Accounting for Batch Reactor Uncertainty in the Nonlinear MPC of End-Use Properties

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There are significant incentives in controlling the end-use properties in batch reactors to reduce the variability in the final product quality. The presence of model errors and other uncertainties poses a problem in achieving this objective using model-based control. A methodology to account for the model uncertainties in nonlinear model predictive control is presented here. This methodology also allows establishing a trade-off between robustness and optimality in the controller. This is based on determining the uncertainty in the predicted final values of the properties, in the form of elliptical confidence regions. The controller then ensures that the complete confidence region is within the target range for the product. A semiinfinite programming problem is solved to find the input values for the rest of the batch, utilizing techniques that reduce the complexity of the problem. A Parameter Adaptive Extended Kalman Filter is used to estimate the important unmeasured and observable properties. An emulsion polymerization process for styrene is chosen as a case study and the methods developed here are demonstrated on this example process.

Introduction

There is a strong incentive in controlling the batch product properties to minimize the variability in the product quality. In most cases, the product quality is decided by the end-use properties. In polymerization processes, the end-use properties are currently controlled indirectly by controlling the molecular properties at target set points. The direct on-line control of end-use properties using a static model that relates these properties to the molecular properties of the product is considered here.

Nonlinear Model Predictive Control (NLMPC) provides an attractive methodology to handle the time varying and highly nonlinear batch processes, where the control actions need to be taken early on in the batch to be effective. In this study, the control objective is formulated so as to attain this target set for the end-use properties at the end of the batch (Valappil and Georgakis, 2001). The approach is well suited to cases where there is insufficient number of manipulated variables to control all the end-use properties at a specific set point. However, if there are extra degrees of freedom, an optimal objective (like maximizing a conversion subject to fixed batch time) can be realized once the target values for the properties are attained. The effect of uncertainty in this scheme and the methodologies for explicit uncertainty consideration are discussed in this communication.

Chemical processes are characterized by significant uncertainties, a limited number of noisy measurements and the fact that the end-use properties that are controlled are usually not measured on-line. The consideration of uncertainty is especially important for the cases where an optimal operation is desired, as this would put the properties at the boundaries of end-use property target region, thus making them susceptible to uncertainty. One of the most widely used approaches to quantify the uncertainties is the use of a state estimator. This can be useful to some extent in handling the unmodeled

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effects in the process. The problem would occur when there are end-use properties that are dependent on the unobservable states (which are estimated in open loop). This would result in inaccurate predictions of these properties, thus making their control difficult. This motivates the use of a method to handle the uncertainties in an explicit way during the control calculation, thus taking control actions that are conservative, but safe.

The incorporation of model and other uncertainties in process design, optimization, and control have appeared in many recent studies. The use of information about the model uncertainty for optimization of batch processes has been discussed (Terwiesch et al., 1998, 1994; Loeblein et al., 1999). These techniques are mostly applied to optimal profiles determined off-line, and are based on the expected value of the objective function or some measure of variability in the objective. In linear and nonlinear model predictive control, a min-max formulation of the controller has been used to incorporate uncertainty (Campo and Morari, 1987; Allwright and Papavasiliou, 1992; Kothare et al., 1996). The motivation for this is to find the inputs that would minimize the worst case objective function. The use of min-max method can result in a very conservative controller. To ensure the satisfaction of hard constraints under model error, chance constrained programming and semi-infinite programming based methods have also been used in MPC (Schwarm and Nikolaou, 1999; Kassman et al., 2000; Meadows and Rawlings, 1991).

A methodology that incorporates the model uncertainty in NLMPC for on-line application is presented here. This is based on the control of end-use properties in target regions. The approach presented here is based on ensuring that the properties are controlled indirectly at a point that is reachable, optimal, and also the one that accounts for the uncertainties in the system. For this, the confidence regions for the predicted values of end-use properties are determined by utilizing an uncertainty propagation. The joint confidence regions for the end-use properties are required to lie completely within the target region for the product, while maximizing an objective function that represents the economic objective. A two-stage strategy is used to accomplish this based on the priorities in the objectives. The first stage focuses on the end-use property specifications, while the second stage utilizes the remaining control degrees of freedom for optimizations.

The NLMPC problem under uncertainty is formulated as a semi-infinite programming problem, since the properties can lie anywhere on the boundary of the confidence region. This semi-infinite programming problem is solved using an outer-approximation algorithm which reduces the computational demands and improves convergence properties. With suitable simplifications, the solution of the semi-infinite program is easily attained making it amenable to on-line implementation.

The emulsion polymerization process for styrene is chosen as an example to study the effectiveness of the above methodology. The properties like the melt index, tensile strength, and weight average particle diameter are controlled within the desired target region using the two manipulated variables, additional rates of the monomer, and chain transfer agent. The optimization objective considered is the conversion attained at the end of the batch. Monte Carlo simulations with uncertain parameters are performed to demonstrate that the consideration of uncertainty in NLMPC can significantly reduce the variability in the final product properties.

A brief description of the nominal control problem is presented. This is followed by the description of the methodology to handle uncertainty. This includes the calculation of confidence regions and the description of the numerical procedure. Finally, the application of the method to emulsion polymerization of styrene is presented.

Control of End-Use Properties in Batch Reactors: Nominal Case

Batch processes are characterized by stringent quality requirements, which makes it very important to reduce the variability in the product properties. Nonlinear model predictive control techniques have found applications for batch product property control. This includes tracking of optimal trajectories and direct control of end of the batch quality. The methodology of Shrinking Horizon Model Predictive Control (SHMPC) is very suitable for the end of the batch property control and is used here (Valappil and Georgakis, 2001).

The studies presented here are based on a dynamic first principle model of the batch process. The actual batch process can be presented in nonlinear state space form as below.

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{f}_p(\boldsymbol{x},\boldsymbol{u},\boldsymbol{p},\boldsymbol{d},t) \tag{1}$$

where $\boldsymbol{x}$ denotes the system states, $\boldsymbol{u}$ denotes the manipulated variables, $\boldsymbol{p}$ denotes the model parameters and $\boldsymbol{d}$ denotes the disturbances entering the process.

Target regions for end-use property control

The product properties in many of the chemical processes can be classified into molecular properties and end-use properties. The molecular properties are related to the molecular architecture of the product, while the end-use properties are properties that characterize the use of a particular product. Examples of molecular properties include molecular weight distribution, particle-size distribution, and polydispersity. Examples of end-use properties include tensile strength, melt index, scrub resistance, film adhesion, and oil resistance.

The desired values of the end-use properties are specified by the intended use of the product. In many practical situations, the interest is in ensuring that the particular product properties lie in a certain range of specification. The end-use properties can be related to the molecular properties of the product at the end of the batch using the available static models. The molecular properties are functions of states at the end of batch. Thus, a nonlinear functional relationship between the end-use product properties and the state values can be obtained as given below

$$z_f = \boldsymbol{q}(\boldsymbol{x}_f,\xi) \tag{2}$$

where z_f is a vector of end-use properties, $\boldsymbol{x}_f$ are the states of the system at the end of the batch, and ξ denotes the

parameters of the end-use property model. The parameters ξ are estimated when fitting the relationship between the two sets of properties. Examples for these parameters include the weights in artificial neural networks or coefficients in a partial least-squares model.

The requirement that the end-use properties lie in the target region Q_t can then be transformed into a set of quality constraints in the form of nonlinear equalities and inequalities. Target regions of arbitrary shapes can be represented this way

$$\boldsymbol{q}(\boldsymbol{x}_f,\xi) \subseteq Q_t \Leftrightarrow \left\{\boldsymbol{q}_1(\boldsymbol{x}_f,\xi) \le \boldsymbol{0};\qquad \boldsymbol{q}_2(\boldsymbol{x}_f,\xi) = \boldsymbol{0}\right\} \quad (3)$$

A single set of inequalities is defined to represent the above set of inequalities and equalities. The representation of the target region in terms of states can be given as

$$\left\{\boldsymbol{r}(\boldsymbol{x}_f,\xi) \le \boldsymbol{0}\right\} \quad (4)$$

and in terms of end-use properties

$$\left\{\boldsymbol{s}(z_f) \le \boldsymbol{0}\right\} \quad (5)$$

Since the states are functions of inputs used in the batch $\boldsymbol{u}$, these inequalities can be represented in terms of inputs as

$$\{\boldsymbol{g}(\boldsymbol{u}) \le \boldsymbol{0}\} \quad (6)$$

Successive target region linearization approach

The control of end-use properties under a nominal condition can be formulated as to find inputs that would bring the final states of the batch to the desired target region. This can be given as

$$\begin{gathered}\left\{\text{Find } \boldsymbol{u} \ni \boldsymbol{r}(\boldsymbol{x}_f) \le \boldsymbol{0}\right\}\\ \frac{d\boldsymbol{x}}{dt} = \boldsymbol{f}(\boldsymbol{x},\boldsymbol{u},\boldsymbol{p},\boldsymbol{d},t)\\ \boldsymbol{x}(t=0) = \boldsymbol{x}_0\\ \boldsymbol{h}(\boldsymbol{x}(\tau)) \le \boldsymbol{0};\qquad t \le \tau \le t_f\\ \boldsymbol{A}\boldsymbol{u}(\tau) \le \boldsymbol{b};\qquad t \le \tau \le t_f\end{gathered} \quad (7)$$

The term $\boldsymbol{h}(\boldsymbol{x})$ represents the nonlinear path constraints on the states. These constraints are augmented with target region constraints for solution. The last term denotes the constraints on the manipulated variables and their rates of change, which are represented as linear inequalities in the manipulated variables $\boldsymbol{u}$.

