Multirate Nonlinear State Estimation with Application to a Polymerization Reactor

Srinivas Tatiraju and Masoud Soroush
Dept. of Chemical Engineering, Drexel University, Philadelphia, PA 19104

Babatunde A. Ogunnaike
DuPont Central Science and Engineering, Wilmington, DE 19880

A method of multirate nonlinear state observer design, which can use directly a nonlinear process model in the observer design without any linear approximation, is presented. The multirate nonlinear state observer is easy to design and implement, and is computationally efficient. Furthermore, for a number of processes, it is possible to prove the global convergence of the multirate state observer analytically. The design, implementation and performance of the state observer design method are shown by a polymerization reactor in which free-radical solution polymerization of styrene takes place. The initiator concentration and three leading moments of the molecular weight distribution (MWD) of the polymer product are estimated continuously from: (i) frequent measurements of the reactor temperature, jacket temperature and reacting-mixture density; (ii) infrequent and delayed measurements of the leading moments of the MWD. Each infrequent measurement has a sampling period and a measurement delay of 0.5 or 1 h. In the presence of model-plant mismatch and measurement noise, the convergence of the multirate state observer is shown by numerical simulations.

Introduction

A polymer product is composed of macromolecules with different molecular weights, and the processability and subsequent utility of a polymer product depend strongly on the molecular weight distribution (MWD) of the macromolecules. Since the MWD is influenced greatly by the polymerization reactor operating conditions, the production of a high quality polymer requires effective monitoring and control of the MWD in the reactor. Both of these can be realized only when sufficient on-line information on the MWD is available.

Polymerization reactors are a class of processes in which many essential process variables related to product quality cannot be measured or can be measured at low sampling rates and with significant time delays. The lack of readily-available, frequent, on-line measurements, from which polymer properties can be inferred, has motivated a considerable research effort in the following research directions: (a) the development of new on-line sensors [lists of many of the currently-available on-line sensors are given in Ray (1986) and Chien and Penlidis (1990)]; (b) the development of qualitative and quantitative relations between readily-available on-line measurements such as density, viscosity and refractive index, and polymer properties such as conversion and average molecular weights (Schork and Ray, 1983; Ohshima and Tomita, 1995; Ohshima et al., 1995); (c) the development of state estimators/observers that are capable of estimating unmeasurable polymer properties.

Since the 1970s, the problem of state estimation in polymerization reactors has been studied extensively (Jo and Bankoff, 1976; Schuler and Suzhen, 1985; Ellis et al., 1988; Adebekun and Schork, 1989; Kim and Choi, 1991; Kozub and MacGregor, 1992; van Dootingh et al., 1992; Ogunnaike, 1994; Robertson et al., 1995; Liotta et al., 1997). The availability of sufficiently-accurate, first-principles, mathematical models of the reactors has made possible the development of the state estimators/observers. State estimation in other chemical/pet-

---

Correspondence concerning this article should be addressed to M. Soroush.

rochemical and biochemical processes has also been studied. Examples are bioreactors and distillation columns (Bastin and Dochain, 1990; Quintero-Marmol et al., 1991). In most of these studies, extended Kalman filters (EKFs) have been used for state estimation.

A major characteristic of polymerization reactors is their complex nonlinear behavior. Phenomena such as multiple steady states in continuous stirred tank reactors, parametric sensitivity, and limit cycles are manifestations of the complex nonlinearity. Thus, reliable state estimation in polymerization reactors requires nonlinear models that can capture the complex nonlinear behavior. Motivated by the need for nonlinear state estimation in many processes such as polymerization reactors, many attempts have been made since the early 1980s to develop nonlinear state estimation methods that can use directly a nonlinear process model in the estimator/observer design without any linear approximation (Krener and Isidori, 1983; Zeitz, 1987; van Dootingh et al., 1992; Ciccarella et al., 1993; Kazantzis and Kravaris, 1996; Robertson et al., 1996; Soroush, 1997).

In polymerization reactors, most of essential measurements related to polymer product quality, such as the leading moments of a MWD obtained by a gel permeation chromatograph (GPC), are available at low sampling rates and with considerable time delays. On the other hand, measurements of process variables such as temperatures, pressures, and densities are usually available at high sampling rates and with almost no delays. Because polymer product quality is usually not observable from the frequent, delay-free measurements alone, one has to design a multirate estimator/observer (that is, one that uses both the frequent and infrequent measurements) to provide reliable estimates of the states, especially in the presence of model-plant mismatch and measurement noise.

The need for multirate estimators has been well recognized in the chemical/petrochemical and biochemical industries (Ellis et al., 1998; Bastin and Dochain, 1990; Kim and Choi, 1991; Stone et al., 1992; Ogunnaike, 1994; Gudi et al., 1995; Mutha et al., 1997; Tatiraju et al., 1998). So far, the problem of multirate state estimation has been studied primarily within the framework of the EKF. For example, Ellis et al. (1988) used a multirate EKF to estimate the unmeasurable process states continuously from the frequently available measurements of temperature and density and the infrequent and delayed measurements of the average molecular weights (obtained by a GPC). Gudi et al. (1995) implemented a two-time-scale EKF on a biochemical reactor. Another multirate state estimation approach commonly used in electrical engineering applications involves using smoothing algorithms (Meditch, 1973) along with a bank of Kalman filters (Hong, 1994; Williamson et al., 1996). Mutha et al. (1997) proposed the use of a fixed-lag smoothing algorithm for multirate state estimation in a polymerization reactor.

In this article we present a multirate nonlinear state-observer design method that can use directly a nonlinear process model in the observer design without any linear approximation. The resulting multirate state observer can be interpreted as a multirate reduced-order Luenberger state observer. Because of its reduced-order nature, (a) the state observer is computationally inexpensive to implement and (b) for many processes it is possible to prove the global convergence of the state observer analytically. The similarities and differences between the multirate nonlinear state-observer design method and EKF are discussed. The design, implementation, and performance of the multirate state estimation method are shown by a continuous polymerization reactor in which free-radical solution polymerization of styrene takes place.

The scope of this work and some preliminaries are given, followed by the multirate nonlinear observer design method. The polymerization system and its mathematical model are then described, followed by the application of the multirate nonlinear state observer to the reactor. Simulation results are presented and discussed.

Scope and Preliminaries

Consider the class of nonlinear processes described by a state-space model of the form

$$\begin{cases} \dot{x}(t) = f[x(t), u(t)] & \\ y_i(t) = h_i[x(t)], & i = 1, \ldots, p \\ Y_i(t_{i_k}) = H_i[x(t_{i_k} - \theta_i)], & i = 1, \ldots, q, \ k = 1, 2, \ldots \end{cases} \tag{1}$$

where $x = [x_1 \ldots x_n]^T$ denotes the vector of state variables, $u = [u_1 \ldots u_m]^T$ represents the vector of measurable inputs (manipulated inputs and measurable disturbances), $y = [y_1 \ldots y_p]^T$ is the vector of "fast" measurable outputs (whose measurements are available so frequently that these measurements can be considered as continuous functions of time), $Y = [Y_1 \ldots Y_q]^T$ is the vector of "slow" measurable outputs (which are measured at lower sampling rates and are available with different time delays), t_{i_k} $(k = 1, 2, \ldots)$ are the time instants at which the measurements of the slow measurable output Y_i are available, θ_i is the dead-time associated with the slow measurable output Y_i, and $f(.,.)$, $h(.) = [h_1(.) \ldots h_p(.)]^T$, and $H(.) = [H_1(.) \ldots H_q(.)]^T$ are smooth vector functions. We make the following assumptions:

(a1) The $p \times n$ matrix $\partial h(x)/\partial x$ has *locally* p linearly independent rows or columns; this condition ensures that none of the available fast measurable outputs are redundant.

(a2) The process state variables are locally detectable from the fast and slow measurable outputs.

Definition 1. (Soroush, 1997): Consider a system of the form of Eq. 1. A state variable x_i is said to be locally detectable from the fast measurable outputs, if there exists a $1 \times p$ smooth vector function $\psi_i(\xi + x, u, y)$ such that the universal equilibrium point of the subsystem

$$\dot{\xi}_i = f_i(\xi + x, u) - f_i(x, u) + \psi_i(\xi + x, u, y)[y - h(\xi + x)],$$
$$\xi_j(t) \equiv 0, j \neq i, j = 1, \ldots, n,$$

that is, $\xi_i = 0$, is locally asymptotically stable.

