Recursive Estimation in Constrained Nonlinear Dynamical Systems

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DOI 10.1002/aic.10355
Published online in Wiley InterScience (www.interscience.wiley.com).

In any modern chemical plant or refinery, process operation and the quality of product depend on the reliability of data used for process monitoring and control. The task of improving the quality of data to be consistent with material and energy balances is called reconciliation. Because chemical processes often operate dynamically in nonlinear regimes, techniques such as extended-Kalman filter (EKF) and nonlinear dynamic data reconciliation (NDDR) have been developed for reconciliation. There are various issues that arise with the use of either of these techniques. EKF cannot handle inequality or equality constraints, whereas the NDDR has high computational cost. Therefore, a more efficient and robust method is required for reconciling process measurements and estimating parameters involved in nonlinear dynamic processes. Two solution techniques are presented: recursive nonlinear dynamic data reconciliation (RNDDR) and a combined predictor–corrector optimization (CPCO) method for efficient state and parameter estimation in nonlinear systems. The proposed approaches combine the efficiency of EKF and the ability of NDDR to handle algebraic inequality and equality constraints. Moreover, the CPCO technique allows deterministic parameter variation, thus relaxing another restriction of EKF where the parameter changes are modeled through a discrete stochastic equation. The proposed techniques are compared against the EKF and the NDDR formulations through simulation studies on a continuous stirred tank reactor and a polymerization reactor. In general, the RNDDR performs as well as the two traditional approaches, whereas the CPCO formulation provides more accurate results than RNDDR at a marginal increase in computational cost. © 2005 American Institute of Chemical Engineers *AIChE J,* 51: 946–959, 2005

Introduction

In any modern chemical plant or refinery, the reliability of data used for process monitoring and control has a major impact on process efficiency and product quality. State and parameter estimation deals with the problem of obtaining accurate estimates of process variables from measured data, consistent with a process model. These estimates can be used either in model predictive and inferential control strategies or to monitor the performance of the process. For a steady-state process, this problem has also been termed as *data reconciliation*. A landmark achievement[1] in state estimation for linear dynamic systems was the development of the Kalman filter. For linear dynamic systems, the Kalman filter (KF) gives

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optimal estimates in the presence of measurement and state uncertainties.[2] The Kalman filter can be extended to obtain simultaneous state and parameter estimates, by treating the parameters to be estimated as augmented states.[3] For nonlinear systems, extended Kalman filters (EKF) have been developed, which are based on linearizing the nonlinear equations and applying the Kalman filter update equations to the linearized system. Again several different variants of this basic strategy have been developed, which are very well described by Muske and Edgar.[4] The advantages of the KF, the EKF, and their variants lie in their predictive–corrective form and the recursive nature of estimation. The recursive form of these estimation methods allows for rapid estimation in real time, which is extremely important for online deployment.

Although the EKF is an efficient estimator because of its recursive nature, several researchers[5] have enumerated the following disadvantages of the EKF:

- The EKF does not take into account bounds and other algebraic constraints on the estimates and can therefore give rise to infeasible estimates. In some processes, this can lead to failure of the EKF.
- The EKF can give poor estimates of unmeasured parameters and disturbance variables.
- It is difficult to tune the EKF (especially the selection of the uncertainty variance associated with the unknown parameter model) to obtain accurate estimates.

To overcome these deficiencies, an alternate class of methods for state and parameter estimation, especially for nonlinear dynamic systems, constitute techniques that are based on moving-horizon optimization.[6,7] Because no explicit model is assumed for parametric variation, they can effectively track deterministic changes in the parameters. Liebman et al.[8] proposed the nonlinear dynamic data reconciliation (NDDR) formulation, in which the moving-horizon optimization approach is extended to handle errors in measured inputs and to take into account algebraic constraints and bounds on variables. The main drawback of moving-horizon–based approaches is that, unlike the EKF, they can be computationally demanding because of their nonrecursive form, thus raising real-time implementation concerns. Furthermore, it is not readily apparent whether these methods can effectively handle uncertainties in state evolution caused by random fluctuations in unmeasured disturbances.

The objective of this paper is to demonstrate that the deficiencies of EKF can be eliminated by making appropriate modifications to it without sacrificing its essential recursive computational nature. We propose two solution techniques—recursive nonlinear dynamic data reconciliation (RNDDR) and the combined predictor–corrector optimization (CPCO) method that takes into account bounds and other constraints imposed on the estimates—to handle uncertainties in the state space model arising from random unmeasured disturbances, and also to provide accurate estimates of unmeasured parameters and disturbances that undergo deterministic changes. Concomitant with these methods we also propose a simple and effective method for choosing the variance (tuning parameter) of uncertainty associated with the model for parameter changes.

The proposed techniques are compared with the EKF and the NDDR methods through simulation studies of a continuous stirred tank reactor (CSTR) and a styrene polymerization reactor. The results show that both proposed techniques provide state and parameter estimates that are as accurate as, or better than, currently used methods. More important, the computational requirements of the proposed methods are 1 to 2 orders of magnitude lower than those of NDDR. Between the two proposed techniques, the CPCO method provides more accurate estimates at a marginal increase in computational cost. Thus these methods are ideally suited for online control and monitoring applications.

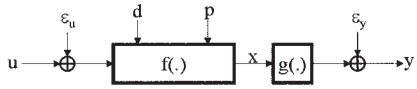

Figure 1. Estimation problem.

Issues and Techniques in State and Parameter Estimation

A general nonlinear dynamic process subject to various disturbances is shown schematically in Figure 1. In this figure, the functions $f(\cdot)$ and $g(\cdot)$, respectively, describe the nonlinearities associated with the process dynamics and measurement model. The variable ε_y represents the errors associated with the measured outputs y, whereas ε_u represents the uncertainties in manipulated inputs caused by errors such as in valve positioning. The variables d and p are the unmeasured disturbances and parameters, respectively, that affect the process. The following assumptions are made in this work:

(1) The process is described by a continuous time state space model with discrete sampled measurements. It is assumed that such a model can be derived from first principles.

(2) The unmeasured disturbances are always subject to random fluctuations. The uncertainties in inputs, random fluctuations in unmeasured disturbances, and measurement errors are assumed to be white Gaussian noise processes with known covariance matrices.

(3) The unmeasured disturbances and parameters may undergo deterministic step changes or drifts. To track these deterministic changes and estimate them, it is assumed that the parameters and unmeasured variables that change are known or specified a priori. In general, for practical implementation it is necessary to identify online the parameter or unmeasured disturbance variable that undergoes a change. A fault detection and identification strategy can be used for this purpose and integrated with the state and parameter estimator as described by Vachhani et al.[9] We would point out that the literature on state and parameter estimation rarely addresses the online implementation issues, although they are extremely important for deploying these methods. The scope of the present work, however, is limited to the development of the estimator, and online implementation issues will be taken up as part of future work.

The task of state and parameter estimation is to determine the best estimates of the states and the parameters at each time using the available measurements and the process and measurement models. Of course, the estimator has to be computationally efficient if it has to be implemented in real time. For the estimator to be of any practical significance it should be easy to design and deploy, and it should also provide reliable and accurate results.

Table 1. Required Capabilities of a Good Estimator

Item	Description
a	Handles uncertainties in both process inputs and outputs, and random unmeasured disturbances
b	Handles nonlinear processes
c	Deals with unknown deterministic changes in parameters and disturbances
d	Handles algebraic equality or inequality constraints
e	Is computationally efficient
f	Is easily implementable
g	Provides accurate estimates

These requirements that have to be satisfied by an estimator are shown in Table 1.

The approaches that have been developed to address the problem of state and parameter estimation fall into two broad categories. The first is recursive in nature and is based on extensions of the Kalman filter, and the second approach is based on a moving-horizon–optimization technique. Both approaches fail to completely satisfy the requirements described above. The primary drawback of the Kalman filter variants is their inability to handle algebraic constraints, and that of the moving-horizon-optimization–based formulations is the computational cost. Herein, we propose two formulations that meet the requirements listed in Table 1 for an estimator. The performance of the proposed methods is compared against the traditional EKF and the NDDR formulation for simultaneous state and parameter estimation with the requirements for an estimator as the guideline. First a brief description of the EKF and NDDR approaches is presented followed by details of the proposed formulations.

