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A methodology for on-line setpoint modification for batch reactor control in the presence of modeling error

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Abstract

Batch and semi-batch reactors are usually highly nonlinear and involve complex reaction mechanisms. Often, the lack of rapid direct or indirect measurements of the properties to be controlled makes the process control task very difficult. It is the usual practice to follow the prespecified setpoint profiles for process variables for which measurements are available, e.g., temperature, in order to obtain desired product properties. Model error can be the cause of poor performance when these setpoint profiles based on a model are implemented on the actual plant. This paper formulates a state estimation model based algorithm for on-line modification of setpoint profiles utilizing infrequent and delayed measurement information of the properties to be controlled, with the goal of obtaining the desired values of the properties in the minimum batch time. The algorithm modifies the setpoint profile for the remainder of the batch after every such measurement by making one step in the right direction instead of attempting to find a completely new optimal profile. This results in robustness with respect to model error and allows improvement even with infrequent product property measurements. The implementation of the setpoint profiles is made via real-time observer based nonlinear quadratic dynamic matrix control, which has been studied extensively in the literature. The modest additional on-line computational requirements of the proposed method offer promise for the practical on-line implementation. The effectiveness of the algorithm is demonstrated with simulations for bulk polymerization of styrene.

Keywords: Batch reactor; Model error; Setpoint profile; Optimal control

1. Introduction

Batch and semi-batch processes are characterized by strong nonlinearities, significant time delays in measuring the properties to be controlled and unmeasured disturbances affecting the system. The lack of instantaneous measurements of the properties to be controlled (e.g., in the case of a polymerization reactor, molecular weights) makes direct control almost impossible. It is the practice to track the setpoint profiles of other variables such as temperature to obtain the desired product properties. Such profiles can be computed by off-line optimization of appropriate objective functions based on the available model using maximum principle [2,13–15], or by a nonlinear programming technique [1,6]. The modeling of batch/semi-batch processes involves complex reaction mechanisms and the presence of model-plant mismatch is unavoidable. Because of the modeling errors and external disturbances, even if the optimal profiles are tracked perfectly, the final properties may significantly differ from the desired values. To account for the modeling errors and disturbances, new optimal profiles may be recomputed once new product property measurements are obtained. Such computations would require solving a computationally intensive nonlinear optimization problem and are not feasible for practical on-line implementation. Furthermore, such a computation implicitly assumes that the new measurement information has been sufficient to fully correct for the model error, which is not likely to be the case.

To avoid reoptimizing the nonlinear objective function, every time new property measurements are obtained, Kozub and Macgregor [7] proposed a method based on the instantaneous properties of the desired product. Palanki et al. [11] derived optimal state feedback laws for a class of nonlinear systems. Ellis et al. [3] adjust the temperature and monomer addition policies in molecular weight distribution (MWD) control of a batch polymerization process. Zafiriou and Zhu [16] proposed an approach for modifying the optimal profile from batch to batch so that an improvement in the objective function is accomplished in every batch. However, they assumed that all the states are measured. Moreover, the

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computation is off-line and the initial few batches need to be discarded until the true optimal profile for the plant is found.

In this paper, a state estimation model based algorithm is proposed for on-line modification of the optimal profile (e.g., temperature setpoint profile to be tracked by the real-time control system) of batch/semi-batch processes. Rather than assuming that the real-time controller perfectly tracks the setpoint, the algorithm is integrated with the observer based nonlinear quadratic dynamic matrix controller (NLQDMC) studied by Gattu and Zafiriou [5] for setpoint tracking. The objective of this work is to propose a systematic model based optimization procedure to update the setpoint profile on-line to compensate for modeling errors and disturbances utilizing the infrequent and delayed product property measurements. Once the delayed direct/indirect measurements of the properties to be controlled are available, the values of the states at current time are estimated. Based on the current state of the process, the values of the properties at the end of the batch are predicted. The concepts of model predictive control algorithms are used in the future prediction. Once the prediction is made, the setpoint profile is updated by carrying out one iteration of a gradient based optimization method. The modified profile is implemented by the real-time control system that utilizes frequently available measurements (e.g., temperature) until the next set of property measurements are available.

2. Methodology

The proposed approach involves (i) on-line modification of setpoint profile and (ii) on-line tracking of setpoint profile. The algorithm for setpoint modification is introduced and discussed in detail in this section. The real-time controller for setpoint tracking utilizes the observer based NLQDMC algorithm [5] and we only provide here a brief summary of the parts that are necessary for the illustration example. The measurements are divided into two categories as primary and secondary measurements. The primary measurements are the frequent measurements (e.g., temperature) used for state estimation in the NLQDMC control algorithm. The secondary measurements are infrequent and delayed measurements of product properties used in the estimation phase of the on-line update of the setpoint profile.

