Enhancing Model Predictive Control Using Dynamic Data Reconciliation

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The use of data reconciliation techniques can considerably reduce the inaccuracy of process data due to measurement errors. This in turn results in improved control system performance and process knowledge. Dynamic data reconciliation techniques are applied to a model-based predictive control scheme. It is shown through simulations on a chemical reactor system that the overall performance of the model-based predictive controller is enhanced considerably when data reconciliation is applied. The dynamic data reconciliation techniques used include a combined strategy for the simultaneous identification of outliers and systematic bias.

Introduction

Data reconciliation, occasionally referred to as measurement error reconciliation, is the adjustment of a set of data in order that the quantities derived from the data obey natural laws, such as material and energy balances. Measurements made on processes, such as flow, tank level, or temperature, are adjusted in some proportion to the standard error of the measurement. The adjustments are made using redundancies in the measurements. After adjustment, the material and, if considered, the energy balances, are exactly satisfied (Bodington, 1995).

Errors in measured process data may occur through a malfunction of instruments, miscalibration, or poor sampling and are usually broadly classified as gross errors or systematic biases. Several researchers have addressed instrumentation malfunction and associated fault detection, using principal component analysis, for example, but this is only one part of the overall data reconciliation process (Rollins et al., 1996; Qin and Li, 1999). Most data reconciliation techniques require that both gross errors, including outliers, and systematic biases be absent from the data before the reconciliation is carried out. An additional difficulty with process data is that not all variables are measured because of cost considerations or technical infeasibility and, therefore, must, if possible, be estimated instead.

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Inaccurate process data can easily lead to poor decisions which will adversely affect many parts of the process. Many process control and optimization activities are also based on small improvements in process performance; errors in process data can easily exceed the actual changes in process performance. Moreover, because of the immense scale of operation, the impact of any error is greatly magnified in absolute terms (Mah et al., 1976).

The main aim of data reconciliation is to reduce or eliminate as much as possible the effect of random measurement error on the analysis of process performance and on the predictions for future operation. Additional objectives are to improve confidence in the calculation of unmeasured variables and to identify process losses and faulty measurements.

Data reconciliation may be performed on a set of steady-state data, using a steady-state model of the process, or it may be applied to dynamic data, using a dynamic model of the process. Methods for reconciling steady-state process data are well developed (Bodington, 1995). However, even so-called "steady-state" processes are never truly at steady state. They continually undergo variations about a nominal steady-state condition (Narasimhan and Mah, 1987). Therefore, dynamic models would undoubtedly better represent the real process. Moreover, some chemical processes are intrinsically dynamic and, in some chemical processes, disturbances with dynamic effects may occur frequently (Becerra et al., 1998b).

For the reasons outlined above and because steady-state conditions are a particular case in a dynamic model, it is desirable to develop dynamic data reconciliation strategies.

A key feature of the dynamic data reconciliation strategy presented here is a combined algorithm for identifying and eliminating systematic bias as well as outliers. Previously, McBrayer and Edgar (1995) developed a method for the identification of systematic bias in dynamic data. Chen and Romagnoli (1998) devised a method for the identification of outliers. Sanchez et al. (1999) presented a method for the simultaneous detection of systematic bias and outliers. However, this method is only applicable to steady-state processes.

The general dynamic data reconciliation problem has been tackled by a number of researchers in the field. Darouach and Zasadzinski (1991) were some of the first researchers to address the issue. They presented an on-line estimation algorithm for linear dynamic systems. Their algorithm involves a recursive solution technique in weighted least squares. Liebman et al. (1992) presented a method for nonlinear dynamic data reconciliation using nonlinear programming (NLP) techniques. Ramamurthi et al. (1993) presented a successively linearized horizon-based estimator (SLHE) for dynamic data reconciliation in closed-loop systems. They compare the performance of SLHE with the extended Kalman filter (EKF) and NLP approaches. Albuquerque and Biegler (1995) proposed a method for dynamic data reconciliation which works by discretizing the set of ordinary differential equations using a one-step integration method and then uses the sequential quadratic programming (SQP) method to solve the resulting NLP.

Karjala and Himmelblau (1996) proposed a procedure for dynamic reconciliation of data using recurrent neural networks and the EKF. Albuquerque and Biegler (1996) presented a study on data reconciliation and gross error detection for dynamic systems. Bagajewicz and Jiang (1997) gave a brief review of data reconciliation using both steady-state and dynamic models. Becerra et al. (1998b) presented a method for dynamic data reconciliation using sequential modular simulators using a bank of extended Kalman filters. Becerra et al. (1999) proposed a dynamic data reconciliation method for nonlinear systems described by differential-algebraic models using the EKF.

In this article, a number of dynamic data reconciliation tools (Abu-el-zeet, 2000) including bias and outlier identification algorithms are used to improve the performance of a model-based predictive control (MPC) scheme. It is shown through simulations using a dynamic model of two continuous stirred tank reactors (CSTRs) that reconciling the process data prior to using it for predictive control does improve the overall performance considerably.

Dynamic Data Reconciliation Problem

Data reconciliation is the adjustment of process measurements—which are subject to error, to obtain values that are consistent with the material and energy balances. The simplest case is a process operating in steady state where all the desired variables are measured and no gross errors are present in the measurements. It is assumed that the measurement error is Gaussian with known variances and that the mean of measurement errors is assumed to be zero. The measurement vector (y_m) can be written as

$$y_m = y_{\text{true}} + \epsilon \tag{1}$$

where y_{true} is the vector of the true values of the variables, ϵ is a vector of random measurement errors that are normally distributed with zero mean, and a covariance matrix V.

