Robust Nonlinear Model Predictive Control of Batch Processes

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NMPC explicitly addresses constraints and nonlinearities during the feedback control of batch processes. This NMPC algorithm also explicitly takes parameter uncertainty into account in the state estimation and state feedback controller designs. An extended Kalman filter estimates the process noise covariance matrix from the parameter uncertainty description and employs a sequential integration and correction strategy to reduce biases in the state estimates due to parameter uncertainty. The shrinking horizon NMPC algorithm minimizes a weighted sum of the nominal performance objective, an estimate of the variance of the performance objective, and an integral of the deviation of the control trajectory from the nominal optimal control trajectory. The robust performance is quantified by estimates of the distribution of the performance index along the batch run obtained by a series expansion about the control trajectory. The control and analysis approaches are applied to a simulated batch crystallization process with a realistic uncertainty description. The proposed robust NMPC algorithm improves the robust performance by a factor of six compared to open loop optimal control, and a factor of two compared to nominal NMPC. Monte Carlo simulations support the results obtained by the distributional robustness analysis technique.

Introduction

Batch processes are widely applied in many sectors of the chemical industries including pharmaceuticals, polymers, food products, biotechnology, and electronic chemicals. Increased competition has motivated the interest in mathematical modeling, optimization, and advanced process control techniques that enable the operation of flexible high-performance production lines (Le Lann et al., 1999; Rippin, 1983). Advanced control techniques have the potential to improve performance. Since the advent of dynamic matrix control (Cutler and Ramaker, 1980), model predictive control (MPC) has been the most popular advanced control strategy. Linear MPC (Garcia et al., 1989) has been heralded as a major advance in industrial control. However, for highly nonlinear systems, which is the case for most batch processes, linear MPC is often subject to severe performance limitations due to the limited validity of the linear model. For these systems, nonlinear MPC (NMPC) is the more appropriate approach. Although most of the reported NMPC applications (Qin and Badgwell, 2000; Mayne, 2000) are based on scheduling multiple models, successive linearization, or empirical nonlinear models (such as artificial neural networks), NMPC based on a first-principles nonlinear model is becoming increasingly feasible in the chemical industries due to improvements in computational power and optimization algorithms (Biegler, 2000; Biegler and Rawlings, 1991; Wright, 1996).

NMPC is an optimization-based multivariable constrained control technique using a nonlinear dynamic process model for the prediction of the process outputs (Allgöwer et al., 1999; Bequette, 1991). At each sampling time, the model is

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updated on the basis of new measurements and state variable estimates. Then, the open-loop optimal manipulated variable moves are calculated over a finite prediction horizon with respect to some cost function, and the manipulated variables for the subsequent prediction horizon are implemented. Then, the prediction horizon is usually shifted by one sampling time into the future and the previous steps are repeated. For batch processes, the objective to be optimized usually is a representative property of the product at the end of the batch. Hence, the control problem usually leads to a shrinking horizon NMPC formulation (Eaton and Rawlings, 1990; Thomas et al., 1994).

NMPC provides a systematic methodology to handle nonlinearity and constraints on manipulated and controlled variables that is not limited to a certain model structure. However, control performance can be strongly dependent on how accurately the specific model describes the real process. Most process models, which are developed from experimental observations of limited quality and quantity, are far from being highly accurate and involve significant uncertainties. The importance of taking model uncertainty into account in the analysis and design of MPC controllers is widely accepted in the control community. While, for linear MPC, both robust stability (Rawlings and Muske, 1993; Badgwell, 1997a,b; Mayne et al., 2000) and robust performance (Lee and Yu, 1994) have been studied, in the case of NMPC, research has been focused on the study of robust stability rather than performance. Although robust performance analysis can identify issues in implementation that need to be addressed for a theoretically-derived algorithm to be readily applied in practice, rigorous robust performance analysis techniques and studies are lacking. Several approaches have been proposed to incorporate uncertainties into NMPC formulations. One of the most straightforward approaches is to repeatedly solve on-line an open-loop optimization whose objective is to minimize the expected value of the performance over the set of perturbations, using updates of the measured (estimated) variables at each sampling time (Terwiesc et al., 1994). Alternative approaches have been presented based on a cascade optimization framework (Visser et al., 2000) or on a receding horizon implementation of an open-loop minimax optimization problem (Scokaert and Mayne, 1998; Alamir and Balloul, 1999). Although the aforementioned approaches address parameter uncertainties to some extent, none of these articles provide a comprehensive robustness analysis of the described techniques. Valapil and Georgakis (2001) proposed an extended Kalman filter (EKF)-based NMPC approach to control the end-use properties in batch reactors. Their 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 NMPC problem. The performance of their approach was assessed via Monte Carlo simulation. The only systematic robust performance analysis for NMPC is presented by Eaton and Rawlings (Eaton et al., 1989; Eaton and Rawlings, 1990). Their technique provides information on the effect of parameter uncertainty on the performance index by computing the sensitivity coefficients with respect to model parameters, however, parameter uncertainty is not implicitly considered in the controller design.

This article presents an NMPC algorithm that also explicitly takes parameter uncertainty into account to improve the robust performance of the state estimation and state feedback controller designs. An extended Kalman filter estimates a time-varying process noise covariance matrix from the parameter uncertainty description and employs a sequential integration and correction strategy to reduce biases in the state estimates due to parameter uncertainty. The shrinking horizon NMPC algorithm minimizes a weighted sum of the nominal performance objective, an estimate of the variance of the performance objective, and an integral of the deviation of the control trajectory from the nominal optimal control trajectory. Robust performance is quantified by estimates of the distribution of the performance index along the batch run obtained by a series expansion about the control trajectory. The performance of the proposed robust NMPC approach is assessed via an application to a simulated batch crystallization process with a realistic uncertainty description, where comparisons are made with nominal NMPC and open-loop optimal control. The robust performance analysis results are compared with Monte Carlo simulations.

