}$ is the vector of model parameters in the uncertainty set $\mathscr{P}$, f is the vector function $f:\mathbb{R}^{n_x}\times\mathscr{U}\times\mathscr{P}\rightarrow\mathbb{R}^{n_x}$ that describes the dynamic equations of the system, $h:\mathbb{R}^{n_x}\times\mathscr{U}\times\mathscr{P}\rightarrow\mathbb{R}^{c}$ is the vector of functions describing the linear and nonlinear, time-varying or end-time algebraic constraints for the system, and c is the number of these constraints. Although we represent here the process model (9) as a set of ordinary differential equations (ODE), the approaches are applicable to process models described by general differential-algebraic equations (DAE) or integro-partial differential equations.

In the nominal case the optimization problem (8)–(10) is solved by fixing $\theta=\hat{\theta}$, yielding the nominal optimal control trajectory $\hat{u}(t)$. In the uncertain case the variation of model parameters is incorporated into the optimization to produce a robust control trajectory. Two formulations for the robust performance objective are considered here.

The first approach is the minmax approach that minimizes the worst-case deviation of the end-point performance index:

$$\min_{u(t)\in\mathscr{U}} \quad \psi_{\text{w.c.}}(x(t_\mathrm{f}),\theta) \tag{11}$$

subject to (9) and (10). The worst-case deviation is computed with the analysis techniques described in the previous section. The main advantage of this approach compared to other minmax optimizations is that it can incorporate all the usual uncertainty descriptions (e.g., independent bounds on each parameter), or situations where different uncertainty descriptions are used for different subsets of the parameters. While this approach provides the best value for the worst-case performance deviation, it may yield poor results in other more likely cases (e.g. the nominal case). A multiobjective optimization avoids this drawback. One of the objectives is the nominal value of the end-point objective computed with the nominal parameter vector and the other is the variance of the objective around the nominal value, caused by parameter uncertainty:

$$J_1 = \psi(\hat{x}(t_\mathrm{f}),\hat{\theta}), \tag{12}$$

$$J_2 = \mathrm{Var}\,(\psi(x(t_\mathrm{f}),\theta)). \tag{13}$$

The objective (13) is computed using the distributional analysis technique presented in the last section. The advantage of this approach is that the computational burden of obtaining the variance of the objective is much smaller than in other probabilistic formulations presented in the literature. When a first-order series expansion is used the variance is computed similarly as in the mean–variance approach described in [11]. However, in the proposed technique the nominal value of the end-point performance is used in the objective function rather than its expected value. This approach provides a better evaluation of the nominal performance since for nonlinear systems the expected value of the performance index can be significantly different from its nominal value (these are equivalent when the performance index is linear in the parameters).

The two main approaches to formulating multiobjective optimization problems are the weighted-sum and ε-constraint techniques. In the former the multiobjective problem of minimizing the vector $J=[J_1 \quad J_2]$ is converted into a scalar problem by using the weighted sum of the objectives:

$$\begin{aligned} &\min_{u(t)\in\mathscr{U}} \quad \{J_1 + wJ_2\}, \\ &\text{s.t.} \quad (9)\ \text{and}\ (10), \end{aligned} \tag{14}$$

where w is the weighting coefficient. The ε-constraint technique minimizes a primary objective, J_1 and expresses the other as an inequality constraint:

$$\begin{aligned} &\min_{u(t)\in\mathscr{U}} \quad J_1, \\ &\text{s.t.} \quad (9)\ \text{and}\ (10), \\ &J_2 \leqslant \varepsilon. \end{aligned} \tag{15}$$

The advantage of the multiobjective approaches is that the tradeoff between nominal and robust performance can be controlled by appropriately weighting the two objectives or choosing the value for the constraint, respectively. Each approach involves a user-specified parameter. The latter approach has the weakness that a poor choice of ε may result in an infeasible problem.