2.1. Modification of setpoint profile

The setpoint profile is modified on-line whenever there is a new set of secondary measurements available. Let T_b be the sample time associated with the secondary measurements, which may be much longer than the sampling time for the primary measurements. It is also assumed that there is a delay of one sample unit in processing the secondary measurements, i.e., at time kT_b of the batch (kth sampling point for secondary measurements), only the measurements at sampling time $k-1$ are available. Based on the measurements at $k-1$, the prior estimates of states at $k-1$ are corrected and the values of states at k are estimated. Using the estimated values of the states and the model, the setpoint profile is then modified.

2.1.1. Estimation

Consider a nonlinear model of the form

$$\dot{x} = f(x,u), \tag{1}$$

$$y = h(x), \tag{2}$$

where x is the state vector, u the setpoint for the on-line control, and y is the vector of secondary measurements. For example, for a polymer reactor where the polymer properties (e.g., molecular weight distribution) are controlled by following a prespecified temperature profile, the temperature is the setpoint for the real-time control system but it is considered the input u in the on-line modification of the setpoint profile.

At time k, a linear model is obtained by linearizing the above nonlinear model at $\hat{x}_{k-1|k-2}$ and u_{k-1} and is given by

$$\dot{z} = A_{k-1}z + B_{k-1}u, \tag{3}$$

$$y = C_{k-1}z, \tag{4}$$

where $A_k = (\partial f/\partial x)|_{x=\hat{x}_{k|k-1},u=u_k}$, $B_k = (\partial f/\partial u)|_{x=\hat{x}_{k|k-1},u=u_k}$, $C_k = (\partial h/\partial x)|_{x=\hat{x}_{k|k-1}}$, and z is used to denote the state vector for the linearized model. Physically it corresponds to the same variables as x, but a different symbol is used to avoid any confusion with the state estimates that are obtained later in this section. The notation $\hat{x}_{k|k-1}$ represents the estimate of x at k based on the information at $k-1$. To account for the persistent disturbances and modeling errors, (3) and (4) are augmented with stochastic states:

$$\dot{z} = A_{k-1}z + B_{k-1}u + G_{k-1}w + w_1, \tag{5}$$

$$\dot{w} = w_2, \tag{6}$$

$$y = C_{k-1}z + v, \tag{7}$$

where w_1, w_2 and v are uncorrelated white noise sequences with $[w_1^T, w_2^T]^T \sim (0, Q_b)$ and $v \sim (0, R_b)$, Q_b and R_b being covariance matrices associated with process and measurement noise. w as integrated white noise corresponds to persistent disturbances. v and w_1 clearly have the dimensions of y and z (or x) correspondingly. In (5), w (and w_2 in (6)) may meaningfully have a dimension from scalar up to that of z, as determined by the selection of G_{k-1}. A further limitation on its dimension based on detectability is discussed in the next paragraph. A selection $G_{k-1}=B_{k-1}$ assumes that such persistent disturbances appear in u and could be the result of imperfect setpoint tracking by the real-time control system for which u is the setpoint. However, another reasonable selection for G_{k-1} would be a matrix of zeros and ones, corresponding to persistent disturbances affecting certain states of the process.

The only technical requirement in using this kind of disturbance model is that the augmented system should

be detectable. In general, it is required that the number of new augmented states w are less than or equal to the number of outputs y for the detectability of the augmented system. For more details on the detectability of the augmented system the reader is referred to [10].

In our development, it is assumed that

$$Q_b \approx \begin{bmatrix} \delta_{w1}^2 & 0 \\ 0 & \delta_{w2}^2 \end{bmatrix}$$

and $R_b \approx \delta_v^2 I$, where δ_{w1}^2, δ_{w2}^2 and δ_v^2 are scalar variances. Define $\delta_1=\delta_{w1}/\delta_v$, $\delta_2=\delta_{w2}/\delta_v$ and let $\delta_v^2 = 1$. The parameters δ_1 and δ_2 are used as tuning parameters which determine the value of estimator gains. Note that the augmented model is similar to the type B augmented model in the observer based NLQDMC algorithm [5]. For the type B augmented model, δ_2 alone is sufficient to deal with open-loop unstable systems and also to account for persistent disturbances and modeling errors. However, we have included δ_1 in the formulation for the sake of completeness and also to have an additional degree of freedom if required. The initial choice, though, should be $\delta_1=0$. Small values for both δ_1 (when used) and δ_2 are recommended in the presence of significant measurement noise.