Definition 2. (Soroush, 1997): A system of the form of Eq. 1 is said to be locally detectable from the fast measurable outputs, if there exists an $n \times p$ smooth matrix function $\psi(\xi + x, u, y)$ such that the universal equilibrium point of the subsystem

$$\dot{\xi} = f(\xi + x, u) - f(x, u) + \psi(\xi + x, u, y)[y - h(\xi + x)],$$

that is, $\xi = 0$, is locally asymptotically stable.

A necessary condition for local detectability (from the fast measurements) of a system of the form of Eq. 1 is the existence of an $n \times p$ smooth matrix function $\psi(\xi + x, u, y)$ such that locally all the eigenvalues of the $(n \times n)$ matrix

$$\left[\frac{\partial f(x,u)}{\partial x} - \psi(x,u,y)\frac{\partial h(x)}{\partial x}\right]$$

lie in the left half of the complex plane.

Definition 3. (Soroush, 1997): Consider a system of the form of Eq. 1. A state variable x_i is said to be locally observable from the fast measurable outputs, if there is an lth-order $(0 \le l \le n-1)$ time-derivative of a fast measurable output y_j, that explicitly depends on the state variable x_i.

Definition 4. (Zeitz, 1987): A system of the form of Eq. 1 is said to be locally observable from the fast measurable outputs, if the following $(np \times n)$ matrix has locally n linearly independent rows or columns

$$\frac{\partial}{\partial x}\begin{bmatrix} h(x) \\ h^1(x, u^{(0)}) \\ h^2(x, u^{(0)}, u^{(1)}) \\ \vdots \\ h^{n-1}(x, u^{(0)}, u^{(1)}, \ldots, u^{(n-2)}) \end{bmatrix}$$

where

$$h^1(x, u^{(0)}) = \frac{\partial h(x)}{\partial x} f(x,u)$$

$$h^2(x, u^{(0)}, u^{(1)}) = \frac{\partial h^1(x, u^{(0)})}{\partial x} f(x,u) + \frac{\partial h^1(x, u^{(0)})}{\partial u}\frac{du}{dt}$$

$$h^{l+1}(x, u^{(0)}, u^{(1)}, \ldots, u^{(l)}) = \frac{\partial h^l(x, u^{(0)}, u^{(1)}, \ldots, u^{(l-1)})}{\partial x} f(x,u) + \sum_{j=0}^{l-1}\frac{\partial h^l(x, u^{(0)}, u^{(1)}, \ldots, u^{(l-1)})}{\partial u^{(j)}}\frac{du^{(j)}}{dt}, \qquad l = 0, \ldots, n-2$$

$$u^{(l)}(t) = \frac{d^l u(t)}{dt^l}, \qquad l = 0, 1, 2, \ldots$$

Multirate Nonlinear Observer Design Method

As a consequence of the assumption of (a1) made in the previous section, one can always find a locally one-to-one change of variables (locally invertible state transformation) of the form

$$\begin{bmatrix} \eta \\ y \end{bmatrix} = \mathfrak{I}(x) = \begin{bmatrix} Qx \\ h(x) \end{bmatrix}$$

where $\eta = [\eta_1, \ldots, \eta_{n-p}]^T$ and Q is a constant $(n-p) \times n$ matrix which, for the sake of simplicity, is chosen such that (c1) each row of Q has only one nonzero term equal to one and (c2) the determinant of the $n \times n$ matrix

$$\begin{bmatrix} Q \\ \dfrac{\partial h(x)}{\partial x} \end{bmatrix}$$

is locally nonzero. Here $\partial h(x)/\partial x$ is a $p \times n$ matrix whose ijth entry is $\partial h_i(x)/\partial x_j$. The new variables $\eta_1, \ldots, \eta_{n-p}$ are simply $(n-p)$ state variables of the original model of Eq. 1, that satisfy the determinant condition of (c2) given in this section.

Using the locally invertible state transformation $[\eta \;\; y]^T = \mathfrak{I}(x)$, we first recast the model of Eq. 1 in terms of the new state variables η and y

$$\begin{cases} \dot{\eta}(t) = F_\eta[\eta(t), y(t), u(t)] \\ \dot{y}(t) = F_y[\eta(t), y(t), u(t)] \\ Y_i(t_{i_k}) = \mathcal{H}_i[\eta(t_{i_k} - \theta_i), y(t_{i_k} - \theta_i)], \end{cases}$$

$$i = 1, \ldots, q, \quad k = 1, 2, \ldots \tag{2}$$

where

$$F_\eta(\eta, y, u) = Qf[\mathfrak{I}^{-1}(\eta, y), u],$$

$$F_y(\eta, y, u) = \left.\frac{\partial h(x)}{\partial x}\right|_{x = \mathfrak{I}^{-1}(\eta, y)} f[\mathfrak{I}^{-1}(\eta, y), u]$$

and

$$\mathcal{H}(\eta, y) = H[\mathfrak{I}^{-1}(\eta, y)]$$

We then design a multirate reduced-order nonlinear state observer/estimator of the form

$$\begin{aligned} \dot{z}(t) &= F_\eta[z(t) + Ky(t), y(t), u(t)] \\ &\quad - KF_y[z(t) + Ky(t), y(t), u(t)] \\ &\quad + L\{Y^*(t) - \mathcal{H}[z(t) + Ky(t), y(t)]\} \\ \hat{x}(t) &= \mathfrak{I}^{-1}[z(t) + Ky(t), y(t)] \end{aligned} \tag{3}$$

where the state observer gains K and L are constant $(n-p) \times p$ and $(n-p) \times q$ matrices, respectively. $Y^*(t)$ is the *predicted* present value of the vector of the slow measurements. Each Y_i^* is obtained by a least-squared-error curve fit of a polynomial of order m_i to the most recent r_i measurements of the slow measurable output Y_i, where m_i is chosen such that $r_i > m_i$. The values of $r_1, \ldots, r_q, m_1, \ldots, m_q$ are set by the designer. As the order of the polynomial m_i is increased, the sensitivity of the state estimates to noise in the slow measurement Y_i decreases. The state observer of Eq. 3 is a multirate version of the state observer design method presented in Soroush (1997).

Remark 1: In the case that $r_i = 3$ and $m_i = 1$, once a measurement of Y_i arrives at a time instant t_{i_k}, a straight line is fitted to the most-recent three measurements of Y_i via linear regression. The equation of this line is given by

$$Y_i^*(t) = A_{i_k} t + B_{i_k}, \qquad t_{i_k} \le t < t_{i_{k+1}}, \qquad i = 1, \dots, q \quad (4)$$

where A_{i_k} and B_{i_k} are respectively the slope and the intercept of the regression line. Equation 4 is used to predict the present value of the slow measurable output Y_i during the intersampling period $t_{i_k} \le t < t_{i_{k+1}}$. As soon as the next measurement of Y_i is available, the slope and intercept of the regression line are recalculated by using the most-recent three measurements of Y_i (including the new measurement). Thus, each $Y_i^*(t)$ is a piece-wise continuous function of time.

State observer tuning

The state observer/estimator should be tuned (that is, the constant matrices L and K should be chosen) properly to ensure that nominally the mismatch between the actual and estimated values of every state variable decays to zero asymptotically. The observer error e, $e \triangleq \hat{\eta} - \eta$ is governed by

$$\dot{e} = F_\eta(e + \eta, y, u) - F_\eta(\eta, y, u) - K\{F_y(e + \eta, y, u) - F_y(\eta, y, u)\} + L\{Y^* - \mathcal{H}[e + \eta, y]\} \quad (5)$$

which has a universal equilibrium point at $e = 0$. Thus, the observer/estimator should be tuned such that the equilibrium point of the observer error dynamics is asymptotically stable. The detectability of the system of Eq. 1 from the slow and fast measurable outputs guarantees the existence of a pair of matrices K and L, which place the $(n - p)$ eigenvalues of the Jacobian matrix of the system of Eq. 5, that is,

$$\frac{\partial F_\eta(\eta, y, u)}{\partial \eta} - K \frac{\partial F_y(\eta, y, u)}{\partial \eta} - L \frac{\partial \mathcal{H}(\eta, y)}{\partial \eta}, \quad (6)$$

in the left half plane.

The two observer/estimator gains K and L provide the designer with enough flexibility to set arbitrarily the extent to which the estimator should rely on a given measurable output, whether it is fast or slow. While the gain K represents a "weight" on the fast measurable outputs, the gain L is a "weight" on the slow measurable outputs. In the case that $K = 0$, the estimator calculates estimates of the state variables on the basis of the slow measurable outputs only. The reduced-order nature of the estimator facilitates the design and implementation of the estimator and reduces the time needed for calculating the state estimates.