The data reconciliation problem can be stated as a constrained least-squares estimation problem where the weighted sum of errors is to be minimized subject to constraints

$$\min_{y_{\text{true}}} (y_m - y_{\text{true}})^T V^{-1} (y_m - y_{\text{true}}) \tag{2}$$

subject to

$$f(y_{\text{true}}) = 0 \tag{3}$$

where $V \in \Re^{n_y \times n_y}$ is the covariance matrix of the measured variables y_m. The constraints arise because the mass balances, energy balances, and any other performance equations must be satisfied, and are encapsulated in the term $f(y_{\text{true}})$.

Systematic bias can be estimated as a parameter (McBrayer and Edgar, 1995). The objective function is formulated as follows

$$J = \left(\frac{\bar{y}_1 - \left(y_{m_1} - \hat{b}_1 \right)}{\sigma_1} \right)^2 + \left(\frac{\bar{y}_2 - \left(y_{m_2} - \hat{b}_2 \right)}{\sigma_2} \right)^2 + \cdots + \left(\frac{\bar{y}_i - \left(y_{m_i} - \hat{b}_i \right)}{\sigma_i} \right)^2$$

subject to

$$\begin{aligned} f(\bar{y}) &= 0. \\ \bar{y}_{l,i} \le \bar{y}_i &\le \bar{y}_{u,i} \quad \forall i, \\ \hat{b}_{l,i} \le \hat{b}_i &\le \hat{b}_{u,i} \quad \forall i, \end{aligned} \tag{4}$$

where y_{m_i} is the ith measured variable, $\bar{y}_i$ is the ith estimate, σ_i is the measurement noise standard deviation of the ith measured variable, and $\hat{b}_i$ is the estimate of bias on the ith measured variable. Note that $\hat{b}_i$ is also included in the inequality constraints. This allows for physical limits on the range of admissible biases.

The dynamic data reconciliation problem is addressed here using a moving horizon estimator (MHE). The following is a formulation of the MHE.

MHE

The moving horizon estimation problem may be defined as a nonlinear dynamic optimization problem with a discrete time performance index and a continuous time model and constraints. It is assumed that the measurements are sampled with a sampling time T_s. The process model is represented as

$$\dot{x}(t) = f_x(x(t), u(t), p, t) \tag{5}$$

where $x \in \Re^{n_x}$, is a differential state vector, $u \in \Re^{n_u}$ is a given input vector, $p \in \Re^{n_p}$ is a vector of physical parameters, f_x is a mapping of n_x state equations, and t denotes continuous time.

Assume that the model outputs are given by

$$y(t) = c(x(t),u(t),b,t) \tag{6}$$

where $y \in \Re^{n_y}$ is the vector of model outputs, $b \in \Re^{n_b}$ is a vector of bias parameters, and c is a mapping of n_y output equations. It is assumed that system 5 is observable through 6.

Assume that a sequence of nh recent output measurements is available: $\{y_m(t_0), y_m(t_0 + T_s), \ldots, y_m(t_f)\}$, where time t_f is assumed to be present time. Assume also that the input variable $u(t)$ is known during the period $t \in [t_0, t_f]$. The moving horizon estimation problem is

$$\min_{x_0,p,b} J = \sum_{k=0}^{nh-1} L\big(y(t_0 + kT_s),\, y_m(t_0 + kT_s),\, b,\, k\big) \tag{7}$$

subject to

$$\dot{x}(t) = f_x(x(t),u(t),p,t) \qquad t \in [t_0,t_f] \tag{8}$$

$$x(t_0) = x_0 \tag{9}$$

$$y(t) = c(x(t),u(t),b,t) \qquad t \in [t_0,t_f] \tag{10}$$

$$\psi(y(t),x(t),u(t),p,t) \le 0 \qquad t \in [t_0,t_f] \tag{11}$$

where $y_m \in \Re^{n_y}$ is the vector of measured outputs, k is a sampling index, L is a weighting function, and ψ is a mapping of n_ψ inequality constraints $t_f = t_0 + (nh - 1)T_s$.

The purpose of the solution is to find the following estimates at the present time: $\hat{y}(t_f), \hat{x}(t_f), \hat{b}(t_f)$, and $\hat{p}(t_f)$.

The weighting function L in a moving horizon estimation problem may be defined as follows

$$L(y,y_m,b,k) = \frac{1}{2}\big(y - (y_m - Sb)\big)^T V^{-1}\big(y - (y_m - Sb)\big) \tag{12}$$

where $S \in \Re^{n_y \times n_b}$ is a bias distribution matrix. Note that bias is not necessarily estimated in all measured variables.

In order to reduce the dynamic optimization problem defined above to a nonlinear programming problem, it is necessary to discretize the continuous equations. This may be done using fourth-order Runge Kutta steps. However, the integration step h will not necessarily be the same as the measurement sampling time T_s (it would be normal to expect that $h \le T_s$). Assume that the integration time is chosen such that $T_s = n_i h$, where n_i is the number of integration steps per sampling period. Given that it is assumed that the input variable $u(t)$ is known during the period $t \in [t_0, t_f]$, then the following input sequence is also known: $\{u(t_0),\, u(t_0 + h),\, u(t_0 + 2h),\, \ldots,\, u(t_f)\}$.

Define the following decision vector

$$X = \begin{bmatrix} x_0 \\ p \\ b \end{bmatrix} \tag{13}$$

where $X \in \Re^{n_x + n_p + n_b}$.

Define the following vector of inequality constraints

$$\Psi = \begin{bmatrix} \psi(y(t_0),x(t_0),u(t_0),p,t_0) \\ \psi(y(t_0+h),x(t_0+h),u(t_0+h),p,t_0+h) \\ \psi(y(t_0+2h),x(t_0+2h),u(t_0+2h),p,t_0+2h) \\ \vdots \\ \psi(y(t_f),x(t_f),u(t_f),p,t_f) \end{bmatrix} \le 0 \tag{14}$$

where $\Psi \in \Re^{(n_i+1)n_\psi}$.