A popular way to solve the infinite-dimensional optimization problems (14) and (15) is by describing the control input $u(t)$ as linear piecewise trajectories by discretizing the batch time in N equal intervals and considering the control values at each intersection as the optimization variables. An alternative is to use Lagrangian polynomials to approximate the control path [11]. The simplest approach to solving the optimization problem is to solve the optimization and model equations sequentially, by integrating the model along the input profile for each iteration of the optimization. This approach is applicable even if the optimal solution is discontinuous due to state and terminal time constraints. The implementation of state constraints is not always straightforward using the sequential solution technique, in which case approaches that solve the model equations simultaneously with the optimization problem can be used [34,35].

The corresponding multiobjective approach when using only hard bounds on the uncertainty is to replace

J_2 with the worst-case value for the performance objective deviations $\delta\psi_{\text{w.c.}}$. This approach behaves similarly to the distributional approach.

3.2. Robust closed-loop optimal control

It is a common opinion that state feedback based on the nominal model improves robust performance compared with open-loop implementation. However this is not always true for a particular system with uncertainty description. Feedback increases coupling between variables, thus in the process of reducing the effects of uncertainty for some of the variables, the sensitivity of other variables to variation in model parameters may be increased. The aforementioned robustness analysis techniques also apply when either linear or nonlinear feedback is present. In this case the controller and the process are treated as one system, and the analysis is performed with the feedback controller incorporated.

Consider the case where the feedback law is provided by an output feedback controller:

$$u(t) = u_{\text{ref}}(t) + \mathbf{K}(y(t) - y_{\text{ref}}(t)), \tag{16}$$

where y represents the measurements, $y_{\text{ref}}(t)$ is the output reference vector obtained with the open-loop optimal input $u_{\text{ref}}(t)$, and $\mathbf{K}$ is the static or dynamic gain matrix of the feedback controller.

The optimal control problem in the closed-loop scenario can be stated similarly as in the open-loop case, except that the decision parameters are the reference control trajectory and the gain matrix of the controller:

$$\min_{\mathbf{K},u_{\text{ref}}(t)} \quad \psi(x(t_f), \theta), \tag{17}$$

$$\text{s.t.} \quad \dot{x}(t) = f(x(t), u(t), \theta), \quad x(0) = x_0, \tag{18}$$

$$y(t) = g(x(t), u(t), \theta), \tag{19}$$

$$u(t) = u_{\text{ref}}(t) + \mathbf{K}(y(t) - y_{\text{ref}}(t)), \quad u(t) \in \mathscr{U}, \tag{20}$$

$$h(x(t), u(t), \theta) \leqslant 0. \tag{21}$$

Solving off-line the optimization problem (17)–(21) with constant parameter vector $\theta = \hat{\theta}$ gives the nominal optimal gain and nominal optimal open-loop control trajectory. With the nominal performance index this approach is similar to that proposed by Bhatia and Biegler [5]. They demonstrate how simple feedback correction can enhance robust performance. However, additional improvement of the robust performance can be achieved when parameter uncertainty is explicitly taken into consideration, as it is illustrated in the case study. To incorporate uncertainties in the optimization, the aforementioned minmax and multiobjective approaches can be used in the closed-loop case, too, to compute a robust optimal feedback gain and associated reference trajectory.

The optimization problem (17)–(21) is solved by discretizing the batch time in N discrete intervals, as described in the open-loop case. The control inputs $u(k)$ at every discrete time $k = 0, \ldots, N$ and the coefficients of the dynamic feedback gain matrix $\mathbf{K}(i,k)$ with $i = \dim(y)$ or static feedback gain vector $\mathbf{K}(i)$, are considered as the optimization variables. In the crystallization example that follows, the optimization was solved iteratively, determining the optimal $u(k)$ by solving an inner optimization problem for each step of the outer optimization loop of obtaining the optimum $\mathbf{K}$. This nested optimization algorithm provided better convergence than simultaneously using $u(k)$ and $\mathbf{K}$ as decision variables in the optimization. The optimization is solved off-line and the robust analysis is performed with the obtained feedback gain. Techniques that repeatedly solve similar optimization problems on-line, which belong to the category of nonlinear model predictive control [36,37], are not treated in this paper although the robust analysis and design approaches are applicable to such control systems.