The model (5)–(7) is used to compute a Kalman gain for state estimation. Since (5) and (6) are continuous but only discrete measurements are available for (7), we use the continuous–discrete Kalman filter formulation. By iterating to steady state the equations for the Kalman gain (Table 3.7-1 in [9]), we can obtain the steady state Kalman gain, which we denote as

$$K_{k-1} \triangleq \begin{bmatrix} K_{k-1}^1 \\ K_{k-1}^2 \end{bmatrix}.$$

The superscript 1 stands for the gain for the subsystem consisting of original states z and 2 stands for the gain for the subsystem consisting of augmented states w. Once the Kalman gain is computed, it is used to correct the states of the nonlinear and of the augmented linearized model. The corrected estimates at $k-1$ are given as

$$\hat{x}_{k-1|k-1} = \hat{x}_{k-1|k-2} + K_{k-1}^1[y_{k-1} - h(\hat{x}_{k-1|k-2})], \tag{8}$$

$$\hat{w}_{k-1|k-1} = \hat{w}_{k-1|k-2} + K_{k-1}^2[y_{k-1} - h(\hat{x}_{k-1|k-2})], \tag{9}$$

where y_{k-1} is the measurement at $k-1$. The model for the future prediction is obtained as

$$\dot{\hat{x}} = f(\hat{x}, u) + G_{k-1}\hat{w}, \tag{10}$$

$$\hat{y} = h(\hat{x}). \tag{11}$$

The values of estimates for states at k are obtained by integrating (10) and (11) over one sample unit T_b.

The procedure is similar to the extended Kalman filter technique, except that we use the steady state Kalman gain, whose computation is based on the linearized model at every k to correct the state estimates. The reason for using the steady state Kalman gain is the following. The Kalman filter equations are derived from the statistics of the added gaussian white noise terms. If the values of Q_b, R_b and the initial estimate of the state covariance matrix P_0 are known exactly, the correct estimates are obtained. However, this information is often unknown and with some simplifications the covariance matrices are essentially used as tuning parameters. Hence, it is desirable to keep the number of tuning parameters as small as possible. By using the steady state Kalman gain, we eliminate the need of choosing P_0.

2.1.2. Determination of optimal profile

The optimal setpoint profile for the remaining time of the batch is determined based on the model described by (10) and (11) and the values of the estimated states at k. The objective of the on-line modification of the setpoint profile at time k is to compute the profile for the remainder of the batch to achieve the desired final properties in the minimum batch time starting from time k. The modified profile will be implemented by the NLQDMC controller until time $k+1$ when a new secondary measurement will become available and the profile will be modified again. One needs to keep in mind that the modification of the setpoint profile is made on-line and should not be computationally expensive. Therefore, the use of minimum time optimal control techniques to obtain the complete solution at every sampling time is ruled out. Furthermore, such a computation implicitly assumes that the new measurement information has been sufficient to fully correct for the model error, which is not likely to be the case. Hence we choose to have the algorithm simply make one step in the right direction instead of attempting to find a completely new optimal profile, which results in robustness with respect to model error.

First the fixed-end-point and free-end-time problem is converted to a free-end-point and fixed-end-time problem through a coordinate transformation [8] which can be solved very efficiently. This method can be applied to any nonlinear system in which at least one of the state variables is monotone. In chemical reactors, normally the conversion is the monotone state variable. In the following, we briefly summarize this method. The state vector $x=(x_1,x_2,\ldots,x_n)$ is rearranged so that x_1 is the monotone state variable which is used as the new independent variable. Then a coordinate transformation is made given by

$$\tau \leftarrow x_1, \qquad q_1 \leftarrow t, \qquad q_i \leftarrow x_i \quad (i > 1). \tag{12}$$

This transforms (1) into

$$\dot{q}(\tau) = F(q, u, \tau) \tag{13}$$

with $F_1=1/f_1$ and $F_i=f_i/f_1$ for $i>1$. The subscripts indicate elements of the vector functions f and F. The initial and terminal conditions are

$$q_1(\tau_0) = t_0, \qquad q_i(\tau_0) = x_{i0} \quad \text{for } i > 1, \tag{14}$$

$$q_1(\tau_f) = \text{free}, \qquad q_i(\tau_f) = x_{if} \quad \text{for } i > 1, \tag{15}$$

$$\tau_0 = x_{10}, \qquad \tau_f = x_{1f}. \tag{16}$$

The transformed problem can be solved using any gradient based optimization method. In this paper, the steepest descent with constraints method is used. As explained, at each k, we carry out one iteration of the algorithm. One iteration is suggested because, once the new secondary measurements are obtained, the model and initial estimates change resulting in a different optimal profile. Therefore, we want to get the local improvement by carrying out one iteration only. It also reduces the on-line computational requirements. When the next set of secondary measurements are available, another iteration is carried out and the updated setpoint profile is implemented by the real-time NLQDMC algorithm that utilizes the primary measurements.