When an ith state variable x_i is not observable from the fast measurable outputs, the decay rate of the mismatch between the actual and estimated values of the state variable is usually not affected by the elements of the ith row of the gain K. In such a case, the entries of that row of the matrix K can simply be set to zero. When such a state variable is observable from the slow measurable outputs, a value of the gain L that locally places the eigenvalues of the matrix of Eq. 6 in the left half plane, ensures the asymptotic convergence of the estimated value of the state variable to its actual value.

Remark 2: When an $F_{y_i}(\eta, y, u)$ (ith component of F_y) is independent of η, $F_{y_i}(\eta + e, y, u) - F_{y_i}(\eta, y, u) = 0$. Thus, in such a case the use of F_{y_i} in the closed-loop observer of Eq. 3 does not affect the local stability of the error dynamics, and no values of $K_{1i}, \dots, K_{(n-p)i}$ will affect the local stability and (maybe) speed of the observer error dynamics. For the sake of simplicity, in these cases, we set $K_{1i} = \dots = K_{(n-p)i} = 0$. This will be illustrated when the observer of Eq. 3 is applied to the jacketed polymerization reactor.

Remark 3: In the case that a process has no fast measurable outputs ($p = 0$), the state observer/estimator of Eq. 3 takes the form

$$\dot{\hat{x}}(t) = f[\hat{x}(t), u(t)] + L\{Y^*(t) - H[\hat{x}(t)]\} \quad (7)$$

that is, the state estimates are calculated solely by using the measurable inputs and the slow measurable outputs. In this case, the observer error is governed by the system

$$\dot{e} = f(e + x, u) - f(x, u) + L\{Y^* - H(e + x)\} \quad (8)$$

Thus, a necessary condition for the local asymptotic convergence of the observer of Eq. 7 is that locally all the eigenvalues of the $n \times n$ Jacobian matrix

$$\frac{\partial f(x, u)}{\partial x} - L \frac{\partial H(x)}{\partial x} \quad (9)$$

lie in the left half of the complex plane. Note that in this case the use of the slow measurable outputs allows one to design a state estimator whose error has an adjustable rate of decay. A multirate observer of the form of Eq. 7 was implemented successfully in real time on a biochemical reactor wherein continuous estimates of the concentrations of biomass, substrates, and products were calculated by using very infrequent and delayed measurements only (Tatiraju et al., 1999).

Comparison with multirate extended Kalman filter

The multirate state observer of Eq. 3 with the gain $L = 0$ is a reduced-order Luenberger state observer with a constant gain, which is a deterministic version of a reduced-order Extended Kalman filter (EKF) with a constant gain. The similarities and differences between the multirate state observer and multirate EKF include:

- An extended Kalman filter is tuned by adjusting covariance matrices of noise signals and initial estimation error, while the multirate state observer of Eq. 3 is tuned by adjusting the gain matrices K and L. In the case of an EKF if a serious error is made in choosing the values of the covariance matrices, the EKF can provide poor and biased estimates of the states. Because of this, much insight and adequate prior simulations are required to arrive at an acceptable set of tuning parameters in the case of an EKF (Kozub and MacGregor, 1992). On the other hand, the gains of the multirate state observer should be chosen such that (a) the observer error dynamics are asymptotically stable and (b) proper "weights" are placed on the model, fast measurements, and slow measurements, depending on the reliability of each of these. In the case of the multirate state observer, simple observability tests of state variables facilitate the observer tuning greatly.

- While for many processes it is possible to prove the global asymptotic convergence of the multirate state observer analytically, the analytical proof of the global asymptotic convergence is, in general, not possible in the case of an EKF.
- For a process with n state variables and p fast measurable output, the state observer will be of order $n-p$, while for the same process a standard EKF will be of order $n(n+1)$.

Free-Radical Polymerization Reactor Model

We use the mathematical model of Schmidt and Ray (1981) to describe the dynamics of free-radical solution polymerization of styrene in a jacketed continuous stirred tank reactor (CSTR). The solvent and initiator are benzene and azo-bis-iso-butyro-nitrile, respectively. The polymerization model has the following form

$$\frac{dC_i}{dt} = -\left[\frac{1}{\tau} + k_i\right] C_i + f_1$$

$$\frac{dC_s}{dt} = -\frac{C_s}{\tau} + f_2$$

$$\frac{d\lambda_0}{dt} = -\frac{\lambda_0}{\tau} + f_3(C_i, C_s, C_m, T)$$

$$\frac{d\lambda_1}{dt} = -\frac{\lambda_1}{\tau} + f_4(C_i, C_s, C_m, T)$$

$$\frac{d\lambda_2}{dt} = -\frac{\lambda_2}{\tau} + f_5(C_i, C_s, C_m, T)$$

$$\frac{dC_m}{dt} = f_6(C_i, C_m, T)$$

$$\frac{dT}{dt} = f_7(C_i, C_m, T, T_j)$$

$$\frac{dT_j}{dt} = f_8(T, T_j) \tag{10}$$

where

$$f_1 = \frac{Q_i C_{i_i}}{V}$$

$$f_2 = \frac{Q_s C_{s_s} + Q_i C_{s_i}}{V}$$

$$f_3(C_i, C_s, C_m, T) = \left[\left(k_{f_m} C_m + k_{t_d} P + k_{f_s} C_s\right)\right] \alpha P + \frac{1}{2} k_{t_c} P^2$$

$$f_4(C_i, C_s, C_m, T) = \left[\left(k_{f_m} C_m + k_{t_d} P + k_{f_s} C_s\right)(2\alpha - \alpha^2) + k_{t_c} P\right] \times \frac{P M_m}{(1-\alpha)}$$

$$f_5(C_i, C_s, C_m, T) = \left[\left(k_{f_m} C_m + k_{t_d} P + k_{f_s} C_s\right)(\alpha^3 - 3\alpha^2 + 4\alpha) + k_{t_c} P(\alpha + 2)\right] \frac{P M_m^2}{(1-\alpha)^2}$$

$$f_6(C_i, C_m, T) = \frac{Q_m C_{m_m} - Q_t C_m}{V} - k_p C_m P$$

$$f_7(C_i, C_m, T, T_j) = \gamma k_p C_m P + \frac{US(T_j - T)}{\rho c_p V} + \frac{Q_t (T_{\text{in}} - T)}{V}$$

$$f_8(T, T_j) = \frac{US}{\rho_w c_{p_w} V_j}(T - T_j) + \frac{Q_c(T_{w_{\text{in}}} - T_j)}{V_j}$$

$$\alpha = \frac{k_p C_m}{(k_p + k_{f_m}) C_m + k_{f_s} C_s + k_t P}$$

$$P = \sqrt{\frac{2 f^* C_i k_i}{k_t}}$$

The number-average and weight-average molecular weights ($\text{kg}\cdot\text{kmol}^{-1}$) (denoted by M_n and M_w, respectively) are related to the moments according to

$$M_w = \frac{\lambda_2}{\lambda_1} \qquad M_n = \frac{\lambda_1}{\lambda_0}$$

We use a value of 7.1 $\text{kmol}\cdot\text{m}^{-3}$ for the concentration of the solvent in the initiator feed stream. The rest of the parameter values are the same as those given in Hidalgo and Brosilow (1990). A sufficiently high fraction of solvent in the feed and the reaction operating conditions given in Table 1 lead to a low steady-state monomer conversion, thereby ensuring that the gel and glass effects are not dominant. At low solvent fractions and high steady-state monomer conversion, it is not possible to measure density of the polymer solution on-line, because the extremely viscous polymer solution clogs the