4. Case study: batch crystallization

4.1. Problem formulation

Here the robust optimization techniques are applied to a batch KNO_3 crystallization process for both the open-loop and closed-loop scenarios. The mathematical model is [38]:

$$x^{\mathrm{T}} = [\mu_0, \ldots, \mu_4, C, \mu_{\text{seed},1}, \ldots, \mu_{\text{seed},3}, T], \tag{22}$$

$$f(x,u,\theta) = \begin{bmatrix} B \\ G\mu_0 + Br_0 \\ 2G\mu_1 + Br_0^2 \\ 3G\mu_2 + Br_0^3 \\ 4G\mu_3 + Br_0^4 \\ -\rho_c k_v(3G\mu_2 + Br_0^3) \\ G\mu_{\text{seed},0} \\ 2G\mu_{\text{seed},1} \\ 3G\mu_{\text{seed},2} \\ \dfrac{-UA(T - T_j) - 3\Delta H_c(C)\rho_c k_v G\mu_2 m_s}{(\rho_c k_v \mu_3 + C + 1)m_s c_p(C)} \end{bmatrix}, \tag{23}$$

where μ_i is the ith moment $(i = 0, \ldots, 4)$ of the total crystal phase and $\mu_{\text{seed},j}$ is the jth moment $(j = 0, \ldots, 3)$ corresponding to the crystals grown from seed, C is the solute concentration, T is the temperature, r_0 is the crystal size at nucleation, k_v is the volumetric shape factor, ρ_c is the density of the crystal, U is the heat transfer coefficient, A is the heat transfer area, m_s is the mass of the solvent, $\Delta H_c(C)$ is the heat of crystallization which is an empirical function of the solute concentration, and $c_p(C)$ is the heat capacity of the slurry [27].

The crystal growth rate (G) and the nucleation rate (B) are [38]:

$$G = k_g S^g, \tag{24}$$

$$B = k_b S^b \mu_3, \tag{25}$$

where $S = (C - C_{\text{sat}})/C_{\text{sat}}$ is the relative supersaturation, and $C_{\text{sat}} = C_{\text{sat}}(T)$ is the saturation concentration. The model parameter vector consists of the kinetic parameters for growth and nucleation

$$\theta^{\mathrm{T}} = [g, \ln(k_g), b, \ln(k_b)] \tag{26}$$

with nominal values

$$\hat{\theta}^{\mathrm{T}} = [1.31, 8.79, 1.84, 17.38] \tag{27}$$

and the uncertainty description (2) characterized by the covariance matrix [7]:

$$V_\theta^{-1} = \begin{bmatrix} 102873 & -21960 & -7509 & 1445 \\ -21960 & 4714 & 1809 & -354 \\ -7509 & 1809 & 24225 & -5198 \\ 1445 & -354 & -5198 & 1116 \end{bmatrix}. \tag{28}$$

The control input is the jacket temperature:

$$u(t) = T_j(t). \tag{29}$$

The temperature profile is described as linear piecewise trajectories obtained by discretizing the batch time in N intervals and considering the temperatures at every discrete time as the optimization variables.

The optimization objective considered is the minimization of the nucleated crystal mass to seed crystal mass ratio at the end of the batch:

$$\psi(x(t_{\mathrm{f}})) = \frac{\mu_3 - \mu_{\text{seed},3}}{\mu_{\text{seed},3}}. \tag{30}$$

Additionally the variation of another CSD parameter, the weight mean size, is also computed:

$$\mathrm{WMS} = \frac{\mu_4}{\mu_3}. \tag{31}$$

The optimization problem as stated in (8)–(10) is solved, with the constraints:

$$h(x, u, \theta) = \begin{bmatrix} \frac{\mathrm{d}T_j(t)}{\mathrm{d}t} - R_{\max} \\ -\frac{\mathrm{d}T_j(t)}{\mathrm{d}t} + R_{\min} \\ C(t_{\mathrm{f}}) - C_{f,\max} \end{bmatrix} \leqslant 0 \text{ and } T_j(t) \in \mathcal{U} = [T_{j,\min}, T_{j,\max}], \tag{32}$$

where $R_{\min}$ and $R_{\max}$ are the minimum and maximum temperature ramp rates, and $C_{f,\max}$ is the maximum solute concentration at the end of the batch that specifies the minimum yield required by economic considerations. The optimization problem was solved using the sequential simulation-optimization approach.