Extended Kalman filter

For linear dynamical processes, the Kalman filter (see the Appendix) or its extensions have been the popular choice and the variants of the Kalman filter are described in this subsection. We use the term extended-Kalman filter (EKF) in a generic sense to refer to any extension of the Kalman filter for handling process nonlinearity or for simultaneous state and parameter estimation. First the EKF as developed to handle process nonlinearity is described. Consider the following continuous nonlinear state space description with discrete measurements sampled at regular intervals with sampling period Δt

$$x_{k+1} = x_k + \int_{k\Delta t}^{(k+1)\Delta t} f[x(\tau),\, u_k]d\tau + w_k \qquad x_k \equiv x(k\Delta t)$$

$$y_{k+1} = g(x_{k+1}) + v_{k+1} \tag{1}$$

where w_k and v_{k+1} are assumed to be independent Gaussian white noise processes with known covariance matrices Q_k and R, respectively. Given the filtered state estimates $\hat{x}_{k\,|\,k}$ and manipulated inputs u_k, the predicted state estimates $\hat{x}_{k+1\,|\,k}$ can be obtained by integration of the nonlinear differential equations. Covariance propagation can be done by linearizing the continuous nonlinear dynamic equation to generate system matrices and integrating a Ricatti equation, or by approximating the state transition matrix and using an equivalent discrete uncertainty variance.[4] Herein the EKF is implemented using a linear time-invariant (LTI) approximation, achieved through linearization, of the system for covariance propagation using Eq. A4 (see the Appendix). A better approximation for the covariance propagation can be chosen, if required, depending on accuracy requirements. The updated state estimates are obtained using the Kalman filter update equation based on

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

where the Kalman gain matrix is obtained using the linearized measurement function at $\hat{x}_{k+1\,|\,k}$, in Eq. A7 (see the Appendix).

Simultaneous state and parameter estimation

The problem of simultaneous state and parameter estimation in the extended Kalman filter formulation is addressed by augmenting the state equations with a fictitious discrete evolution equation of the form $p_{k+1} = p_k + w_{pk}$, for the parameters that have to be estimated. Unmeasured disturbance variables that undergo deterministic changes are treated in a similar manner.

The continuous nonlinear state space description, with dependency on the changing parameters shown explicitly, can be written as

$$x_{k+1} = x_k + \int_{k\Delta t}^{(k+1)\Delta t} f[x(\tau),\, u_k,\, p_k]d\tau + w_k$$

$$y_{k+1} = g(x_{k+1}) + v_{k+1} \tag{3}$$

The parameter estimation problem is addressed by augmenting the state space equation with parameter uncertainty

$$\begin{bmatrix} x_{k+1} \\ p_{k+1} \end{bmatrix} = \begin{bmatrix} x_k \\ p_k \end{bmatrix} + \begin{bmatrix} \int_{k\Delta t}^{(k+1)\Delta t} f[x(\tau),\, u_k,\, p_k]d\tau \\ 0 \end{bmatrix} + \begin{bmatrix} w_k \\ w_{pk} \end{bmatrix} \tag{4}$$

Given the filtered state and parameter estimates at the kth instant $\hat{x}_{k\,|\,k}$ and $\hat{p}_{k\,|\,k}$, and the uncertainty in filtered estimates $P_{k\,|\,k,a}$, the propagated state estimate is determined as follows (the prediction part)

$$\begin{bmatrix} \hat{x}_{k+1|k} \\ \hat{p}_{k+1|k} \end{bmatrix} = \begin{bmatrix} \hat{x}_{k|k} + \int_{k\Delta t}^{(k+1)\Delta t} f[x(\tau),\, u_k,\, \hat{p}_{k/k}]d\tau \\ \hat{p}_{k/k} \end{bmatrix} \qquad \hat{x}_{k|k} \equiv \hat{x}(k\Delta t) \tag{5}$$

For covariance propagation, the nonlinear state space model is linearized around $[\hat{x}_{k\,|\,k}, \hat{p}_{k\,|\,k}, u_k]$. The resulting augmented matrix in the continuous domain is given by:

Table 2. Estimator Properties for EKF

Property	a	b	c	d	e	f	g
Status	Yes	Yes	Yes	No	Yes	Q_p selection?	Unrealistic estimates

$$\bar{A}_{k,a} = \begin{bmatrix} A_k & \Gamma_{pk} \\ 0 & 0 \end{bmatrix} \tag{6}$$

and the corresponding discrete state-transition matrix is approximated by $\bar{A}_{k,a} = \exp(A_{k,a}\Delta t)$. Using this linearized approximation, the covariance matrix of estimation errors is propagated as

$$P_{k+1|k,a} = [\bar{A}_{k,a}]P_{k|k,a}[\bar{A}_{k,a}]^T + \begin{bmatrix} Q_k & 0 \\ 0 & Q_{pk} \end{bmatrix} \tag{7}$$

The updated estimates are obtained by linearizing the measurement model around $\hat{x}_{k+1\,|\,k}$ and using the standard Kalman filter update equation

$$\begin{bmatrix} \hat{x}_{k+1|k+1} \\ \hat{p}_{k+1|k+1} \end{bmatrix} = \begin{bmatrix} \hat{x}_{k+1|k} \\ \hat{p}_{k+1|k} \end{bmatrix} + K_{k+1}[y_{k+1} - g(\hat{x}_{k+1|k})] \tag{8}$$

where

$$K_{k+1} = P_{k+1|k,a}G_{k+1,a}^T(G_{k+1,a}P_{k+1|k,a}G_{k+1,a}^T + R)^{-1}$$

$$G_{k+1,a} = \left[\left.\frac{\partial g}{\partial x}\right|_{x=[\hat{x}_{k+1|k}]} \quad \mathbf{0} \right]$$

The uncertainty in filtered estimates can be calculated as

$$P_{k+1|k+1,a} = (I - K_{k+1}G_{k+1,a})\,P_{k+1|k,a} \tag{9}$$

It should be noted that the evolution equation for parameters essentially describes the parameters as being constant, which clearly is a poor choice if the intention is to track and accurately estimate changes in parameters. To offset this, usually the uncertainty associated with the parameter evolution equation (represented by its variance Q_p) is used as a tuning parameter and chosen to be a sufficiently high value to enable the changing parameter value to be tracked by the estimator. However, a very high value of Q_p leads to a higher weight being given to the measurements in obtaining the estimates, which in turn decreases the accuracy of the state estimates. Thus the overall performance of the EKF is sensitive to the choice of Q_p, and some effort is required to tune this parameter. Some researchers such as Jang et al.[6] have found that the EKF does not track parameter changes very well. A main reason for their findings can be attributed to the fact that these authors choose the uncertainty associated with the augmented evolution equation for the parameters to be zero.

In summary, the EKF approach can deal with nonlinear processes, handle uncertainties in the process model caused by random disturbances and uncertainty in inputs/outputs, and is efficient because of the recursive computation scheme. Although it can track deterministic changes in parameters and/or unmeasured disturbances, it relies on a poor description of their evolution, which can pose difficulties in tuning the method to obtain accurate estimates. The main drawback of the EKF is that it can give unrealistic or infeasible estimates because it does not take into account bounds or other algebraic constraints. The features of the EKF are summarized in Table 2.

Table 3. Estimator Properties for NDDR

Property	a	b	c	d	e	f	g
Status	No	Yes	Yes	Yes	No	Window size?	OK

Dynamic data reconciliation

For state and parameter estimation in nonlinear dynamic processes, a moving-horizon-optimization–based method can be used as an alternative to EKF. These were developed more than three decades ago and have been used by several researchers for nonlinear chemical processes.[6,7] This approach allows bounds and other algebraic constraints on the state and parameter estimates to be incorporated. Liebman et al.[8] developed the nonlinear dynamic data reconciliation (NDDR) approach based on this strategy, which can also deal with input uncertainties and provide state and parameter estimates at each time that satisfy all algebraic constraints imposed on them. The NDDR problem can be formulated as a nonlinear optimization problem as follows[8] (where $\hat{x}$, $\hat{y}$ are the reconciled states and outputs at all collocation points; p_k had the estimated parameter)

$$\min_{\hat{x},\hat{p}_k} \sum_{j=k-(N-1)}^{k} (y_j - \hat{y}_j)^T R^{-1} (y_j - \hat{y}_j) \tag{10}$$

subject to

$$\frac{d\hat{x}}{dt} = f(\hat{x}, \hat{p}_k)$$

$$\hat{y} = g(\hat{x})$$

$$h(\hat{x}, \hat{p}_k) \le 0$$

$$e(\hat{x}, \hat{p}_k) = 0$$

$$x_L \le \hat{x} \le x_U$$

$$p_L \le \hat{p}_k \le p_U$$

The NDDR optimization problem can be solved in two ways. One approach is to incorporate the nonlinear differential equations in the solution strategy by embedding—also called the sequential approach—in which only the initial state estimates are treated as decision variables, and the differential