Table 1. Operating Conditions of the Reactor

$C_m(0) = 3.00 \times 10^0$	$\text{kmol}\cdot\text{m}^{-3}$
$C_i(0) = 5.00 \times 10^{-2}$	$\text{kmol}\cdot\text{m}^{-3}$
$C_s(0) = 5.00 \times 10^0$	$\text{kmol}\cdot\text{m}^{-3}$
$T(0) = 3.30 \times 10^2$	K
$T_j(0) = 2.95 \times 10^2$	K
$\lambda_0(0) = 0.0$	$\text{kmol}\cdot\text{m}^{-3}$
$\lambda_1(0) = 0.0$	$\text{kg}\cdot\text{m}^{-3}$
$\lambda_2(0) = 0.0$	$\text{kg}^2\cdot\text{kmol}^{-1}\cdot\text{m}^{-3}$
$C_{m_m} = 8.698 \times 10^0$	$\text{kmol}\cdot\text{m}^{-3}$
$C_{i_i} = 5.888 \times 10^{-1}$	$\text{kmol}\cdot\text{m}^{-3}$
$C_{s_i} = 7.100 \times 10^0$	$\text{kmol}\cdot\text{m}^{-3}$
$C_{s_s} = 7.500 \times 10^0$	$\text{kmol}\cdot\text{m}^{-3}$
$Q_c = 6.550 \times 10^{-5}$	$\text{m}^3\cdot\text{s}^{-1}$
$Q_i = 1.550 \times 10^{-5}$	$\text{m}^3\cdot\text{s}^{-1}$
$Q_m = 5.250 \times 10^{-5}$	$\text{m}^3\cdot\text{s}^{-1}$
$Q_s = 6.3750 \times 10^{-5}$	$\text{m}^3\cdot\text{s}^{-1}$
$T_{\text{in}} = 3.300 \times 10^2$	K
$T_{w_{\text{in}}} = 2.950 \times 10^2$	K

densitometer. This operational constraint has forced many, who have studied in real-time control and monitoring of polymerization reactors by using on-line densitometers and/or viscometers, to operate the reactors in nonviscous regions (Ellis et al., 1988).

The first-principles mathematical model of the process described by Eq. 10 is used to represent the actual process. The state estimation problem is to calculate continuous estimates of the number-average and weight-average molecular weights of the polymer and the concentrations of the initiator and solvent from:

- The frequent, delay-free, on-line "measurements" of the reacting mixture density, reactor temperature (T) (K), and jacket temperature (T_j) (K). The monomer conversion (and, thereby, the monomer concentration C_m ($\mathrm{kmol \cdot m^{-3}}$)) can be inferred from the density measurement, and thus can be available on-line at high sampling rates. These measurements are assumed to be made on-line at very high sampling frequencies, and, hence, they are considered as continuous functions of time.
- The infrequent and delayed "measurements" of the three leading MWD moments, which are assumed to be obtained with a GPC at sampling periods of 0.5 or 1 h and with corresponding measurement delays of 0.5 or 1 h.

Multirate Observer Design for the Polymerization Reactor

For this process, the vector of fast measurable outputs $y = [C_m \; T \; T_j]^T$ and the vector of slow measurable outputs $Y = [\lambda_0 \; \lambda_1 \; \lambda_2]^T$. The system of Eq. 10 is already of the form of Eq. 2; the first five differential equations representing the η subsystem ($\eta = [C_i \; C_s \; \lambda_0 \; \lambda_1 \; \lambda_2]^T$), and the last three differential equations form the y subsystem.

The local observability and detectability of each state variable from each measurable output as defined by Definitions 1 and 3 are indicated in Table 2. For example, the zeroth moment is detectable but not observable from the monomer concentration measurement. While all the state variables of the polymerization process are observable from the fast and slow measurable outputs, only four of the state variables (T, T_j, C_m, C_i) are observable from the fast measurements alone. However, all the state variables are detectable from the fast measurements. Thus, the slow measurements allow for calculating reliable estimates of all the state variables by making all the state variables observable.

Application of the estimation method of Eq. 3 to this polymerization reactor leads to the following multirate nonlinear reduced-order state observer/estimator

$$\begin{bmatrix}\dot z_1\\ \dot z_2\\ \dot z_3\\ \dot z_4\\ \dot z_5\end{bmatrix} = \begin{bmatrix} -\left[\dfrac{1}{\tau}+k_i\right]\hat C_i + f_1 \\ -\dfrac{\hat C_s}{\tau}+f_2 \\ -\dfrac{\hat\lambda_0}{\tau}+f_3\left(\hat C_i,\hat C_s,C_m,T\right) \\ -\dfrac{\hat\lambda_1}{\tau}+f_4\left(\hat C_i,\hat C_s,C_m,T\right) \\ -\dfrac{\hat\lambda_2}{\tau}+f_5\left(\hat C_i,\hat C_s,C_m,T\right)\end{bmatrix} - K\begin{bmatrix} f_6\left(\hat C_i,\hat C_s,C_m,T\right)\\ f_7\left(\hat C_i,\hat C_s,C_m,T,T_j\right)\\ f_8\left(T,T_j\right)\end{bmatrix} + L\begin{bmatrix}\lambda_0^*-\hat\lambda_0\\ \lambda_1^*-\hat\lambda_1\\ \lambda_2^*-\hat\lambda_2\end{bmatrix} \qquad (11)$$

where

$$\hat C_i = z_1 + K_{11}C_m + K_{12}T + K_{13}T_j$$

$$\hat C_s = z_2 + K_{21}C_m + K_{22}T + K_{23}T_j$$

$$\hat\lambda_0 = z_3 + K_{31}C_m + K_{32}T + K_{33}T_j$$

$$\hat\lambda_1 = z_4 + K_{41}C_m + K_{42}T + K_{43}T_j$$

$$\hat\lambda_2 = z_5 + K_{51}C_m + K_{52}T + K_{53}T_j$$

and $\lambda_0^*(t)$, $\lambda_1^*(t)$ and $\lambda_2^*(t)$ are the predicted present values of the infrequent measurable outputs. Each of the predicted present values is obtained by fitting a least-squared-error line to the most recent three measurements of the moment (here $r_i = 3$, $m_i = 1$, $i = 1, \ldots, 3$). These linear regressions are always carried out except when only one measurement of each slow measurable output is available. In the exceptional case, the predicted present value of each slow measurable output is set equal to the single available measurement. A flow diagram of the proposed multirate observer/estimator is shown

Table 2. Observability/Detectability of the State Variables of the Reactor

State Variable/Measurement	Reactor Temp.	Jacket Temp.	Monomer Concentration	0th Moment	1st Moment	2nd Moment
Reactor temperature	Yes/Yes	Yes/Yes	Yes/Yes	Yes/Yes	Yes/Yes	Yes/Yes
Jacket temperature	Yes/Yes	Yes/Yes	Yes/Yes	Yes/Yes	Yes/Yes	Yes/Yes
Monomer concentration	Yes/Yes	Yes/Yes	Yes/Yes	Yes/Yes	Yes/Yes	Yes/Yes
Initiator concentration	Yes/Yes	Yes/Yes	Yes/Yes	Yes/Yes	Yes/Yes	Yes/Yes
Solvent concentration	No/Yes	No/Yes	No/Yes	Yes/Yes	Yes/Yes	Yes/Yes
0th Moment	No/Yes	No/Yes	No/Yes	Yes/Yes	No/Yes	No/Yes
1st Moment	No/Yes	No/Yes	No/Yes	No/Yes	Yes/Yes	No/Yes
2nd Moment	No/Yes	No/Yes	No/Yes	No/Yes	No/Yes	Yes/Yes

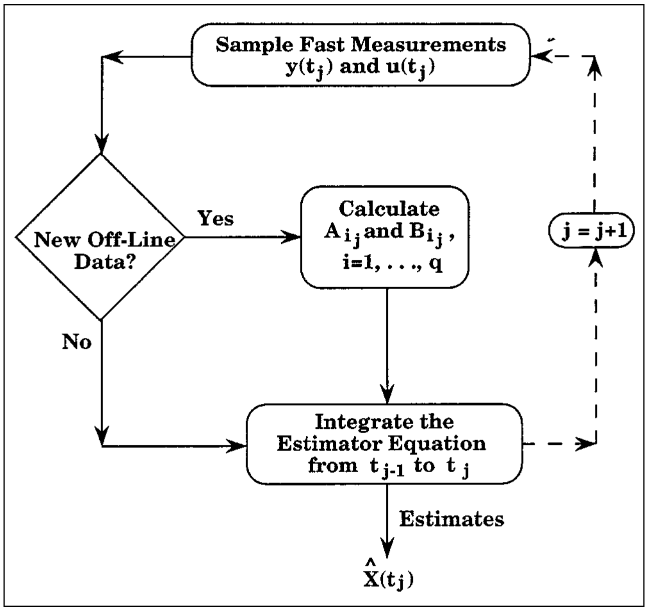

Figure 1. Flow diagram of the multirate estimator.

in Figure 1. The observer/estimator initial conditions are given in Table 3.