Problem Formulation and Solution Strategy

EKF-based NMPC approach

The optimal control problem to be solved on-line in every sampling time in the NMPC algorithm can be formulated as

$$\min_{u(t)\in\mathfrak{U}} \mathfrak{K}[x(t),u(t),p] \tag{1}$$

subject to

$$\dot{x}(t) = f[x(t),u(t),p] \tag{2}$$

$$y(t) = g[x(t),u(t),p] \tag{3}$$

$$x(t_k) = \hat{x}(t_k), \quad x(t_0) = \hat{x}_0 \tag{4}$$

$$h[x(t),u(t),p] \le 0, \quad t\in[t_k,t_F] \tag{5}$$

where $\mathfrak{K}$ is the performance objective, t is the time, t_k is the time at sampling instance k, t_F is the final time at the end of the prediction, $x(t)\in\mathbb{R}^{n_x}$ is the n_x vector of states, $u(t)\in\mathfrak{U}$ is the n_u set of input vectors with $\mathfrak{U}=\mathfrak{U}_1\times\mathfrak{U}_2\times\ldots\times\mathfrak{U}_{n_u}$ representing the set of all possible trajectories of each control input, $y(t)\in\mathbb{R}^{n_y}$ is the n_y vector of measured variables used to compute the estimated states $\hat{x}(t_k)$, and $p\in\mathfrak{P}\subset\mathbb{R}^{n_p}$ is the n_p vector of uncertain parameters, where the set $\mathfrak{P}$ can be either defined by hard bounds or probabilistic, characterized by a multivariate probability density function. The function $f:\mathbb{R}^{n_x}\times\mathfrak{U}\times\mathfrak{P}\to\mathbb{R}^{n_x}$ is the vector function of the dynamic equations of the system, $g:\mathbb{R}^{n_x}\times\mathfrak{U}\times\mathfrak{P}\to\mathbb{R}^{n_y}$ is the measurement equations function, and $h:\mathbb{R}^{n_x}\times\mathfrak{U}\times\mathfrak{P}\to\mathbb{R}^{c}$ is the vector of functions that describe all linear and nonlinear, time-varying or end-time algebraic constraints for the system, where c denotes the number of these constraints. The objective function can have the following general form

$$\mathfrak{K}[x(t),u(t),p] = \mathfrak{M}[x(t_F),p] + \int_{t_k}^{t_F}\mathfrak{L}[x(t),u(t),p]dt \tag{6}$$

The form of Eq. 6 is general enough to express a wide range of objectives encountered in NMPC applications (moving or shrinking horizon approach on regulation and/or set point tracking, direct minimization of the operation time, optimal initial conditions, multiple simultaneous objectives, treatment of soft constraints, and so on). For batch processes with end-point optimization the objective usually reduces to the Mayer form ($\mathfrak{L}(\cdot)=0$), however, the Lagrange term ($\mathfrak{L}(\cdot)$) still may be used, such as to implement soft constraints on control rate (Sage and White III, 1977).

In order to incorporate uncertainties in the NMPC approach, several approaches have been proposed mainly based on minmax formulation of the performance objective (usually a representative property of the product), that is, minimization of the worst-case deviation of some performance index (ψ) caused by parameter uncertainty (Alamir and Balloul, 1999). Although this formulation usually does improve robust performance in the worst-case scenario, it may lead to poor results in the nominal case. To overcome this problem, another approach is based on a multiobjective optimization. According to this approach, the weighted sum of the expected or nominal value of the end-point performance index and the variance of the performance index around the nominal or expected value, caused by parameter uncertainty, is minimized

$$\mathfrak{M}\left[x(t_F),p\right]=E\left\{\psi\left[x(t_F),p\right]\right\}+w\mathrm{Var}\left\{\psi\left[x(t_F),p\right]\right\} \tag{7}$$

where E represents either the expected or nominal value and w is the weighting factor that can be used to control the trade-off between robustness and nominal performance. The expected or nominal value and the variance of the end-point performance index can be computed using the distributional robustness analysis technique presented in the next section. A third term that improves the trade-off between nominal performance and robustness is described in the case study section.

The aforementioned NMPC approach assumes knowledge of the states. In practice not all states can be measured and the rest of the states need to be estimated from available measurements. There are many state estimators described in the literature. In this article a continuous-discrete extended Kalman filter (EKF) (Jazwinsky, 1970) is implemented in conjunction with the NMPC strategy. Although EKF-based NMPC techniques have been described in the literature (Lee and Ricker, 1993, 1994; Lakshmanan and Arkun, 1999) with several industrial applications (Ahn et al., 1999; Seki et al., 2001; Qin and Badgwell, 2000), we will briefly present the approach used in this article to emphasize the differences compared to other techniques.

The EKF gain is designed using the following stochastic representation of the process

$$\dot{x}(t)=f\left[x(t),u(t),p\right]+q(t) \tag{8}$$

$$y(t)=g\left[x(t),u(t),p\right]+r(t) \tag{9}$$

where $q(t)$ and $r(t)$ are the process noise vector and measurement noise vector, respectively. Both $q(t)$ and $r(t)$ are assumed to be white noises with zero mean and covariance $\boldsymbol{Q}(t)$ and $\boldsymbol{R}(t)$, respectively. The appropriate choice of these parameters is important for the performance of the estimator. While the measurement covariance matrix $\boldsymbol{R}$ can be directly derived from the accuracy of the measurement device and can be easily obtained experimentally, the appropriate choice of $\boldsymbol{Q}$ is much less straightforward. Ali and Zafiriou (1993) proposed a nonlinear optimization based technique to obtain the process covariance matrix $\boldsymbol{Q}$. For large systems, this technique is computationally very expensive and only produces a constant covariance matrix. However, it has been shown for batch processes that the use of a time-varying full covariance matrix $\boldsymbol{Q}$ leads to a better performance than the constant diagonal matrix (Valapil and Georgakis, 1999, 2000). An estimate of the time-varying $\boldsymbol{Q}$ can be obtained by assuming that the process noise vector $q(t)$ mostly represents the effects of parametric uncertainty, in which case (Valapil and Georgakis, 1999, 2000)

$$q(t)=f\left[x(t),u(t),p\right]-f\left[x_{\mathrm{nom}}(t),u(t),P_{\mathrm{nom}}\right] \tag{10}$$

Performing a first-order series expansion of the righthand side of Eq. 10 around the nominal state (x_{nom}) and nominal parameter (p_{nom}) vectors, and computing the covariance of the resulting $q(t)$, give the following expression for the process noise covariance matrix (Valapil and Georgakis, 1999, 2000)

$$\boldsymbol{Q}(t)=\boldsymbol{S}_p(t)\boldsymbol{V}_p\boldsymbol{S}_p^T(t) \tag{11}$$

where $\boldsymbol{V}_p\in\mathbb{R}^{n_p\times n_p}$ is the parameter covariance matrix, and $\boldsymbol{S}_p(t)$ is the Jacobian computed using the nominal parameters and estimated states

$$\boldsymbol{S}_p(t)=\left(\frac{\partial f}{\partial p}\right)_{\hat{x}(t),u(t),p_{\mathrm{nom}}} \tag{12}$$

Equation 11 provides an easily implementable way to estimate the process noise covariance matrix, since the parameter covariance matrix $\boldsymbol{V}_p$ is usually available from parameter estimation (Beck and Arnold, 1977), and the sensitivity coefficients in $\boldsymbol{S}_p$ can be computed by finite differences or via sensitivity equations (Caracotsios and Stewart, 1985; Feehery et al., 1997).