Then, the moving horizon estimation problem defined above can be reduced to the following nonlinear programming (NLP) problem

$$\min_X \quad J(x) \tag{15}$$

subject to

$$\Psi(X) \le 0 \tag{16}$$

Notice that, given the decision vector X and the input sequence $\{u(t_0), u(t_0 + h), u(t_0 + 2h), \ldots, u(t_f)\}$, it is possible to integrate the model differential Eq. 8 to obtain the state sequence $\{x(t_0), x(t_0 + h), x(t_0 + 2h), \ldots, x(t_f)\}$. With X and the state sequence, it is possible to calculate, via the output Eq. 10, the output sequence $\{y(t_0), y(t_0 + h), y(t_0 + 2h), \ldots, y(t_f)\}$. Given X, the measured output sequence $\{y_m(t_0), y_m(t_0 + T_s), \ldots, y_m(t_f)\}$, and the computed output sequence $\{y(t_0), y(t_0 + T_s), \ldots, y(t_f)\}$, it is possible to compute $J(X)$. Thus, given X, it is possible to compute JX and $\Psi(X)$.

The solution to the above nonlinear programming problem can be obtained using a standard SQP algorithm. Furthermore, given that the objective $J(X)$ is often chosen to be a sum of quadratic functions such as Eq. 12, then a nonlinear least-squares algorithm is probably a good choice for the solution.

Detection and identification of systematic bias

Systematic biases occur when measurement devices provide consistently erroneous values, either too high or too low, and may be caused by incorrect installation or calibration of the measurement systems. It is important that data containing such bias is identified and either treated or removed prior to the data reconciliation stage. If the measurements are adjusted in the presence of such biases, all of the adjustments will be greatly affected by them and would not be reliable indicators of the true state of the process.

Surprisingly few researchers have explicitly addressed the problem of identification of systematic bias. Most of the limited previous work has focused on steady-state processes (Narasimhan and Mah, 1987; Mah and Tamhane, 1982; Rollins and Davis, 1992, for example). Work involving nonlinear dynamic systems has been published by McBrayer and Edgar (1995). Their technique uses the model-based nonlinear dynamic data reconciliation (NDDR) method developed by Liebman (1991) and requires the calculation of a set of base statistics. These serve as a *base case* with which statistics from the actual data can be compared. The base statistics are calculated using base case data generated by adding Gaussian noise to the calculated estimates. To determine whether or not a bias is present, the residuals are examined.

A new approach for the detection and identification of systematic bias is presented in the following algorithm (Abu-el-zeet, 2000).

A new bias detection and identification algorithm

The new algorithm, based on the easy to implement, moving horizon concept, operates by assuming just one of the measurements to be biased. The appropriate flags are set in order for bias on that particular variable to be estimated as a free parameter. Then, the bias estimate of that variable is analyzed and checked in two simple ways. The first is a check on the magnitude of the bias which is compared to a pre-set threshold value. The second test checks the bias against the standard deviation of the measurements in the current data window. Again, this is checked against a preset threshold value. In order for the algorithm to flag a possible presence of bias on that particular measurement, the results from both tests must exceed their respective threshold values. If the chosen measurement is deemed to be free of bias, a different measurement is chosen and assumed to be biased and the procedure is repeated. This is done sequentially for all the measurement variables until the biased individual (if any) is found. In other words, if the algorithm has not found a biased individual, it will assume a different measurement to be biased each time the reconciliation procedure is run. The algorithm is summarized in Figure 1.

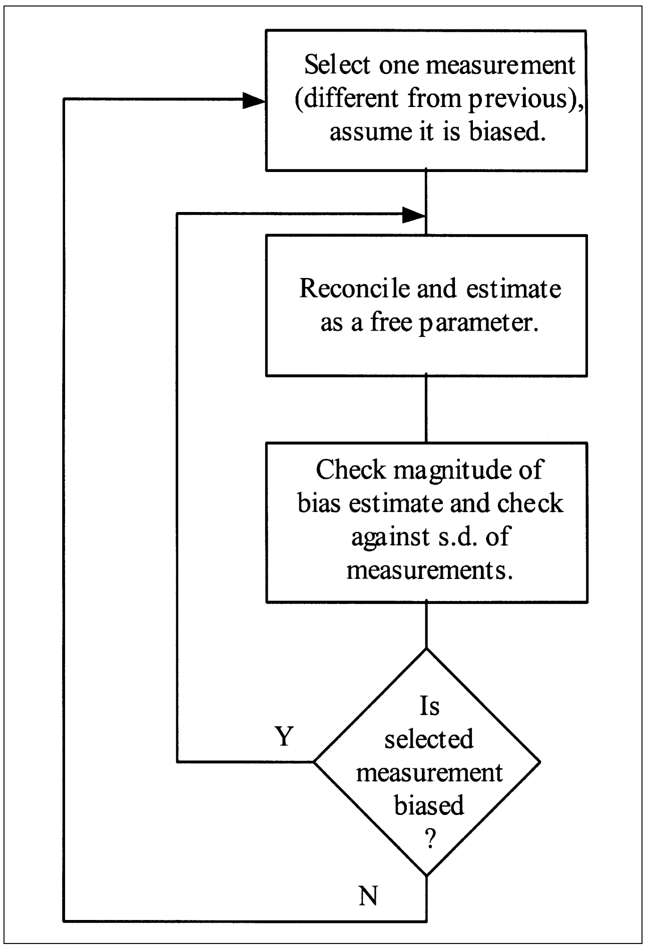

Figure 1. New bias detection and identification algorithm.

