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State Estimation Model Based Algorithm for On-line Optimization and Control of Batch Processes

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State Estimation Model Based Algorithm for On-line Optimization and Control of Batch Processes[1]

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Abstract

Batch/semi-batch processes are highly nonlinear and involve complex reaction mechanisms. Model-plant mismatch always exists. The lack of rapid direct or indirect measurements of the properties to be controlled makes the control task difficult. It is the usual practice to follow the prespecified setpoint profiles for process variables for which measurements are available, in order to obtain desired product properties. Modeling error can be the cause of bad performance when optimal profiles computed for the model, are implemented on the actual plant. In this paper, a state estimation model based algorithm is presented for on-line modification of the optimal profile and control with the goal of obtaining the desired properties at the minimum batch time. The effectiveness of the algorithm is demonstrated by its application to bulk polymerization of styrene.

1. Introduction

Batch/semi-batch processes are characterized by strong nonlinearities, significant time delay in the measurements of the properties to be controlled and external unmeasured disturbances entering the system. The lack of instantaneous measurements of the properties to be controlled (e.g., in a polymerization reactor, the control of 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 are computed by off-line optimization of appropriate objective functions based on the available model [1,9]. 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 the new measurements are obtained. Such computations require solving a computationally intensive nonlinear optimization problem and are not feasible for practical on-line implementation.

To avoid reoptimizing the nonlinear objective function every time the new measurements are obtained, Kozub and Macgregor [4] proposed a method based on the instantaneous properties of the desired product. Palanki *et al.* [7] derived optimal state feedback laws for a class of nonlinear systems. Zafiriou and Zhu [10] 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 the controller tracks the optimal profiles perfectly and all the states are measured. Moreover, the 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., setpoint profile to be tracked) and control (e.g., to track the setpoint profile) of batch/semi-batch processes. 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 setpoint profile is updated by carrying out one iteration of a gradient based optimization method. The modified profile is implemented till the next set of measurements are available. State estimation NLQDMC algorithm [2] is used as a control algorithm for setpoint tracking.

2. Methodology

The proposed algorithm involves (i) on-line modification of setpoint profile (ii) on-line tracking of setpoint profile. The measurements are divided into two categories as primary and secondary measurements. The primary measurements are used for state estimation in the control algorithm. The secondary measurements are used in the estimation phase of on-line update of 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. It is assumed that there is a delay of one sample unit in processing the secondary measurements, i.e., at the sampling time k the information about the measurements at sampling time $k-1$ is available. Based on the measurements at $k-1$ the 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 modified.

Estimation

Consider the nonlinear model of the form

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

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

where x is the state vector, u is the setpoint for the on-line control, y is the vector of secondary measurements. For example, in a polymerization process where the polymer properties (e.g., molecular weights) are controlled by following a prespecified temperature profile, the temperature is the setpoint in the on-line control and is the input in the on-line modification of setpoint profile.

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

$$\begin{aligned} \dot{z} &= A_{k-1}z + B_{k-1}u \\ y &= C_{k-1}z \end{aligned} \tag{3}$$

where $A_k = (\frac{\partial f}{\partial x})|_{x=x_{k|k-1},u=u_k}$, $B_k = (\frac{\partial f}{\partial u})|_{x=x_{k|k-1},u=u_k}$, $C_k = (\frac{\partial h}{\partial x})|_{x=x_{k|k-1}}$. 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) is augmented with stochastic states and is given as:

$$\begin{aligned} \dot{z} &= A_{k-1}z + B_{k-1}u + G_{k-1}w + w_1 \\ \dot{w} &= w_2 \\ y_j &= C_{k-1}z_j + v_j \end{aligned} \tag{4}$$

where w_1, w_2 and v_j are uncorrelated white noise sequences with $[w_1^T, w_2^T]^T \sim (0, Q_b)$ and $v_j \sim (0, R_b)$, Q_b and R_b being covariance matrices associated with process and measurement noise. y_j is the measurement. The only technical requirement in using this kind of disturbance model is that the augmented system is detectable. In general, it is required that the number of new augmented states are less than or equal to the number of outputs for the detectability of the augmented system. For more details the reader is referred to [2].

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 $\delta_{w1}^2, \delta_{w2}^2$ 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.