Table 4. Estimator Properties for RNDDR

Property	a	b	c	d	e	f	g
Status	Yes	Yes	Yes	Yes	Yes	Q_p?	Yes

Table 5. Estimator Properties for CPCO

Property	a	b	c	d	e	f	g
Status	Yes	Yes	Yes	Yes	Yes	Yes	Yes

equations are integrated using an initial value ODE (ordinary differential equation) solver to generate the estimates for all instants within the time window.[10] The alternative is to use a simultaneous approach in which the differential equations are converted to algebraic equations by some form of discretization, and solving the resulting constrained optimization problem.[8] In general, the simultaneous approach is computationally more efficient than the sequential strategy, and is used in this paper. It should be noted that the size of the optimization problem in the simultaneous approach is significantly larger because the decision variables consist of all variables that need to be estimated at each discretization point and each sampling instant within the time window. At each time instant, the optimization problem is solved for the chosen window size and only the estimates for the current time are used. The procedure is repeated at each sampling instant by moving one sampling period forward, and thus the designation *moving horizon* approach.

Liebman et al.[8] used a collocation method based on Legendre polynomials to discretize the differential equations. Instead, in this work we make use of Lagrangian polynomials because they are simpler and provide the same accuracy. The solution for $y(t)$ in each sampling period of the time window is represented as a sum of orthogonal (here Lagrangian) polynomials as follows:

$$\hat{y}(t) = \sum_{i=1}^{n_c} \Upsilon_i(t)\,\hat{y}(t_i)$$

$$\Upsilon_i(t) = \prod_{j=1, j\neq i}^{n_c} \frac{t - t_j}{t_i - t_j} \tag{11}$$

where n_c represents the total number of collocation points in each sampling period (including the end points representing the sampling instants) and t_j represents the collocation roots. Using the above solution the nonlinear differential equations are converted to linear algebraic equations that, together with the other algebraic and bound constraints, form the constraints of the nonlinear optimization problem to be solved.

To deal with input uncertainties, the inputs are grouped along with the measured variables and are also estimated; that is, they are also treated as decision variables in the optimization formulation. If parameters and unmeasured disturbance variables need to be estimated, then they are usually assumed to be constant within the time window to reduce the size of the optimization problem. However, if manipulated inputs are also estimated, then they can be assumed to be constant only within each sampling instant, and not for the entire time window. Although NDDR can deal with measurement and input uncertainties, Liebman et al.[8] do not discuss how well their approach handles random fluctuations in unmeasured disturbance variables. Such unmeasured disturbances, which are subject to random fluctuations, may also have to be treated in a similar manner as parameters and estimated as part of the optimization problem. This essentially implies that NDDR does not distinguish between deterministic and stochastic changes in unmeasured variables or parameters, and treats them in the same manner in the estimation approach. In contrast, the EKF approach models random variations in disturbances as process noise, whereas deterministic changes are modeled as integrated white noise and tracked by augmented states.

The main advantage of the NDDR formulation, as against the EKF, is its capability of handling algebraic constraints. In addition, it also does not assume any model for changes in

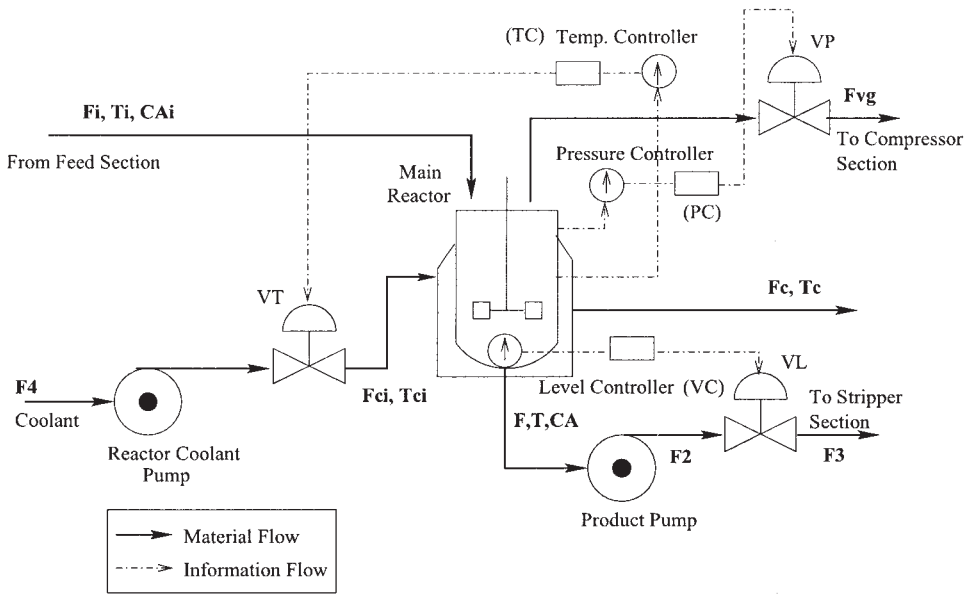

Figure 2. CSTR.

Table 6. Parameters for the CSTR of Figure 2

Notation	Variable	(Steady State/Constant) Value
V	Volume of liquid in reactor	48 ft^3
C_A	Reactant concentration in reactor	0.2345 lb · mol A/ft^3
T	Reactor temperature	600 °R
n	Number of moles in gas phase of reactor	28.3656 lb · mol C
V_g	Volume of gas phase (constant)	16 ft^3
F_i	Inlet feed flow rate	40 ft^3/h
C_{Ai}	Inlet reactant concentration	0.50 lb · mol A/ft^3
T_c	Jacket temperature	590.51 °R
F_c	Coolant flow rate	56.626 ft^3/h
T_i	Inlet feed temp.	530 °R
V_j	Volume of jacket	3.85 ft^3
k_o	Frequency factor	7.08×10^{10} h^{-1}
C_d	Catalyst activity	1
E	Activation energy	29,900 Btu/lb · mol
R	Universal gas constant	1.99 Btu/lb · mol °R
U	Heat transfer coefficient	150 Btu/h ft^2 °R
A	Heat transfer area	150 ft^2
T_{ci}	Inlet coolant temperature	530 °R
ΔH	Heat of reaction	−30,000 Btu/lb · mol
C_p	Heat capacity (process side)	0.75 Btu/lbm °R
C_j	Heat capacity (coolant side)	1.0 Btu/lbm °R
ρ	Density of process mixture	50 lbm/ft^3
ρ_j	Density of coolant	62.3 lbm/ft^3
K_v	PI controller parameter for volume	1 h^{-1}
T_v	PI controller parameter for volume	1 h^{-2}
K_t	PI controller parameter for temperature	4.3 ft^3 h^{-1} °R^{-1}
T_t	PI controller parameter for temperature	4.3 ft^3 h^{-2} °R^{-1}
K_p	PI controller parameters for pressure	0.5 ft^3 h^{-1} (Btu ft^{-3})$^{-1}$
T_p	PI controller parameters for pressure	0.5 ft^3 h^{-2} (Btu ft^{-3})$^{-1}$

parameters and unmeasured disturbances, and thus there is no tuning required to track these deterministic changes. The chief drawback of NDDR is that its optimization-based estimation technique can be computationally demanding, especially if uncertainties in inputs and unmeasured disturbances have to be taken into account. This may pose problems in using it for real-time applications. Another issue that arises is the choice of window size. A summary of the advantages and disadvantages of NDDR is presented in Table 3.

Proposed Recursive Formulations

Current methods for state and parameter estimation do not satisfactorily meet the desired requirements listed in Table 1. To overcome the disadvantages of existing techniques, we propose two novel recursive dynamic data reconciliation methods. These methods are developed by suitably combining the advantages of EKF and NDDR methods.

The first method we propose is referred to as the recursive nonlinear dynamic data reconciliation (RNDDR) technique. It is basically developed from EKF by providing it with the capability of handling algebraic constraints, without sacrificing the recursive estimation characteristic of the technique.