In the closed-loop case the following measured states are considered in the feedback control law:

$$y = [\mu_1, \mu_2, \mu_3, C, T]^{\mathrm{T}}. \tag{33}$$

The first, second, and third-order moments can be measured using laser backscattering [39]. The solute concentration can be measured using several techniques (e.g. conductivity, attenuated total reflection Fourier transform infrared spectroscopy, etc. [39]). Temperature measurements are readily available using thermocouples. The zeroth order moment cannot be measured accurately since it strongly depends on the number of very small particles that are not perceivable even under an optical microscope. The measurements of higher order moments are not reliable due to their strong dependence on the statistics of the larger particles in solution. Measurements of the seed moments is not possible because they characterize only the part of the crystals grown from seed and cannot be distinguished in the mixture of seed and nucleated crystals.

4.2. Results and discussion

The nominal and robust optimal open-loop jacket temperature profiles are shown in Fig. 2. The nominal and the worst-case values of the performance index at the end of the batch are presented in Table 1. Robustness analysis results based on the first- and second-order series expansions are very similar, indicating that the first-order analysis produces good quantitative results for this process. From Table 1 it can be observed that parameter uncertainty causes performance degradation (above 12%) if the nominal optimal trajectory is implemented. The worst-case (minmax) control trajectory reduces the worst-case performance degradation, but at the cost of substantial degradation of the nominal performance. The weighted-sum approach achieves improved robustness with negligible loss in nominal performance. The optimal control trajectory obtained

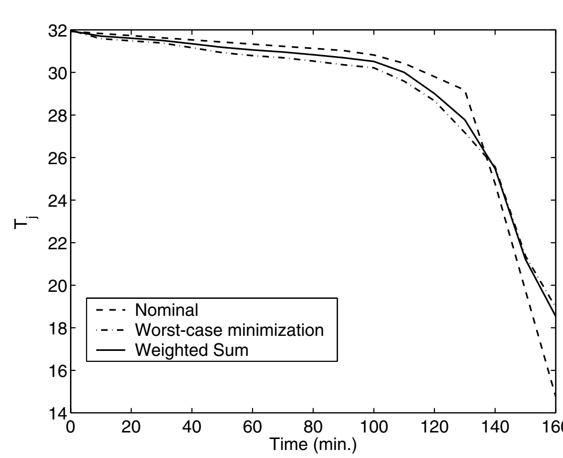

Fig. 2. Optimal temperature profiles for the end-point optimization of the open-loop system in the nominal case as well as using two robust optimization approaches.

Table 1
Nominal and worst-case performance indices (associated with a confidence level $\alpha = 0.95$) for open-loop end-point optimization[a]

Optimization approach	$\psi(t_f)$	$\psi_{w.c.}(t_f); (\delta\psi_{w.c.}(t_f))$ First order expansion	$\psi_{w.c.}(t_f); (\delta\psi_{w.c.}(t_f))$ Second order expansion
Nominal case	8.26	9.28 (12.3%)	9.31 (12.7%)
Worst-case minimization	8.67	8.98 (8.7%)	9.04 (9.4%)
Multiobjective minimization (weighted-sum approach, $w = 0.3$)	8.26	9.13 (10.5%)	9.18 (11.1%)

[a] The relative worst-case performance degradation compared to the nominal value is shown in parentheses.

with the weighted-sum approach is between the control trajectories obtained in the nominal and worst-case optimizations. Similar results as the weighted-sum approach was obtained by the ε-constraint approach with $\varepsilon = 0.14$, which is equal to the variance of the performance index obtained with the weighted-sum control trajectory. The nominal temperature profile has a steep decrease in the last third of the batch period. The robust control trajectories do not drop as fast near the end of the batch run, reducing the potential for excessive nucleation which directly affects the performance index (the nucleated to seed mass ratio). Fig. 3 shows the variation of the solute concentration corresponding to the three different optimal control profiles. All three trajectories provide the required minimum yield.