Detection and identification of outliers

Outliers which are often loosely referred to as gross errors are usually caused by nonrandom events where the measurement bears little or no relation to the true measurement value. Gross errors can be subdivided into measurement-related errors, such as malfunctioning sensors, and process-related errors such as process leaks. In general, data reconciliation schemes assume that the error is normally distributed. A gross error severely violates that assumption. It is therefore paramount that gross errors are identified and removed from the data prior to (or simultaneously with) the data reconciliation step.

Considerable effort has been expended on developing methods for gross error identification in steady-state chemical processes. Some of the first researchers to publish work on the subject were Almasy and Sztano (1975). Other prominent researchers in the field are Mah and Tamhane (1982), Serth and Heenan (1986), Narasimhan and Mah (1987), among many others. A number of good review articles are available on the subject (Mah, 1982; Mah, 1987; Crowe, 1996).

Only a handful of researchers have addressed the problem of gross error detection in dynamic process data. The method proposed by Chen and Romagnoli (1998), which is based on the moving horizon concept, is adopted in this work with some modification.

By making use of cluster analysis techniques, Chen and Romagnoli (1998) propose a method which successfully distinguishes outliers from normal data. They use a clustering technique proposed by Yin and Chen (1994) in which each object is assigned to the cluster of its nearest neighbor within a certain distance. The method is straightforward, the formulation of which is reproduced here.

Given a set of *nh* objects $y_1, y_2, \ldots, y_{nh}$, in a d dimensional space which refers to the number of measurement variables, the mean minimum distance (MMD) is defined as

$$MMD = \frac{1}{nh} \sum_{i=1}^{nh} \min_{j \neq i} \left[\left(\sum_{k=1}^{d} (y_{ik} - y_{jk})^2 \right)^{1/2} \right] \tag{17}$$

Because, in practice, the variations of individual measurements may be different, it is necessary to weigh each variable by its own variance. If this is not done, the result may be that some outliers might end up hidden within a smoother variable containing normal variations of noisy variables. Thus, Eq. 17 should be rewritten as

$$MMD = \frac{1}{nh} \sum_{i=1}^{nh} \min_{j \neq i} \left[\left(\sum_{k=1}^{d} \frac{(y_{ik} - y_{jk})^2}{\nu_k} \right)^{1/2} \right] \quad (18)$$

where ν_k is the kth diagonal element of the covariance matrix V.

In order to incorporate outlier information into the data reconciliation procedure, the objective function of dynamic data reconciliation is modified as

$$J = \sum \frac{1}{2} \{ W_i [y_i - \bar{y}_i] \}^T V^{-1} \{ W_i [y_i - \bar{y}_i] \} \quad (19)$$

where $\bar{y}_i$ is the estimate of the measurement y_i, W_i is the trust degree of y_i and is defined as

$$W_i = \begin{cases} 1 & \text{if } DIST_i \le 2 * MMD \\ \dfrac{2 * MMD}{DIST_i} & \text{if } DIST_i > 2 * MMD \end{cases} \quad (20)$$

Chen and Romagnoli define $DIST_i$ as being equal to the minimum distance between measurement y_i and any other measurements in the moving window. This is where this algorithm is slightly modified. The definition of $DIST_i$ is modified to being the distance from measurement y_i to the mean of all measurements $y_1, y_2, \ldots y_{nh}$ in the data window.

The reason for this modification is intuitive. Consider the situation where measurement y_i is an outlier and assume that in the present data window a measurement y_{i-k} has the same value or a value close to y_i. Using Chen and Romagnoli's definition of $DIST_i$, the algorithm would fail to detect this outlier. However, by using the mean of all the measurements in the data window as a basis for calculating $DIST_i$, the modified algorithm will detect the outlier y_i, and the appropriate value of W_i will be determined by Eq. 20.

The modified version was implemented along with the original method as outlined by Chen and Romagnoli (1998). Preliminary results on the CSTR case study discussed further in this article have shown that the slight modification does indeed improve the overall performance of the method.

Model-Based Predictive Control (MPC)

Model-based predictive control has been the subject of intensive research for about 20 years. Although the theoretical solutions have been available for some time, industrial application took place only recently due mainly to the lack of availability, at an acceptable price, of computing capacity (Balchen et al., 1992).

MPC has become a powerful tool for dynamic optimization and control. There are a number of different MPC schemes available, however, the basic idea behind them all is essentially the same and can be summarized as follows (Lee and Ricker, 1994).

- Predictions of future output behavior are calculated using a dynamic model of the process, based on past and predicted manipulated input moves and current and past output measurements.
- Optimization is then performed, based on the prediction, to find a sequence of input moves that minimizes a chosen measure of the output deviation from their respective reference values while satisfying all the given constraints.

Since the quality of prediction may improve as more measurements are collected, only the first of the calculated input sequences is implemented and the whole optimization is repeated at the next sampling time. This *receding horizon* implementation makes MPC a feedback control algorithm.

Various versions of MPC exist, but they are differentiated by the type of model they use and the cost function. The most well-known MPC algorithms are dynamic matrix control (DMC), model algorithmic control (MAC), and generalized predictive control (GPC). DMC was developed by Cutler and Ramaker (1980). MAC was developed by Richalet et al. (1978) and was originally known as model predictive heuristic control. GPC was developed by Clarke et al. (1987). There are a number of review articles on MPC such as Qin and Badgwell (1996), Garcia et al. (1989), and Eaton and Rawlings (1992) to name a few. A number of textbooks are also available on the subject, for example, Camacho and Bordons (1999).

For the purpose of this work, an MPC algorithm developed by Becerra et al. (1998a) has been used. This algorithm is based on state-space models, and the following is a brief outline of the algorithm.