A solution method suitable for the end-use property control at target regions was introduced in Valappil and Georgakis (2001). This is based on a Newton's method that successively linearizes the target region until a solution is obtained (Mayne and Sahba, 1985). The main step in the problem is to linearize the target region constraints in terms of inputs $\boldsymbol{g}(\boldsymbol{u})$ to find a step towards the solution via a quadratic program as given below

$$\begin{gathered}\min_{\Delta \boldsymbol{u}} \{\Delta \boldsymbol{u}'\Delta \boldsymbol{u}\}\\ \boldsymbol{g}(\boldsymbol{u}) + \nabla \boldsymbol{g}(\boldsymbol{u})\Delta \boldsymbol{u} \le \widetilde{\psi\epsilon}^{0}(\boldsymbol{u})\\ \boldsymbol{A}\boldsymbol{u} + \boldsymbol{A}\Delta \boldsymbol{u} \le \boldsymbol{b}\end{gathered} \quad (8)$$

Here, $\widetilde{\psi\epsilon}^{0}$ is a parameter that is used to ensure feasibility in the quadratic program. A linear program determines this value if there is no feasible solution to the linearized problem. The nominal controller finds the inputs that would bring the properties to the interior of the target region. The stopping criterion that is used for this problem is to minimize the maximum among all the constraints that represent the target region.

It is computationally demanding to determine all the future control moves using NLMPC. The solution is to parameterize the inputs with the appropriate, reduced number of variables (control vector parameterization). A Lagrange polynomial approach is used here for input parameterization, whereby the parameters are the values of inputs at certain future time intervals. The details of this parameterization scheme and the solution of the nominal control problem are given in Valappil and Georgakis (2001).

Incorporation of Uncertainty in the Control of End-use Properties

The nominal control problem discussed in a previous section was solely based on controlling the properties. In many processes, there are also benefits to be realized from operating the batch in an optimal manner. The explicit consideration of the uncertainties in NLMPC is important in such cases. In most situations, the optimum lies in the intersection of the constraints. Target region constraints can become active, which results in the end of the batch properties at the boundaries of the target region. The consideration of model and other uncertainties in the process is important in maintaining the product quality in these cases. This would also allow a trade-off between robustness and the optimal operation of the process.

Two different approaches for incorporating uncertainty are the open-loop and closed-loop techniques. In the open-loop methods, the information about the uncertainty is used to determine policies that account for them. Closed-loop techniques, on the other hand, utilize the information about the system from on-line measurements. It is desirable to utilize the features of both open- and closed-loop methods for uncertainty handling in the control of end-use properties. The stochastic state estimator (EKF in this case) incorporates the effect of unmeasured disturbances and other uncertainties. As the measurements come in during the batch, the estimator uses these measurements to reduce the uncertainties that occur from the recipe and the unmeasured sources. The unmeasured disturbances are estimated using the adapted parameters. Apart from this, the process model is used for the prediction of the end of the batch properties. Both the uncertainty in the current states and the model uncertainty has its effect on the final property predictions. Both these effects are considered by determining the confidence regions on the final property predictions.

The methodology developed here has three main components. First is quantifying the state uncertainty via the use of an Extended Kalman Filter. The second component is the establishment of uncertainty in the future prediction, which is done with confidence regions. The third part is the solution of the NLMPC problem using semi-infinite programming.

State estimation

The state estimator plays an important role in the methodology for the control of end-use properties with uncertainty. Apart from an estimate of states and unmeasured disturbances, the information about the current state uncertainty is obtained from a stochastic state estimator (EKF for example). These values are necessary for calculating the uncertainty in the final property predictions.

For state estimation and control purposes, the batch process is represented in the first principle model form as below

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{f}(\boldsymbol{x},\boldsymbol{u},\boldsymbol{p},\boldsymbol{d},\theta,t) + \boldsymbol{w} \tag{9}$$

where θ denotes certain adapted parameters in the model and $\boldsymbol{w}$ denotes the process noise.

The state estimator used here is a Parameter Adaptive Extended Kalman Filter (PAEKF) where certain fictitious parameters are estimated along with the states using the available measurements. This is analogous to adding integral action in a controller, thus eliminating the offset in the estimated variables. The system states are augmented with adapted parameters to form the augmented state space system given below

$$\frac{d}{dt}\begin{pmatrix}\boldsymbol{x}\\ \theta\end{pmatrix} = \begin{pmatrix}\boldsymbol{f}\\ \boldsymbol{0}\end{pmatrix} + \begin{pmatrix}\boldsymbol{w}\\ \boldsymbol{w}\theta\end{pmatrix} \tag{10}$$

The linearized version of this augmented state space form is used in the EKF and for propagation of covariance. This can be given as

$$\frac{d\boldsymbol{x}_a}{dt} = \boldsymbol{A}_a\boldsymbol{x}_a + \boldsymbol{B}_a\boldsymbol{u} \tag{11}$$

The covariance matrix for the augmented system $\boldsymbol{P}_a$ and the augmented state space matrix $\boldsymbol{A}_a$ are appropriately given by

$$\boldsymbol{P}_a = \begin{bmatrix}\boldsymbol{P}_x & \boldsymbol{P}_{x\theta}\\ \boldsymbol{P}_{\theta x} & \boldsymbol{P}_\theta\end{bmatrix};\ \boldsymbol{A}_a = \begin{bmatrix}\dfrac{\delta \boldsymbol{f}}{\delta \boldsymbol{u}} & \dfrac{\delta \boldsymbol{f}}{\delta \theta}\\ \boldsymbol{0} & \boldsymbol{0}\end{bmatrix};\ \boldsymbol{B}_a = \begin{bmatrix}\dfrac{\delta \boldsymbol{f}}{\delta \boldsymbol{u}}\\ \boldsymbol{0}\end{bmatrix} \tag{12}$$

The performance of the EKF depends on the specification of covariance of $\boldsymbol{w}$ and $\boldsymbol{w}_\theta$. The former is obtained by a procedure that was presented in Valappil and Georgakis (2000). This uses the information about model uncertainty to obtain time varying and non-diagonal process noise covariance matrix. The covariance for $\boldsymbol{w}_\theta$ is obtained by trial and error with different values.

The selection of process noise covariance matrix, $\boldsymbol{Q}$ is quite important in this application, as these values impact the state covariance at the end of the batch. If this is selected too low, apart from the possibility of filter divergence, the control actions would be very aggressive as the end-use property covariance predictions are an underestimate. On the other hand, if this is quite high, the control actions would be too conservative and the optimal objective is not completely realized. The uncertainty in the initial conditions of the batch is reflected in the covariance of states from the EKF, $\boldsymbol{P}$. This covariance decreases as time progresses since more measurements become available during the batch.

Calculation and use of joint confidence regions for end-use properties

The methodology presented here involves estimating and using the uncertainty in the predictions of end-use properties at the final time. This uncertainty is in the form of covariance for each property and their cross-covariance. The main disadvantage of using confidence intervals for individual properties is that it does not account for the correlations in end-use properties. The use of joint confidence regions that accounts for property correlations are much more suitable for the problem examined here.

Calculation of Confidence Regions (Subproblem A-1). The uncertainty in the final states needs to be calculated from the information about the current state uncertainty from EKF and the process-model mismatch. Since the system is nonlinear and of high dimensions, it is computationally demanding to do a complete nonlinear uncertainty propagation. An alternative is to use a linear approximation to do the propagation of uncertainty. (See Figure 1.) This is customarily used in the uncertainty analysis for nonlinear systems. The states and their associated covariance are propagated foward in time using a linear approximation for the system as given below

$$\frac{d\boldsymbol{P}_a}{dt} = \boldsymbol{A}_a\boldsymbol{P}_a + \boldsymbol{P}_a\boldsymbol{A}_a^T + \boldsymbol{B}_a\boldsymbol{C}_u\boldsymbol{B}_a^T + \boldsymbol{J}_p\boldsymbol{C}_p\boldsymbol{J}_p^T - \boldsymbol{P}_a\boldsymbol{C}_a^T\left[\boldsymbol{C}_a\boldsymbol{P}_a\boldsymbol{C}_a^T + \boldsymbol{R}\right]^{-1}\boldsymbol{C}_a\boldsymbol{P}_a \tag{13}$$

where $\boldsymbol{J}_p$ is the sensitivity of system equations to parameters, $\boldsymbol{C}_p$ is the parameter covariance matrix, and $\boldsymbol{C}_u$ is the covariance of the input values. The first two terms account for the

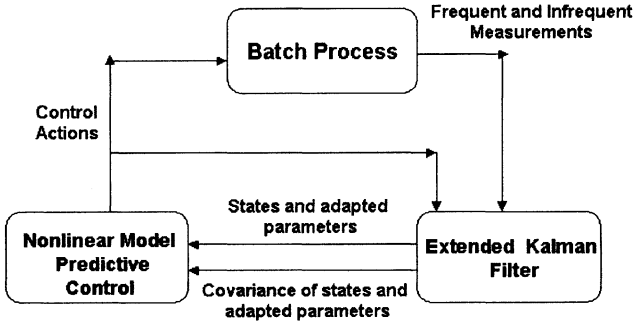

Figure 1. Use of information about model uncertainty in state estimation and NLMPC.