2.1.3. Algorithm

$$\min_{u(\tau)} \phi(q(\tau_f)) \tag{17}$$

subject to (13) where τ_f is the desired value of x_1 at the end of the batch and ϕ is the selected performance index.
(a) Set $\tau_0 = \hat{x}_{1,k|k-1}$, $q_1 = t_k$ and $q_i = \hat{x}_{i,k|k-1}$ for $i > 1$.
(b) Forward integration of model

$$u_{\text{old}}(\tau) \rightarrow \dot{q}(\tau) = F(q, u, \tau) \rightarrow q(\tau).$$

(c) Linearize $F(q,u,\tau)$ at $u_{\text{old}}(\tau)$, $q(\tau)$ to obtain $F_q(q,u_{\text{old}})$ and $F_u(q,u_{\text{old}})$.
(d) Backward integration of adjoint system

$$\dot{\lambda} = -F_q(q, u_{\text{old}})\lambda; \ \lambda(\tau_f) = \nabla_q \phi(q(\tau_f)).$$

(e) Compute gradient

$$g(\tau) = F_u^{\text{T}}(q, u_{\text{old}})\lambda(\tau).$$

(f) Line search

$$u_{\text{new}}(\tau) = u_{\text{old}}(\tau) - \alpha \tilde{P} g(\tau), \quad 0 \leq \alpha \leq \min[\alpha_e, \alpha_{\max}],$$

where $\tilde{P}$ is the constraint projection matrix, $\alpha_{\max}$ the limit imposed by constraints and α_e is the limit on maximum adjustment on successive updates.

Optimal step size α is computed using Armijo step size rule [12]. The user defined limit α_e can be used to tune the algorithm. By decreasing it the algorithm will become less aggressive in making changes in the setpoint profile. The updated u_{new} is used as the setpoint for the on-line control algorithm.

2.2. Setpoint tracking

The real-time controller that implements the setpoint profile and utilizes the more frequent primary measurements is also based on a nonlinear process model that overlaps with the one used for setpoint modification ((1) and (2)). Let us denote it as

$$\dot{x}_c = f_c(x_c, u_c), \tag{18}$$

$$y_c = h_c(x_c), \tag{19}$$

where u_c is the manipulated variable for and y_c is the controlled variable that corresponds to the primary measurements. The state vectors x in (1) and x_c in (18) partially overlap. This will become more clear in the example section. The model (18) and (19) is the state space description of the primary measurement variables and the related input variables, whereas (1) and (2) is the state space description of the secondary measurement variables and the related input variables. The setpoint for the controlled variable y_c in (19) is the input vector u in (1). In a polymer reactor, y_c and u may be the reactor temperature and u_c may correspond to the cooling water which controls the modified temperature profile obtained by the procedure described in the previous section. u_c would not appear in (1) and (2).

The observer based NLQDMC algorithm [5] is used for implementing the setpoint profile. It utilizes a repeated linearization after every primary measurement and state augmentation similar to (3)–(7). This linearized model is used in solving on-line at every primary sampling point, a predictive control problem. The requirement of solving only one quadratic program (QP) at each sampling time makes this algorithm an attractive option for industrial implementation. Here, we briefly summarize aspects of the algorithm needed for following the example in Section 3. For more details, the reader is referred to [5].

The following optimization problem is solved after each primary measurement to obtain the future manipulated variables:

$$\min_{\Delta u_{c,k},\ldots,\Delta u_{c,k+M-1}} \sum_{l=1}^{P} e_{k+l}^{\text{T}} \Gamma^2 e_{k+l} + \Delta u_{c,k+l-1}^{\text{T}} \Lambda^2 \Delta u_{c,k+l-1}, \tag{20}$$

where Δu_c is the change in manipulated variables, defined as $\Delta u_{c,k} \triangleq u_{c,k} - u_{c,k-1}$. P is the prediction horizon and M is the number of future moves to be optimized. Γ and Λ are diagonal weight matrices. e is the predicted deviation of the output y_c from its reference setpoint value computed as u in the previous section. Note that the reference setpoint is updated whenever the setpoint profile is modified as described in the previous section. Constraints on system variables can also be included. The full nonlinear model is used for estimating the effect of past inputs to the predicted error. However, the linearized model is used for the prediction of the effects of the future inputs, which are the optimization variables. This yields a standard quadratic programming problem. The standard approach in all model predictive control algorithms is that M future manipulated variables are computed, but only the first move is implemented [4], and the optimization is repeated after the next primary measurement is obtained.

Two different types of augmented linearized models are utilized in [5], referred as Types A and B. In the example in the next section we use the Type B augmentation that is similar to the one described by (5)–(7). Persistent disturbances are assumed to enter in the process inputs u_c. Two

tuning parameters σ_1, σ_2 of the same nature as δ_1, δ_2 can be used, and general tuning guidelines are discussed in [5]. The reader is referred there for additional details and for the formulation of the use of the linearized models for the P-step ahead prediction.