To study how feedback influences the robust performance of the system the linear feedback controller expressed by (16) is implemented using the measurement vector (33). To fairly compare the robust performance in the closed-loop and open-loop scenarios, the reference trajectories were obtained from the nominal open-loop optimization, so that the closed-loop system has a similar nominal performance index as the open-loop system. The results of the end-point optimization of the closed-loop system for both the nominal and the worst-case model parameters are presented in Table 2. The robustness of the end-point objective is improved by more than a factor of two, even when the feedback controller is designed ignoring model uncertainty. The feedback controller designed ignoring model uncertainty yields better robust performance than the robust open-loop approaches. Using the robust end-point optimization algorithms for feedback controller design further improves the robust performance. With the feedback controller obtained from either robust optimization technique the worst-case performance deviation at the end of the batch was reduced to only 1.2%, which represents a factor of 5 improvement compared to that obtained by the "nominal" feedback controller, and a factor of 10 improvement compared to the nominal open-loop implementation. All three feedback controllers provide the same nominal performance as in the open-loop implementation. Although the feedback controllers obtained using the worst-case and multi-objective robust optimization approaches are somewhat different, their nominal performance and robust performance are the same. Normally some fine-tuning of the weighting parameter w may be required to yield a feedback controller with similar robustness as in the worst-case minimization approach. For this example similar nominal and worst-case end-point performance indices were obtained for a wide range for the weighting parameter, although the controller gains, the dynamic

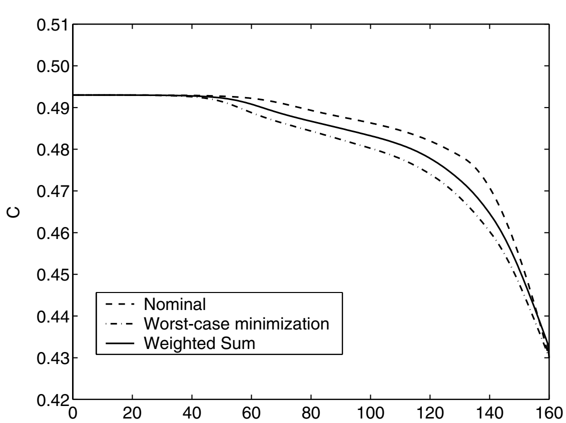

Fig. 3. Solute concentration profiles for temperature trajectories obtained from the end-point optimization of the open-loop system in the nominal case as well as using two robust optimization approaches.

Table 2
Nominal and worst-case performance indices (associated with a confidence level $\alpha = 0.95$) for closed-loop end-point optimization[a]

Optimization approach	**K**	$\psi(t_f)$	$\psi_{w.c.}(t_f); (\delta\psi_{w.c.}(t_f))$
Nominal case	[1.6e−2, 0.02, 1.1e−5, 2.3, −8.3e−5]	8.26	8.77 (6.2%)
Worst-case minimization	[4.4e−2, 5.0e−7, 3.1e−8, 10.1, −0.30]	8.26	8.36 (1.2%)
Multiobjective minimization (weighted-sum approach $w = 1$)	[0.12, 7.8e−7, 7.1e−8, 9.8, −0.36]	8.26	8.36 (1.2%)

[a] In parentheses the relative worst-case performance degradation compared to the nominal value is shown.

Table 3
Nominal and worst-case performance indices (associated with a confidence level $\alpha = 0.95$) for closed-loop control strategies in the case of measurement noise

Standard deviation [%]	0.5		1.5	
Performance index and worst case deviation	$\psi(t_f)$	$\psi_{w.c.}(t_f)$	$\psi(t_f)$	$\psi_{w.c.}(t_f)$
Nominal feedback controller	8.34	9.87	8.47	27.51
Robust feedback controller (worst-case minimization)	8.26	9.52	8.31	21.39

variations, and the sensitivity of the states and the other CSD properties varied widely.