In the time update phase of the estimation, the states and state covariance are propagated by integrating the model equations augmented with the covariance propagation equation for one sampling time ($t\in[t_{k-1},t_k]$)

$$\dot{x}(t)=f\left[x(t),u(t),p\right] \tag{13}$$

$$\dot{\boldsymbol{P}}(t)=\tilde{\boldsymbol{A}}(t)\boldsymbol{P}(t)+\boldsymbol{P}(t)\tilde{\boldsymbol{A}}^T(t)+\boldsymbol{Q}(t) \tag{14}$$

with initial conditions $\hat{x}(t_{k-1})$ and $\boldsymbol{p}(t_{k-1})$ obtained from the last estimation, and the jacobian $\tilde{\boldsymbol{A}}(t)$ defined by

$$\tilde{\boldsymbol{A}}(t)=\left(\frac{\partial f}{\partial x}\right)_{\hat{x}(t),u(t),p_{\mathrm{nom}}} \tag{15}$$

Define the solutions of Eqs. 13–14 as $\hat{x}^-(t_k)$ and $\boldsymbol{P}^-(t_k)$, respectively. With these values the Kalman gain $\boldsymbol{K}$ is com-

puted, and then the measurement update stage is performed according to

$$\boldsymbol{K}(t_k) = \boldsymbol{P}^-(t_k)\tilde{\boldsymbol{C}}^T(t_k)\left[\tilde{\boldsymbol{C}}(t_k)\boldsymbol{P}^-(t_k)\tilde{\boldsymbol{C}}^T(t_k) + \boldsymbol{R}\right]^{-1} \quad (16)$$

$$\boldsymbol{P}(t_k) = \left[\boldsymbol{I} - \boldsymbol{K}(t_k)\tilde{\boldsymbol{C}}(t_k)\right]\boldsymbol{P}^-(t_k) \quad (17)$$

$$F_K(t_k) = \boldsymbol{K}(t_k)\left[(y_m(t_k) - g(\hat{x}^-(t_k), u(t_k), p_{\text{nom}})\right] \quad (18)$$

$$\hat{x}(t_k) = \hat{x}^-(t_k) + F_K(t_k) \quad (19)$$

where $y_m(t_k)$ corresponds to the measurements obtained from the real process at time t_k, $F_K(t_k)$ is the Kalman filter correction factor, and $\tilde{\boldsymbol{C}}$ is the jacobian of the measurement equations with respect to the states

$$\tilde{\boldsymbol{C}}(t) = \left(\frac{\partial g}{\partial x}\right)_{\hat{x}(t),u(t),p_{\text{nom}}} \quad (20)$$

The estimated states in Eq. 19 are used as the initial value for the model prediction stage in the optimization algorithm. Note, however, that in the presence of constant parameter uncertainty the prediction results in biased state and/or output values. To diminish this problem, a sequential integration and correction approach is used instead of performing the prediction by integrating the model equations over the whole prediction horizon $t \in [t_k, t_F]$. According to this technique, the state equations are integrated over one sampling time with the initial values $\hat{x}(t_k)$ obtained from the estimator, and then the initial values for the next sampling period are computed by adding the Kalman filter correction factor $[F_K(t_k)]$ to the values obtained from the integration. This procedure is repeated until the end of the prediction t_F. This sequential integration and correction strategy represents the main difference of our technique compared to the aforementioned approaches.

Distributional robustness performance analysis

The robust NMPC algorithm incorporates the distributional approach of Nagy and Braatz (2002), which is an extension of earlier worst-case analysis techniques developed for finite-time nonlinear systems (Ma et al., 1999; Ma and Braatz, 2000, 2001).

With δp defined as the perturbation about the nominal parameter vector (p_{nom}) with dimension ($n_p \times 1$), the real parameter vector is

$$p = p_{\text{nom}} + \delta p \quad (21)$$

with mean and covariance given by

$$E[p] = p_{\text{nom}} \quad (22)$$

$$Cov[p - p_{\text{nom}}] = \boldsymbol{V}_p \quad (23)$$

A popular way to describe the uncertainty of parameters is by defining the hyperellipsoidal confidence region that quantifies the accuracy of the parameters. Assuming zero mean, normal measurement errors, and known covariance matrix, the hyperellipsoidal confidence region is given by

$$\mathcal{P}(\alpha) \triangleq \left\{p : (p - p_{\text{nom}})^T \boldsymbol{V}_p^{-1} (p - p_{\text{nom}}) \le \chi^2_{n_p}(\alpha)\right\} \quad (24)$$

where α is the confidence level, and $\chi^2_{n_p}(\alpha)$ is the chi-squared distribution function with n_p degrees of freedom. Using the Hölder 2-norm, the ellipsoidal set (Eq. 24) can be written as

$$\mathcal{P}(\alpha) \triangleq \left\{p : \|\boldsymbol{W}_p \delta p\|_2 \le 1,\ p \in \mathbb{R}^{n_p}\right\} \quad (25)$$

where $\boldsymbol{W}_p \in \mathbb{R}^{n_p \times n_p}$ is a positive-definite weighting matrix of the form

$$\boldsymbol{W}_p = \left[\chi^2_{n_p}(\alpha)\right]^{-1/2} \boldsymbol{V}_p^{-1/2} \quad (26)$$

The variation of the performance index caused by parameter uncertainty is

$$\delta\psi = \psi - \psi_{\text{nom}} \quad (27)$$

where ψ_{nom} is the nominal performance for the nominal model parameters p_{nom}, and ψ as its value for the uncertain parameters p.