Let $K_{k-1} \triangleq \begin{bmatrix} K_{k-1}^1 \\ K_{k-1}^2 \end{bmatrix}$ be the steady state kalman gain obtained by using the continuous-discrete kalman filter formulation [6]. The superscript 1 stands for the gain for the subsystem consisting of original states and 2 stands for the gain for the subsystem consisting of augmented states. Once the kalman gain is computed, it is used to correct the states of nonlinear and augmented linear model. The corrected estimates at $k-1$ are given as

$$\hat{x}_{k-1|k-1} = \hat{x}_{k-1|k-2} + K_{k-1}^1[y_{k-1} - h(\hat{x}_{k-1|k-2})] \tag{5}$$

$$\hat{w}_{k-1|k-1} = \hat{w}_{k-1|k-2} + K_{k-1}^2[y_{k-1} - h(\hat{x}_{k-1|k-2})] \tag{6}$$

The model for the future prediction is given as:

$$\begin{aligned} \dot{\hat{x}} &= f(\hat{x}, u) + G_{k-1}\hat{w} \qquad (7) \\ \hat{y} &= h(\hat{x}) \qquad (8) \end{aligned}$$

The values of estimates for states at k are obtained by integrating (7 – 8) over one sample unit T_b.

Determination of optimal profile

The optimal setpoint profile for the remaining time of the batch is determined based on the model described by (7 – 8) 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 setpoint profile to achieve the final desired properties in the minimum batch time starting from time k. One has to be reminded that the modification of setpoint profile is 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. First, we utilize the technique proposed by Kwon and Evans [3] to convert the fixed-end-point and free-end-time problem to a free-end-point and fixed-end-time problem through coordinate transformation. This method can be applied to any nonlinear system in which at least one of the state variables is monotone. In the following, we briefly summarize this method. First, the state variable $x = (x_1, x_2, \ldots, x_n)$ is rearranged such that x_1 is the monotone state variable which is used as new independent variable. Then a coordinate transformation is made given by

$$\tau \leftarrow x_1 \quad q_1 \leftarrow t \quad q_i \leftarrow x_i \ (i > 1) \tag{9}$$

It results in a system

$$\dot{q}(\tau) = F(q, u, \tau) \tag{10}$$

with $F_1 = 1/f_1$ and $F_i = f_i/f_1$ for $i > 1$. The transformed problem can be solved using any gradient based optimization method. In our approach, the steepest descent with constraints method is used. At each k, we carry out one iteration of the algorithm. One iteration is justified because, once the new measurements are obtained, the model and initial estimates change resulting in a different optimal profile. Therefore, to reduce the on-line computational requirements, only one iteration is carried out at each k and the updated profile is implemented.

Algorithm:

$$\min_{u(\tau)} \ \phi(q(\tau_f)) \tag{11}$$

subject to (10) where τ_f is the desired value of x_1 at the end of the batch.

(a) Set $\tau_0 = x_{1,k|k-1}$, $q_1 = t_k$ and $q_i = x_{i,k|k-1}$ for $i > 1$.

(b) Forward integration of model.
$u_{old}(\tau) \rightarrow \dot{q}(\tau) = F(q, u, \tau) \rightarrow q(\tau)$

(c) Linearize $F(q, u, \tau)$ at $u_{old}(\tau), q(\tau)$ to obtain $F_q(q, u_{old})$ and $F_u(q, u_{old})$

(d) Backward integration of adjoint system
$\dot{\lambda} = F_q(q, u_{old})\lambda; \quad \lambda(\tau_f) = \Delta_q\phi(q(\tau_f))$

(e) Compute gradient
$g(\tau) = F_u^T(q, u_{old})\lambda(\tau)$

(f) Line search:
$u_{new}(\tau) = u_{old}(\tau) - \alpha\bar{P}g(\tau)$
$0 \leq \alpha \leq min[\alpha_e, \alpha_{max}]$
where $\bar{P}$ is the constraint projection matrix, α_{max} is 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 [8] stepsize rule. The updated u is used as the setpoint for the on-line control algorithm.

2.2. Setpoint tracking

State estimation NLQDMC [2] is used as a control algorithm for tracking and disturbance rejection. 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 the algorithm. For more details, the reader is referred to [2]. Lee and Ricker [5] proposed a slightly different algorithm based on Extended Kalman Filter formulation.