Tuning the state observer

As indicated in Table 2, while the initiator concentration C_i is observable from the fast measurable outputs, the four state variables C_s, λ_0, λ_1, and λ_2 are not observable from the fast measurable outputs C_m, T, and T_j. Since the rate of convergence of the estimates of these unobservable (from the fast measurable outputs) state variables is not affected by the gain components K_{ij}, $i = 2, \ldots, 5$, $j = 1, \ldots, 3$, we simply set

$$K_{i1} = K_{i2} = K_{i3} = 0, \qquad i = 2, \ldots, 5 \tag{12}$$

The gain component K_{13} is also set to zero, because the function f_8 is independent of the initiator concentration C_i (see Remark 2). Note that the use of non-zero values for these gain components can change the shape of the profiles of the estimates of the four state variables C_s, λ_0, λ_1, and λ_2, but not the time needed for the convergence of each estimate. All the components of the gain L, except for L_{31}, L_{42}, and L_{53}, are also set to zero.

Table 3. Initial Conditions of the Estimator

$\hat{C}_i(0) = 2.50 \times 10^{-2}$	$\text{kmol}\cdot\text{m}^{-3}$
$\hat{C}_s(0) = 4.00 \times 10^{0}$	$\text{kmol}\cdot\text{m}^{-3}$
$\hat{\lambda}_0(0) = 1.00 \times 10^{-3}$	$\text{kmol}\cdot\text{m}^{-3}$
$\hat{\lambda}_1(0) = 5.00 \times 10^{0}$	$\text{kg}\cdot\text{m}^{-3}$
$\hat{\lambda}_2(0) = 5.00 \times 10^{4}$	$\text{kg}^2\cdot\text{kmol}^{-1}\cdot\text{m}^{-3}$

Once the gains K and L are set accordingly, the observer error will be governed by

$$\begin{aligned}
\dot{e}_1 &= -\left[k_i + \frac{1}{\tau}\right]e_1 - K_{11}\Delta f_6(e_1, C_i, C_m, T) \\
&\qquad - K_{12}\Delta f_7(e_1, C_i, C_m, T, T_j) \\
\dot{e}_2 &= -\frac{1}{\tau}e_2 \\
\dot{e}_3 &= -\frac{1}{\tau}e_3 + \Delta f_3(e_1, e_2, C_i, C_s, C_m, T) \\
&\qquad - L_{31}e_3 + L_{31}(\lambda_0^* - \lambda_0) \\
\dot{e}_4 &= -\frac{1}{\tau}e_4 + \Delta f_4(e_1, e_2, C_i, C_s, C_m, T) \\
&\qquad - L_{42}e_4 + L_{42}(\lambda_1^* - \lambda_1) \\
\dot{e}_5 &= -\frac{1}{\tau}e_5 + \Delta f_5(e_1, e_2, C_i, C_s, C_m, T) \\
&\qquad - L_{53}e_5 + L_{53}(\lambda_2^* - \lambda_2)
\end{aligned} \tag{13}$$

where

$$\begin{aligned}
\Delta f_3(e_1, e_2, C_i, C_s, C_m, T) &= f_3(C_i + e_1, C_s + e_2, C_m, T) \\
&\qquad - f_3(C_i, C_s, C_m, T) \\
\Delta f_4(e_1, e_2, C_i, C_s, C_m, T) &= f_4(C_i + e_1, C_s + e_2, C_m, T) \\
&\qquad - f_4(C_i, C_s, C_m, T) \\
\Delta f_5(e_1, e_2, C_i, C_s, C_m, T) &= f_5(C_i + e_1, C_s + e_2, C_m, T) \\
&\qquad - f_5(C_i, C_s, C_m, T) \\
\Delta f_6(e_1, C_i, C_m, T) &= f_6(C_i + e_1, C_m, T) - f_6(C_i, C_m, T) \\
\Delta f_7(e_1, C_i, C_m, T, T_j) &= f_7(C_i + e_1, C_m, T, T_j) \\
&\qquad - f_7(C_i, C_m, T, T_j)
\end{aligned}$$

Since the Jacobian of the system represented by Eq. 13 is lower triangular

$$J = \begin{bmatrix}
J_{11} & 0 & 0 & 0 & 0 \\
0 & -\frac{1}{\tau} & 0 & 0 & 0 \\
J_{31} & J_{32} & -\left(L_{31} + \frac{1}{\tau}\right) & 0 & 0 \\
J_{41} & J_{42} & 0 & -\left(L_{42} + \frac{1}{\tau}\right) & 0 \\
J_{51} & J_{52} & 0 & 0 & -\left(L_{53} + \frac{1}{\tau}\right)
\end{bmatrix}$$

the five eigenvalues of the Jacobian are the principal diagonal elements of the matrix. The real eigenvalue J_{11} depends only on K_{11} and K_{12}, and it can be shown easily that J_{11} will be negative, if K_{11} and K_{12} are chosen such that

$$K_{11} \le \gamma K_{12}$$

The eigenvalue J_{22} is inherently negative and independent of the gains. Thus, the rate of convergence of the estimate of the solvent concentration is not adjusted and is set by the process model itself. The other three eigenvalues will also be negative, if the gain components L_{31}, L_{42}, and L_{53} are set such that

$$L_{31} \ge 0, \qquad L_{42} \ge 0, \qquad L_{53} \ge 0$$

Furthermore, the higher the values of L_{31}, L_{42}, and L_{53}, the higher the rate of decay of the corresponding errors and the more sensitive the estimates of the corresponding state variables to the slow measurable outputs. The selection of the gains K and L according to the aforementioned conditions ensures that the observer error dynamics are asymptotically stable. The gain values given in Table 4 will be used in the simulation study presented in the Simulation Results section.

Comparison with multirate EKF

The designed multirate state observer for the polymerization reactor consists of only five first-order ordinary differential equations which should be integrated in real time numerically. However, a standard extended Kalman filter for the same reactor will consist of seventy-two $(8+8\times8)$ first-order ordinary differential equations. Sixty-four of the state variables of the EKF are the entries of the error covariance matrix. In the case of the state observer the gain matrices K and L were set on the basis of: (a) the observability of the state variables; (b) asymptotic stability of the observer error dynamics; (c) our insight into the degree of the accuracy of the model used for estimator design, the reliability of fast measurable inputs and outputs, and how noisy the measurements are. In an EKF, however, much insight and adequate prior simulations are needed to arrive at an acceptable set of tuning parameters (noise and error covariance matrices).

Simulation Results

In this section, simulation results are presented to show the performance of the multirate reduced-order nonlinear state observer in calculating continuous estimates of the state variables of the polymerization reactor. The model of Eq. 10 is used to generate the slow and fast "measurements." The simulated "measurements" are then fed to the estimator/observer, as if they are coming from an actual plant. A step size of 10 s (equivalent to the sampling period of the frequent measurements) is used in all numerical integrations.

Table 4. Values of the Non-Zero Estimator Gain Components

	K_{11}	K_{12}	L_{31}	L_{42}	L_{53}
Figure 2	40	1	5.0×10^{-4}	5.0×10^{-4}	5.0×10^{-7}
Figure 3	40	1	2.0×10^{-4}	2.0×10^{-4}	2.0×10^{-7}
Figure 4	40	1	9.0×10^{-4}	9.0×10^{-4}	1.0×10^{-6}
Figure 5	40	1	9.0×10^{-4}	1.0×10^{-3}	2.0×10^{-6}
Figure 6	40	1	9.0×10^{-5}	9.0×10^{-5}	9.0×10^{-8}
Figure 7	40	1	4.0×10^{-4}	4.0×10^{-4}	4.0×10^{-7}

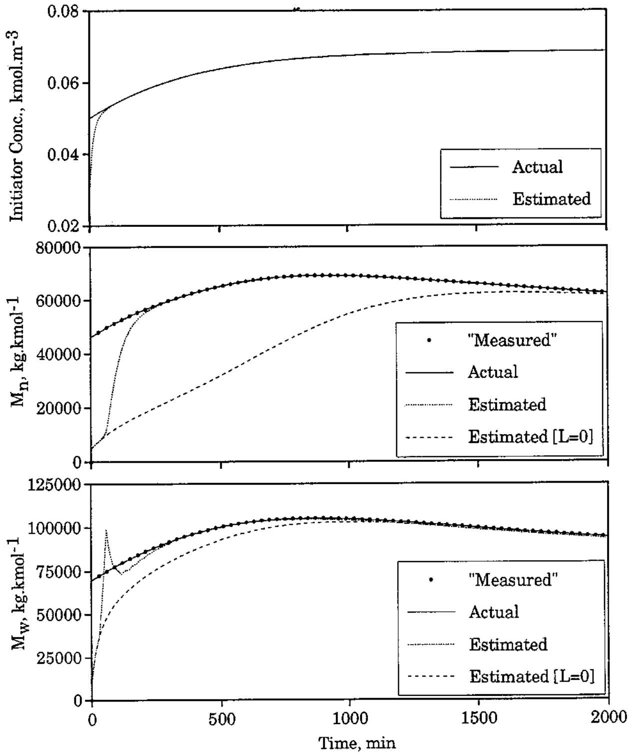

Figure 2. Measured, actual and estimated values of the initiator concentration, and number- and weight-average molecular weights (case a).