The robust performance analysis is based on the series expansion of $\delta\psi$

$$\delta\psi = L\,\delta p + \delta p^T \boldsymbol{M} \delta p + \ldots \quad (28)$$

where the jacobian $L \in \mathbb{R}^{n_p}$, and hessian $\boldsymbol{M} \in \mathbb{R}^{n_p \times n_p}$ are

$$L(t) = \left(\frac{\partial \psi(t)}{\partial p}\right)_{p_{\text{nom}}} \quad (29)$$

$$\boldsymbol{M}(t) = \left(\frac{\partial^2 \psi(t)}{\partial p^2}\right)_{p_{\text{nom}}} \quad (30)$$

The elements of the time-varying sensitivity vector $L(t)$ and matrix $\boldsymbol{M}(t)$ can be computed using finite differences or by integrating the model's differential-algebraic equations augmented with an additional set of differential equations known as sensitivity equations (Caracotsios and Stewart, 1985). The extra computational expense in simulating the sensitivity equations can be reduced substantially by exploiting their structure (Feehery et al., 1997).

When a first-order series expansion is used, analytical expressions of the worst-case deviation in the performance index ($\delta\psi_{w.c.}$) can be computed and the analysis can be performed with low computational cost (Matthews, 1997). In the case of an ellipsoidal uncertainty description the worst-case deviation is defined by

$$\delta\psi_{w.c.}(t) = \max_{\|W_p \delta p\|_2 \le 1} |L(t)\,\delta p| \quad (31)$$

The analytical solution of this optimization problem can be determined using Lagrange multipliers

$$\delta\psi_{w.c.}(t) = \left[\chi^2_{n_p}(\alpha) L(t) \boldsymbol{V}_p L^T(t)\right]^{1/2} \quad (32)$$

$$\delta p_{w.c.}(t) = \frac{\left[\chi^2_{n_p}(\alpha)\right]^{1/2}}{\left[L(t)\boldsymbol{V}_p L^T(t)\right]^{1/2}} \boldsymbol{V}_p L^T(t) \quad (33)$$

The worst-case uncertainty vector in Eq. 33 is not unique. For example, another solution vector is obtained by multiplying by minus one. While both vectors achieve the same maximum deviation $\delta\psi_{w.c}$, one of the vectors is associated with a worst-case increase in ψ and another with a worst-case decrease. The first-order series expansion has provided acceptable accuracy for several batch processes (Ma et al., 1999; Ma and Braatz, 2001; Mathews, 1997). Improved accuracy can be obtained using a higher-order series expansion, but with the cost of a higher computational burden. This approach uses the structured singular value to compute the worst-case deviation in ψ and the associated worst-case parameter vector for second- or higher-order series expansions (Ma and Braatz, 2001). A less computationally expensive estimate of $\delta\psi_{w.c.}$ is the magnitude of the difference between the nominal value and the performance index obtained by applying a nonlinear dynamic simulation using the estimated worst-case parameter vector computed from the first-order analysis (Eq. 33).

The parameter uncertainty description (Eq. 25) is characterized by a multivariate normal distribution with the following probability density function (*pdf*)

$$f_{p.d.}(p) = \frac{1}{(2\pi)^{n_p/2}\det(V_p)^{1/2}} \times \exp\left(-\frac{1}{2}\left[(p-p_{\text{nom}})^T V_p^{-1}(p-p_{\text{nom}})\right]\right) \quad (34)$$

This will be used to estimate the distribution of the performance variable ψ of interest. When a first-order series expansion is used, the *pdf*, of ψ can be estimated as

$$f_{p.d.}(\psi) = \frac{1}{\sqrt{2\pi V_\psi}}\exp\left(-(\psi-\psi_{\text{nom}})^2/(2V_\psi)\right) \quad (35)$$

with the mean and covariance of ψ given by

$$E[\psi] = \psi_{\text{nom}} \quad (36)$$

$$Var[\psi] = V_\psi = LV_pL^T \quad (37)$$

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

A more accurate estimate of the *pdf* of ψ can be computed numerically. One way to do this is to use the higher-order series expansion (Eq. 28) to map the contours of the uncertainty sets $\mathcal{P}(\alpha)$ obtained for different α-levels to the bounds on ψ, and construct the *pdf*, of ψ from the contours on ψ. The contour mappings can be performed by structured singular value analysis applied to the terms in the series expansion (Nagy and Braatz, 2002). Another way to obtain the distribution of ψ is to perform Monte Carlo nonlinear simulations with random samples from the multivariate distribution (Eq. 34). This technique is straightforward to implement and does not have the truncation error caused by the series expansion, however, it is computationally very expensive, as is illustrated in the case study. In the next section Monte Carlo simulations is used to assess the accuracy of the first-order distributional robustness analysis of the NMPC of a batch crystallization process.

Although the above equations were in terms of a particular performance index, note that the robust performance analysis techniques can be applied to any state variable or function of the state variables.

Case Study: Batch Crystallization

The dynamic model of a batch crystallizer with the KNO_3-H_2O system is only briefly described here, as a detailed description of the system is available elsewhere (Miller and Rawlings, 1994). The KNO_3 product crystals can be characterized by one characteristic length z for which the population balance equation is given by

$$\frac{\partial f_d(z,t)}{\partial t} + \frac{\partial\{G_c(S,p_g,z)f_d(z,t)\}}{dz} = B_c(S,p_b) \quad (38)$$

where $f_d(z,t)$ is the crystal size distribution (CSD), t is time, $G_c(S,p_g,z)$ is the rate of crystal growth, $B_c(S,p_b)$ is the nucleation rate, $S=(C\text{-}C_{\text{sat}})/C_{\text{sat}}$ is the relative supersaturation, C is the solute concentration, $C_{\text{sat}}=C_{\text{sat}}(T)$ is the saturation concentration, which is a function of the crystallizer temperature T, and p_g and p_b are the growth and nucleation kinetic parameters, respectively.