Consider the nonlinear model of the form

$$\dot{x} = f_c(x, u) \tag{12}$$

$$y = h(x) \tag{13}$$

where x is the state vector, u is the manipulated variable in the on-line control, y is the controlled variable. The states of the model described by (12) partly consist of the states of the model described by (2) and vice-versa. The model (12 – 13) is the state space description of the primary measurement variables and the related input variables, whereas the (1 – 2) is the state space description of the secondary measurement variables and the related input variables. The controlled variable y in (13) is the input vector u in (1). Referring to the polymerization example, the controlled variable is the temperature and the manipulated variable is the cooling water which controls the optimally modified temperature profile obtained by the procedure described the previous subsection. A linear model is obtained by linearizing (12 – 13) at $x_{k|k-1}$ and u_{k-1}. Let Φ_k and Γ_k be discrete state space matrices, obtained from the linearized model. Let y_k be the measurement of the plant at k and $f(x_k, u_k)$ is denoted as the value of the state when the system model $\dot{x} = f_c(x, u)$ is integrated over one sampling time from the initial conditions x_k and u_k.

The idea is to approximate the nonlinear process as a linear model around the sampling instant, augment the linear model with additional linear states to describe the appropriate disturbances, then compute the estimator gains for the augmented system. Once the estimator gains have been computed, we use them to update the nonlinear states and the augmented linear states to capture the effect of nonlinearity and disturbances. We consider the two sets of linear discrete models given as

Type A:

$$\begin{aligned} z_{j+1} &= \Phi_k z_j + \Gamma_k u_j + w_{1j} \\ \eta_{j+1} &= \eta_j + w_{2j} \\ y_j &= C_k z_j + \eta_j + v_j \end{aligned} \tag{14}$$

Type B:

$$\begin{aligned} z_{j+1} &= \Phi_k z_j + \Gamma_k u_j + \Gamma_k w_j + w_{1j} \\ w_{j+1} &= w_j + w_{2j} \\ y_j &= C_k z_j + v_j \end{aligned} \tag{15}$$

where w_{1j}, w_{2j} and v_j are uncorrelated white noise sequences with $[w_{1j}^T, w_{2j}^T]^T \sim (0, Q)$ and $v_j \sim (0, R)$, Q and R being covariance matrices associated with process and measurement noises. z is the state vector of the linearized model, y_j is the measurement and η and w represent additional linear states to describe the disturbances.

The type A model represents the process model augmented with the disturbance model for disturbances which are step-like at the output. Type B model represents the augmented process and disturbance models for step-like disturbances at the input. In type B model, w going through Γ_k makes it optimal for input disturbances, however, that matrix can be any general matrix as long as the augmented system satisfies the detectability requirement discussed in the previous subsection. Offset-free tracking in the presence of model-plant mismatch can be handled in an effective manner by the use of either type of models. Also, an observer designed based on the description of either type can stabilize the open-loop unstable processes by putting the closed-loop observer poles inside the unit disk, provided that the controller is designed such that the regulator poles are inside the unit disk.

As discussed in the previous subsection it is assumed that $Q \approx \begin{bmatrix} \sigma_{w1}{}^2 & 0 \\ 0 & \sigma_{w2}{}^2 \end{bmatrix}$ and $R \approx \sigma_v{}^2 I$ where $\sigma_{w1}{}^2, \sigma_{w2}{}^2$ and $\sigma_v{}^2$ are scalar variances. Define $\sigma_1 = \sigma_{w1}/\sigma_v, \sigma_2 = \sigma_{w2}/\sigma_v$ and let $\sigma_v{}^2 = 1$. The parameters σ_1 and σ_2 are used as tuning parameters which determine the value of estimator gains.

Let $K_k \triangleq \begin{bmatrix} K_k^1 \\ K_k^2 \end{bmatrix}$ be the steady state kalman gain computed using the discrete Kalman filter [6]. The future prediction equations are given by:

Type A augmented system:

$$\begin{aligned} \hat{x}_{k+1|k} &= \Phi_k \hat{x}_{k|k-1} + \Gamma_k u_k + \\ &\quad K_k^1 [y_k - C_k \hat{x}_{k|k-1} - \hat{\eta}_{k|k-1}] \end{aligned} \tag{16}$$

$$\hat{\eta}_{k+1|k} = \hat{\eta}_{k|k-1} + K_k^2 [y_k - C_k \hat{x}_{k|k-1} - \hat{\eta}_{k|k-1}] \tag{17}$$

$$\hat{y}_{k+1|k} = C_k \hat{x}_{k+1|k} + \hat{\eta}_{k+1|k} \tag{18}$$

By taking the conditional mean, the P-step ahead predictions are

$$\hat{x}_{k+i|k} = \Phi_k \hat{x}_{k+i-1|k} + \Gamma_k u_{k+i-1} \quad i = 2, \ldots, P \tag{19}$$

$$\hat{\eta}_{k+i|k} = \hat{\eta}_{k+i-1|k} \quad i = 2, \ldots, P \tag{20}$$

$$\hat{y}_{k+i|k} = C_k \hat{x}_{k+i|k} + \hat{\eta}_{k+i|k} \quad i = 2, \ldots, P \tag{21}$$