The performance of the multirate state observer is evaluated in three cases: (a) when there is no measurement noise or model-plant mismatch; (b) when the slow measurements are corrupted by noise but there is no model-plant mismatch; (c) when the slow measurements are corrupted by noise and there is model-plant mismatch. A white noise signal is added to each of the moments calculated by the process model to simulate measurement noise. Each white noise signal has a standard deviation of 6% of the steady-state value of the corresponding moment. The noisy measurements of the leading moments that give rise to an average molecular weight measurement that differs by more than 10,000 from the previous average molecular weight measurement are discarded and not used for state estimation. The plant-model mismatch is of the form of a 5% discrepancy in the propagation reaction rate constant k_p ($m^3 \cdot kmol^{-1} \cdot s^{-1}$); the value of k_p used in the state estimator is 5% higher than the value used in the reactor model representing the process. The values of the nonzero estimator gain components are given in Table 4.

Figure 2 depicts the continuous estimates obtained using the multirate state estimator for the case a. The solid lines represent the actual values of the variables, the dotted lines denote the continuous estimates obtained via the multirate estimation, the dashed lines are the continuous estimates obtained by single-rate estimation (when $L=0$), and the bullets represent the "measured" values (sampled actual values plus

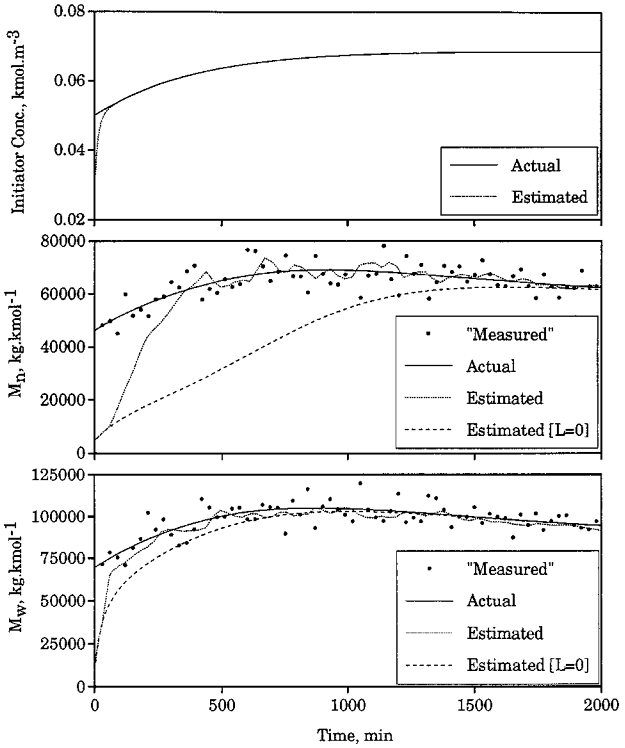

Figure 3. Measured, actual and estimated values of the initiator concentration, and number- and weight-average molecular weights in the presence of measurement noise (case b).

noise signal, if noise is present) of the molecular weights. Note that the "measured" values depicted in Figures 2–4 are available for state estimation 0.5 h after the time shown in these figures.

As Figure 2 shows, the estimates agree well with the actual values. The benefit of using the infrequent and delayed measurements in the estimation algorithm is evident from the dashed curve representing the estimates calculated using only the fast measurements (when $L = 0$). In this case, the estimates do converge to the process steady-state values at a rate set by the process dynamics; the slow measurements (though delayed) are not utilized to correct the estimation error. Since the initiator concentration is observable from the frequent measurements, the use of a nonzero value in the component of gain K corresponding to this state variable causes the estimates to rapidly converge to the actual value. The estimate of the initiator concentration is calculated by using only the fast measurements.

The performance of the multirate estimator in the presence of slow measurement noise is depicted in Figure 3 (case b). Again, the estimator is able to provide sufficiently accurate estimates of the molecular weights even in the presence of considerable noise in the measurements of the moments of the MWD. The estimate of the initiator concentration also rapidly converges to the actual value. The use of the past three slow measurements in the prediction step seemed to be sufficient. Extrapolation on the basis of a higher number of past measurements will increase the computational load, whereas extrapolation using only the past two data points can result in greater error in the prediction in the presence of a noise signal with a larger standard deviation, due to the greater sensitivity to the measurements.

Figure 4 depicts the performance of the multirate estimator in the presence of the measurement noise and the model-plant mismatch (case c). In this case, the estimator is also able to provide sufficiently accurate estimates of the molecular weights while the infrequent measurements play a key role in the estimation. An estimation only based on the fast measurements provides an inaccurate estimate at each step, and, when a slow measurement arrives, the estimate is driven towards the "measured" value until the next sampling interval. The components of the gain L used for this case are higher than those for Figure 2 (see Table 1), since under the plant-model mismatch, the estimator should rely more on the information provided by the measurements than on the model. In the case of the initiator concentration, there is a permanent mismatch between the actual and the estimated values. When $L = 0$ (state variables are estimated from the fast measurements only), there is a permanent mismatch between the actual values and the corresponding state estimates for all the state variables. The permanent mismatch can be taken care of by adding adaptive features ("integral" action) to the state observer.

Figure 5 depicts the performance of the multirate estimator when the slow measurements are available at a lower

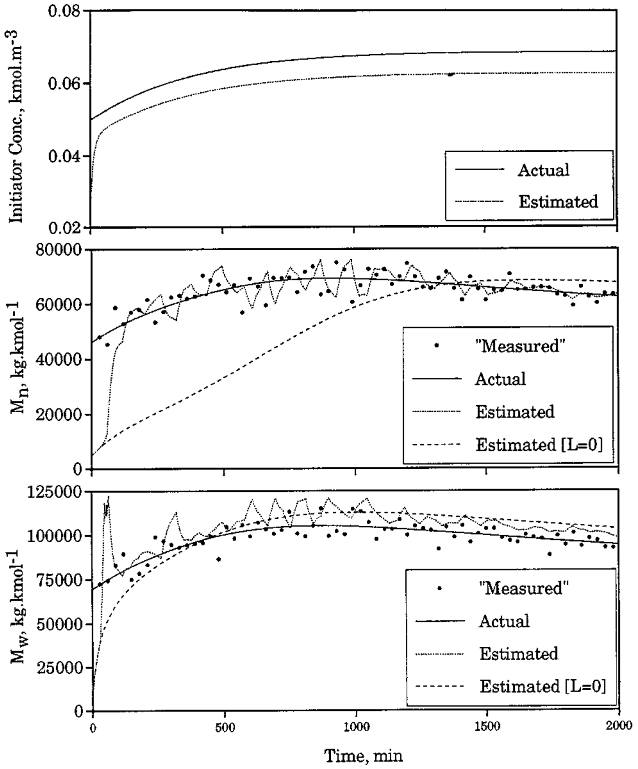

Figure 4. Measured, actual and estimated values of the initiator concentration, and number- and weight-average molecular weights in the presence of measurement noise and plant-model mismatch (case c).

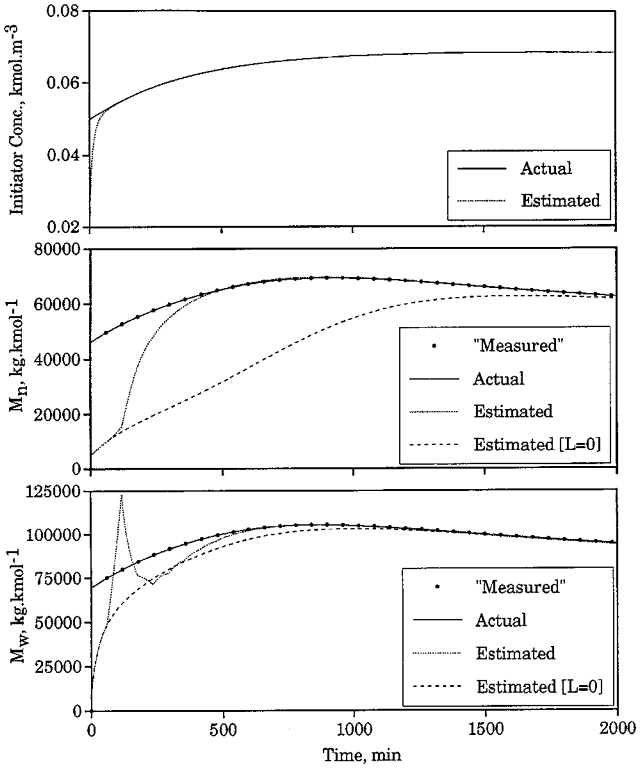

Figure 5. Measured, actual and estimated values of the initiator concentration, and number- and weight-average molecular weights for lower rates of sampling and greater time delays in the slow measurable outputs (case a).