A popular method of simplifying the simulation and optimization is based on the moments, which replaces the partial differential Eq. 38 with a set of ordinary differential equations (Hulbert and Katz, 1964)

$$\frac{d\mu_0}{dt} = B_c \quad (39)$$

$$\frac{d\mu_j}{dt} = jG_c\mu_{j-1} + B_c z_0^j, \quad j=1,2,\ldots \quad (40)$$

where z_0 is the crystal size at nucleation, which is assumed to be constant, and μ_j is the jth moment defined by

$$\mu_j = \int_0^\infty z^j f_d(z,t)dz \quad (41)$$

A similar material balance tracks only the crystals grown from seed. These moment equations can be derived similarly as Eqs. 39–40.

$$\frac{d\mu_{\text{seed},j}}{dt} = jG_c\mu_{\text{seed},j-1}, \quad j=0,1,\ldots \quad (42)$$

Assuming constant volume, the solute concentration C satisfies

$$\frac{dC}{dt} = -3\rho_c k_v G_c \mu_2 - \rho_c k_v B_c z_0^3 \quad (43)$$

where ρ_c is the density of the crystal, and k_v is the volumetric shape factor, defined as the volume of a crystal divided by z^3.

For a jacketed batch cooling crystallizer, the energy bal-

ance is written

$$\frac{dT}{dt} = \frac{-UA(T - T_j) - 3\Delta H_c(C)\rho_c k_v G_c \mu_2 m_s}{(\rho_c k_v \mu_3 + C + 1) m_s c_p(C)} \quad (44)$$

where U is the heat-transfer coefficient, A is the heat-transfer area, T_j is the jacket temperature, 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.

Several models for growth and nucleation kinetics have been developed and are available in the literature (Garside, 1984; Nyvlt et al., 1985; Rawlings et al., 1993). The most common kinetic models when nuclei form from existing crystals are given by the equations

$$G_c = k_g S^g \quad (45)$$

$$B_c = k_b S^b \int_0^\infty z^3 f_d(z,t)\, dz \quad (46)$$

where $p = [g, \ln(k_g), b, \ln(k_b)]^T$ are the kinetic parameters for growth and nucleation.

In Eqs. 39–46 the moments and concentration are defined on a per mass of solvent basis. In the dynamic simulation, the solute concentration, temperature, and moments $\mu_0, \ldots, \mu_4$ and $\mu_{\text{seed},0}, \ldots, \mu_{\text{seed},3}$ are computed, resulting in ten ordinary differential equations.

From practical considerations, the following measurements are considered

$$y = [\mu_1, \mu_2, \mu_3, C, T]^T \quad (47)$$

The first three variables (moments μ_1, μ_2, and μ_3) can be measured using video microscopy or laser backscattering (Braatz, 2002; Fujiwara et al., 2002; Patience and Rawlings, 2001). Several on-line techniques are available for the solution concentration measurements such as conductivity or attenuated total reflection Fourier transform infrared spectroscopy (Rawlings et al., 1993; Braatz and Hasebe, 2002). Temperature measurements are readily available using common thermocouples.

The nominal model parameters p are reported in Table 1. These values were determined by maximum likelihood, with the details reported by Miller and Rawlings (1994). The inverse of the parameter covariance matrix was estimated as (Ma et al., 1999)

$$V_p^{-1} = \begin{bmatrix} 102{,}873 & -21{,}960 & -7{,}509 & 1{,}445 \\ -21{,}960 & 4{,}714 & 1{,}809 & -354 \\ -7{,}509 & 1{,}809 & 24{,}225 & -5{,}198 \\ 1{,}445 & -354 & -5{,}198 & 1{,}116 \end{bmatrix} \quad (48)$$

Table 1. Nominal Kinetic Parameters of the KNO_3 System (Miller and Rawlings, 1994)

g	k_g (μm/min)	b	k_b (particles/cm^3/min)
1.31	exp(8.79)	1.84	exp(17.38)

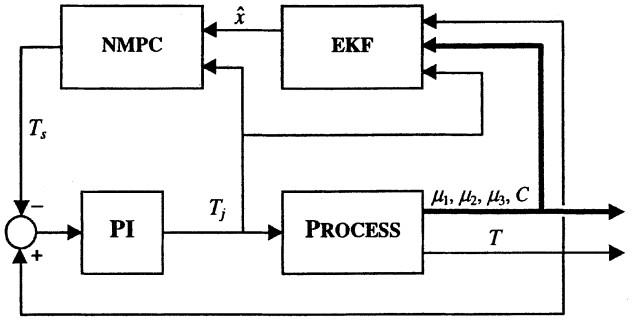

Figure 1. Hierarchical NMPC structure coupled with the EKF.

This matrix was estimated from dynamic data collected for four batch simulation experiments as described by Chung et al. (2000). In brief, Eq. 48 was computed from the measurement noise covariance matrix, whose diagonal elements were specified by experimental data reported by Miller and Rawlings (1994), and the jacobian of the model predictions with respect to the parameters using expressions for computing approximate covariance matrices for nonlinear systems (Beck and Arnold, 1977).

The hierarchical implementation of the NMPC algorithm for the batch cooling crystallizer is shown in Figure 1. The EKF estimates the entire state vector from the current measurements taken from the process. The estimated states are used to initialize the optimal control problem in the NMPC algorithm, which is used to compute the set point on the crystallizer temperature that is sent to a lower level PI controller that manipulates the jacket temperature to achieve the desired temperature. Not shown or modeled is the local flow controller that manipulates a valve position to achieve the jacket temperature, since the dynamics of this loop are so fast that a high gain controller ensures that the local flow control loop has a neglible effect on the higher level control loops.