Rewriting (16) and (19) as

$$\begin{aligned} \hat{x}_{k+1|k} &= \Phi_k \hat{x}_{k|k-1} + \Gamma_k u_{k-1} + \Gamma_k \Delta u_k + \\ &\quad K_k^1 [y_k - C_k \hat{x}_{k|k-1} - \hat{\eta}_{k|k-1}] \end{aligned} \tag{22}$$

$$\hat{x}_{k+i|k} = \Phi_k \hat{x}^*_{k+i-1|k} + \Gamma_k u_{k-1} + \sum_{l=1}^{i} \Phi_k^{l-1} \Gamma_k \Delta u_{k+i-l} \tag{23}$$

for $i = 2, \ldots, P$, where $\hat{x}^*_{k+i-1|k}$ is the estimate computed using (16) or (19) by setting $u_{k+i} = u_{k-1}$ for $i = 0, \ldots, P-1$ and Δu is the change in manipulated variables, defined as $\Delta u_k \triangleq u_k - u_{k-1}$.

Now, to account for the nonlinearity in the future predictions, the computations related to the past information are carried out using the available nonlinear model. However, the contribution of the future manipulated variables is computed by using the linear model inorder to formulate the optimization as a QP. Then, the future predictions are given by:

Type A augmented system:

$$\hat{x}_{k+1|k} = f(\hat{x}_{k|k-1}, u_{k-1}) + \Gamma_k \Delta u_k +$$

$$K_k^1[y_k - h(\hat{x}_{k|k-1}) - \hat{\eta}_{k|k-1}] \quad (24)$$

$$\hat{\eta}_{k+1|k} = \hat{\eta}_{k|k-1} + K_k^2[y_k - h(\hat{x}_{k|k-1}) - \hat{\eta}_{k|k-1}] \quad (25)$$

$$\hat{y}_{k+1|k} = h(\hat{x}_{k+1|k}) + \hat{\eta}_{k+1|k} \quad (26)$$

The P-step ahead predictions are

$$\hat{x}_{k+i|k} = f(\hat{x}^*_{k+i-1|k}, u_{k-1}) + \sum_{l=1}^{i} \Phi_k^{l-1}\Gamma_k \Delta u_{k+i-l} \quad (27)$$

$$\hat{\eta}_{k+i|k} = \hat{\eta}_{k+i-1|k} \quad (28)$$

$$\hat{y}_{k+i|k} = h(\hat{x}_{k+i|k}) + \hat{\eta}_{k+i|k} \quad (29)$$

for $i = 2, \ldots, P$

By the similar procedure, the prediction equations for the type B augmented model are given by:

Type B augmented system:

$$\hat{x}_{k+1|k} = f(\hat{x}_{k|k-1}, u_{k-1}) + \Gamma_k \hat{w}_{k|k-1} + \Gamma_k \Delta u_k + K_k^1[y_k - h(\hat{x}_{k|k-1})] \quad (30)$$

$$\hat{w}_{k+1|k} = \hat{w}_{k|k-1} + K_k^2[y_k - h(\hat{x}_{k|k-1})] \quad (31)$$

$$\hat{y}_{k+1|k} = h(\hat{x}_{k+1|k}) \quad (32)$$

The P-step ahead predictions are

$$\hat{x}_{k+i|k} = f(\hat{x}^*_{k+i-1|k}, u_{k-1}) + \Gamma_k \hat{w}_{k+i-1|k} + \sum_{l=1}^{i} \Phi_k^{l-1}\Gamma_k \Delta u_{k+i-l} \quad (33)$$

$$\hat{w}_{k+i|k} = \hat{w}_{k+i-1|k} \quad (34)$$

$$\hat{y}_{k+i|k} = h(\hat{x}_{k+i|k}) \quad (35)$$

for $i = 2, \ldots, P$, with $\hat{x}_{0|-1} = x_0$, $\hat{\eta}_{0|-1} = 0$ and $\hat{w}_{0|-1} = 0$. P is the prediction horizon. To avoid complexity in notation, we used the same notation for estimator gains for both Type A and Type B systems. But in actuality they come from solving ARE's with different system matrices.