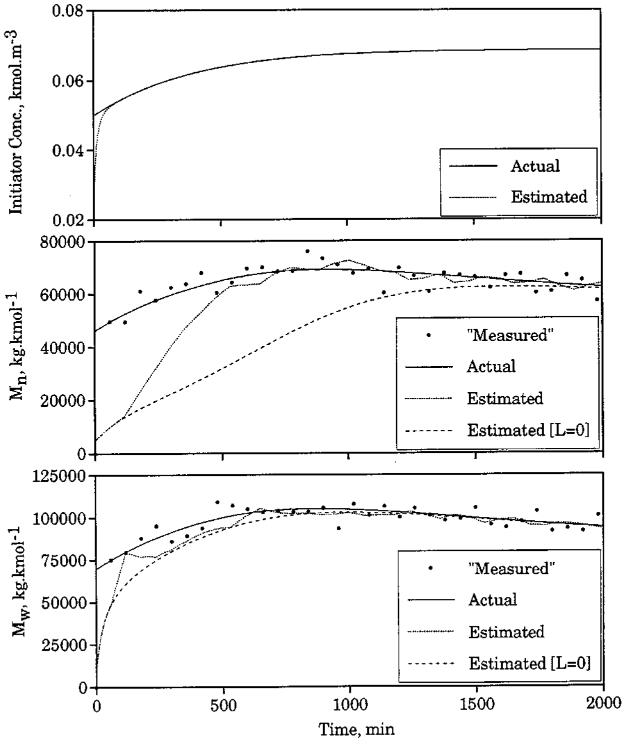

Figure 6. Measured, actual and estimated values of the initiator concentration, and number- and weight-average molecular weights for lower rates of sampling and greater time delays in the slow measurable outputs in the presence of measurement noise (case b).

sampling frequency of 1 h^{-1} and with a greater measurement delay of 1 h for the case a. As this figure shows, in spite that the measurements arrive at a slower rate, the estimator is able to provide continuous estimates of the number-average and weight-average molecular weights with sufficient accuracy. This is attributed to the fact that the multirate estimator relies on a combination of the fast measurements and the predicted trend of the slow measurements, thereby providing reliable estimates even under such conditions. However, the estimates of the number-average and weight-average molecular weights calculated by using only the fast measurements take a considerable time to converge to the actual process steady state (shown by the dashed line). As stated earlier, the state estimates (of the unobservable states) calculated by using only the fast measurements converge at a rate set by the process itself.

The performance of the multirate estimator in the presence of measurement noise is depicted in Figure 6 (case b). Even in the presence of the measurement noise, the estimator provides sufficiently accurate estimates of the average molecular weights. Figure 7 shows the performance of the multirate estimator in the presence of measurement noise and model-plant mismatch for the case c. In this case also, while the estimation by using only the fast measurements (shown by the dashed line) yields a permanent mismatch between the actual value and the corresponding state estimate, the estimation from both fast and slow measurements (shown by the dotted line) provides more accurate estimates of the molecular weights.

Conclusions

A multirate nonlinear state estimator design method was presented. It was implemented on a simulated continuous polymerization reactor to estimate the three leading moments of the MWD, and solvent and initiator concentrations from: (a) the frequent "measurements" of monomer concentration, reactor temperature, and jacket temperature; (b) the infrequent and delayed "measurements" of the leading moments.

The estimator can directly use a nonlinear process model without any linearization. It provides the designer with sufficient flexibility to design a reliable multirate state estimator with adjustable reliance on the fast and slow measurements. The multirate estimator is robust enough to provide sufficiently accurate, continuous, state estimates in the presence of common problems such as measurement noise and plant-model mismatch, frequently encountered in practice. Compared to multirate EKF state estimation methods, the reduced-order estimator is easier to design and implement and is computationally more efficient. Furthermore, for many processes, it is possible to prove the global convergence of the state estimator/observer analytically.

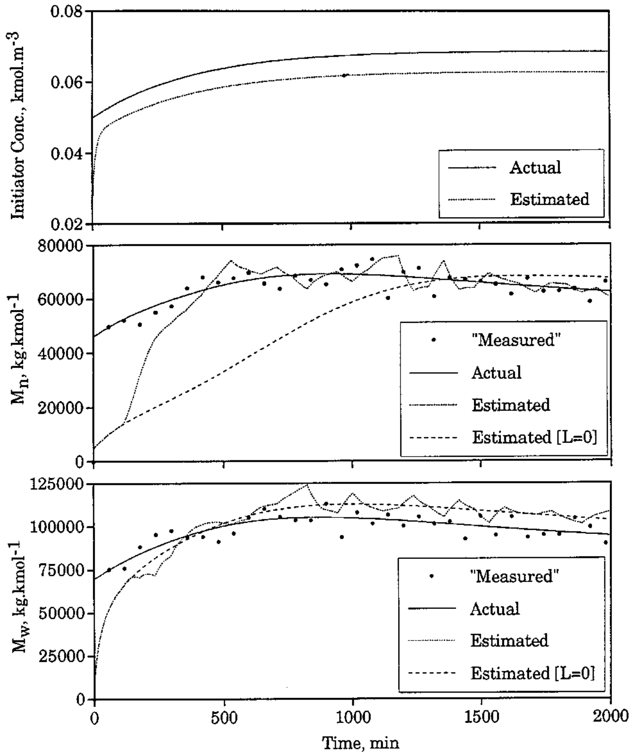

Figure 7. Measured, actual and estimated values of the initiator concentration, and number- and weight-average molecular weights for lower rates of sampling and greater time delays in the slow measurable outputs in the presence of measurement noise and plant-model mismatch (case c).

Acknowledgment

Financial support from the National Science Foundation through the grant CTS-9703278 is gratefully acknowledged.

Notation

c_p = heat capacity of reacting mixture, $\text{kJ}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$
c_{p_w} = heat capacity of the jacket fluid, $\text{kJ}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$
C_{i_i} = concentration of the initiator in the initiator inlet stream, $\text{kmol}\cdot\text{m}^{-3}$
C_{m_m} = concentration of the monomer in the monomer inlet stream, $\text{kmol}\cdot\text{m}^{-3}$
C_{s_i} = concentration of the solvent in the initiator inlet stream, $\text{kmol}\cdot\text{m}^{-3}$
C_{s_s} = concentration of the solvent in the solvent inlet stream, $\text{kmol}\cdot\text{m}^{-3}$
f^* = initiator efficiency
k_{f_m} = rate constant for chain-transfer-to-monomer reactions, $\text{m}^3\cdot\text{kmol}^{-1}\cdot\text{s}^{-1}$
k_{f_s} = rate constant for chain-transfer-to-solvent reactions, $\text{m}^3\cdot\text{kmol}^{-1}\cdot\text{s}^{-1}$
k_i = dissociation rate constant for initiator, s^{-1}
k_t = rate constant for termination reactions ($k_t = k_{t_c} + k_{t_d}$), $\text{m}^3\cdot\text{kmol}^{-1}\cdot\text{s}^{-1}$
k_{t_c} = rate constant for termination by combination reactions, $\text{m}^3\cdot\text{kmol}^{-1}\cdot\text{s}^{-1}$
k_{t_d} = rate constant for termination by disproportionation reactions, $\text{m}^3\cdot\text{kmol}^{-1}\cdot\text{s}^{-1}$
P = live polymer molar concentration, $\text{kmol}\cdot\text{m}^{-3}$
Q_c = inlet flow rate of the coolant, $\text{m}^3\cdot\text{s}^{-1}$
Q_i = flow rate of the initiator inlet stream, $\text{m}^3\cdot\text{s}^{-1}$
Q_m = flow rate of the monomer inlet stream, $\text{m}^3\cdot\text{s}^{-1}$
Q_s = flow rate of the solvent inlet stream, $\text{m}^3\cdot\text{s}^{-1}$
S = jacket-reactor heat-transfer surface area, m^2
t = time, s
T_{in} = temperature of the reactor inlet stream, K
$T_{w_{\text{in}}}$ = inlet coolant temperature, K
U = overall jacket-reactor heat-transfer coefficient, $\text{kJ}\cdot\text{m}^{-2}\cdot\text{s}^{-1}\cdot\text{K}^{-1}$
V = reactor volume, m^3
V_j = volume of jacket holdup, m^3
$-\Delta H_p$ = heat of propagation reactions, $\text{kJ}\cdot\text{kmol}^{-1}$
$\gamma = (-\Delta H_P)/(\rho c_p)$, $\text{m}^3\cdot\text{K}\cdot\text{kmol}^{-1}$
λ_0 = 0th moment of the MWD, $\text{kmol}\cdot\text{m}^{-3}$
λ_1 = 1st moment of the MWD, $\text{kg}\cdot\text{m}^{-3}$
λ_2 = 2nd moment of the MWD, $\text{kg}^2\cdot\text{kmol}^{-1}\cdot\text{m}^{-3}$
ρ = density of the reacting mixture, $\text{kg}\cdot\text{m}^{-3}$
ρ_w = density of the jacket fluid, $\text{kg}\cdot\text{m}^{-3}$
τ = reactor residence time $[V/(Q_i + Q_m + Q_s)]$, s