The performance of the nominal and worst-case minimization feedback controllers were investigated by simulations using normally-distributed random measurement noise on all measurements with standard deviations (σ) 0.5% and 1.5%, respectively. Table 3 shows that even small measurement noise ($\sigma = 0.5\%$) can significantly decrease the performance of the feedback controllers. Although measurement noise was not taken into consideration in its design, the robust feedback controller provided better nominal and robust performance than the nominal feedback controller. The nominal performance achieved by the robust feedback controller when there is noise with $\sigma = 0.5\%$ is the same as when there is no noise ($\psi = 8.26$), and the degradation in nominal performance is small when there the standard deviation of the noise is 1.5%. The degradation in robust performance for both feedback controllers is quite large when there is noise with $\sigma = 1.5\%$. This illustrates two points. First, it serves as a reminder that the potential benefits of feedback control over open-loop control for batch processes depends on the availability of accurate and reliable sensors. Second, significant measurement noise should be taken into consideration in the controller design, e.g., by introducing a properly designed filter on the measurements.

Figs. 4–6 show the variation of probability distribution function for the performance index along the entire batch run for the nominal open-loop, nominal feedback, and robust feedback cases without measurement noise. The distribution is much narrower in both closed-loop scenarios. The feedback controller obtained from the robust optimization provides a very narrow distribution at the end of the batch, however it provides a wider distribution in the third quarter of the batch run than for the nominal feedback controller. This supports the perspective that the goal of robust optimal control is to *manage* where and when the effects of uncertainty occur, rather than to *suppress* the effects of uncertainty. The robust feedback controller manages uncertainty by concentrating its effects for intermediate times in such a manner that it has small effects at the final time.

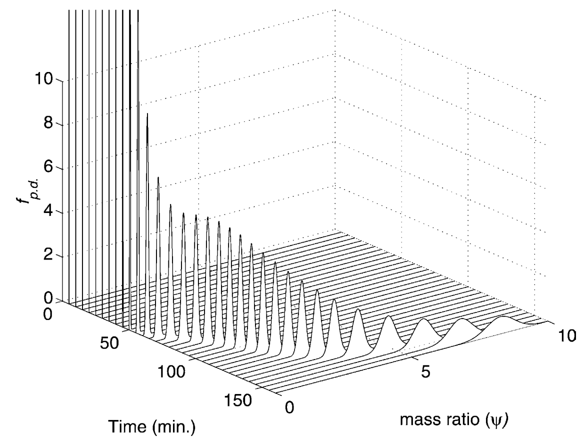

Fig. 4. The variation of the PDF of the performance objective (nucleated mass to seed mass ratio) for the whole batch run, in the case of the optimal control trajectory obtained by the optimization of the nominal open-loop system.

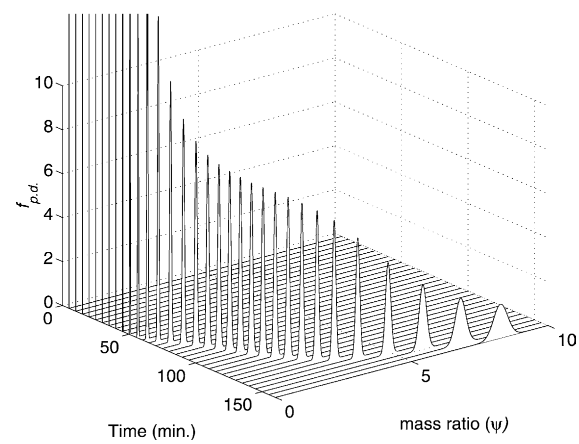

Fig. 5. The variation of the PDF of the performance objective (nucleated mass to seed mass ratio) for the whole batch run, in the case of the optimal feedback control law obtained by the optimization of the nominal closed-loop system.