3. Illustration

In this section, the algorithm is tested through simulations for the thermally initiated bulk polymerization of styrene in a batch reactor. The differential equations describing the polymerization system are given by Kwon and Evans [8]. We have added equations for the reactor jacket that is used to control the reactor temperature through manipulation of the cooling water flow rate.

$$\dot{x}_1 = f_1 = \frac{\rho_0^2 \rho}{M_m}(1-x_1)^2 \exp(2x_1 + 2\chi x_1^2) A_m \exp\left(-\frac{E_m}{x_4 T_{\text{ref}}}\right), \tag{21}$$

$$\dot{x}_2 = f_2 = \frac{f_1 x_2}{1+x_1}\left(1 - \frac{1400 x_2}{A_w \exp(B/x_4 T_{\text{ref}})}\right), \tag{22}$$

$$\dot{x}_3 = f_3 = \frac{f_1}{1+x_1}\left(\frac{A_w \exp(B/x_4 T_{\text{ref}})}{1500} - x_3\right), \tag{23}$$

$$\dot{x}_4 = \frac{\rho_0(-\Delta H_p) f_1}{M_m \rho c_p T_{\text{ref}}} - \frac{U_c A_c}{\rho c_p V}(x_4 - x_5), \tag{24}$$

$$\dot{x}_5 = \frac{q_{\text{c ref}} q_{\text{c}}}{V_c}\left(\frac{T_{\text{j,in}}}{T_{\text{ref}}} - x_5\right) + \frac{U_c A_c}{(\rho c_p)_c V_c}(x_4 - x_5), \tag{25}$$

$$\rho = \frac{1-x_1}{r_1 + r_2 T_c} + \frac{x_1}{r_3 + r_4 T_c},$$

$$\rho_0 = r_1 + r_2 T_c,$$

$$c_p = 1.256 + 0.004404(x_4 - 50)\ \text{kJ/kg K},$$

$$T_c = x_4 T_{\text{ref}} - 273.15,$$

where x_1 is the conversion, $x_2 = x_n/x_{nf}$ and $x_3 = x_w/x_{wf}$ are dimensionless number average and weight average chain lengths (NACL and WACL), respectively, $x_4 = T/T_{\text{ref}}$ is the dimensionless reactor temperature, $x_5 = T_{\text{j}}/T_{\text{ref}}$ the dimensionless jacket temperature, $q_{\text{c}} = Q_{\text{c}}/q_{\text{c ref}}$ the dimensionless cooling water flow rate, T the reactor temperature, T_{j} is the jacket temperature and Q_{c} is the cooling water flow rate. The initial values of the states are $x_{10}=0.0$, $x_{20}=1.0$, $x_{30}=1.0$, $x_{40}=1.0$ and $x_{50}=0.975$. Table 1 gives several reference values used to obtain the dimensionless variables as well as the values of process parameters.

The objective of the batch is to achieve a conversion of 0.8 (80%) with values of dimensionless NACL and WACL equal to 1.0 in the minimum amount of time. The objective is achieved by tracking the optimal temperature profile which is modified on-line utilizing the delayed measurements of NACL, WACL and conversion. The model described by (21)–(23) is used for on-line modification of temperature setpoint profile and it corresponds to (1). The secondary measurements are the measurements of conversion, NACL and WACL, so in this case $y=x$ in (2). x_4 is the input variable u in the on-line modification phase. A coordinate transformation [8] given by

$$\tau \leftarrow x_1, \quad q_1 \leftarrow t, \quad q_2 \leftarrow x_2, \quad q_3 \leftarrow x_3 \tag{26}$$

is made to transform the free-end-time and fixed-end-point problem to free-end-point and fixed-end-time problem. In the new coordinates the objective function (performance index) for on-line modification of the temperature profile can be stated mathematically as

$$\min_{x_4(\tau)} q_1^2(\tau_f) + \gamma[(q_2(\tau_f) - 1)^2 + (q_3(\tau_f) - 1)^2]. \tag{27}$$

This function was proposed for optimizing the process in [8], where the value for the weight coefficient was gradually increased to $\gamma=10\,000$. Here we use this value throughout. The use of such a large value makes the optimization drive the NACL and WACL properties very close to the desired value of 1.0 (scaled). It does not mean that the minimization of batch time is ignored. As the results indicate in the rest of this section, the batch time is greatly decreased through the use of this objective function. Through appropriate scaling of the time variable, the first term in (27) can be made dimensionless and of order of magnitude unity. Here we scale time by dividing it by a reference time of 300 min. One can incorporate this directly into the model equations by multiplying the right-hand side of (21) by this reference time. Finally, note that lower and upper operational limits on the temperature can be added as constraints on the optimization variable x_4, and handled through the constraint projection matrix and $\alpha_{\max}$ in step (f) of the algorithm in Section 2.1.3. Here we have not incorporated such con-

Table 1
Parameter values

A_w	0.033454
B	4364 K
M_m	104 kg/kmol
χ	0.33
r_1	0.9328×10^3 kg/m^3
r_3	1.0902×10^3 kg/m^3
r_2	-0.87902 kg/m^3 °C
r_4	-0.59 kg/m^3 °C
E_m	10 103.5 K
A_m	4.266×10^5 m^3/kmol s
A_c	1.0 m^2
V_c	0.02 m^3
V	0.2 m^3
$T_{\text{j,in}}$	330 K
T_{ref}	399.15 K
$(\rho C_p)_c$	4.17×10^3 kJ/m^3 K
$(-\Delta H_p)$	67 400 kJ/kmol
U_c	0.5 kJ/K m^2 s
$q_{\text{c ref}}$	0.16667×10^{-4} m^3/s
x_{nf}	700
x_{wf}	1500

straints because the limits given in [8] did not come close to being violated in the simulations.