The CSD property considered as the performance index in the NMPC is the nucleated crystal mass to seed crystal mass ratio at the end of the batch

$$\psi[x(t_f)] = \frac{\mu_3 - \mu_{\text{seed},3}}{\mu_{\text{seed},3}} \quad (49)$$

The main objective of the robust NMPC algorithm is to minimize this CSD property, while being robust to parameter uncertainty. The optimization problem solved in the NMPC approach at every sampling time is

$$\min_{T(t)} \left\{ \psi(x(t_F), p_{\text{nom}}) + wVar[\psi(x(t_F), p)] + \lambda \int_{t_k}^{t_f} \| T(t) - T_{\text{nom}}(t) \|_2 dt \right\} \quad (50)$$

subject to the model equations and the following inequality

constraints

$$T_{\min}(t) \le T(t) \le T_{\max}(t) \tag{51}$$

$$R_{T,\min}(t) \le \frac{dT(t)}{dt} \le R_{T,\max}(t) \tag{52}$$

$$C(t_f) \le C_{\max}(t_f) \tag{53}$$

where $T_{\min}$, $T_{\max}$, $R_{T,\min}$, and $R_{T,\max}$ are the minimum and maximum temperatures and temperature ramp rates, respectively, during the batch and t_f is the end time of the batch. In the last term of the objective function (Eq. 50), $T_{\text{nom}}(t)$ is the nominal optimal temperature profile obtained with the nominal parameters. The inclusion of this term in the objective function improves the nominal performance of the robust NMPC scheme. By setting the appropriate weight λ, similar nominal performance can be achieved for larger values of the weighting coefficient on the variance (w) as in the case of NMPC without uncertainty. When $\lambda = 0$ is used, the same nominal performance can be achieved by only significantly reducing w, which leads to significant degradation of the robust performance of the NMPC algorithm. Constraints 51 and 52 ensure that the temperature profile stays within the operating range of the crystallizer. The final constraint 53 ensures that the minimum yield required by economic considerations will be met. The temperature profile is described as linear piecewise trajectories by discretizing the batch time in N equal intervals and considering the temperatures at every time as the optimization variables. The NMPC with the EKF is implemented in Matlab using the sequential solution approach, in which a stiff ODE integrator is used in combination with an optimization subroutine (*fmincon*). The optimal temperature profile $T_s(t)$ is used as the set point for the lower level PI controller, which tracks the desired optimal set point using the jacket temperature. To reduce on-line computations, the jacobian matrices $\tilde{\boldsymbol{A}}$, $\tilde{\boldsymbol{C}}$, and $\boldsymbol{S}_p$ used in the EKF are computed symbolically off-line using the Matlab symbolic toolbox. Since the estimation is faster than the optimization, a smaller estimation sampling time (1 min) is used in the EKF than for control discretization (10 min), achieving a faster convergence of the estimator.

The overall performance of the control approach directly depends on the performance of the EKF, which is determined by the tuning parameters $\boldsymbol{Q}$ and $\boldsymbol{R}$, the initial values of the state estimates $\hat{x}_0$, and the initial value of the state covariance matrix $\boldsymbol{P}(t_0)$. In the simulations it was assumed that the state-of-the-art sensors and associated chemometric analysis tools are used (Braatz and Hasebe, 2002) so that the measurements are relatively accurate, which corresponds to diagonal elements of $\boldsymbol{R}$ that are small ($\boldsymbol{R} = 0.001\ \boldsymbol{I}$). The time-varying state covariance matrix $\boldsymbol{Q}(t)$ given by Eq. 11 is designed to take into account the effect of parameter uncertainties on the state equation Eq. 8. Like any estimator, the performance of the EKF can be sensitive to poor estimates of $\hat{x}_0$. The initial value of $\boldsymbol{P}(t_0)$ is the measure of the accuracy of the initial state estimates. In the case of large errors in $\hat{x}_0$, choosing too small values for $\boldsymbol{P}(t_0)$ can cause poor performance or even divergence of the estimator. If large errors in the initial states are expected, then the diagonal elements of $\boldsymbol{P}(t_0)$ should be selected to be larger. To account for this, the elements of the diagonal $\boldsymbol{P}(t_0)$ are computed as $[x_i(t_0) - \hat{x}_{0,i}]^2$. Using this approach to estimate $\boldsymbol{P}(t_0)$, the robust NMPC algorithm was run for $\pm 5\%$ and $\pm 10\%$ errors in the initial values of the unmeasured state estimates (see Table 2). An error of $+5\%$ or -5% in $\hat{x}_0$ leads to an offset in the end-point performance of 10.2% or 16.6%, respectively, compared to the ideal case when all states are perfectly known. In the case of $\pm 10\%$ errors in $\hat{x}_0$, the EKF does not converge. Convergence for larger errors in the initial states could be achieved by increasing the magnitude of the diagonal elements of $\boldsymbol{P}(t_0)$. This example also illustrates the improved estimation provided by the implemented EKF compared to the conventional EKF. When the conventional EKF was used with diagonal and constant $\boldsymbol{Q}$ (using the diagonal elements of $\boldsymbol{Q}(t_0)$ given by Eq. 11) and without using the sequential integration and correction strategy, its state estimates diverged even for the $\pm 5\%$ errors in $\hat{x}_0$.

Table 2. Performance of Robust NMPC with EKF for 0, 5, and 10% Errors in the Initial Values of the State Estimates

$\hat{x}_0$	$x(t_0)$	$0.95x(t_0)$	$1.05x(t_0)$	$0.90x(t_0)$	$1.10x(t_0)$
$\psi(t_f)$	7.8	8.6	9.1	*	*

*Indicates that the EKF diverged.

Figure 2 shows the nominal profiles obtained by nominal NMPC and robust NMPC, respectively. In the latter case $\lambda = 0.01$ is used to achieve a similar nominal performance as in the former case. To focus attention on the effects of parameter uncertainty, the initial states are considered known; hence, $\boldsymbol{P}(t_0)$ is set small ($0.01\ \boldsymbol{I}$). The open-loop optimal trajectory is also shown, and seen to have nearly the same temperature profile as NMPC. The trajectories presented in Figure 2 are used as the set point for the PI controller. The PI controller tracks the profiles accurately (within ± 0.05°C), and a variation less than 0.5% in the final performance index is achieved compared to the ideal controller case (when the set point profile is implemented perfectly). When the controller was detuned to provide a set point tracking error of ± 0.1°C a

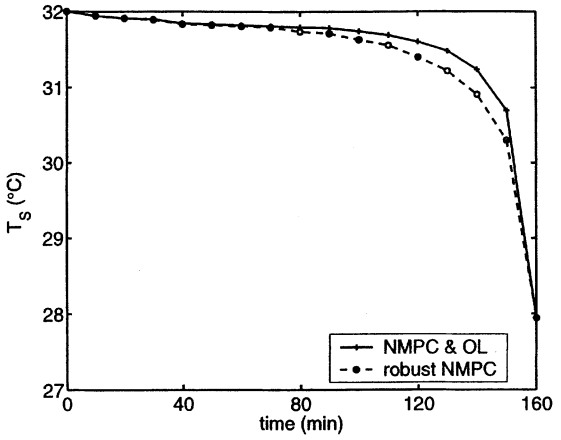

Figure 2. Optimal temperature profiles for nominal NMPC ($w = 0$), robust MPC ($w = 0.2$), and for open-loop optimal control.