Recursive Nonlinear Dynamic Data Reconciliation

In KF and EKF, the estimation procedure at each sampling instant can be regarded as being composed of two steps (as described in the Appendix). In the first step, the state estimates from the previous time instant are propagated using the process dynamic equation (along with its error covariance matrix), whereas in the second step the predicted state estimates are corrected using the measurements made at the current time instant. It is shown in the Appendix that the optimal updated state estimates for KF (as also in EKF) are obtained by solving an unconstrained optimization problem for which the objective function is given in Eq. A5. In the absence of any constraints the solution of this optimization problem is given by the standard Kalman filter update equation for the state estimates. If algebraic constraints or bound constraints have to be imposed on the state estimates, these can be conveniently included in this optimization problem. In this case, the solution of the optimization problem has to be obtained numerically. This forms the basis for the proposed RNDDR method described below.

Consider the system given by Eq. 3 with bounds and algebraic constraints imposed on the states and parameters. Let $\hat{x}_{k\,|\,k}$, $\hat{p}_{k\,|\,k}$, and $P_{k\,|\,k}$ be given at time instant k. The predicted state estimates $\hat{x}_{k+1\,|\,k}$ and $\hat{p}_{k+1/k}$ are determined by integration, and the variance in the predicted estimates is calculated by covariance propagation using Eq. 7 as with EKF.

To obtain the updated state estimates, the following optimization problem is solved:

$$\underset{\hat{x}_{k+1|k+1},\,\hat{p}_{k+1|k+1}}{\text{Minimize}} \left(\begin{bmatrix}\hat{x}_{k+1|k+1}\\ \hat{p}_{k+1|k+1}\end{bmatrix} - \begin{bmatrix}\hat{x}_{k+1|k}\\ \hat{p}_{k+1|k}\end{bmatrix}\right)^T (P_{k+1|k,a})^{-1} \left(\begin{bmatrix}\hat{x}_{k+1|k+1}\\ \hat{p}_{k+1|k+1}\end{bmatrix} - \begin{bmatrix}\hat{x}_{k+1|k}\\ \hat{p}_{k+1|k}\end{bmatrix}\right) + [y_{k+1} - g(\hat{x}_{k+1|k+1})]^T R^{-1} [y_{k+1} - g(\hat{x}_{k+1|k+1})] \quad (12)$$

subject to the following constraints:

$$x_L \le \hat{x}_{k+1|k+1} \le x_U$$

$$p_L \le \hat{p}_{k+1|k+1} \le p_U$$

$$h(\hat{x}_{k+1|k+1}, \hat{p}_{k+1|k+1}) \le 0$$

$$e(\hat{x}_{k+1|k+1}, \hat{p}_{k+1|k+1}) = 0$$

The solution obtained using EKF is used as an initial guess for solving the above optimization problem. It should be noted that if the measurement model is linear and constraints are absent, then the solution for the updated state estimates obtained will be the same as the one computed using Eq. A6. The covariance

Table 7. Bounds on States and Catalyst Activity for CSTR Case Study

Variable	Lower Bound	Upper Bound
V	0	60
C_A	0	1
T	0	750
T_c	0	750
n	0	50
C_d	0	1

Table 8. Catalyst Deactivation

RMS Error	V	P	T	Ca	Tc	Parameter Estimation
Data	0.4892	1.9373	0.6913	0.0050	0.6553	—
RNDDR	0.1528	1.9023	0.4056	0.0018	0.3768	0.0271
CPCO	0.1512	1.6323	0.2435	0.0009	0.2229	0.0206
EKF	0.1629	2.0122	0.4419	0.0020	0.4128	0.0297
NDDR	0.1774	1.8176	0.4598	0.0027	0.4375	0.0488

matrix of the error in the updated state estimates is computed using Eq. 9. By using this equation, the effect of the constraints on the covariance matrix of estimation errors is neglected. In any case, for nonlinear systems, the covariance matrix of estimation errors represents only an approximation and, therefore, there is insufficient justification for trying to account for the effect that constraints have on it.

The advantages of RNDDR are similar to those of EKF, when it comes to handling uncertainties, nonlinearity, and tracking deterministic changes in parameters and unmeasured disturbances. The computational efficiency of this algorithm is also of the same order as that of the EKF. In addition, like NDDR, it has the ability to handle algebraic constraints and bounds on states and parameters. However, the augmentation strategy for parameter estimation is still a limitation. Table 4 summarizes the features of the RNDDR method.

Combined predictor–corrector optimization

The combined predictor–corrector optimization (CPCO) formulation is motivated from both the EKF and the nonlinear dynamic data reconciliation formulation to model parametric variation as deterministic changes. The prediction and correction steps over a sampling period used in the EKF are combined and solved as a single optimization problem in this technique: thus the name "combined predictor–corrector optimization " is used to denote this method. Similar to the NDDR method, no explicit model is required for estimating unmeasured parameters. However, to effectively use the parameter estimates obtained in the preceding sampling instant, changes from the previous estimates are penalized by using a weight matrix (Q_p) in the optimization problem. This also directly controls the variability in the parameter estimates. The nonlinear dynamic equations can either be embedded in the optimization problem or converted to algebraic equations using orthogonal collocation. Unless otherwise stated, we use the second approach in our implementation.

Consider the following system

$$x_{k+1} = x_k + \int_{k\Delta t}^{(k+1)\Delta t} f[x(\tau),\, u_k,\, p_k]d\tau + w_k$$

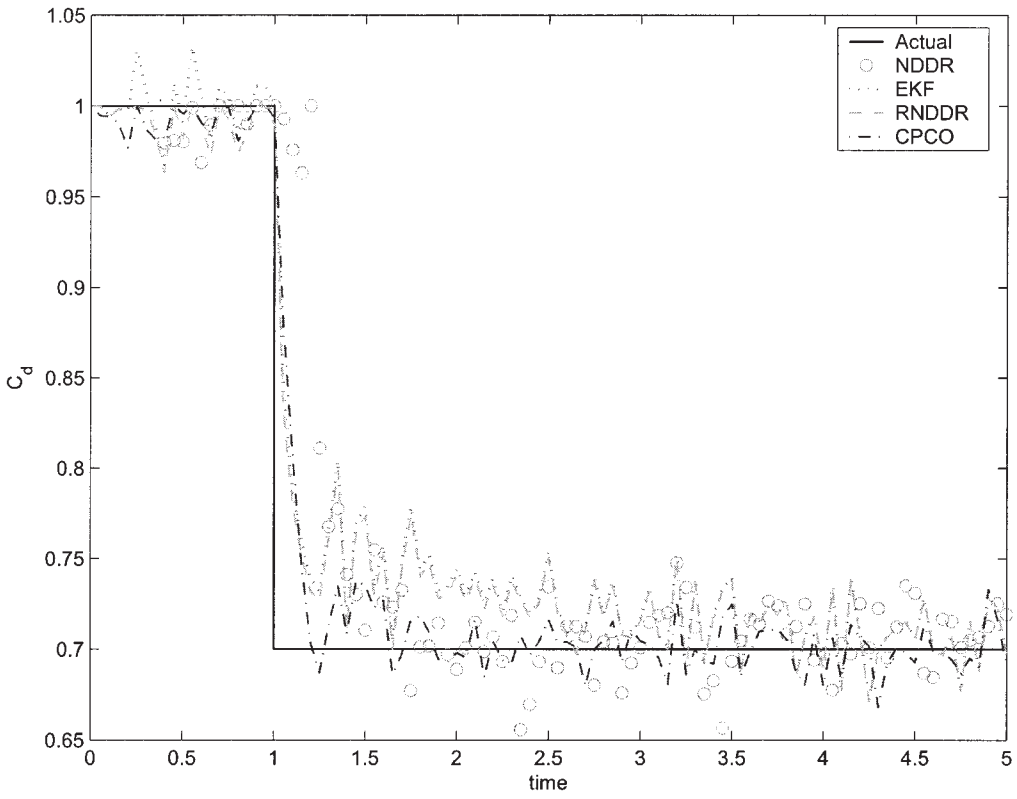

Figure 3. Catalyst activity estimate: step change (NDDR, EKF, RNDDR, CPCO).