The states, adapted parameters, and their covariance from the EKF are used in model predictive control.

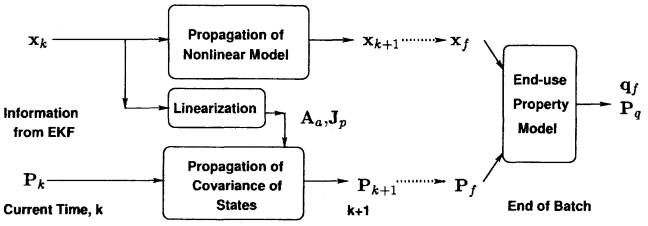

Figure 2. Propagation of uncertainty to the end of batch using nonlinear model and linearized covariance propagation equations.

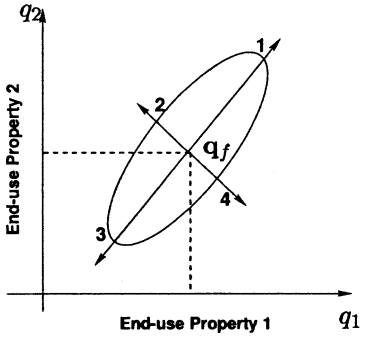

Figure 3. Points in the elliptical confidence region that are required to lie in target set for a case with two end-use properties.

propagation of state uncertainty via the dynamics of the system, the third term accounts for the control implementation uncertainty, and the fourth term accounts for the effects of the model uncertainty. The final term represents the feedback due to the measurements. The above equation is propagated from current time to the end of the batch to obtain the state covariance at the end of the batch. The initial conditions for the above integration are the state covariance at the end of the batch. The initial conditions for the above integration are the state covariance matrix from EKF. The matrices $\boldsymbol{A}_a$, $\boldsymbol{B}_a$, $\boldsymbol{C}_a$, $\boldsymbol{J}_p$ depend on the states of the system and change with time during the propagation. The system is repeatedly linearized every 1 min. during this calculation to get the above matrices using the state values. This calculation is given in Figure 2.

This gives the covariance of the states at the end of the batch. The covariance of end-use properties are obtained using the nonlinear relationship between the states and the end-use properties given in Eq. 2. A linear approximation is used to perform the calculation of the covariance of the end-use properties $\boldsymbol{P}_q$ by

$$\boldsymbol{P}_q = \left(\frac{\partial \boldsymbol{q}}{\partial \boldsymbol{x}}\right)\boldsymbol{P}_x\left(\frac{\partial \boldsymbol{q}}{\partial \boldsymbol{x}}\right)^T + \left(\frac{\partial \boldsymbol{q}}{\partial \xi}\right)\boldsymbol{P}_\xi\left(\frac{\partial \boldsymbol{q}}{\partial \xi}\right)^T \tag{14}$$

where $\boldsymbol{P}_\xi$ is the covariance matrix for the parameters of the end-use property model. The uncertainty of the static end-use property model is, thus, incorporated in this step of the calculation.

The covariance of the end-use properties at the end of the batch is utilized to obtain the 95% confidence regions for the end-use properties. Joint confidence regions are obtained in the form of hyper-ellipsoids centered at the nominal value. This assumes the multivariate normal distribution of the end-use properties. The hyper-ellipsoidal confidence regions (with $100(1-\alpha)\%$ confidence) are characterized by the equation

$$(z - z_f)^T \boldsymbol{P}_q^{-1}(z - z_f) \le n_p F_{(\alpha, n_p, n_f - n_p)} \tag{15}$$

where n_p is the number of end-use properties, n_f is the number of degrees of freedom, and z denotes the properties that lie anywhere within the confidence region. The righthand side contains the statistical F distribution that depends on the number of properties and the level of confidence α.

The boundaries of the hyper-ellipsoidal confidence region can be obtained by using the equality signs in Eq. 15. There is an infinite number of points in this boundary and a finite representation of this is necessary for control purposes. The points in the confidence region that are considered are the ones where the axes of the confidence region intersect its boundary (Figure 3). These points are obtained by an eigenvalue decomposition of the inverse of the end-use property covariance matrix $\boldsymbol{P}_q$.

$$\boldsymbol{P}_q^{-1} = \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^T \tag{16}$$

where $\boldsymbol{V}$ is the matrix of eigenvectors and $\boldsymbol{\Lambda}$ is the matrix with diagonal elements are eigenvalues. The length of each axis of the hyper-ellipsoid is obtained from the eigenvalue and eigenvector, and is used to find the points of interest on the boundary. For each eigenvalue λ_i (axis), there are two such points of intersection, which are given by

$$z_{1,i} = z_f + \boldsymbol{v}_i\sqrt{\frac{n_p F_{(\alpha, n_p, n_f - n_p)}}{\lambda_i}}\ ;$$

$$z_{2,i} = z_f - \boldsymbol{v}_i\sqrt{\frac{n_p F_{(\alpha, n_p, n_f - n_p)}}{\lambda_i}}\ ; \qquad i = 1, 2, ..., n_p \tag{17}$$

where $\boldsymbol{v}_i$ and λ_i denote the ith eigenvector and the eigenvalue of the inverse of the end-use property covariance matrix $\boldsymbol{P}_q$. A single vector $\boldsymbol{e}$ is used to represent the set of all the above $2n_p$ points. The vector $\boldsymbol{e}_i$ thus denotes the ith point on the confidence region where the axes intersect the boundary.

Dependence of Confidence Region on Future Inputs (Subproblem A-2). The confidence regions calculated via uncertainty propagation are dependent on the values of the inputs during the batch. Both the size of the region and the orientation of the axes can vary significantly with the variation in the future input values. In the iterative calculations, it is computationally infeasible to update their values by the complete uncertainty propagation each time the input values change. To handle this problem, a linear approximation is used for the dependence of final end-use property covariance to the inputs. The covariance of the end-use properties for the in-

puts $\boldsymbol{u}_2$ are obtained using the values at $\boldsymbol{\mu}_1$ as given below

$$\boldsymbol{P}_q(\boldsymbol{u}_2) = \boldsymbol{P}_q(\boldsymbol{u}_1) + \left(\frac{\partial \boldsymbol{P}_q}{\partial \boldsymbol{u}}\right)_{\boldsymbol{u}_1} (\boldsymbol{u}_2 - \boldsymbol{u}_1) \tag{18}$$

where the values of $\partial \boldsymbol{P}_q/\partial \boldsymbol{u}$ are obtained by sensitivity analysis. Since higher-order terms are ignored in this approximation, the resulting confidence region is an underapproximation. The correlation structure in the properties is adequately well captured by the linear approximation, which is sufficient for the purposes studies here.

Formulation of the NLMPC problem under uncertainty

The main objective of the NLMPC under uncertainty is to control the entire confidence region within the target region for the product (Figure 4). The secondary objective is to realize the optimal operation of the batch. This formulation can be mathematically represented at time t_k as

$$\begin{gathered}
\min_{\boldsymbol{u}(\tau)} J_k(\boldsymbol{x}_f, t_f) \\
\boldsymbol{s}(\boldsymbol{z}) \le \boldsymbol{0} \\
(\boldsymbol{z} - \boldsymbol{z}_f)^T \boldsymbol{P}_q^{-1} (\boldsymbol{z} - \boldsymbol{z}_f) = pF_{(\alpha,p,n-p)} \\
\boldsymbol{z}_f = \boldsymbol{q}(\boldsymbol{x}_f, \xi) \\
\frac{d\boldsymbol{x}}{dt} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{u}, \boldsymbol{p}, \boldsymbol{d}, \theta, t) \\
\boldsymbol{h}(\boldsymbol{x}(\tau)) \le \boldsymbol{0}; \qquad t \le \tau \le t_f \\
\boldsymbol{A}\boldsymbol{u}(\tau) \le \boldsymbol{b}; \qquad t \le \tau \le t_f
\end{gathered} \tag{19}$$

where $\boldsymbol{J}$ denotes the objective function (this could be, for example, batch time, batch conversion, yield, and so on), $\boldsymbol{z}$, the properties on the boundary of the confidence region, and $\boldsymbol{s}$ denotes the target region constraints on the properties. The property covariance matrix, $\boldsymbol{P}_q$ in the above is obtained by the covariance propagation given in Eq. 14. The desired confidence value for the properties α is specified by the user and, if this is not achievable, the controller determines the level of confidence that can be handled within the target region. The above problem is repeated at time t_{k+1}.

The formulation presented above results in a semi-infinite programming problem since the values of the end-use properties $\boldsymbol{z}$ can lie anywhere on the confidence region. Semi-infinite programming problems represent the class of problems where one or more of the variables belong to an infinite set. The general form of semi-infinite program can be given as

$$\begin{gathered}
\min_{\boldsymbol{u}} h(\boldsymbol{u}) \\
\boldsymbol{g}(\boldsymbol{u}, \zeta) \le \boldsymbol{0}; \qquad \zeta \subset \boldsymbol{\Psi}
\end{gathered} \tag{20}$$

where $\boldsymbol{u}$ represents the independent variables, and ζ represents the parameter, which belongs to the set $\boldsymbol{\Psi}$. The variable $\boldsymbol{u}$ in the above equation represents the inputs in Eq. 19. The variable ζ represents the infinite variable, which can be the angle covering the hyper-ellipsoid that spans from 0 to 360. Semi-infinite programming problems appear in many areas in engineering (Hettich and Kortanek, 1993). Many of the robust optimization and control problems can be cast in the semi-infinite form for solution (Reemsten and Ruckmann, 1998; Kassman et al., 2000). The solution to the above semi-infinite program is difficult, and there is no guarantee that the algorithm would converge. The solution to this problem is accomplished in two stages keeping in mind the priorities in objectives. These stages are listed below.