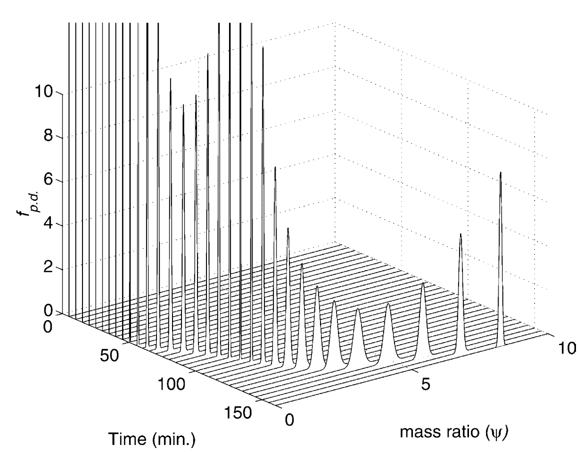

Fig. 6. The variation of the PDF of the performance objective (nucleated mass to seed mass ratio) for the whole batch run, in the case of the optimal robust feedback control law obtained by the worst-case optimization of the uncertain closed-loop system.

To illustrate how feedback influences the effects of perturbations in model parameters on process variables that are not included in the objective, the variation of all the states and CSD properties are computed for different confidence levels α. The results are plotted as distribution bands in Figs. 7–9, for nominal open-loop, nominal feedback, and robust feedback implementations. In addition to increasing the robustness of the performance index, feedback reduces considerably variations in the first three moments (μ_0, μ_1, μ_2). The variations of the rest of the states due to perturbations in the model parameters, however, are larger for the feedback controllers than in the open-loop implementation. This should not be surprising, since the feedback controllers manipulate the jacket temperature which has a rather direct effect on the temperature, and increased variations in the temperature are expected to lead to increased variations in some of the other states. Also, feedback increases cou-

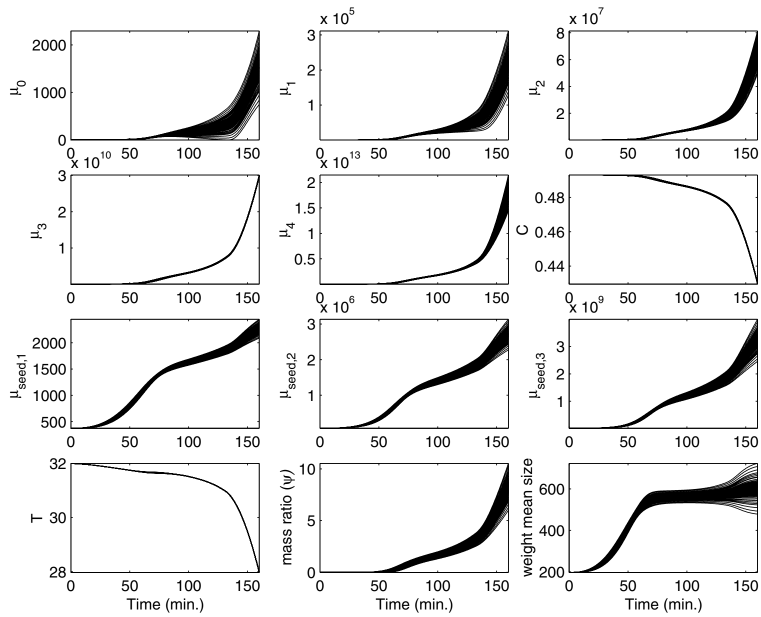

Fig. 7. Distribution bands caused by parameter uncertainty, obtained for different confidence levels α with the optimal control trajectory resulted from the optimization of the nominal open-loop system.