The temperature setpoint profile is implemented by using the NLQDMC algorithm to manipulate the cooling water flow rate. The modeling equations of reactor dynamics augmented with modeling equations of jacket dynamics (21)–(25) are used in the on-line control and they correspond to (18). The primary measurement is the reactor temperature. Hence, x_4 is the controlled variable and (19) is $y_c=x_4$. q_c is the manipulated variable u_c in the on-line control phase.

In all the simulations it is assumed that there is modeling error in the heat transfer coefficient, U_c, and parametric uncertainty in the parameter A_w. A value of 0.04 is used for the plant heat transfer coefficient instead of the value in Table 1 used in the model. A value of $A_{w,\text{plant}}=1.2A_w$ is used in simulations.

If the model is perfect, i.e., if there is no parametric uncertainty in A_w, then the desired values of NACL and WACL with 80% conversion are achieved in 313 min by implementing the temperature profile which is optimal for the model. This profile is used as the initial temperature setpoint profile applied to the plant equations that include modeling error as described above. Fig. 1 demonstrates the tracking of temperature profile which is optimal for the model without modifying it on-line. The observer based NLQDMC algorithm is used for on-line control to track the temperature setpoint profile. Tuning parameter values of $\Gamma=1$, $\Lambda=0.015$, $P=5$, $M=1$, $\sigma_1=0$ and $\sigma_2=10$ are used in the control algorithm. A sample time of 1.0 min is used for the primary measurement, i.e., for temperature measurements. A lower constraint of 0.0 is imposed on the cooling water flow rate. It can be seen that the control algorithm can track the setpoint profile almost perfectly even in the presence of error in the heat transfer coefficient. However, due to the modeling error in A_w, as shown in Table 2, values of NACL=1.08 and WACL=1.09 are obtained at the end of the batch with a conversion of 0.801.

Table 2
Product properties at the end of the batch

Setpoint	t_f	Properties at t_f		
		NACL	WACL	Conversion
No modification	313	1.080	1.090	0.801
Modified on-line	220	1.003	1.006	0.804

Fig. 2 demonstrates the tracking of temperature profile with on-line modification utilizing the delayed secondary measurement information of conversion and WACL, NACL. Tuning parameter values of $\delta_1=0.0$, $\delta_2=0.1$ and $G_k = G = [0\ 1\ 1]^{\mathrm{T}}$ are used in the estimation phase of on-line modification of the temperature setpoint profile. As mentioned in the guidelines earlier in the paper, a $\delta_1=0$ is used. The selection of G_k corresponds to a persistent disturbance affecting both the second and third state, i.e., NACL and WACL, respectively. A sample time of 20 min is used for the secondary measurements, i.e., for molecular weights and conversion. It is further assumed that they are delayed by 20 min. The selection of sample time is based on the approximate time to obtain the measurements through a chromatograph [3]. It is assumed that the first secondary measurement sample is taken 5 mm after the start of the batch. A constraint of $\pm 2K$ (± 0.005 in dimensionless units) is imposed on the change of optimal profile at each step of modification through the selection of α_e. The same tuning parameters as before are used for the control algorithm. The online modification algorithm results in step-like changes in the setpoint every 20 min. The NLQDMC controller does a very good job in responding to the setpoint

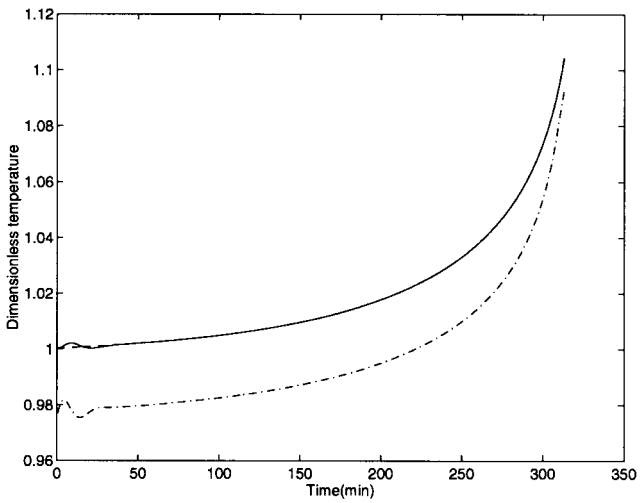

Fig. 1. Temperature vs. time. Setpoint tracking without on-line modification. Dashed line – setpoint, solid line – reactor temperature, dashed and dotted line – jacket temperature.