- The first stage is to find the inputs that would bring the end-use properties and associated confidence region inside the target set. This is due to the fact that the quality comes first, and the satisfaction of product specifications is of utmost importance.
- Once first-stage objectives are accomplished, the inputs are manipulated to move the process towards the optimum, while making sure that the complete confidence region still remains in the target set.

The problem given in Eq. 19 can also be solved in one step, without recourse to feasibility and optimization subproblems. The solution of the feasibility problem is done to ensure the property constraints are satisfied first and only the remaining degrees of freedom are used for optimization.

The first-stage problem is one of solving semi-infinite inequalities. This is a difficult problem and the solution method for this is addressed in detail here. The second-stage problem is a semi-infinite optimization problem. Since the initial guess from the first stage satisfies the target region constraints, the problem is solved without much difficulty. It is transformed here into a constrained nonlinear optimization problem for the solution.

Integration of dynamic system and calculation of the gradients

The solution of the nonlinear model predictive control involves the integration of the dynamic system into the future. Further, the gradient of the end of the batch states and covariance with respect to the inputs are needed in each step. Finite difference gradients are not recommended for use in Newton type methods, since the convergence depends on gradient information. The gradients here are obtained by sensitivity analysis. The equation for the time evolution of the sensitivity of states with respect to the inputs can be given as

$$\begin{gathered}
\frac{d}{dt}\frac{\partial \boldsymbol{x}}{\partial \boldsymbol{u}} = \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}\frac{\partial \boldsymbol{x}}{\partial \boldsymbol{u}} + \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{u}} \\
\frac{\partial \boldsymbol{x}}{\partial \boldsymbol{u}_{(t=0)}} = \boldsymbol{0}
\end{gathered} \tag{21}$$

The sensitivity equations are solved simultaneously along with the nonlinear equations using the program ODESSA (Leis and Kramer, 1988). Runge-Kutta method is used for the integration. The same procedure is used to obtain the sensitivity of state covariance with respect to the inputs. The nonlinear relationship between the end-use properties and the inputs are used to determine the gradient of target region constraints with respect to the inputs.

Solution Method for the Control of End-Use Properties with Uncertainty Consideration

The NLMPC problem presented in the previous section needs to be solved at each time step with the information available on-line. This makes it important to use a method that is computationally efficient and has good convergence properties. The following features of the formulation have an important impact on the method used for solution.

- The feasibility of the problem depends on α, the level of confidence. If the desired level of confidence is not achievable, a conservative and realistic value has to be determined.
- The dependence of confidence region on inputs and the frequency of linearization in calculating the confidence regions have to be established. Furthermore, the propagation of state covariance into the future has to be computationally feasible, as it is performed on-line at each controller execution.

The above issues are addressed systematically in the methodology presented here.

Semi-infinite programming solution (Subproblem B-1)

The first-stage problem of bringing the complete confidence region for the properties into the target set is formulated as one of solving semi-infinite inequalities as given below

$$\begin{gathered}
\{\text{Find } \boldsymbol{u} \ni \boldsymbol{s}(\boldsymbol{z}) \le \boldsymbol{0}\} \\
(\boldsymbol{z}-\boldsymbol{z}_f)^T \boldsymbol{P}_q^{-1}(\boldsymbol{z}-\boldsymbol{z}_f) = pF_{(\alpha,n_p,n_f-n_p)} \\
\boldsymbol{z}_f = \boldsymbol{q}(\boldsymbol{x}_f,\xi) \\
\frac{d\boldsymbol{x}}{dt} = f(\boldsymbol{x},\boldsymbol{u},\boldsymbol{p},\boldsymbol{d},\theta,t) \\
\boldsymbol{h}(\boldsymbol{x}(\tau)) \le \boldsymbol{0}; \qquad t \le \tau \le t_f \\
\boldsymbol{A}\boldsymbol{u}(\tau) \le \boldsymbol{b}; \qquad t \le \tau \le t_f
\end{gathered} \tag{22}$$

The solution of a nonlinear semi-infinite programming problem has to be done by approximating the infinite set of parameters by a finite one. A number of approaches have been proposed to do this finite approximation, including exchange methods, discretization methods, and the method of local reduction (Hettich and Kortanek, 1993). A simplification of this semi-infinite problem is achieved by making an assumption about the nature of the target region. It needs to be noted that in most cases the target regions tend to be convex, since these are either simple independent bounds on the individual properties or other convex shapes. Also, the joint confidence regions are hyper-ellipsoidal in shape due to the linearized approach in their calculation, and, hence, convex. With this assumption, it becomes necessary to consider only the points where the principal axes intersect the boundaries of the confidence region. The notion of convexity implies that, once these points are in the target region, the intermediate points in the straight line connecting them are also within the target set. The problem given in Eq. 22 can be reformulated in terms of the finite number of points of intersection as

$$\begin{gathered}
\{\text{Find } \boldsymbol{u} \ni \boldsymbol{s}(\boldsymbol{e}_i) \le \boldsymbol{0} \qquad i = 1, 2, ..., 2n_p\} \\
\boldsymbol{z}_f = \boldsymbol{q}(\boldsymbol{x}_f,\xi) \\
\frac{d\boldsymbol{x}}{dt} = \boldsymbol{f}(\boldsymbol{x},\boldsymbol{u},\boldsymbol{p},\boldsymbol{d},\theta,t) \\
\boldsymbol{h}(\boldsymbol{x}(\tau)) \le \boldsymbol{0}; \qquad t \le \tau \le t_f \\
\boldsymbol{A}\boldsymbol{u}(\tau) \le \boldsymbol{b}; \qquad t \le \tau \le t_f
\end{gathered} \tag{23}$$

where $\boldsymbol{e}_i$ is calculated by the procedure given in the subsection on calculation of confidence regions (Subproblem A-1).

It is possible to formulate the problem as a solution of one nonlinear inequality problem by putting all the $2n_p$ points under consideration together. However, this has the disadvantage that the number of constraints in the problem would be very large with an increase in the number of properties. This is understandable, as with simple upper and lower bound constraints on properties, a problem with n properties would result in $2n^2$ constraints. This prompts the application of an efficient semi-infinite programming solution strategy that adaptively formulates a reduced problem. An efficient solution technique suitable for the problem and based on the outer approximation method is described below.

Outer Approximation Method. The semi-infinite program problem presented in Eq. 20 has to be solved in an iterative fashion. At each iteration, an approximate problem is formulated that considers only a finite subset of the $2n_p$ points at the target region boundary (Figure 5). The outer approximation is a systematic way of forming the approximate problem (Gonzaga and Polak, 1979). These methods help to reduce the computational complexity of the semi-infinite program and has desirable convergence characteristics (Reemsten, 1994; Mayne et al., 1979).

The application of out-approximation is aided by the fact that we are interested only in the finite number of points where the axes of the hyper-ellipsoid intersect the confidence region. The outer approximation procedure used here is based on adaptive constraint addition without the removal of constraints. The procedure is started with only the nominal point for the properties under consideration (finding inputs that will bring the nominal values to the target region). For the formulation of the approximate problem at each step, each target region constraint is examined in turn. The points where the axes intersect the confidence region boundary ($2n_p$ points) are examined to find the point which violates that constraint by the maximum amount. This point of maximum constraint violation is appended to the problem for the next step. This procedure is repeated until a solution is obtained that satisfies the target region constraints for all the $2n_p$ points at the confidence region boundary (Figure 5).

It needs to be noted that as the number of iterations increase, the approximate problem would approach the complete problem with all the constraints. However, the procedure actually stops well before this happens. Thus, the number of constraints that are handled are much less than treating the complete confidence region ($2n_p$ constraints). The algorithm for forming the approximate problem is given below.

(1) Start with the previously determined set of constraints representing the approximate problem. The procedure is initialized with the nominal point as the sole point of consideration ($Q = \{\boldsymbol{s}(\boldsymbol{z}_f) \le \boldsymbol{0}\}$).

(2) For $i = 1, 2, ..., n_c$ (Examine target region constraints successively).

(a) Find the point of maximum violation of the constraint under consideration $k = m$ such that $q_m = \max\{s_i(z_j),\ j = 1, 2, ..., 2n_p\}$

(b) If this does not satisfy the target region constraint, append it to the constraint set if $q_i(z_k) > 0$; $Q = \{Q, s_i(z_k)\}$

(3) Solve the above approximate problem using target region linearization.

Determination of the Level of Confidence. The feasibility of solving the semi-infinite program presented before depends on the level of confidence α that is used, the tightness of the constraints on the end-use properties, and the number and range of the available inputs, as well as on the magnitude of the disturbance that is currently acting on the process. Consequently, the initially selected values of α need to be updated on-line to avoid reaching an infeasible situation. This way, there is a trade off between this confidence demanded from the controller and the optimum that is attained.