Table 3. Worst-Case Performance (for Parameter Uncertainty with Confidence Level $\alpha = 0.95$) for the Performance Index (the Nucleation to Seed Mass Ratio) Obtained by Open Loop Optimal Control, Nominal NMPC ($w = 0$), Robust NMPC ($w = 0.2$) with EKF, and robust NMPC ($w = 0.2$) with Perfect Knowledge of the States*

Control Approach	Nominal $\psi(t_f)$	$\psi_{w.c.}(t_f)$ Est. with First-Order Expansion	$\psi_{w.c.}(t_f)$ Improved Value from Dynamic Simulation
Open-loop optimal control	7.7	9.3	9.6
NMPC (nominal, with EKF)	7.7	9.0	8.3
Robust NMPC (with EKF)	7.8	8.8	8.1
Robust NMPC (with known states)	7.8	8.5	8.0

*The worst-case deviation was estimated using first-order robustness analysis, with the improved value computed by performing dynamic simulation for the worst-case parameter computed from first-order analysis.

significantly larger variation (2.7%) in the performance index was observed.

Table 3 shows the effects of parameter uncertainty on the performance index for open-loop optimal control, nominal NMPC with EKF, robust NMPC with EKF, and robust NMPC when the states are perfectly known. Nominal NMPC with EKF considerably reduces the worst-case deviation in the performance index by a factor of three compared to open-loop optimal control. Robust NMPC with EKF provides an additional factor of two reduction in the worst-case performance deviation, while providing nearly the same nominal performance as open-loop optimal control. The state estimates obtained by the EKF were sufficiently accurate to provide the same nominal performance and a small degradation in robust performance compared to having perfect state information. The first-order series expansion gave more accurate results for open-loop optimal control than for the NMPC approaches. The larger differences for the NMPC algorithms indicate the usefulness of improving the accuracy of the worst-case performance estimates via nonlinear simulation.

Distributional analysis provides a more comprehensive assessment of the robust performance. Figures 3–5 show the

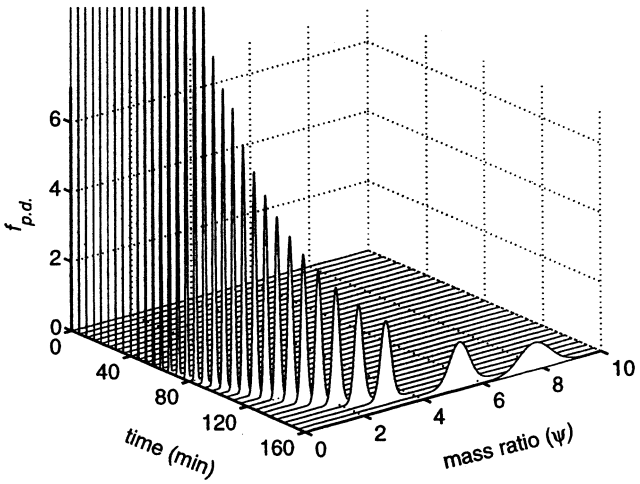

Figure 4. Variation of the p.d.f. of the performance index (the nucleation to seed mass ratio) during the batch when nominal NMPC with EKF is implemented.

The p.d.f was determined using first-order distributional analysis.

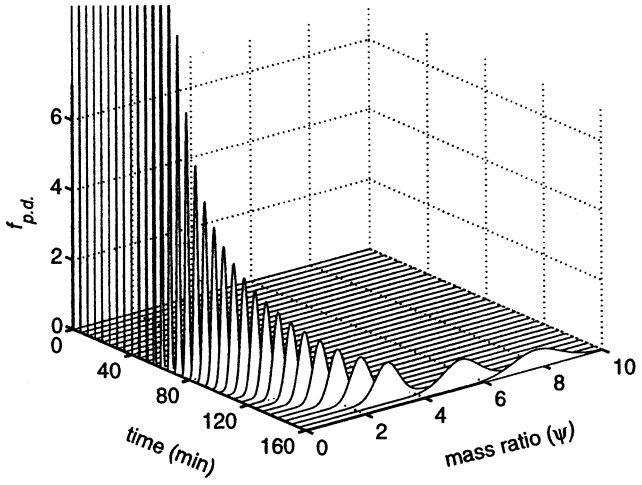

Figure 3. Variation of the p.d.f. of the performance index (the nucleation to seed mass ratio) during the batch when open-loop optimal control is implemented.

The p.d.f was determined using first-order distributional analysis.

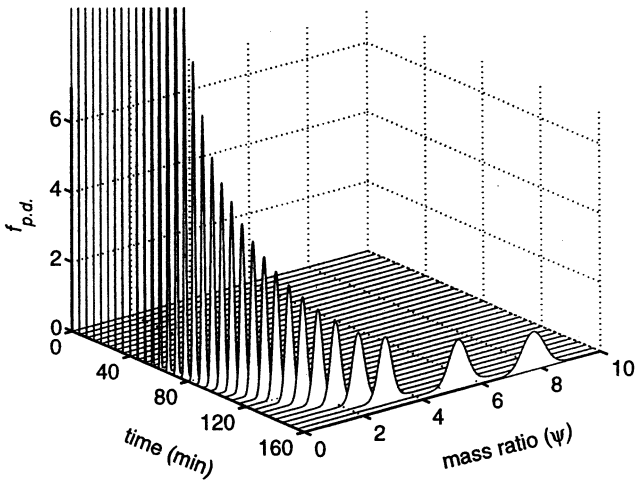

Figure 5. Variation of the p.d.f. of the performance index (the nucleation to seed mass ratio) during the batch when robust NMPC with EKF is implemented.

The p.d.f was determined using first-order distributional analysis.