Table 9. Approximate Time Required

Estimator	Time (s)
EKF	0.05
RNDDR	0.2
CPCO (warm start)	1–2
CPCO (cold start)	3–4
NDDR	30–600

$$e(x, p) = 0$$

$$h(x, p) \leq 0$$

$$y_{k+1} = g(x_{k+1}) + v_{k+1} \tag{13}$$

The state estimate $\hat{x}_{k \mid k}$ with the uncertainty $P_{k \mid k}$ is available. The two stages of Kalman filter are solved simultaneously using collocation to capture the process dynamics, whereas the filtered state and parameter estimates are the decision variables in the CPCO problem. The differential equations are converted to algebraic equations to describe the process behavior within the sampling interval. The CPCO formulation is posed as

$$\min_{\substack{\hat{x}_{k+1|k+1} \\ \hat{p}_{k+1|k+1}}} (\hat{x}_{k+1|k+1} - x_{n_c})^T P_{k+1|k}^{-1} (\hat{x}_{k+1|k+1} - x_{n_c}) + [y_{k+1} - g(\hat{x}_{k+1|k+1})]^T R^{-1} [y_{k+1} - g(\hat{x}_{k+1|k+1})] + (\hat{p}_{k+1} - \hat{p}_k)^T Q_p^{-1} (\hat{p}_{k+1} - \hat{p}_k) \tag{14}$$

subject to the following constraints

$$D_i(x_1, \ldots, x_{n_c}) = f(x_i, u_k, \hat{p}_{k+1}) \qquad i = 2, \ldots, n_c$$

$$h(x_i, \hat{p}_{k+1}) < 0 \qquad i = 1, \ldots, n_c$$

$$h(\hat{x}_{k+1|k+1}, \hat{p}_{k+1}) \leq 0$$

$$e(x_i, \hat{p}_{k+1}) = 0 \qquad i = 1, \ldots, n_c$$

$$e(\hat{x}_{k+1|k+1}, \hat{p}_{k+1}) = 0$$

$$x_L \leq \{x_i \text{ and } \hat{x}_{k+1|k+1}\} \leq x_U$$

$$p_L \leq \hat{p}_{k+1} \leq p_U$$

where n_c is the number of collocation points used (including the end points or the sample instants). In this formulation x_1 is $\hat{x}_{k \mid k}$ and x_{n_c} is equivalent to $\hat{x}_{k+1 \mid k}$. The first set of equality constraints is the result from analytical differentiation of the Lagrangian polynomial.

It should be noted that, unlike the NDDR method, uncertainties in the state equations arising from the random fluctuations in disturbances or from inaccuracies in the parameter estimates are explicitly accounted for by the estimate error covariance matrix $P_{k+1 \mid k}$ in the objective function 14. Similar to the EKF, the error covariance matrix $P_{k+1 \mid k}$ is obtained as

$$P_{k+1|k} = \bar{A}_k P_{k|k} \bar{A}_k^T + \bar{\Gamma}_{pk} Q_p \bar{\Gamma}_{pk}^T + Q_k \tag{15}$$

where $\bar{A}_k$ and $\bar{\Gamma}_{pk}$ are the system matrices of the linearized discrete state space model representation given by

$$\bar{A}_k = \exp(A_k \Delta t)$$

$$\bar{\Gamma}_{pk} = \int_{k\Delta t}^{(k+1)\Delta t} \exp[A_k(t - \tau)] \Gamma_{pk} d\tau$$

$$A_k = \left. \frac{\partial f(x, u, p)}{\partial x} \right|_{x=\hat{x}_{k|k}, u=u_k, p=\hat{p}_k}$$

$$\Gamma_{pk} = \left. \frac{\partial f(x, u, p)}{\partial p} \right|_{x=\hat{x}_{k|k}, u=u_k, p=\hat{p}_k} \tag{16}$$

Whereas in the EKF formulation, an explicit model for the evolution of the parameter is used with associated uncertainty Q_p, in the above formulation Q_p is used as a weight to penalize large changes in the parameter estimates. In the following section a method is proposed for choosing Q_p for all recursive formulations.

The uncertainty in filtered-state estimates can be calculated as shown previously for the extended-Kalman filter by linearizing the measurement function around the filtered-state estimates ($\hat{x}_{k+1 \mid k+1}$).

The advantages of this formulation are that the differential and algebraic constraints, and the deterministic nature of parametric changes are directly taken into account through integration of the prediction part with the optimization formulation for correction. The CPCO algorithm satisfies all requirements of a good estimator and is duly noted in Table 5. This approach can be interpreted as a two-point window-based NDDR formulation with the past information being accounted for by the use of the state uncertainty propagation, thus combining the concepts of NDDR and EKF.

Uncertainty variance selection

In all the recursive formulations for joint state and parameter estimation, the choice of weight matrix Q_p has a significant impact on the accuracy of the estimates. We propose a general method for selecting this tuning parameter. We note that the uncertainty in a measurement is caused both by uncertainty in the parameter value and by sensor errors. Because Q_p is a measure of the uncertainty in the parameter evolution we choose its value such that the uncertainty it causes in a measurement is approximately equal to the measurement error variance. This choice essentially gives equal weight to the process model and the measurements in deriving the estimates. For a nonlinear process, where several variables of different types are measured, a balanced choice of Q_p can be obtained by minimizing the following objective function

$$\min_{Q_p} \sum_{i=1}^{M} \left\{ \frac{[(\mathbf{C_i} \bar{\mathbf{\Gamma}}_p \mathbf{Q}_p \bar{\mathbf{\Gamma}}_p^T \mathbf{C_i^T}) - R_{ii}]}{R_{ii}} \right\}^2 \tag{17}$$

Table 10. Inlet Concentration Change

RMS Errors	V	P	T	Ca	Tc	Parameter Estimation
Data	0.4738	1.8968	0.6536	0.0048	0.6649	—
RNDDR	0.052	1.4254	0.2033	0.0034	0.1663	0.0541
CPCO	0.0529	1.3894	0.1888	0.0030	0.1585	0.0309
NDDR	0.1307	1.7374	0.4113	0.0032	0.4002	0.0252

where M is the number of sensors, $\mathbf{C_i}$ is the **i**th row vector of the linearized measurement matrix, and $\bar{\Gamma}_p$ is defined as in Eq. 16. The linearized system matrices ($\mathbf{\Gamma}_p$ and $\mathbf{C}$) are obtained by linearizing the nonlinear equations around the steady-state values.

CSTR Case Study

Two popular case studies drawn from literature are used to evaluate the performance of the different formulations presented. The CSTR case study has been used previously for simultaneous state and parameter estimation as well as for dynamic data reconciliation studies.[9] It is also a popular case study for diagnostic studies.[11,12]

CSTR description

The schematic of the CSTR system is shown in Figure 2. The process involves an exothermic reaction $A_{(l)} \rightarrow B_{(l)} + C_{(g)}$. The temperature in the reactor is controlled by manipulating the flow rate of the coolant flowing through the jacket. The level in the reactor is controlled by manipulating the outlet flow rate from the reactor. The pressure in the reactor is controlled by changing the vent gas flow rate. PI controllers are used to control the temperature, volume, and pressure of the reactor. Both the reactor and the jacket are modeled with perfectly mixed tank dynamics.

The reactor holdup at any time is given by

$$\frac{dV}{dt} = F_i - F \tag{18}$$

The reactant concentration C_A is given by

$$\frac{dC_A}{dt} = \frac{F_i}{V}(C_{Ai} - C_A) - r_A \tag{19}$$

Assuming constant heat capacities and densities, an overall heat balance on the reactor gives the reactor temperature as

$$\frac{dT}{dt} = \frac{F_i}{V}(T_i - T) + \frac{r_A(-\Delta H)}{\rho C_p} - \frac{UA(T - T_c)}{V\rho C_p} \tag{20}$$

Overall heat balance on the jacket gives the coolant temperature, as follows

$$\frac{dT_c}{dt} = \frac{F_c}{V_j}(T_{ci} - T_c) + \frac{UA(T - T_c)}{V_j\rho_j C_{pj}} \tag{21}$$

The pressure in the reactor depends on the number of moles of vapor n. This in turn depends on the rate of reaction and vent (molar) flow rate F_{vg}. The vapor space V_g is assumed to be constant and the vapor is assumed to behave ideally

$$\frac{dn}{dt} = r_A V - F_{vg} \tag{22}$$

$$PV_g = nRT \tag{23}$$

The reaction rate is given as

$$r_A = C_d C_A k_o e^{-E/RT} \tag{24}$$

Assuming no accumulation in the pumps, valves, and jacket, the following relations are obtained:

$$F_3 = F_2 = F \tag{25}$$

$$F_4 = F_c = F_{ci} \tag{26}$$

It is assumed that in addition to the three controlled variables, the reactor concentration and coolant outlet temperature are also measured, using a regular sampling period of 3 min. It may be noted that four of the state variables—V, T, T_c, and C_A—are measured directly, whereas the measured pressure is a nonlinear function of the state variables n and T.