The level of confidence that can be handled with the procedure is determined during the linear program step in the successive target region linearization approach. This step is used in the algorithm to determine the feasibility of the linearized constraint set, and can also be used to establish the appropriate level of confidence. A modified linear program is used to accomplish this, as given below

$$\begin{aligned} &\min_{\boldsymbol{u},c} \{c\} \\ &\boldsymbol{g}_c(\boldsymbol{u}) + \nabla \boldsymbol{g}_c(\boldsymbol{u})\,\Delta \boldsymbol{u} \le c \\ &\boldsymbol{A}\boldsymbol{u} + \boldsymbol{A}\,\Delta \boldsymbol{u} \le \boldsymbol{b} \\ &\|\Delta \boldsymbol{u}\|_\infty \le L \end{aligned} \tag{24}$$

where $\boldsymbol{g}_c(\boldsymbol{u})$ denote the target region constraints for all the $2n_p$ points on the confidence region, represented in terms of the input values.

The solution of the above problem depends on the confidence value α, since the value of $\boldsymbol{g}_c$ depends on α. If $c > 0$, the linearized confidence region cannot be enclosed in the target set. Hence, an iterative procedure becomes necessary in the algorithm. The above problem is solved repeatedly starting with the desired confidence level (95% usually) and reducing it by 10% each iteration, until a feasible solution to the above LP is obtained ($c < 0$). This value of the confidence α is then used in the remaining steps of the algorithm along with c.

The level of trade-off between optimality and robustness would depend on the process under study and the objectives. If the process is highly constrained by quality and safety concerns, it would be desirable to keep the value of α high. On the other hand, if there is a certain amount of flexibility in maintaining the properties, one can choose lower values of α and achieve higher economic returns.

Second-stage optimization (Subproblem B-2)

The purpose of the second-stage optimization is to move the confidence region to the optimal point within the target region, while maintaining the level of confidence that has been obtained in the first stage. This is accomplished by solving a nonlinear programming problem that minimizes (or maximizes) the objective function subject to target region constraints

$$\begin{aligned} &\min_{\boldsymbol{u}} J(\boldsymbol{x}_f, t_f) \\ &\boldsymbol{s}(\boldsymbol{e}_i) \le \boldsymbol{0} \qquad i = 1, 2, ..., 2n_p \\ &z_f = \boldsymbol{q}(\boldsymbol{x}_f, \xi) \\ &\frac{d\boldsymbol{x}}{dt} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{u}, \boldsymbol{p}, \boldsymbol{d}, \theta, t) \\ &\boldsymbol{h}(\boldsymbol{x}(\tau)) \le \boldsymbol{0}; \qquad t \le \tau \le t_f \\ &\boldsymbol{A}\boldsymbol{u}(\tau) \le \boldsymbol{b}; \qquad t \le \tau \le t_f \end{aligned} \tag{25}$$

The solution to the above problem is easily attained with a simplification, as the initial guess is the value from the first-stage semi-infinite inequality problem (Subproblem B-1). These input values already satisfy the target region constraints (they are feasible). This makes it desirable to use a feasible directions method which ensures that the constraints are satisfied in each iteration of the algorithm. The problem can be solved by transforming it into a conventional constrained optimization problem considering all the $2n_p$ points of interest (corresponds to points where the axes intersect the boundary of hyper-ellipsoid for the n_p properties) as nonlinear constraints. The solution is accomplished by using Feasible Sequential Quadratic Programming (FSQP). FSQP utilizes a sequential quadratic programming method, which ensures that each iterate in the problem is feasible for the target region constraints. This is quite desirable as even if the algorithm fails to converge to the optimum, the quality specifications are met since the target region constraints are always satisfied.

Algorithm for MPC of batch processes under uncertainty

(1) Start with the initial guess for inputs $\boldsymbol{u}_0(\tau)$, $t \le \tau \le t_f$.

(2) Propagate the nonlinear model and the covariance propagation equations to get the expected values and expected covariance of the properties at the end of the batch $\boldsymbol{P}_q$ and its gradient $\partial \boldsymbol{P}_q / \partial \boldsymbol{u}$.

(3) Use the outer approximation procedure given earlier to formulate the approximate reduced problem.

(4) Solve the approximate problem using the target region linearization method with the steps given below.

(a) Solve the LP to find the maximum possible level of confidence α (Eq. 24).

(b) Solve the QP and determine the direction to move the inputs, $\Delta \boldsymbol{u}$ (Eq. 8).

(c) Update $\boldsymbol{u}$ using $\Delta \boldsymbol{u}$ calculated in the above step.

(d) If the reduced problem converged, go to step 5; else go back to step (a).

(5) If the complete confidence region is within the target region, go to step 6. Otherwise, go back to step 3 to add the appropriate constraints using the outer-approximation method.

(6) Solve the second-stage optimization problem using the input values from above to find the optimal input values (Subproblem B-2).

(7) Implement the first control move in the plant.

Case Study: Emulsion Polymerization of Styrene

Emulsion processes are widely used for the manufacture of latex paints, adhesives, coatings, and textile products. The control of end-use properties in these processes is very important (Dimitratos et al., 1994), as many of the products from emulsion processes are value added and customers demand strict quality. Economic objectives like minimizing the batch time or maximizing production can also be of great benefit in such processes due to the value added nature of the products. These processes are characterized by complex mechanisms which are rarely completely captured in a mathematical model. These features motivate the use of uncertainty handling methods in the control of emulsion polymerization processes.

Mathematical model for emulsion polymerization of styrene

Different approaches can be used for developing a mathematical model for emulsion polymerization. The level of detail that is adopted depends on the intended use of the model. The process model used here is an extension of a previous model by Liotta et al. (1997) and described in detail in Valappil and Georgakis (2001). A brief overview of the model and the important features of the process are given below.

The particle-size distribution (PSD) of the latex is an important characteristic due to its impact on the end-use properties. The molecular weight distribution also influences the end-use properties to a great extent and are decided by the development of molecular architecture during the batch. In the modeling approach used, the PSD is discretized into a reduced number of populations (chosen based on statistical and physical arguments). For the styrene case study presented here, three populations were considered. The growth of these populations is modeled individually. The molecular weight part is handled by using moment transformation with the first three moments of MWD. The moments for each population are modeled and the cumulative effect is used to find the moments of MWD for the final polymer. This is sufficient to predict the number and weight average molecular weights, and, hence, the end-use properties that depend on these average molecular weights.

The number of states in the model developed with the discretization of PSD depends on the number of populations considered. For the case with three populations, 26 states are to be considered. Some of the parameters that are used for the above model were validated at 50°C. Thus, the control studies are done by maintaining the temperature in the vicinity of 50°C. The important states, measurements, and end-use properties in this process are listed below.

States

- Monomer, initiator and CTA concentrations
- Volume of individual populations
- Average number of radicals per particle for each population
- Moments of live radical distribution
- Moments of dead polymer chain distribution

Manipulated Variables

- Monomer addition rate
- Chain transfer agent addition rate
- Coolant flow rate

On-line Measurements

The measurements available in this process are listed below.

- **Density of reaction mixture:** Density can be related to the conversion of the instantaneous reaction mixture and is measured every minute.
- **Reactor and jacket temperatures**
- **Infrequent measurement of PSD:** The sampling is considered infrequent and the measurements are assumed to be available with a delay. Both the frequency of sampling and the measurement delay is assumed to be 10 min.

End-Use Properties

- **Melt Flow Index:** This property is given by a correlation with the weight average molecular weight (Bremner and Rudin, 1990).
- **Tensile Strength:** The relationship between number average molecular weight and tensile strength reported in Bernsted and Anderson (1990) is used.
- **Weight Average Particle Diameter:** The weight average particle diameter ($\overline{D}_W$) of the product is considered as an end-use property that is controlled.

Control Objectives and Uncertainties. The primary objective in this process is to ensure that the three end-use properties satisfy the target region constraints. This has to be accomplished while maintaining the temperature of the batch within the acceptable bounds (50 ± 1°C). These path constraints are considered in the NLMPC along with the target region. The optimization objective used here is the maximization of conversion at the end of the batch. Hard constraints on both the manipulated variables are also considered in this study.

Different types of uncertainties are considered here to test the effectiveness of the methodology presented in this article. This includes model uncertainty in the form of parametric error in two of the model parameters k_{adj} and k_t. Also, uncertainty in the initial conditions of the batch (concentrations of initiator and monomer) is considered. The unmeasured disturbances that are treated here are the heat-transfer fouling and the impurities that affect the initiator decomposition efficiency.

The observability property of this process has an impact on the application of both EKF and NLMPC. The molecular

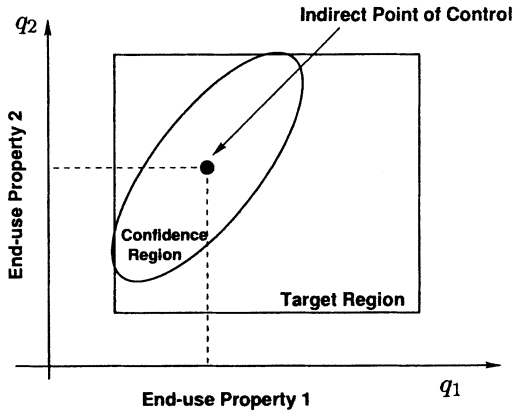

Figure 4. Control of two end-use properties under uncertainty.

The complete confidence region is enclosed in the target set for the product properties.