Optimization

$$\min_{\Delta u_k, \ldots, \Delta u_{k+M-1}} \sum_{l=1}^{P} ||\Gamma(\hat{y}_{k+l|k} - r_{k+l})||^2 + ||\Lambda \Delta u_{k+l-1}||^2 \quad (36)$$

where $||\bullet||^2$ is defined by $||x||^2 = x^T x$. M is the number of future moves to be optimized. It is assumed that $u_{k+M-1} = u_{k+M} = \ldots = u_{k+P-1}$. Γ and Λ are diagonal weight matrices and r is the reference setpoint. The reference setpoint is updated whenever the setpoint profile is modified as described in section 2.1

M future manipulated variables are computed, but only the first move is implemented. The optimization is subject to input and other possible constraints. The estimate $\hat{x}_{k+1|k}$ is computed by the following equations.

Type A augmented system:

$$\hat{x}_{k+1|k} = f(\hat{x}_{k|k-1}, u_k) + K_k^1[y_k - h(\hat{x}_{k|k-1}) - \hat{\eta}_{k|k-1}] \quad (37)$$

Type B augmented system:

$$\hat{x}_{k+1|k} = f(\hat{x}_{k|k-1}, u_k) + \Gamma_k \hat{w}_{k|k-1} + K_k^1[y_k - h(\hat{x}_{k|k-1})] \quad (38)$$

3. Illustration

In this section, the algorithm is applied to thermally initiated bulk polymerization of styrene in a batch reactor. The differential equations describing the system are given by,[3]:

$$\dot{x}_1 = f_1 = \frac{\rho_0 p}{M_m}(1-x_1)^2 exp(2x_1 + 2\chi x_1^2) A_m exp(-\frac{E_m}{x_4 T_{ref}}) \quad (39)$$

$$\dot{x}_2 = f_2 = \frac{f_1 x_2}{1+x_1}(1 - \frac{1400 x_2}{A_w exp(\frac{B}{x_4 T_{ref}})}) \quad (40)$$

$$\dot{x}_3 = f_3 = \frac{f_1}{1+x_1}(\frac{A_w exp(\frac{B}{x_4 T_{ref}})}{1500} - x_3) \quad (41)$$

$$\dot{x}_4 = \frac{\rho_0(-\Delta H_p) f_1}{M_m \rho c_p T_{ref}} - \frac{U_c A_c}{\rho c_p V}(x_4 - x_5) \quad (42)$$

$$\dot{x}_5 = \frac{q_{cref} q_c}{V_c}(\frac{T_{j,in}}{T_{ref}} - x_5) + \frac{U_c A_c}{(\rho c_p)_c V_c}(x_4 - x_5) \quad (43)$$

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

$$\rho_0 = r_1 + r_2 T_c$$

$$c_p = 1.256 + .004404(x_4 - 50) \ J/(gm\ K)$$

$$T_c = x_4 T_{ref} - 273.15$$

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, $x_4 = T/T_{ref}$ is the dimensionless reactor temperature, $x_5 = T_j/T_{ref}$ is the dimensionless jacket temperature, x_n is NACL, x_w is WACL, $q_c = Q_c/q_{cref}$ is the dimensionless cooling water flow rate, T is the reactor temperature, T_j is the jacket temperature and Q_c is the cooling water flow rate. The parameter values used are, $A_w = .033454$, $B = 4364\ K$, $M_m = 104$, $\chi = .33$, $r_1 = .9328\ gm/cc$, $r_3 = 1.0902\ gm/cc$, $r_2 = -.00087902\ gm/cc\ C$, $r_4 = -.00059\ gm/cc\ C$, $e_m = 10,103.5\ K$, $A_m = 4.266e08\ cc/g\ mol\ s$, $A_c = 1.0\ m^2$, $V_c = .02\ m^3$, $V = 0.2\ m^3$, $T_{j,in} = 330\ K$, $T_{ref} = 399.15\ K$, $(\rho c_p)_c = 4.17 J/cc\ K$, $(-\Delta H_p) = 67,400 J/mol$, $U_c = .05 J/K\ cm^2\ s$, $q_{cref} = 1000 cc/min$, $x_{nf} = 700$ and $x_{wf} = 1500$. The initial values of the states are $x_{10} = 0.0, x_{20} = 1.0, x_{30} = 1.0, x_{40} = 1.0, x_{50} = 0.975$.