Table 4. Worst-Case Performance (for Parameter Uncertainty with Confidence Level $\alpha = 0.95$) for the Weight Mean Size (WMS) Obtained by Open-Loop Optimal Control, Nominal NMPC ($w = 0$), Robust NMPC ($w = 0.2$) with EKF, and Robust NMPC ($w = 0.2$) with Perfect Knowledge of the States*

Control Approach	Nominal $WMS(t_f)$	$WMS_{w.c.}(t_f)$ Est. with First-Order Expansion	Improved Value from Dynamic Simulation
Open-Loop Optimal Control	590	535	538
NMPC (Nominal, with EKF)	591	558	543
Robust NMPC (with EKF)	594	563	545
Robust NMPC (with Known States)	591	570	551

*The worst-case deviation was estimated using first-order robustness analysis, with the improved value computed by performing dynamic simulation for the worst-case parameter computed from first-order analysis.

variation of the probability density function of the performance index along the batch run for open-loop optimal control, nominal NMPC, and robust NMPC. The distributions of ψ increase monotonically during the batch run for all three cases. The NMPC approaches provide a considerably narrower distribution for the entire batch compared to the open-loop optimal control. Compared to nominal NMPC, robust NMPC has a narrower endpoint distribution, which is expected since the endpoint variance is included in its optimization objective, while providing a slightly wider distribution in the third quarter of the batch run.

Although not included explicitly in the NMPC optimization objective, the variation of the weight mean size

$$WMS = \frac{\mu_4}{\mu_3} \tag{54}$$

was also computed. Table 4 shows the effect of parameter uncertainty on the *WMS* at the end of the batch. The *WMS* at the end of the batch is not significantly more robust for the NMPC algorithms than for open-loop implementation. Hence, a batch control strategy can be highly robust for some product quality variables, while being less robust for others. This illustrates the importance of considering in the objective function (Eq. 50) all product quality variables for which increased robustness is desired. As in Table 3, the small differences of the results obtained with robust NMPC with EKF compared to the case where the states are perfectly known indicate the good performance of the EKF.

To assess the accuracy of the above robustness analysis, Monte Carlo simulations were performed by dynamic simulation with 100 random parameter vectors generated from the multivariate normal distribution function 34. Figures 6–8 show the effects of parameter uncertainty on the two CSD properties (ψ and *WMS*) at the end of the batch run for open-loop optimal control, nominal NMPC, and robust NMPC. These results are quantitatively consistent with the analysis results reported in Figures 3–5 and the last columns of Tables 3–4, with the agreement for open-loop optimal control being somewhat better than for the NMPC algorithms. The computational burden for the Monte Carlo approach, however, is much greater than for series expansion-based robustness analysis. Even with the fairly limited set of data, the Monte Carlo simulations for the NMPC approaches took approximately one week on a 800 MHz Pentium III computer, which is about 25 times longer than the computational time required for the series expansion-based robustness analysis. The series expansion-based robustness analysis

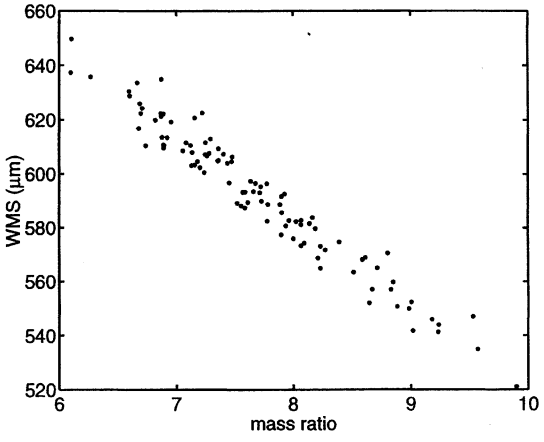

Figure 6. Weight mean size and nucleated to seed mass ratio at the end of the batch for 100 Monte Carlo simulations, when open-loop optimal control is implemented.

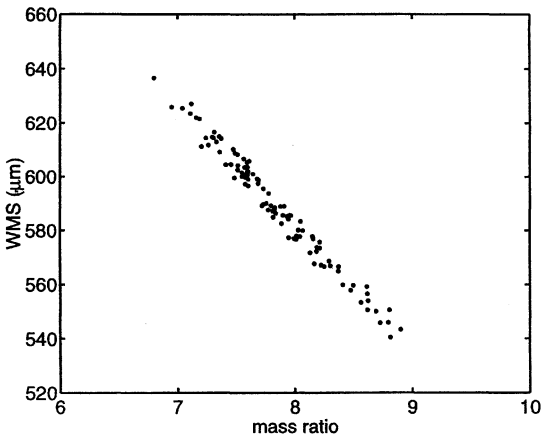

Figure 7. Weight mean size and nucleated to seed mass ratio at the end of the batch for 100 Monte Carlo simulations, when nominal NMPC with EKF is implemented.

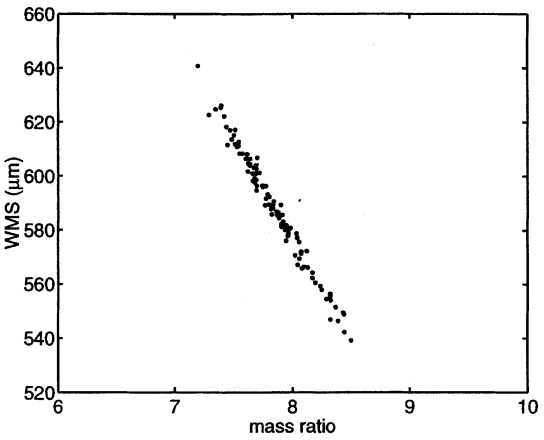

Figure 8. Weight mean size and nucleated to seed mass ratio at the end of the batch for 100 Monte Carlo simulations, when robust NMPC with EKF is implemented.

technique is a computationally efficient approach that can provide valuable information concerning robust performance even for advanced control architectures, such as the combined EKF and NMPC approach used in this article.

Conclusions

A robust EKF-based NMPC algorithm for batch processes is presented which incorporates parameter uncertainty into both the EKF and NMPC algorithms. A series expansion of the performance index is used to estimate the distribution of the process output for the whole batch run. For a simulated batch crystallization process, NMPC considerably improved robust performance compared to open-loop optimal control. Robust performance is significantly enhanced when parameter uncertainty is taken into account in the objective function of the NMPC. The conclusions obtained from the series-based analysis approach are verified through Monte Carlo simulation.

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