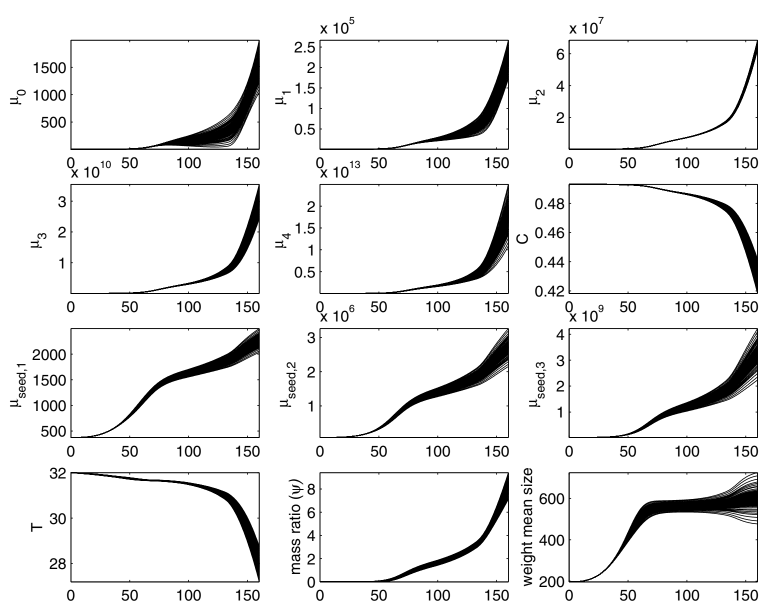

Fig. 8. Distribution bands caused by parameter uncertainty, obtained for different confidence levels α with the optimal control law resulted from the optimization of the nominal closed-loop system.

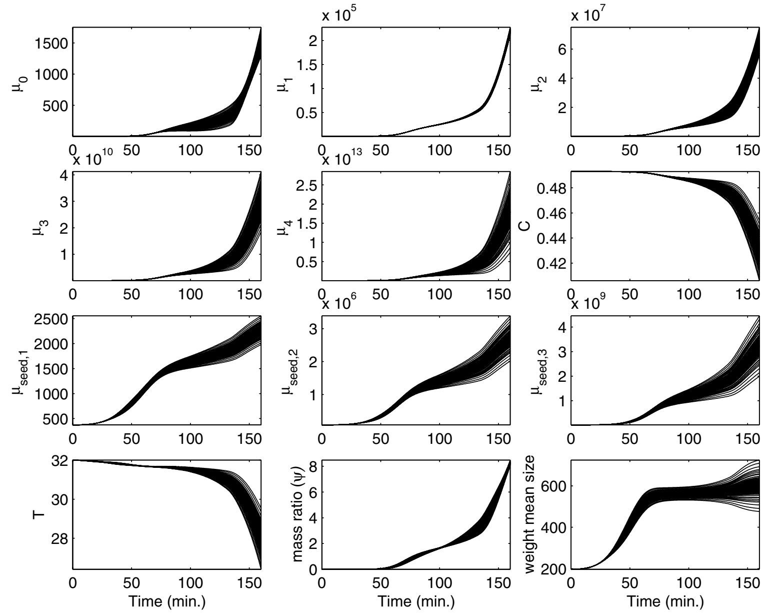

Fig. 9. Distribution bands caused by parameter uncertainty, obtained for different confidence levels α with the optimal control law resulted from the worst-case optimization of the uncertain closed-loop system.

pling of the variables within the system, which is expected to increase variations in some variables. The different feedback gains have quite different effects on the states. While the controller obtained from the optimization of the nominal closed-loop system reduces significantly the distribution of μ_2 the robust feedback controller greatly reduced the variations in μ_0 and μ_1 The two feedback controllers narrow the distribution of the weight mean size in the first third of the batch compared to open loop implementation, while the weight mean size are very similar for all implementations for the rest of the batch run. As before, these results support the notion that the goal of robust optimal control is to manage the effects of model uncertainty, rather than to uniformly suppress them.

The robustness analysis technique provided distributional information on the effects of parameter uncertainties for all states along the entire batch at low computational cost. The distributions in Figs. 4–9 were computed within 4 s using first-order analysis and $\sim$2 h with second-order analysis, whereas Monte Carlo simulations to a similar level of accuracy would take $\sim$21 h (all computations performed on a PIII-800MHz computer running Matlab).

5. Conclusions

Worst-case and distributional robustness analysis techniques were incorporated into open and closed-loop end-point optimization algorithms to provide robust performance. These techniques were applied to a batch crystallization process to quantify the effects of uncertainties in the kinetic parameters, and to compute control trajectories that minimize these effects. It is shown that feedback can considerably reduce the effect of parameter uncertainty on the end-point objective, however, due to increased coupling the sensitivity of other state variables can be increased. This supports the notion that the goal of robust optimal control is to redistribute the effects of model uncertainty away from important variables towards unimportant variables, rather than to uniformly suppress its effects.

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