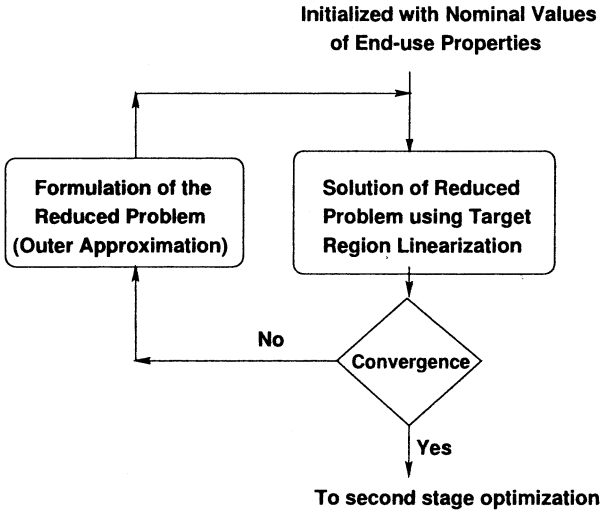

Figure 5. Iterative approach for the solution of semi-infinite problem for first stage of control under uncertainty.

The reduced problem is formulated at each iteration until the complete confidence region is in the target region.

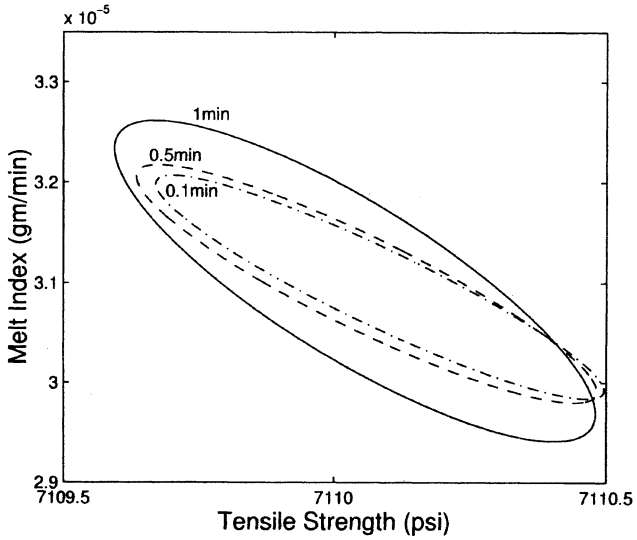

Figure 6. Dependence of confidence regions on frequency of linearization used in the propagation of covariance.

The property confidence region with three values of frequency of linearization (1, 0.5 and 0.1 min) are shown.

weights are affected by the PSD and other states, but there is no effect from MWD back to the measurements. Hence, these states are unobservable and estimated open loop in the state estimation. The covariance of these states are thus not reduced directly by the information from the measurements. There is only an indirect effect of using the observable and estimated states for their open-loop prediction.

Results

The confidence regions for the properties are calculated based on linear approximation to the nonlinear system. Linearization of the system at frequent intervals is utilized while doing this calculation as demonstrated in Figure 2 (Subproblem A-1). The confidence region for two properties, tensile strength and melt index with different frequencies of linearization, are presented in Figure 6. The case study presented here utilizes linearization every 1 min, which is adequately accurate compared to those obtained with 0.5 min and 0.1 min. It needs to be noted that the computational demands increase substantially by reducing the time interval, which makes it impractical to use 0.1 min. It is possible to reduce the interval between linearizations as we reach the end of the batch.

As described earlier, a linear updating scheme is utilized to account for the dependence of the confidence region on inputs. The adequacy of this approximation is examined here. The comparison between the actual confidence region and the linear approximation is shown in Figure 7. The actual nonlinear confidence region is obtained by Monte Carlo simulation. The linear approximation (Subproblem A-2) at the flow rate of CTA equal to 2×10^{-5} gmmol/min is obtained using the covariance calculated at CTA flow equal to 5×10^{-5} gmmol/min. Here, the linear approximation is close to the actual one, and is a slight underestimate of the uncertainty due to the higher-order terms that are ignored. However, as is clear from this plot, the correlation among the two properties is adequately well captured with this approximation. This is what is more important, as the underestimation of the size of confidence region can be compensated by using a higher level of confidence in the controller.

The time evolution of the confidence region for the two end-use properties is shown in the Figure 8. Here, the confidence regions calculated online at three points in the batch are given. The time points of calculation are 1 min, 100 min, and 200 min into the batch. As can be seen from Figure 8, the uncertainty in the properties reduces between 1 min and 100 min. It needs to be noted that these properties are not

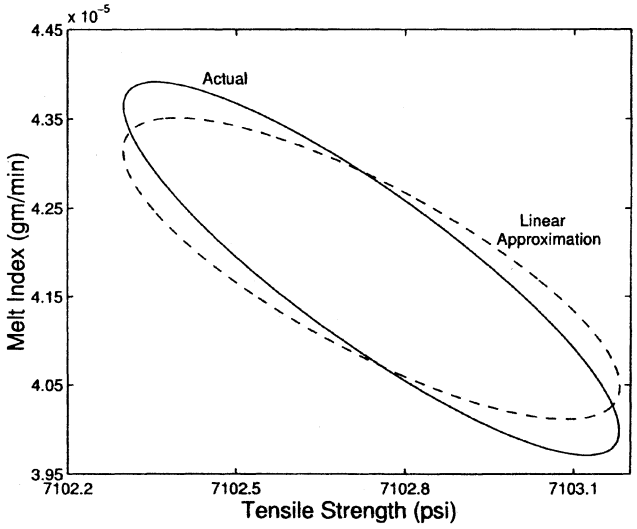

Figure 7. Comparison between actual and linear approximations of confidence regions.

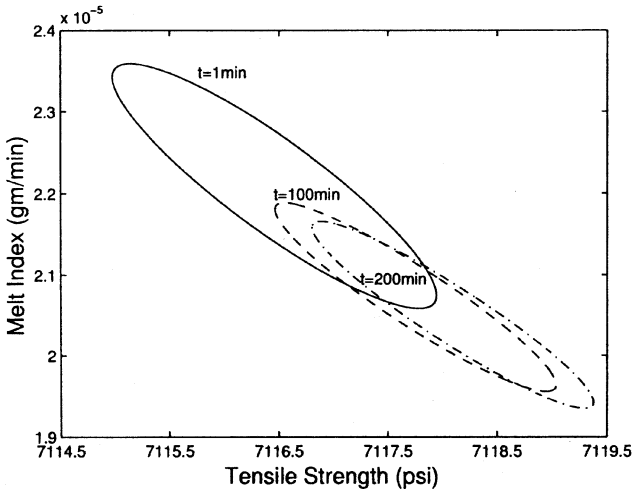

Figure 8. Confidence region for properties at different time points in the batch.

Confidence regions at 1 min, 100 min, and 200 min in the batch are shown.

observable from the available measurements. However, they are determined using the estimated value of the average number of radicals per particle, which are observable from the measurements available. Hence, there is an indirect effect on the covariance of these two properties as the batch progresses. There is not much difference between the covariance at 100 min and 200 min, as most information has already been obtained in the initial stages of the batch.

Monte Carlo simulations are used to demonstrate the effect of uncertainty in the combined state esimation and NLMPC and the result is shown in Figure 9. These simulations used a controller that does not account for the uncertainty. Here, the properties are indirectly controlled at the boundaries of the target region to attain the maximum conversion. This corresponds to the upper limit of the tensile strength and the lower limits of the weight average particle diameter and the melt index. This result is obtained due to the fact that the optimum also corresponds to the lower limit on the chain transfer agent addition. For the Monte Carlo simulations, two of the process parameters k_{adj} and k_t are assumed to be normally distributed with standard deviation equal to 25% of the parameter value. The parameters are sampled from this distribution and the simulation of the complete batch run is performed. The controller uses a model with the nominal value of the two parameters. As can be seen in Figure 9, the end-use property specifications are violated in a number of cases for all the three properties.

The same Monte Carlo analysis is repeated with model predictive controller that considers uncertainty explicitly and the result is shown in Figure 10. Here, the controller moves the properties to the interior of the target region to handle the uncertainty. 95% is the confidence level handled in the controller. The number of constraint violations are much lower than in the previous case. It needs to be noted that not all the values properties are entirely in the specification region, probably due to the linearized confidence region being an underestimate of the uncertainty compared to the actual

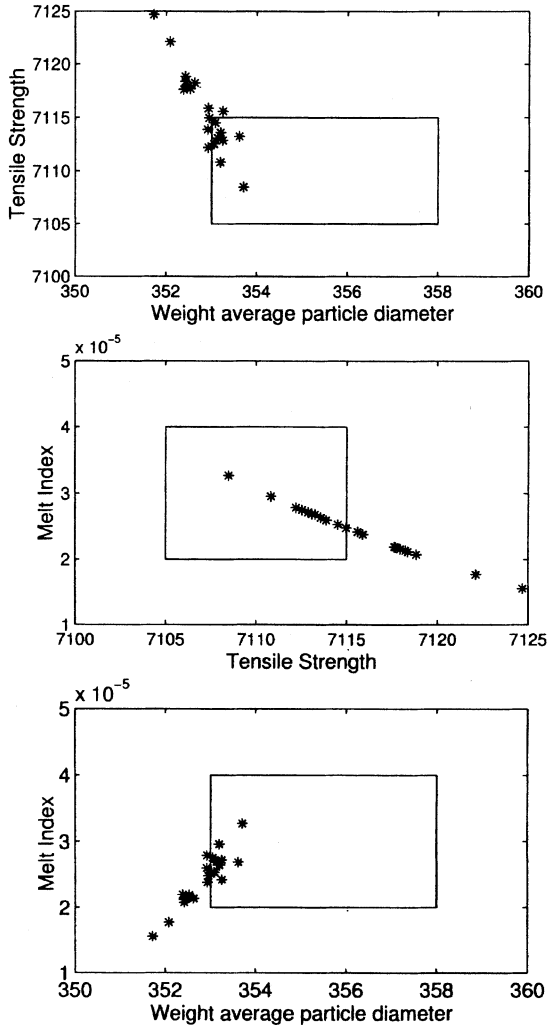

Figure 9. Monte Carlo simulation of the end-use property control without explicit consideration of uncertainty.