The objective of the batch is to achieve a conversion of 0.8 (80%) with values of NACL and WACL equal to 1 in the minimum amount of time. Therefore, the objective function for on-line modification of the setpoint profile can be stated mathematically as

$$\min_{u(t)} \ t_f + \gamma[(x_2(t_f) - 1)^2 + (x_2(t_f) - 1)^2] \quad (44)$$

The primary measurement is the reactor temperature. The secondary measurements are conversion, NACL and WACL. x_4 is the controlled variable in the on-line control phase and is the input variable in the on-line setpoint modification phase, and q_c is the manipulated variable in the on-line control. The model for on-line modification of setpoint profile is described by (39 – 43) and the model for on-line setpoint tracking is described by (39 – 41). A value of $\gamma = 10,000$ is used in simulations.

In all the simulations it is assumed that there is modeling error in the heat transfer coefficient, U_c. A value of 0.04 is used for the plant heat transfer coefficient. Parametric uncertainty is assumed in A_w to demonstrate the on-line modification procedure. A value of $A_{w,plant} = 1.2A_w$ is used in simulations.

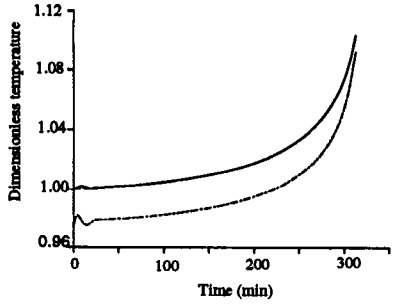

Figure 1: Temperature vs. time. Setpoint tracking without on-line modification; Dashed line –setpoint; Solid line —reactor temperature; Dashed and dotted line – jacket temperature

setpoint	t_f	properties at t_f		
		NACL	WACL	conv.
no modification	313	1.080	1.090	0.801
modified on-line	218	1.002	1.004	0.803

Table 1: Product properties at the end of the batch

For the ideal case with no model-plant mismatch in A_w, the desired properties and conversion are achieved in 313 min. Figure 1 demonstrates the tracking of temperature profile which is optimal for model, without modifying it on-line. Tuning parameter values of $\Lambda = .015, P = 5, M = 1$ and Type B estimator with $\sigma_1 = 0$ and $\sigma_2 = 10$ are used in the control algorithm. A sample time of 1.0 min is used for primary measurement, i.e., for temperature. A lower constraint of 0.0 is imposed on the cooling water flow. It can be seen that the control algorithm can track the setpoint profile almost perfectly even in the presence of uncertainty in the heat transfer coefficient. However, due to the modeling error in A_w, as shown in table 1, values of NACL = 1.08 and WACL = 1.09 are obtained at the end of the batch with a conversion of 0.801.

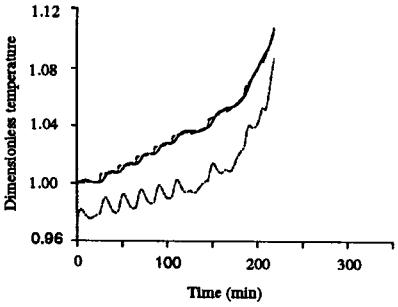

Figure 2: Temperature vs. time. Setpoint tracking with on-line modification; Dashed line –setpoint; Solid line — reactor temperature; Dashed and dotted line – jacket temperature

Figure 2 demonstrates the tracking of temperature profile with on-line modification. Tuning parameter values of $\delta_1 = .1$, $\delta_2 = .1$ and $G_k = G = [0\ 1\ 1]^T$ are used in the estimation phase of on-line modification of setpoint profile. A sample time of 20 min are used for the secondary measurements, i.e., for molecular weights and conversion. It is assumed that the first secondary measurement sample is taken 5 min 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. The same tuning parameters as before are used for the control algorithm. It can be seen that, because of the on-line modification and sudden step like changes, the setpoint is not tracked perfectly. However, at the end of the batch, as shown in table 1, values of NACL = 1.002 and WACL = 1.004 are obtained with a conversion of 0.803. Another important aspect to note is that there is a significant decrease in the batch time from 313 min to 218 min.

4. Conclusions

A state estimation model based algorithm is presented for on-line optimization and control of batch/semi-batch processes. Based on the delayed measurements of the properties to be controlled, the setpoint profile is updated on-line. State estimation NLQDMC algorithm is used for on-line control. The effectiveness of the algorithm is demonstrated by its application to bulk polymerization of styrene. It is observed that by the use of the proposed algorithm, the desired values of molecular weights are achieved with a significant decrease in the batch time, despite the presence of modeling error.

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