In this model predictive control framework, a *receding horizon optimization problem* (RHOP) is solved at every sampling instant. The problem is formulated as follows

RHOP

$$\min_{\Delta u(k)} J(i) = \frac{1}{2} \Delta x(i+N)^T \Phi \Delta x(i+N) + \sum_{k=i}^{i+N-1} \Big\{ F(y(k), u_m(k)) + \frac{1}{2} \Delta x(k)^T Q \Delta x(k) + \frac{1}{2} \Delta u(k)^T R \Delta u(k) + P(y(k)) \Big\} \quad (21)$$

subject to

$$\Delta x(k+1) = A \Delta x(k) + B_m \Delta u_m(k) + \delta(k-i) B_d \Delta u_d(i) \quad (22)$$

$$\Delta y(k) = C \Delta x(k) \quad (23)$$

$$u_l \le u_m \le u_h \quad (24)$$

$$|\Delta u_m| \le u_r \quad (25)$$

$$\Delta u_m(k) = 0, \; M \le k \le N \quad (26)$$

where $F(y)$ is a steady-state objective, Φ, Q, R are weighting matrices of the appropriate dimensions, Δ is the increment operator (that is, $\Delta u(k+1) = u(k) - u(k-1)$), u_m is the vector of manipulated variables, u_d is the disturbance input, $\delta(k-i)$ is 1 when $k=1$ (0 otherwise (so the disturbance is assumed to be a step)), B_m, B_d are submatrices of the identified B matrix, $B=[B_m \quad B_d]$, N is the prediction horizon in samples, M is the control horizon in samples, and i denotes current time.

Output constraint violations along the predictions are corrected in Eq. 21 by means of the term $P(y(k))$. This implies that output constraints are treated as soft constraints. The penalty term is calculated from

$$P(y(k))=\sum_j \rho\left(P_\epsilon\left(\Psi_j(y(k))\right)\right)^2+\mu P_\epsilon\left(\Psi_j(y(k))\right) \quad (27)$$

where ρ and μ are scalar penalty factors. The output constraints are given by

$$\Psi(y(k))\leq 0 \quad (28)$$

and

$$P_\epsilon(\chi)=\begin{cases} \chi & \text{if } \chi>\epsilon \\ -(\chi-\epsilon)^2/4\epsilon & \text{if } -\epsilon\leq\chi\leq\epsilon \\ 0 & \text{if } \chi<-\epsilon \end{cases} \quad (29)$$

This type of penalty term, which combines quadratic and exact (linear) penalties, helps avoid problems when the output constraints are infeasible, but attempts to enforce active and feasible output constraints.

The steady-state objective function used in this work may be expressed as a linear function of inputs and outputs with combined economic and regulatory terms

$$F(y(k))=\frac{1}{2}(y(k)-y_r)^T Q_y(y(k)-y_r)+q^T y(k) + r^T u(k) \quad (30)$$

where Q_y is a weighting matrix of the appropriate dimensions, q and r are weighting vectors, and y_r is a vector of reference values for the outputs.

The optimization algorithm used to solve the receding horizon problem formulated above was Dynamic Integrated System Optimization and Parameter Estimation DISOPE (Becerra and Roberts, 1996).

Simulation Case Study

Simulations were carried out on a dynamic model of two continuous stirred tank reactors (CSTR) connected in series where an exothermic autocatalytic reaction takes place (Figure 2). The two units interact in both directions due to the recycle of a 50% fraction of the product stream into the first reactor. Regulatory controllers are used to control the temperature in both reactors, and the dynamics of these controllers are neglected. Full details of this model can be found in Garcia and Morari (1981) and are briefly outlined below.

The reaction that takes place in the reactors is

$$A+B \underset{k^-}{\overset{k^+}{\Leftrightarrow}} 2B \quad (31)$$

where one molecule of species A reacts with one molecule of species B to produce two molecules of species B and this reaction is reversible.

The dynamic equations describing the model are as follows

$$\left\{\begin{aligned} \frac{dC_{a1}}{dt}&=\frac{0.5}{\tau_1}(C_{a0}+C_{a2})-\frac{C_{a1}}{\tau_1}-\left(k_{1+}C_{a1}C_{b1}-k_{1-}C_{b1}^2\right)\\ \frac{dC_{b1}}{dt}&=\frac{0.5}{\tau_1}C_{b2}-\frac{C_{b1}}{\tau_1}+\left(k_{1+}C_{a1}C_{b1}-k_{1-}C_{b1}^2\right)\\ \frac{dC_{a2}}{dt}&=\frac{C_{a1}}{\tau_2}-\frac{C_{a2}}{\tau_2}-\left(k_{2+}C_{a2}C_{b2}-k_{2-}C_{b2}^2\right)\\ \frac{dC_{b2}}{dt}&=\frac{C_{b1}}{\tau_2}-\frac{C_{b2}}{\tau_2}+\left(k_{2+}C_{a2}C_{b2}-k_{2-}C_{b2}^2\right) \end{aligned}\right\} \quad (32)$$