Implementation Details. The steady-state values used to initialize all the simulation runs are shown in Table 6. The standard deviations of the measurement errors in the five measured variables are, respectively, chosen as 0.5 ft^3, 2 lbf/ft^2, 0.708 °R, 0.005 lb·mol A/ft^3, and 0.708 °R.

For implementing EKF and the two proposed recursive techniques, the initial estimation error covariance matrix P_0 is

Table 11. Catalyst Deactivation with Input Uncertainty

RMS Error	V	P	T	Ca	Tc	Parameter Estimation
Data	0.481	2.0156	0.6874	0.0048	0.6484	—
RNDDR	0.0942	1.6983	0.3168	0.0022	0.2728	0.0232
CPCO	0.0088	1.6776	0.2675	0.0013	0.2274	0.0195
NDDR	0.1400	1.8898	0.4194	0.0028	0.4016	0.0473

Table 12. Parameters for Polymerization Reactor

Parameter	Value
A_i	7.142×10^3 K
B_i	-18.36
A_{f_m}	2.310×10^6 m^3 kmol^{-1} s^{-1}
E_{f_m}/R	6.377×10^3 K
A_p	9.5×10^6 m^3 kmol^{-1} s^{-1}
E_p/R	3.6×10^3 K
A_t	1.25×10^9 m^3 kmol^{-1} s^{-1}
E_t/R	8.43×10^2 K
k_{t_d}	$0.15 \times k_t$
k_{t_c}	$0.85 \times k_t$
A_{f_s}	9.95×10^{10} m^3 kmol^{-1} s^{-1}
E_{f_s}/R	1.1×10^4 K
f	0.63
M_m	104 kg mol^{-1}

chosen to be diagonal. The standard deviations of the errors in the initial estimates of state variables V, T, T_c, and C_A were chosen to be equal to the standard deviations of their respective measurement errors, whereas the standard deviation of error in the initial estimate of n was chosen to be equal to 0.1 lb·mol.

In both the NDDR and the CPCO methods, the nonlinear differential equations are discretized by fitting a Lagrangian polynomial of order 3 for every sampling period. The state estimates required at the collocation roots are initialized by integration from $\hat{x}_{k \mid k}$ and parameter estimate p_k. The moving-horizon window size used in NDDR is 9 for both C_d and C_{Ai} examples. Two alternative strategies are compared to initialize the optimizer for the CPCO formulation. The warm start uses a KF-based correction of state estimates as an initial guess for $\hat{x}_{k+1 \mid k+1}$ and the cold start uses the propagated state estimate $\hat{x}_N$. All numerical computations were carried out on a P4 1.8-GHz Machine, using MATLAB software, unless otherwise indicated.

Results and discussion

The first simulation result we present is the case when the catalyst activity undergoes a step change, and it is required to simultaneously estimate the five state variables and the unknown catalyst activity parameter. In this simulation, no uncertainties in the manipulated inputs or unmeasured disturbances are introduced. For applying the recursive estimation techniques (EKF, RNDDR, and CPCO) the selection of Q_p is based on the procedure described in the section on uncertainty variance selection. The order of magnitude of Q_p obtained using this procedure is 10^{-3}. To evaluate the effectiveness of our proposed method, this value of Q_p is used for all three methods, with no further fine-tuning. Because NDDR, RNDDR, and the CPCO methods are capable of taking bounds into account, upper and lower bounds on the estimated variables and catalyst activity parameter are imposed, as given in Table 7.

Three different step changes in catalyst activity from 1 to 0.7, 1 to 0.8, and 1 to 0.9 at sampling instant 20 were introduced. The process is simulated for 100 sampling instants corresponding to each of these step changes, and the four different methods for state and parameter estimation applied. The root-mean square (RMS) errors in the measurements (difference between measured and true values) and the RMS errors in the estimates (difference between estimated and true values) of both measured variables and parameters are computed and averaged over the three simulation runs for each of the methods, the results of which are reported in Table 8.

A comparison of the methods in terms of accuracy of the estimates shows that the two proposed methods—RNDDR and CPCO—perform better than EKF and NDDR, with the CPCO being marginally better than RNDDR. Although EKF provides better estimates than NDDR on an average, it should be noted that the estimates it provides do not always satisfy the imposed bounds. This is clearly seen in Figure 3, which shows the estimates of the catalyst activity parameter obtained by the four methods for a step change in the parameter from 1 to 0.7. Although the estimates obtained using EKF violate the upper bound of 1.0 for some sampling instants, the other three methods all maintain the estimates within the imposed bounds. Although the EKF does not provide realistic estimates, it does not seriously impair the ability of the method to provide accurate estimates at other time instants for this process. This may not be valid in general, as will be shown subsequently in the second example.

The NDDR method was specifically developed for handling bounds on the variables. Even though it fulfills this requirement, it achieves this at the expense of a tremendous increase in computational time. Table 9 shows the range of computation times required per sampling period for each of the four methods. Because EKF does not require the solution of a constrained optimization problem it consumes the least computation time, whereas NDDR, which requires a large constrained optimization problem to be solved at each sampling instant, takes about 3 to 4 orders of magnitude more computation time compared to that of EKF. The proposed methods fulfill the same objective as NDDR, requiring only about 4–40 times more computation time than that of EKF. This is made possible by judiciously combining the best features of EKF and optimization-based approaches. A further point to be noted is that the computation time required by NDDR exceeds the sampling time period of 180 s in some cases, which renders it unsuitable for real-time applications when the estimates are required for control purposes.

A similar study was also conducted with step changes introduced in inlet concentration (step changes of -0.1, -0.05, 0.05, and 0.1 around a nominal value of 0.5). In this case the inlet concentration is the unmeasured disturbance parameter that has to be estimated along with the other measured variables. The RMSE values for all the methods averaged over the four simulation runs are presented in Table 10. In this case, RNDDR and CPCO give more accurate estimates than does

Table 13. Operating Conditions for Polymerization Reactor

Parameter	Value
C_m	1.9408 kmol m^{-3}
C_i	1.9854×10^{-3} kmol m^{-3}
C_s	5.475 kmol m^{-3}
T	393 K
F_i	1.5414×10^{-4} kmol s^{-1}
F_m	1.5414×10^{-4} kmol s^{-1}
C_{m_m}	7.208 kmol m^{-3}
C_{i_i}	0.1138 kmol m^{-3}
C_{s_i}	9.2 kmol m^{-3}
C_{s_m}	1.75 kmol m^{-3}
V	0.48 m^3

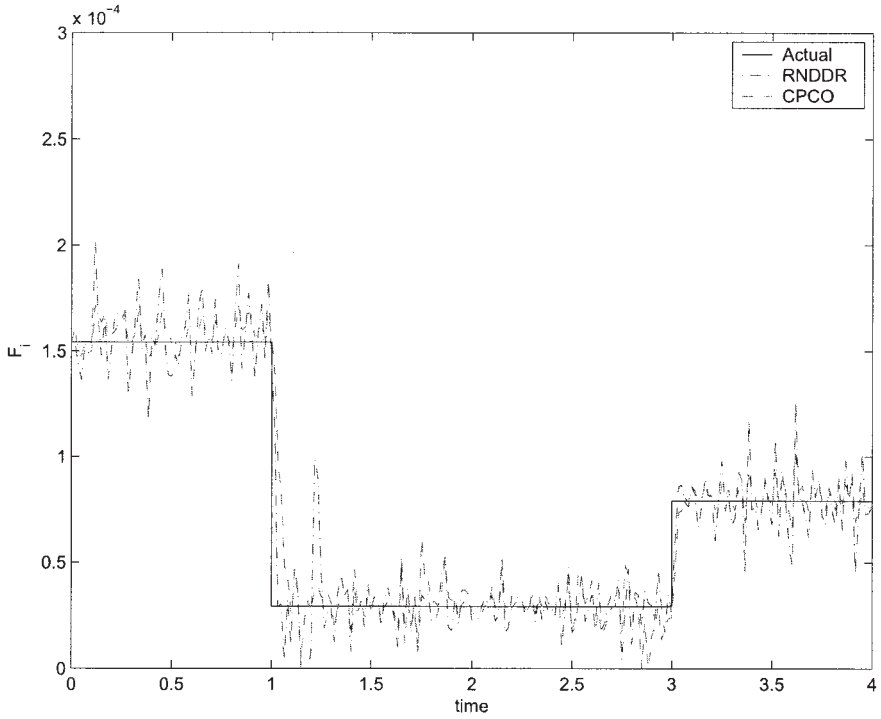

Figure 4. Initiator flow rate estimate.