The end of the batch properties are shown for different parameter values from the assumed normal distribution.

values obtained by Monte Carlo simulations. A way to handle this problem is to increase the level of confidence that is used.

The execution of the controller at the first time instant in the batch ($t = 0$) for the control of three properties is shown in Figure 11. Only the first calculated input value is shown in Figure 11, since these are the values that are implemented in the plant. Here, only CTA is used as the only manipulated variable, which constrains the properties to lie in a specific line in the end-use property space. With the initial guess of the inputs, all three properties are outside the target region (Point 1 in the figure). The second point represents the inputs that bring the complete confidence region within the specifications. The third point corresponds to the optimum, which is at the upper limit for the tensile strength.

The control of three end-use properties with both monomer flow and CTA as the manipulated variables is shown in Figure 12. Here, the initial guess results in the properties that significantly violate the target region constraints. The second input values calculated by the controller results in the com-

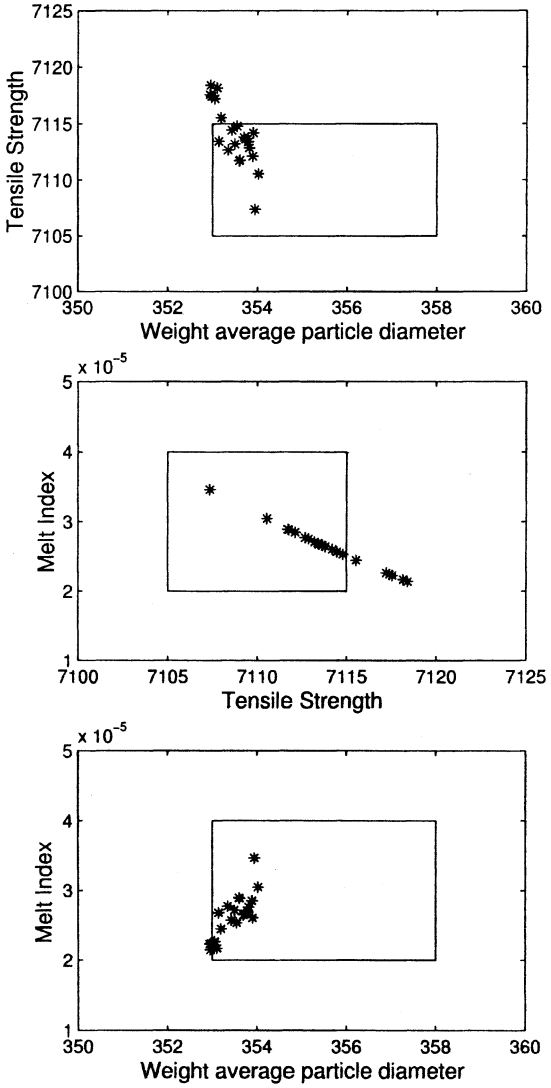

Figure 10. Monte Carlo simulation repeated with the consideration of uncertainty.

The point of control is moved to the interior adequately to reduce the variability in properties.

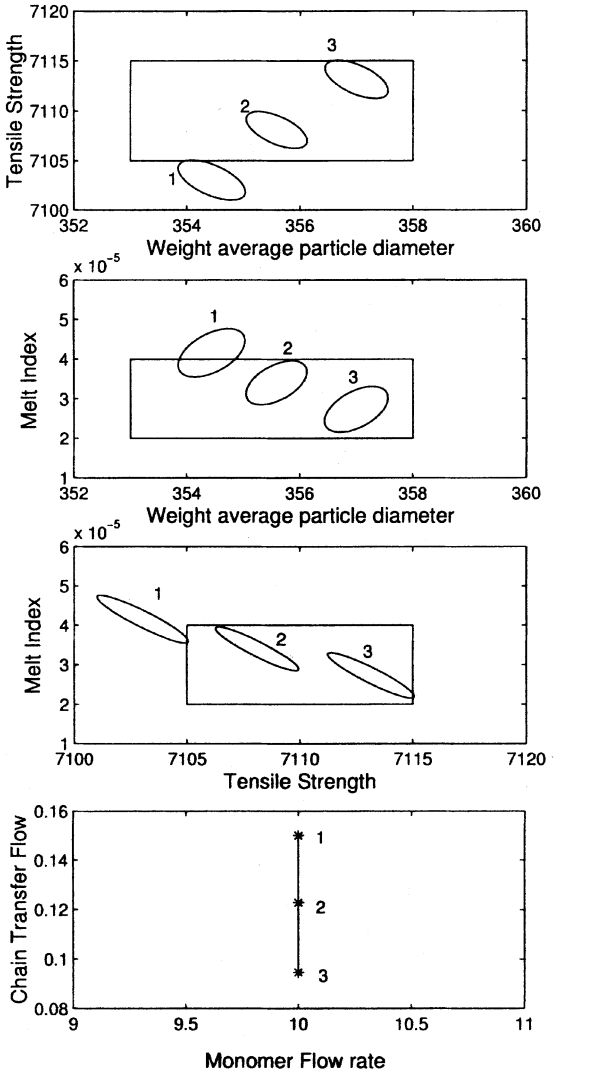

Figure 11. Control of three properties using CTA as the sole manipulated variable.

The properties at the end of the batch are at the boundary of the tensile strength.

plete confidence region in the target specifications, and the third value corresponds to the optimum at the boundary of constraints. Since two manipulated variables are used in this case, the controller has improved the optimum by moving it to the boundary for both tensile strength and particle diameter. The lower limit on the melt index would correspond to a more optimal operating point than the one realized here. However, the controller does not have enough freedom to attain that point, since only two manipulated variables are used with three properties to control.

The case where the desired 95% confidence cannot be handled by the controller is shown in Figure 13. The lower bound on the melt index value is changed here from 2×10^{-5} to 3×10^{-5}. Hence, the controller has to reduce the confidence to 45%, which is the best that could be handled in this case because of the reduced bounds on the melt index and substantial uncertainty of the model. This value is adequately accurate, and the complete confidence region is enclosed in the target set. It can be seen from Figure 13 that a slightly higher confidence can be handled, but this would require smaller increments for calculation in the linear programming step. The increments of 10% were used in this calculation.

The complete simulation of using one manipulated variable (CTA) for the control of two end-use properties is shown in Figure 14. The uncertainty considered here is a 25% mismatch in the adjustable parameter k_{adj}. The first plot shows the target region along with the final point that is attained by the process. The properties that the controller aimed at is the center of the confidence region that is also shown. It can be seen that this point is completely within the 95% confidence region for the properties as shown in the top plot. The figure also shows the CTA flow rate used during the batch. This decreases as time progresses, as the controller moves the process closer to the optimum.

The control of three end-use properties using both the monomer flow and CTA as manipulated variables is demonstrated in Figure 15. The main uncertainty that is studied here is the mismatch in the concentration of initiator in the recipe, along with the parametric uncertainties. The properties that are attained at the end of the batch are well within the specifications, as is clear from the figure. Also, the confidence region for the properties that are calculated by the controller is shown. The end of the batch properties are within or close to these confidence regions. The three adapted parameters are also shown in the figure. They all take positive values to compensate for the decrease in initiator amount that was fed to the batch.

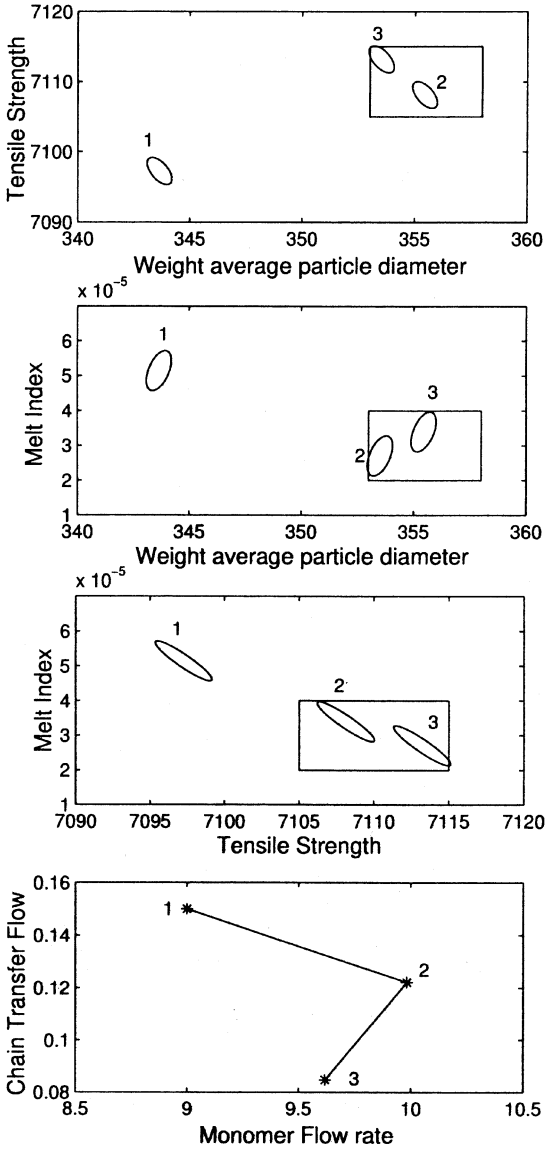

Figure 12. Control of three properties using monomer flow and CTA as the manipulated variables.