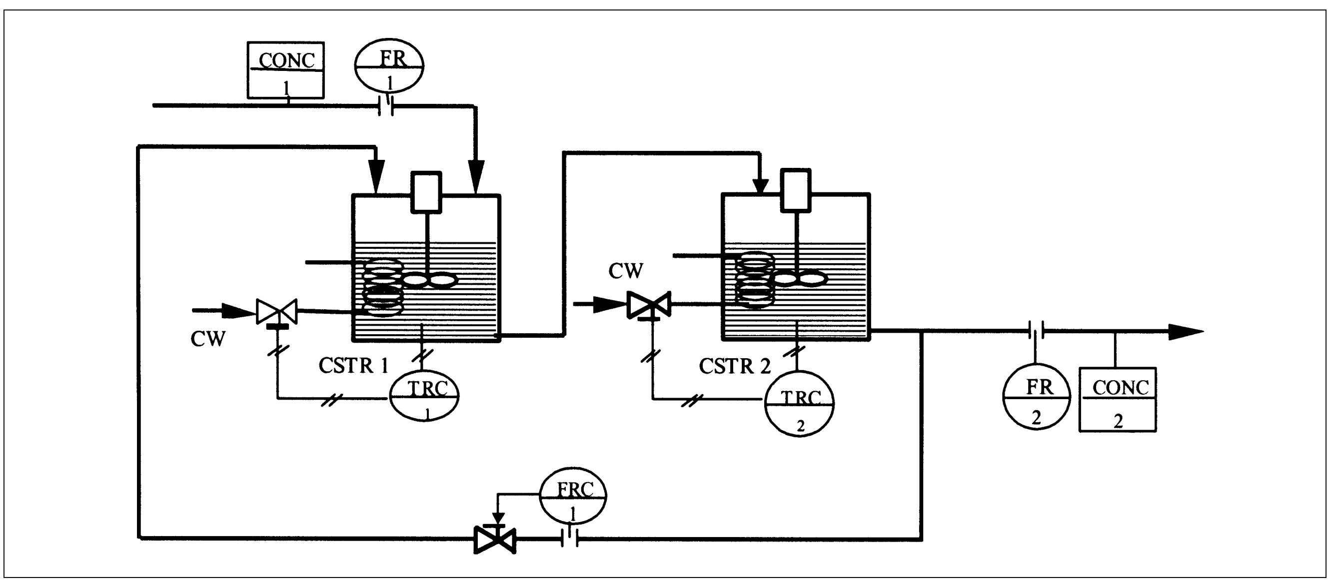

Figure 2. Simulation case study: two CSTRs connected in series.

where C_{xi} is the concentration of species x in tank i, $\tau_1 = 30$ [min] is the residence time of reactor 1, $\tau_2 = 25$ [min] is the residence time of reactor 2, $k_{i\pm} = A_{\pm}\ \exp(-E_{\pm}/RT_i)$ are the reaction rates, $E_{+}/R = 17{,}786$ [K], $E_{-}/R = 23{,}523$ [K], $A_{+} = 9.73\times10^{22}$ [m^3/Kmol s], $A_{-} = 3.1\times10^{30}$ [m^3/Kmols], $C_{a0} = 0.1$ [Kmol/m^3] is the feed concentration of A, T_1 is the temperature in reactor 1, T_2 is the temperature in reactor 2. Note that both temperatures are limited within the range

$$299.5 \le T_i \le 312.5,\ i = 1,2 \qquad (33)$$

In all the simulation cases that follow, the system was started from the steady-state condition given by the set points $T_1(0) = 307K$ and $T^2(0) = 302K$, which yield steady-state values $C_{b1}(0) = 0.05165[Kmol/m^3]$, $C_{b2}(0) = 0.05864$ $[Kmol/m^3]$. The sampling time for the measurements was 1 min. Note that the overall open-loop time constant of the process is approximately 40 min (Garcia and Morari, 1981). It is worth noting that the simulation times which appear in the results that follow relate to the real plant. The simulations would typically run at speeds of between 10 to 100 times faster depending on the computational load on the algorithm.

Implementation issues

The algorithms presented in this article have been implemented in C++ and interfaced to an industrial process simulator known as Aspen-OTISS from Aspen Tech (U.K.) Ltd. (SAST, 1993). OTISS is an interactive dynamic simulation system that allows its modular expansion by the user. Two case studies have been set up to show the benefits of using dynamic data reconciliation together with a model predictive control scheme. In the first case study (Figure 3) the model predictive controller acts directly upon the biased measurements from the plant. However, in the second case study

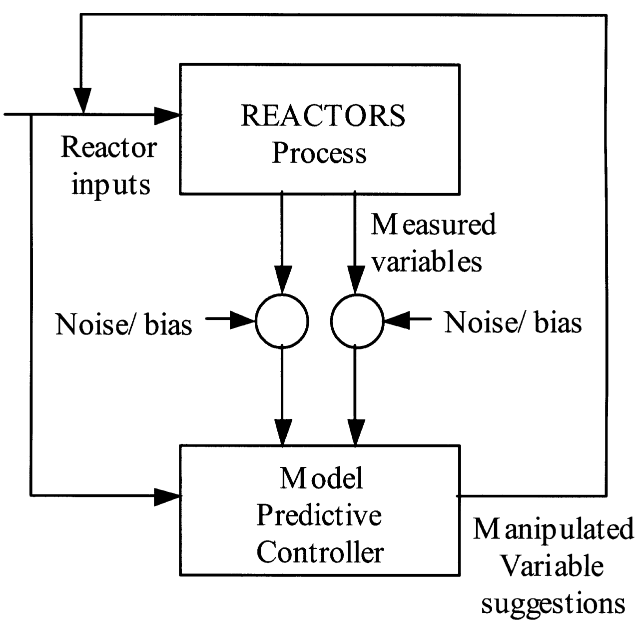

Figure 3. Case study 1: MPC without the use of dynamic data reconciliation.