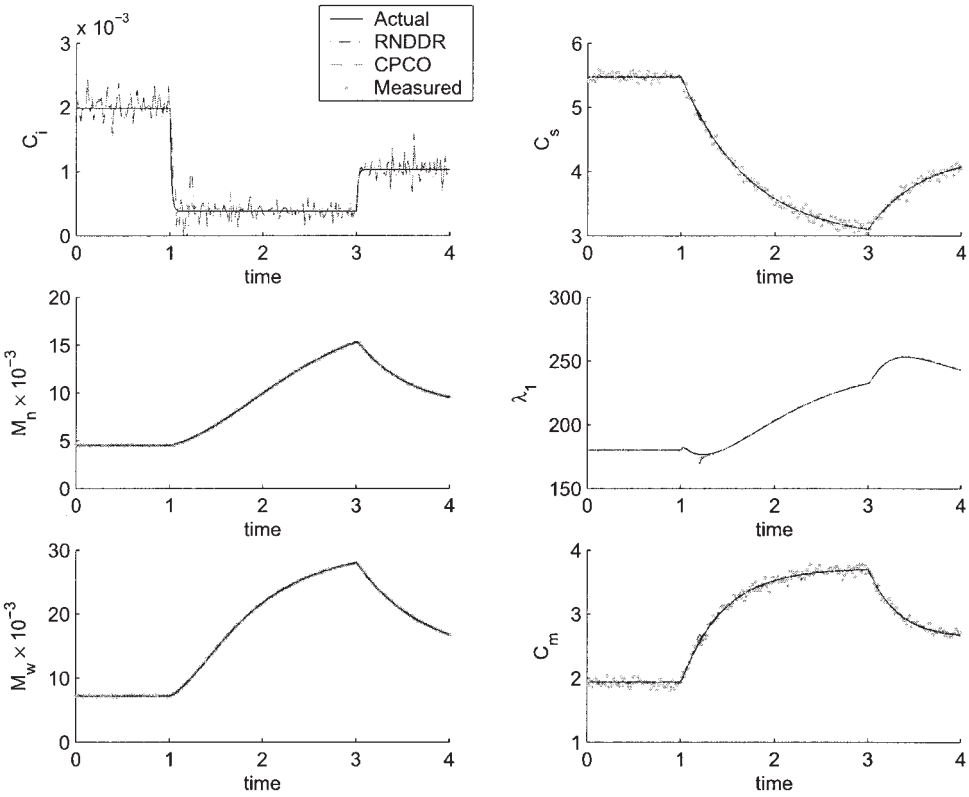

Figure 5. State estimate for initiator flow rate change.

Table 14. Bounds on States and Initiator Flow Rate for Polymerization Case Study

Variable	Lower Bound	Upper Bound
C_i	0	1
C_s	0	15
M_n	100	25,000
λ_1	0.01	500
M_w	100	40,000
C_m	0	10
F_i	0	0.001

NDDR of the measured variables, but provide less-accurate parameter estimates. Overall, the CPCO method provides the best balance between accuracy of estimates and computational time requirements.

The computational limitation of NDDR is more forcefully brought in the presence of input uncertainties. Similar to EKF, the proposed recursive formulations can easily account for input uncertainties by modeling them as state noise without any increase in the computational complexity of the problem. However, in NDDR the input variables also have to be estimated by treating them as decision variables of the optimization problem, thus leading to a significant increase in the complexity of the problem.

The catalyst deactivation simulation study as described earlier was repeated by adding normally distributed random errors of variance 0.04 (units same as square of inputs) in all manipulated variables, and NDDR along with the two proposed methods were applied. Because of the presence of this uncertainty, the Q_p computed using the procedure described earlier in this case was found to be 10^{-3}. This value was used in both proposed formulations without any further tuning. The results of this simulation are presented in Table 11. Because of the size of the optimization problem, it was not possible to execute NDDR under the MATLAB environment. Instead, this method was implemented using a successive quadratic programming (SQP) solver running under a LINUX operating system. Although it is not possible to make a direct comparison of the computation times in this case because of the different environments used, we note that the proposed methods required the same computational time as reported in Table 9, whereas NDDR now required between 60 and 1000 s for each sampling instant. Furthermore, at several sampling instants the SQP failed to converge to the required degree of tolerance. In Table 11 the RMS errors in measured and estimated values are presented. Again, it can be observed that the proposed formulations provide more accurate estimates compared to those of NDDR, with the CPCO method providing marginally better estimates than those of RNDDR.

Polymerization Reactor Case Study

The polymerization reactor[13] is a popular example in the literature for state estimation[14] and reconciliation studies[15] because of its inherent complexity and nonlinearities. The case study used here is that of a styrene polymerization in a CSTR.[16] The objective of this case study is to demonstrate the importance of using bounds to obtain a working estimator.

Polymerization reactor description

The dynamic equations for initiator, solvent, and monomer concentrations in the reactor are as follows:

$$\frac{dC_i}{dt} = -\left(\frac{F_i}{V} + k_i\right)C_i + \frac{F_i C_{i_i}}{V} \tag{27}$$

$$\frac{dC_s}{dt} = -\frac{F_t C_s}{V} + \frac{F_i C_{s_i} + F_m C_{s_m}}{V} \tag{28}$$

$$\frac{dC_m}{dt} = -k_p C_m P + \frac{F_m C_{m_m} - F_t C_m}{V} \tag{29}$$

where

$$P = \sqrt{\frac{2fC_i k_i}{k_t}} \tag{30}$$

is the concentration of live polymer and

$$F_t = F_i + F_m \tag{31}$$

The rate constants used above are as follows:

$$k_i = 0.693/\{60 \times 10^{[(A_i/T)+B_i]}\} \tag{32}$$

$$k_p = A_p \exp\left(\frac{-E_p}{RT}\right) \tag{33}$$

$$k_{f_m} = A_{f_m} \exp\left(\frac{-E_{f_m}}{RT}\right) \tag{34}$$

$$k_{f_s} = A_{f_s} \exp\left(\frac{-E_{f_s}}{RT}\right) \tag{35}$$

$$k_t = A_t \exp\left(\frac{-E_t}{RT}\right) \tag{36}$$

$$k_{t_d} = 0.15 \times k_t \tag{37}$$

$$k_{t_c} = 0.85 \times k_t \tag{38}$$

Table 15. Initiator Flow Rate Change

RMS Error	C_s	$M_n \times 10^{-3}$	$M_w \times 10^{-3}$	C_m	Parameter Estimation
Data	0.0533	0.0310	0.0431	0.0530	—
RNDDR	0.0158	0.0155	0.0253	0.0126	1.8807×10^{-5}
CPCO	0.0114	0.0122	0.0216	0.0095	9.2506×10^{-6}

Polymer molecular weight distribution (MWD) is an important property monitored during polymer production because a polymer's end-use properties are strongly dependent on its MWD. The average molecular weight of a polymer solution is correlated to the reacting mixture viscosity, which can be measured online. The dynamic equations for the MWD are dependent on the first moment of the MWD, which is also a state variable

$$\frac{d\lambda_1}{dt} = -\frac{F_t\lambda_1}{V} + [(k_{f_m}C_m + k_{t_d}P + k_{f_s}C_s)(2\alpha - 2\alpha^2) + k_{t_c}P]\frac{PM_n}{(1-\alpha)} \quad (39)$$

$$\frac{dM_n}{dt} = \{[(k_{f_m}C_m + k_{t_d}P + k_{f_s}C_s)(2\alpha - \alpha^2) + k_{t_c}P]M_m - [(k_{f_m}C_m + k_{t_d}P + k_{f_s}C_s)\alpha + 0.5k_{t_c}P] \times M_n(1-\alpha)\}\frac{PM_n}{\lambda_1(1-\alpha)} \quad (40)$$

$$\frac{dM_w}{dt} = \{[(k_{f_m}C_m + k_{t_d}P + k_{f_s}C_s)(\alpha^3 - 3\alpha^2 + 4\alpha) + k_{t_c}P(\alpha+2)]M_m - [(k_{f_m}C_m + k_{t_d}P + k_{f_s}C_s) \times (2\alpha - \alpha^2) + k_{t_c}P]M_w(1-\alpha)\}\frac{PM_m}{\lambda_1(1-\alpha)^2} \quad (41)$$

where

$$\alpha = \frac{k_pC_m}{(k_p + k_{f_m})C_m + k_{f_s}C_s + k_tP} \quad (42)$$

The relevant parameters for simulating the polymerization reactor are provided in Table 12. For the steady state of the reactor the relevant operating conditions are given in Table 13. The measured variables are C_s, M_n, M_w, and C_m.