The 95% confidence is successfully handled by the controller and the properties are pushed to the boundaries of the target region.

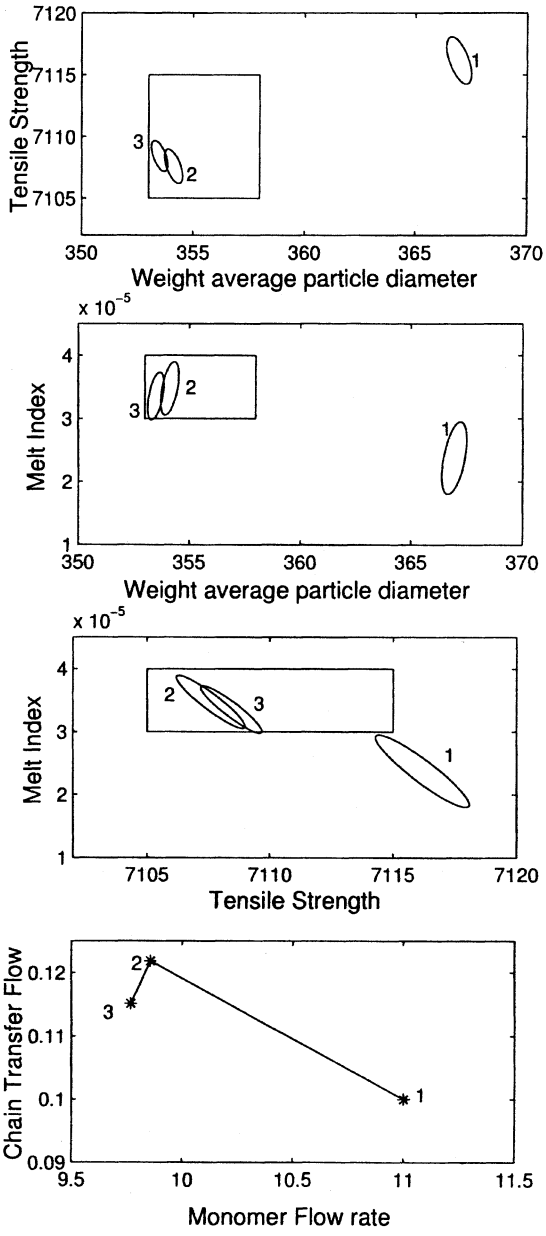

Figure 13. Case where the 95% confidence cannot be handled in control.

The controller determines 55% as the confidence level that can be handled and controls the properties at the appropriate points in the target region.

Conclusions

A methodology to incorporate model uncertainty in the control of batch product properties is presented in this article. This methodology uses the information about the model uncertainty in the form of covariance matrix for the parameters. The advantage of the proposed methodology is that it allows a trade-off between robustness and optimality in a direct manner.

The confidence region for properties is calculated using a linear propagation for the state covariance, as this is computationally feasible to be done on-line. The alternative to this

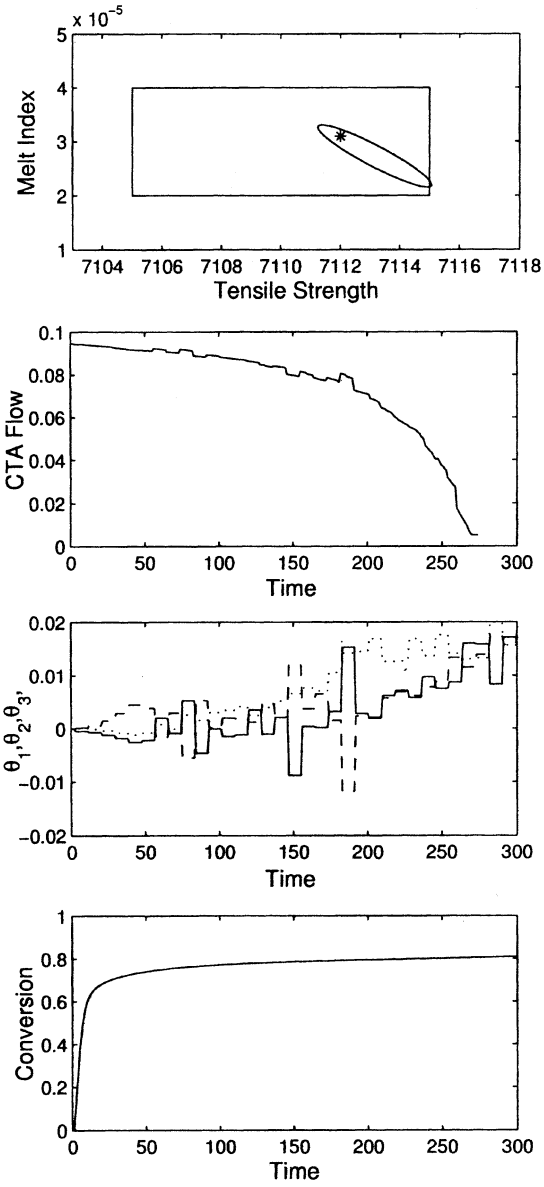

Figure 14. Results of controlling two properties using CTA as the manipulated variable.

Top plots show the end of the batch properties attained (asterisk) and the confidence region calculated by the controller. The adapted parameters and the conversion during the batch are also shown.

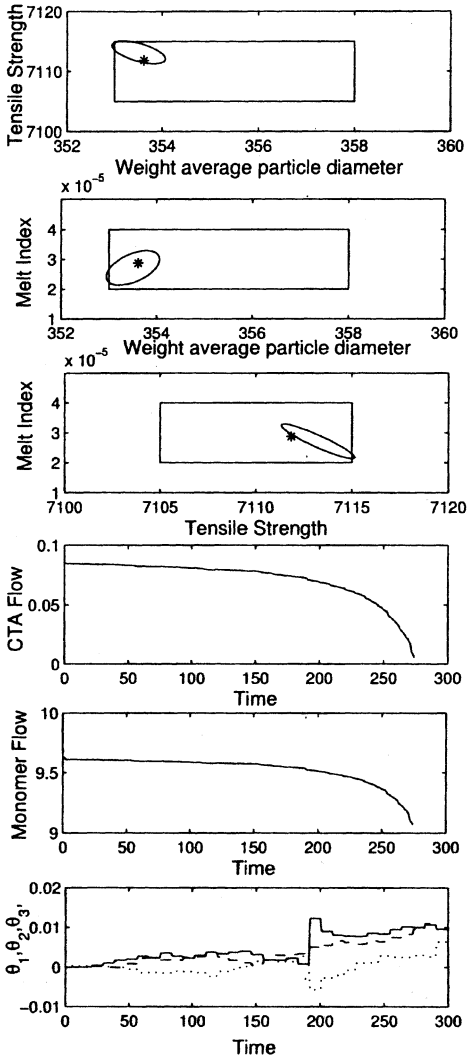

Figure 15. Results of controlling three properties using monomer and CTA as the manipulated variables.

The plots show the end of the batch properties attained (asterisk) and the confidence regions calculated by the controller. The adapted parameters are also shown. The bottom plots show the manipulated variable profiles during the batch.

is the use of a nonlinear model, which appears computationally very intensive and impractical to use on-line at present. Hence, the confidence regions at the end of the batch are approximations of the actual values. The user can compensate for this by increasing the amount of confidence demanded from the controller.

The feasibility of solving the NLMPC under an uncertainty problem on-line is an important issue that had to be addressed. The semi-infinite formulation problems are notoriously time consuming to solve, especially the discretization and the maximization over an infinite set of parameters. Another important factor is the covariance propagation step, which is also computationally intensive. To handle this, a linear updating scheme is used to determine the end-use property covariance. This way, the propagation of state covariance has to be performed only once per control execution.

The benefits of using the methods developed here are demonstrated via Monte Carlo simulations. The chances of not meeting the target region constraints for the end-use properties are greatly reduced with the adoption of these methods. Some improvements are possible in the methodology presented here. First, the more accurate calculation of the end-use property confidence region is possible with more computationally intensive methods. These methods may become feasible to do on-line with further computational power. Otherwise, only an infrequent calculation of the accurate confidence region by complete nonlinear uncertainty propagation could be possible. It needs to be noted that such non-

linear confidence regions will be nonconvex. This would demand more rigorous treatment in the semi-infinite programming.

The time requirements to do the controller calculations online were found to be very reasonable. This analysis was done in an SGI-IRIX workstation. The semi-infinite inequality step for the case study used in this article took, on an average, 16 s to complete. The second-stage optimization by itself took on average 7 s to complete. It needs to be noted that the optimization step can be performed more infrequently depending on the process characteristics. With computational power increasing rapidly, these methods can easily be incorporated in real-time implementations of nonlinear model predictive control in an industrial environment.

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