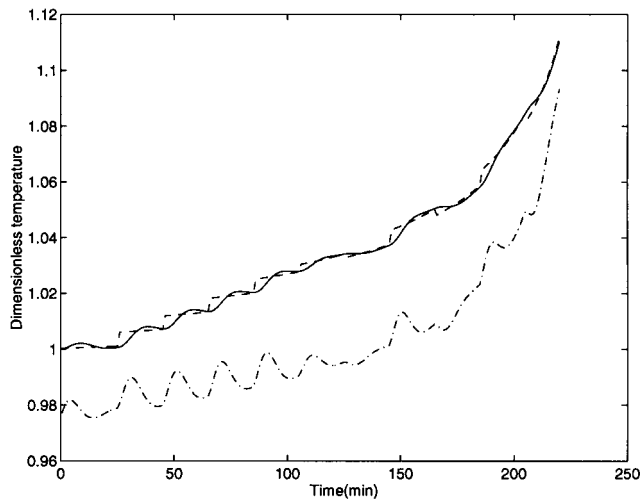

Fig. 2. Temperature vs. time. Setpoint tracking with on-line modification, no measurement noise. Dashed line – setpoint, solid line – reactor temperature, dashed and dotted line – jacket temperature.

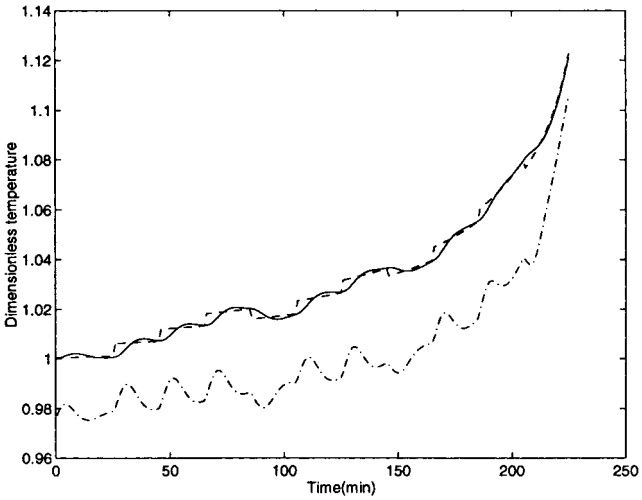

Fig. 3. Temperature vs. time. Setpoint tracking with on-line modification and measurement noise. Dashed line – setpoint, solid line – reactor temperature, dashed and dotted line – jacket temperature.

changes but is not able to track the setpoint perfectly. However, at the end of the batch, as shown in Table 2, values of NACL=1.003 and WACL=1.006 are obtained with a conversion of 0.804. There is a slight deviation in the values of the NACL and WACL from the desired value of 1.0. This is because, in the last 20–40 min of the batch, there is no feedback from secondary measurements because of the assumed delay. Another important aspect to note is that there is a significant decrease in the batch time from 313 to 220 mm. For the simulated plant (with $A_{w,\text{plant}}=1.2A_w$), it takes much less than 313 min to achieve the desired values of NACL and WACL with 80% conversion if the temperature path tracked is optimal for the true plant. The proposed method was able to modify the temperature setpoint profile to reduce the necessary batch time, in spite of the model coefficient errors that are still present at the end of the batch.

Fig. 3 demonstrates the tracking of the temperature setpoint profile with on-line modification using the delayed and noise-corrupted secondary measurements of conversion and molecular weights. One percent error under the normal distribution is introduced in conversion and WACL, NACL measurements. The response is similar to the response observed in the case of measurements without noise. As can be seen in Table 3, the end values of the properties are very close to the desired values. Figs. 4–6 show the conversion, dimensionless NACL and dimensionless WACL measurements as a function of time.

Table 3
Product properties with and without measurement noise

Properties	t_f	Properties at t_f		
		NACL	WACL	Conversion
Without measurement noise	220	1.003	1.006	0.804
With measurement noise	225	1.004	1.011	0.805

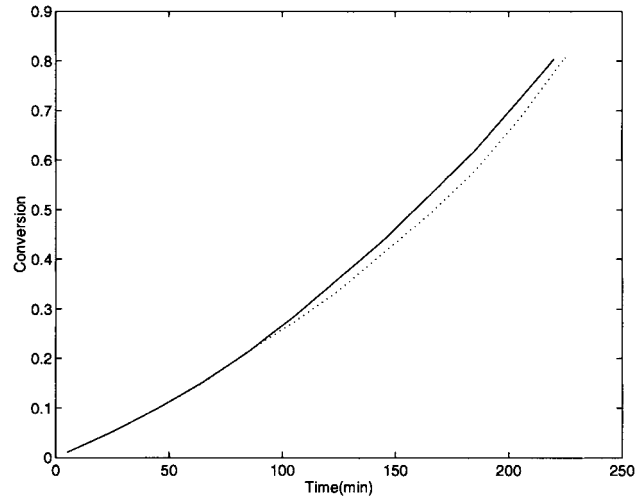

Fig. 4. Conversion vs. time. Solid – no measurement noise, dotted – with measurement noise.