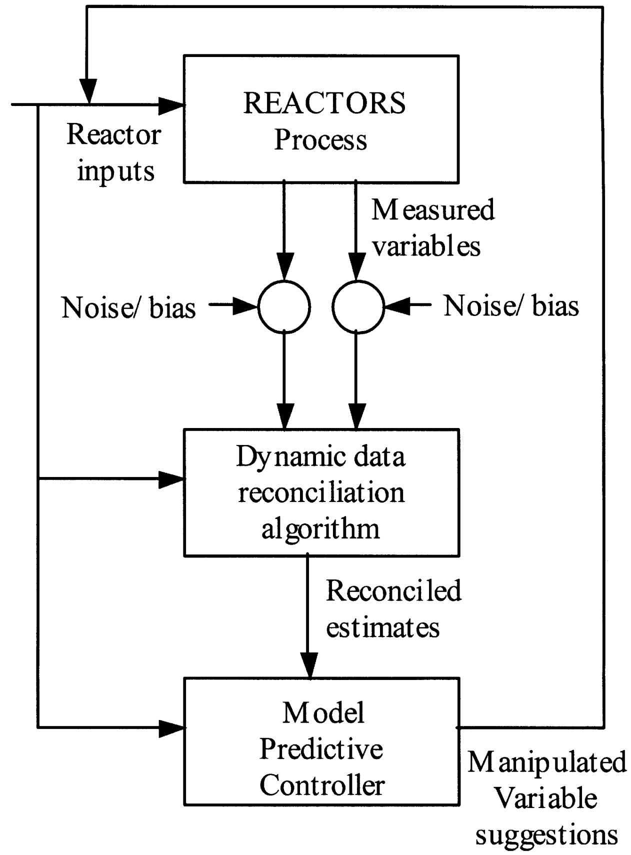

Figure 4. Case study 2: MPC using dynamic data reconciliation techniques.

(Figure 4) the measurements are first treated by the dynamic data reconciliation module before being passed to the model predictive controller.

The following tuning parameters for the predictive controller were used in the simulations: prediction horizon $N = 25$, incremental scaled state weight, $Q = I$, incremental weights on the scaled manipulated variables $R = diag(20000, 20000)$. The predictive controller used is adaptive and uses a moving horizon least-squares identifier (Becerra et al., 1998a). When data reconciliation was enabled, the reconciled values were passed to the module that implements the predictive controller and identification algorithm. A moving data window of reconciled values was used for periodically identifying the linear model. Therefore, the identified model benefited from data reconciliation. Data reconciliation was also active during the initial identification period. The tuning parameters used for the moving horizon scheme were: data window length $nh = 15$, integration step $= 10$ s and the covariance matrix $V = diag(0.5,0.5)$.

In order to simulate the effect of an outlier on the measurements, a bias was added to the measurement in question for a short period of time and then removed. The bias detection and identification algorithm works by applying two simple tests: the first tests the magnitude of the estimated bias and the second tests the bias against the standard deviation of the measurements. For a selected measurement to be suspected of bias, results from both tests must exceed some

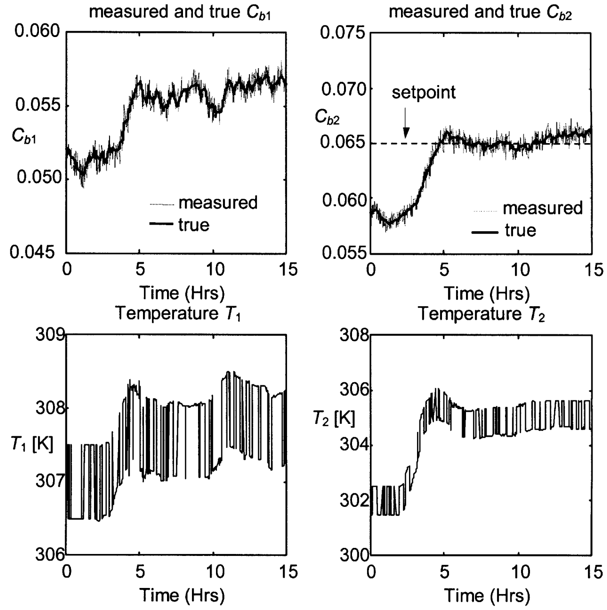

Figure 5. Measured and true C_{b1} and C_{b2}, as well as trends of the manipulated variables T_1 and T_2 when measurements are not biased; data reconciliation is disabled.

Objective: regulatory ($C_{b2} = 0.065$).

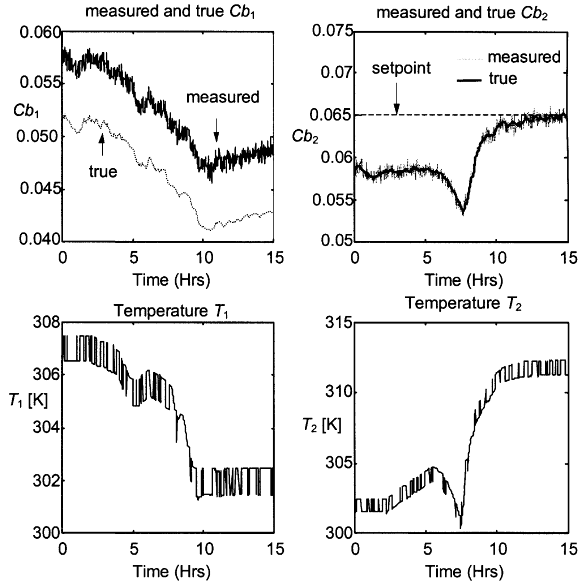

Figure 6. Measured and true C_{b1} and C_{b2}, as well as trends of the manipulated variables T_1 and T_2, bias on $C_{b1} = 0.00585$; data reconciliation disabled.

Objective: regulatory ($C_{b2} = 0.065$).