Superscripts

-1 = inverse of a function [such as $x = \mathfrak{J}^{-1}(\eta, y)$]
T = transpose of a matrix

Literature Cited

Adebekun, D. K., and F. J. Schork, "Continuous Solution Polymerization Reactor Control: 2. Estimation and Nonlinear Reference Control during Methyl Methacrylate Polymerization," *Ind. Eng. Chem. Res.*, **28**, 846 (1989).

Bastin, G., and D. Dochain, *Online Estimation and Adaptive Control of Bioreactors*, Elsevier, New York (1990).

Chien, D. C. H., and A. Penlidis, "On-Line Sensors for Polymerization Reactors," *JMS-Rev. Macromol. Chem. Phys.*, **C30**(1), 1 (1990).

Ciccarella, G., M. Dalla Mora, and A. Germani, "A Luenberger-Like Observer for Nonlinear Systems," *Int. J. Contr.*, **57**, 537 (1993).

Ellis, M. F., T. W. Taylor, V. Gonzalez, and K. F. Jensen, "Estimation of the Molecular Weight Distribution in Batch Polymerization," *AIChE J.*, **34**, 1341 (1988).

Gudi, R. D., S. L. Shah, and M. R. Gray, "Adaptive Multirate State and Parameter Estimation Strategies with Application to a Bioreactor," *AIChE J.*, **41**, 2451 (1995).

Hidalgo, P. M., and C. B. Brosilow, "Nonlinear Model Predictive Control of Styrene Polymerization at Unstable Operating Points," *Comput. Chem. Eng.*, **4**, 481 (1990).

Hong, L., "Approximating Multirate Estimation using a Filter Bank," *Proc. of IEEE Conf. on Decision and Control*, 1232 (1994).

Jo, J. H., and S. G. Bankoff, "Digital Monitoring and Estimation of Polymerization Reactors," *AIChE J.*, **22**, 361 (1976).

Kazantzis, N., and C. Kravaris, "A Nonlinear Luenberger-Type Observer with Application to Catalytic Activity Estimation," *Proc. of ACC*, 1756 (1996).

Kim, K. J., and K. Y. Choi, "On-Line Estimation and Control of a Continuous Stirred Tank Polymerization Reactor," *J. Process Contr.*, **1**, 96 (1991).

Kozub, D., and J. F. MacGregor, "State Estimation for Semi-Batch Polymerization Reactors," *Chem. Eng. Sci.*, **47**, 1047 (1992).

Krener, A. J., and A. Isidori, "Linearization by Output Injection and Nonlinear Observers," *Systems Control Lett.*, **3**, 47 (1983).

Liotta, V., C. Georgakis, and M. S. El-Aasser, "Real-Time Estimation and Control of Particle Size in Semi-Batch Emulsion Polymerization," *Proc. of ACC*, 1172 (1997).

Meditch, J. S., "A Survey of Data Smoothing for Linear and Nonlinear Dynamic Systems," *Automatica*, **9** 151 (1973).

Mutha, R. K., W. R. Cluett, and A. Penlidis, "On-Line Nonlinear Model-Based Estimation and Control of a Polymer Reactor," *AIChE J.*, **43**, 3042 (1997).

Ogunnaike, B. A., "On-Line Modeling and Predictive Control of an Industrial Terpolymerization Reactor," *Inter. J. Contr.*, **59**, 711 (1994).

Ohshima, M., A. Koulouris, S. Tomita, and G. Stephanopoulos, "Wave-Net Based On-Line Quality Inference System for Polymerization Processes,'' *IFAC Symp. on Dynamics and Control of Chemical Reactors, Distillation Columns and Batch Processes*, Copenhagen, Denmark, Preprints, 275 (Jun. 7–9, 1995).

Ohshima, M., and S. Tomita, ''Model-Based and Neural-Net-Based On-Line Quality Inference System for Polymerization Processes,'' AIChE Meeting, Miami, FL (1995).

Quintero-Marmol, E., W. L. Luyben, and C. Georgakis, ''Application of an Extended Luenberger Observer to the Control of Multicomponent Batch Distillation,'' *Ind. Eng. Chem. Res.*, **30**, 1870 (1991).

Ray, W. H., ''Polymerization Reactor Control,'' *IEEE Control Systems Magazine*, **6**, 3 (1996).

Robertson, D. G., J. H. Lee, and J. B. Rawlings, ''A Moving Horizon-Based Approach for Least Squares State Estimation,'' *AIChE J.*, **42**(8), 2337 (1996).

Roberston, D. G., P. Kesavan, and J. H. Lee, ''Detection and Estimation of Randomly Occurring Deterministic Disturbances,'' *Proc. of ACC*, 4453 (1995).

Schmidt, A. D., and W. H. Ray, ''The Dynamic Behavior of Continuous Polymerization Reactors: I,'' *Chem. Eng. Sci.*, **36**, 1401 (1981).

Schork, F. J., and W. H. Ray, ''On-Line Measurement of Surface Tension and Density with Application to Emulsion Polymerization,'' *J. of Appl. Poly. Sci.*, **25**, 407 (1983).

Schuler, H., and Z. Suzhen, ''Real-Time Estimation of Chain Length Distribution in a Polymerization Reactor,'' *Chem. Eng. Sci.*, **40**, 1891 (1985).

Soroush, M., ''Nonlinear State-Observer Design with Application to Reactors,'' *Chem. Eng. Sci.*, **52**, 387 (1997).

Stone, K. M., N. F. Thornhill, F. W. Roche, and N. M. Fish, ''A Method of Using Off-line Measurements in an On-line Estimator of Biomass Concentration for a Penicillin Fermentation and Its Effects on the Quality of the Estimates,'' *Proc. IFAC Symp. on Modeling and Control of Biotechnological Processes and Int. Conf. on Control Applications to Fermentation Technology*, Keystone, CO (1992).

Tatiraju, S., M. Soroush, and B. A. Ogunnaike, ''Multi-Rate Nonlinear State Estimation in a Polymerization Reactor,'' *Engineering Foundation Conf. Polymer Reaction Engineering: III*, Palm Coast, FL (1997).

Tatiraju, S., M. Soroush, and R. Mutharasan, ''Multi-Rate Nonlinear State and Parameter Estimation in a Bioreactor,'' *Biotechnol. Bioeng.*, **63**, 22 (1999).

van Dootingh, M., V. D. Rakotopara, J. P. Gauthier, and P. Hobbes, ''Nonlinear Deterministic Observer for State Estimation: Application to a Continuous Free Radical Polymerization Reactor,'' *Comput. Chem. Eng.*, **16**, 777 (1992).

Williamson, G. A., S. Dasgupta, and F. Minyue, ''Multistage Multirate Adaptive Filters,'' *Proc. of IEEE ICASSP*, 1534 (1996).

Zeitz, M., ''The Extended Luenberger Observer for Nonlinear Systems,'' *Systems Control Lett.*, **9**, 149 (1987).

Manuscript received Dec. 30, 1997.