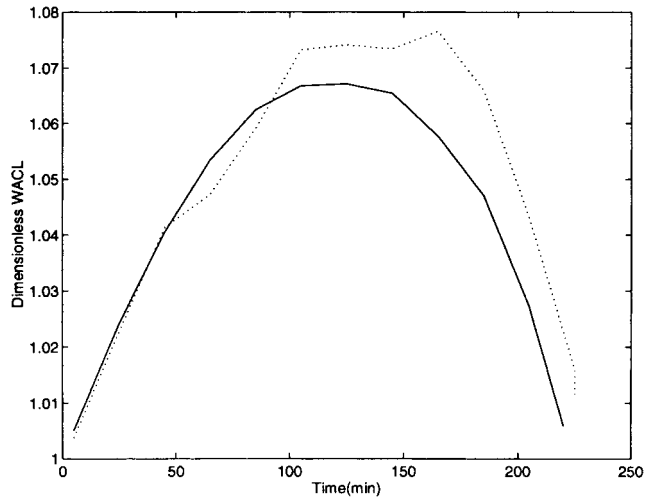

Fig. 5. Dimensionless WACL vs. time. Solid – no measurement noise, dotted – with measurement noise.

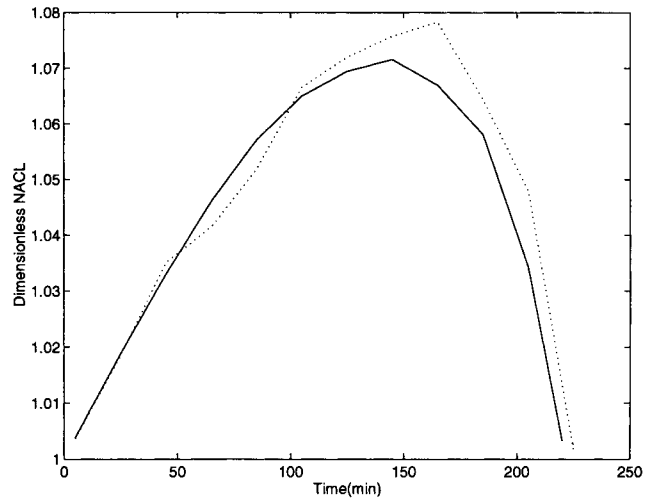

Fig. 6. Dimensionless NACL vs. time. Solid – no measurement noise, dotted – with measurement noise.

4. Conclusions

A state estimation model based algorithm was developed for the on-line modification during the batch of the setpoint time profiles used in the standard real-time reactor control system. It utilizes infrequent and delayed measurements of the product properties that are indirectly controlled through the implementation of the selected time profiles of other process variables like reactor temperature for which frequent measurements are available. The algorithm is integrated with observer based NLQDMC used for real-time control in order to track the modified setpoint profiles. The effectiveness of the algorithm is demonstrated by simulation of bulk polymerization of styrene. It is observed that by the use of the proposed algorithm, the desired values of molecular weights are achieved at the end of the batch despite the presence of significant modeling errors. In addition to obtaining the desired values of final product properties, the algorithm was able to modify the temperature profiles to accomplish the task while minimizing batch time. The algorithm also performed well in the presence of measurement noise without requiring any additional tuning of its parameters. The modest additional on-line computational requirements of the procedure offer promise for practical implementation.

5. Notation

A_k, B_k, C_k	continuous state space matrices
A_c, A_m, A_w, B	parameters in polymerization model
c_p	heat capacity
D	diagonal weight matrix
E_m	Arrhenius constant
G_k	coefficient matrix for disturbance model
$k+1\|k$	estimate at $k+1$ based on information at k
K	estimator gain
M	no. of future moves
P	prediction horizon
$\tilde{P}$	constraint projection matrix
q	transformed state variable
Q, R	covariance matrices
r_1, r_2, r_3, r_4	constants
t	time
u, u_c	input vector
w, v	white noise processes
V, V_c	reactor and jacket volumes
x, x_c	state vector
y, y_c	output vector
z	state vector for linearized models

Greek letters

α	step size
γ	penalty coefficient
Γ, Λ	diagonal weight matrices
Γ_k, Φ_k	discrete state space matrices
ϕ	objective function
ρ	density
τ	transformed independent variable
δ	ratio δ_w/δ_v
δ_w^2, δ_v^2	scalar variances

Subscript

0	initial or nominal value
k	sampling time index

Superscript

^	estimated value
T	transpose

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Support for this project was provided by the National Science Foundation (PYI grant CTS-9057292) and Exxon Chemical.

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