Results and discussion

Open-loop simulation results for decrease in inlet flow rate of initiator stream are presented. The variances of error in the measurements of C_s, M_n, M_w, and C_m are chosen to be, respectively, 0.003, 1000, 2000, and 0.003. Corresponding to these values, the value of Q_p for estimating the unmeasured disturbance variable (inlet flow rate of initiator) is computed using our procedure to be $O(10^{-9})$, which is used in the RNDDR and CPCO methods.

A decrease in inlet initiator flow rate was simulated and the parameter estimates for the same are shown in Figure 4 and the state estimates are shown in Figure 5. In the CSTR catalyst deactivation case study the EKF does not fail, even though the estimate of catalyst activity exceeds the upper bound of unity. However, in this example, if algebraic constraints are not incorporated, the initiator concentration and initiator flow rate estimates can become negative, leading to a mathematically unsolvable problem. Thus it is not possible to use EKF for state estimation for this process. Because of the inclusion of bound constraints (Table 14) both of the proposed methods are able to provide reliable estimates. The CPCO formulation at a relative increase in computation cost performs better than the RNDDR formulation in terms of parameter and state estimates, as can be observed from the RMS estimation errors given in Table 15.

Conclusion

A list of properties has been presented that enumerates the requirements of a good estimator. This is used as a guideline to show the efficacy of the proposed recursive nonlinear dynamic data reconciliation (RNDDR) and the combined predictor–corrector optimization (CPCO) formulations against the traditional approaches of recursive estimation, that is, the extended-Kalman filter (EKF) and the window-based approach, nonlinear dynamic data reconciliation (NDDR). A brief description of the EKF and the NDDR is presented along with the implementation details. The basis toward formulating RNDDR in a predictor–corrector form is presented. The motivation for use of the CPCO is to estimate parameters in a deterministic setting (involving no augmentation), thus requiring simultaneous solution of the prediction and the correction problem.

Extensive simulations are carried out with the continuous stirred tank reactor and the polymerization reactor. The following conclusions can be inferred from the studies. The RNDDR is identical to EKF if there are no bounds on variables or algebraic constraints. In the case of dynamic systems involving algebraic, equality, or inequality constraints the proposed RNDDR and the CPCO formulation are an order of magnitude faster than the traditional NDDR approach and give equally accurate estimates. Therefore, the proposed formulations can be implemented on large nonlinear systems for real-time dynamic data reconciliation.

Another important feature of the proposed formulations, unlike the NDDR, is that input uncertainty and random disturbances can be accounted for through state noise with no increase in the computational complexity (degree of freedom) of the problem. Simulation results are presented for the CSTR in the presence of input uncertainty, in which case the NDDR formulation requires more time, whereas the computational cost of the RNDDR and the CPCO remains the same. Also, the RNDDR and CPCO give results that are as equally accurate as those of NDDR.

In summary, recent literature seems to suggest that the moving-horizon estimator is superior to the EKF approach in chemical engineering systems mainly because of the presence of bounds and constraints that the EKF cannot handle.[5] Further, there are also a number of papers that suggest convergence problems and difficulty in tuning of EKF in a few cases. Through this paper, we have demonstrated that incorporation of bounds and constraints is not as severe a problem as perceived in the literature, and a minor modification of the EKF formulation can handle bounds and constraints. Further, many of the cases where EKF has been shown to fail in the literature can be quite easily handled by a judicious choice of the Q_p matrix. The choice of Q_p does not seem to be difficult either, contrary to what the literature suggests. We have shown that Q_p can be chosen quite systematically. We believe that the advantages of a recursive formulation, in terms of computational superiority and strong fundamental basis, far outweigh the number of cases in which the proposed approaches might fail. Further, by retaining the basic EKF formulation, it will be possible to address other issues such as covariance propagation in nonlinear constrained systems, through advances made such as the incorporation of unscented transformation in the EKF formulation.

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Appendix: Kalman Filter

Let the discrete linear stochastic state-space system be of the form

$$x_{k+1} = \bar{A}_{k+1}x_k + w_k$$

$$y_{k+1} = \bar{C}_{k+1}x_{k+1} + v_{k+1} \tag{A1}$$

where w_k and v_{k+1} are independent normally distributed random variables with covariance Q_k and R_{k+1}, respectively.

Assume unbiased estimates of the state at time instant k ($\hat{x}_{k\,|\,k}$) and the measurement at time instant $k+1$ (y_{k+1}) are available. The state estimate for time instant $k+1$ ($\hat{x}_{k+1\,|\,k+1}$) can be expressed as a linear combination of the two:

$$\hat{x}_{k+1|k+1} = K'_{k+1}\hat{x}_{k|k} + K_{k+1}y_{k+1} \tag{A2}$$

Table A1. Estimator Properties for KF

Property	a	b	c	d	e	f	g
Status	Yes	No	No	No	Yes	Yes	Unrealistic estimates

For $\hat{x}_{k+1\,|\,k+1}$ to be an unbiased estimate of x_{k+1}, we require $K'_{k+1} = (I - K_{k+1}\bar{C}_{k+1})\bar{A}_{k+1}$. Thus the recursive estimator can be rewritten in two parts, first for prediction and the second for correction.

$$\hat{x}_{k+1|k} = \bar{A}_{k+1}\hat{x}_{k|k}$$

$$\hat{x}_{k+1|k+1} = \hat{x}_{k+1|k} + K_{k+1}(y_{k+1} - \bar{C}_{k+1}\hat{x}_{k+1|k}) \tag{A3}$$

We also assume $P_{k|k}$, the uncertainty in the state estimate $\hat{x}_{k\,|\,k}$, is known. Therefore, the uncertainty in $\hat{x}_{k+1\,|\,k}$ can be calculated as

$$P_{k+1|k} = \bar{A}_{k+1}P_{k|k}\bar{A}^T_{k+1} + Q_k \tag{A4}$$

The Kalman gain matrix is obtained by solving the following unconstrained optimization problem:

$$\min_{\hat{x}_{k+1|k+1}} (\hat{x}_{k+1|k+1} - \hat{x}_{k+1|k})^T(P_{k+1|k})^{-1}(\hat{x}_{k+1|k+1} - \hat{x}_{k+1|k}) + (y_{k+1} - \bar{C}_{k+1}\hat{x}_{k+1|k+1})^T(R_{k+1})^{-1}(y_{k+1} - \bar{C}_{k+1}\hat{x}_{k+1|k+1}) \tag{A5}$$

giving the filtered state estimate as

$$\hat{x}_{k+1|k+1} = \hat{x}_{k+1|k} + [(P_{k+1|k})^{-1} + \bar{C}^T_{k+1}(R_{k+1})^{-1}\bar{C}_{k+1}]^{-1}\bar{C}^T_{k+1}(R_{k+1})^{-1}(y_{k+1} - \bar{C}_{k+1}\hat{x}_{k+1|k}) = \hat{x}_{k+1|k} + K_{k+1}(y_{k+1} - \bar{C}_{k+1}\hat{x}_{k+1|k}) \tag{A6}$$

where the Kalman gain matrix K_{k+1} is defined as

$$K_{k+1} = (P_{k+1|k})\bar{C}^T_{k+1}(R_{k+1} + \bar{C}_{k+1}P_{k+1|k}\bar{C}^T_{k+1})^{-1} \tag{A7}$$

The covariance matrix of errors in the filtered state estimates is given by

$$P_{k+1|k+1} = (I - K_{k+1}\bar{C}_{k+1})\,P_{k+1|k} \tag{A8}$$

The KF is meant for state estimation in linear dynamic system with uncertain inputs and outputs and is easy to implement, advantages that are duly noted in Table A1.

Manuscript received Dec. 5, 2003, and revision received July 10, 2004.