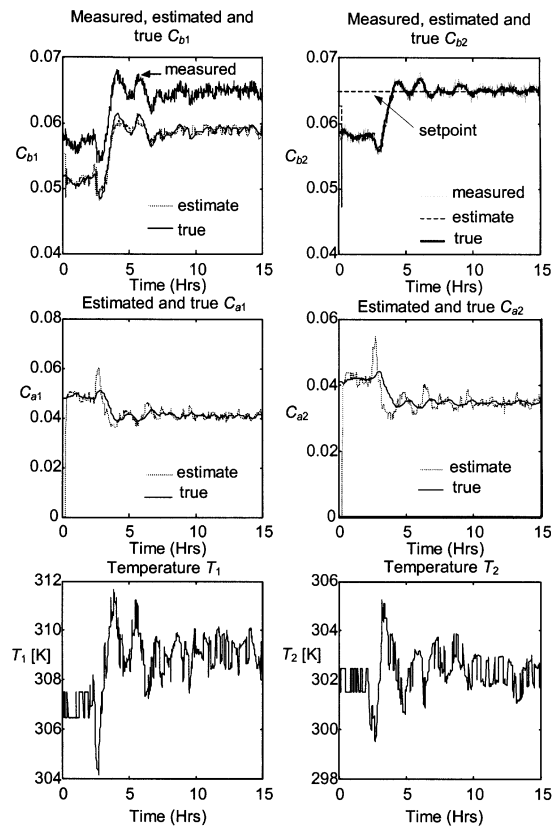

Figure 7. Measured, estimated and true C_{b1} and C_{b2}, estimated and true C_{a1} and C_{a2}, trends of manipulated variables T_1 and T_2, bias on C_{b1}, data reconciliation enabled.

Objective: regulatory ($C_{b2} = 0.065$).

pre-selected threshold values. A small absolute value of 0.00050 was selected for the first test while the second test is specifically

$$\text{if} \frac{\text{bias}}{\sigma} < 5.0 \tag{34}$$

where σ is the standard deviation of the measurements. Then, it is unlikely that bias is present on this particular measurement. The selection of the value 5.0 was inspired by the simulation results obtained by McBrayer and Edgar (1995).

The measured variables are assumed to be C_{b1} and C_{b2}, the concentrations of species B in the first and second tank, respectively. The unmeasured variables are assumed to be C_{a1} and C_{a2}, the concentrations of species A in the first and second tank, respectively.

Simulation Results

An objective function of the type $F(y_m,u_m) = (C_{b2} - 0.065)^2$ was first used. This reflects the desire to regulate the measurement C_{b2} at the value 0.065. Figure 5 shows the measured and true values of C_{b1} and C_{b2}, as well as the temperatures which are the manipulated variables of the plant. The excitation signal, which can be seen superimposed on the manipulated variables, is due to the fact that the MPC scheme used is adaptive and uses a moving horizon least-squares identifier. In this instance there are no bias or outliers on the measurements. It can be seen that in this case the controller manages to regulate C_{b2} about the set point. This behavior should be compared to Figure 6 where a systematic bias of magnitude 0.00585 is present on measurement C_{b1}. The deterioration in response due to the bias is evident. Figure 7 shows the same case where this time the data is first reconciled prior to the model predictive control stage. It can be observed that, by using data reconciliation, the predictive controller is able to meet the required regulatory objective with increased accuracy and speed. The other sub-figures in Figure 7 show the true and estimated values of the unmeasured variables C_{a1} and C_{a2}, as well as the trends of the manipulated variables T_1 and T_2. Notice that there is an initial identification period of 2 h when the predictive controller is not in operation. Although the reactors start from the same steady-state conditions in Figures 5 and 7, the final steady-state conditions are different, despite using the same predictive control algorithm with the same controller settings. In the case of Figure 7, the only difference is the presence of the moving horizon estimator (plus a bias in the measurement of C_{b1}). Although the bias is correctly estimated, the system is driven by the controller to a different steady state as compared with Figure 5 that also provides the desired value for C_{b2} (= 0.065). It may be noticed that the control problem in the regulatory case has one controlled variable C_{b2} and two manipulated variables T_1 and T_2. The fact that the system is driven to a different steady state by the controller makes the response of C_{b2} look different in Figures 5 and 7 due to the nonlinear nature of the reactors, despite the controller having the same tuning in both cases. The steady-state solutions can be checked by specifying the reactor temperatures T_1 and T_2, and solving the resulting system of nonlinear Eqs. 32 with the time derivatives set to zero.

The second type of objective function tested is a combined economic and regulatory objective. This is of the form $F(y_m, u_m) = (C_{b1} - 0.060)^2 - C_{b2}$ and reflects the desire to

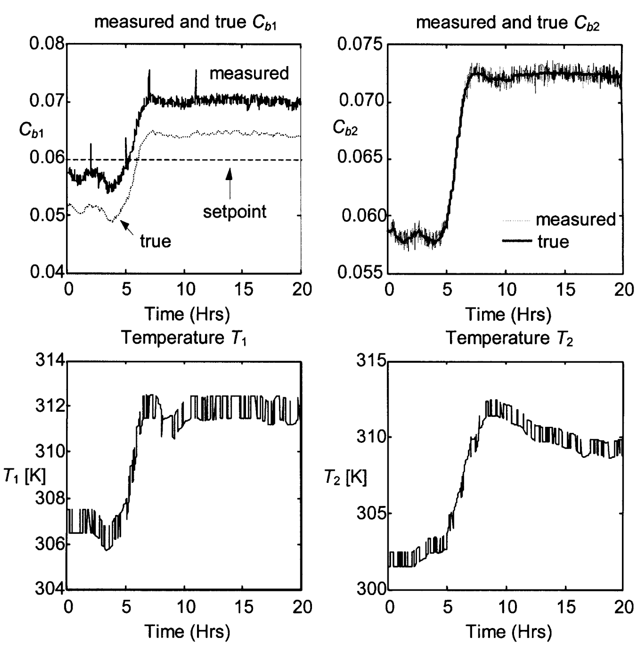

Figure 8. Measured and true C_{b1} and C_{b2}, as well as trends of the manipulated variables T_1 and T_2, bias and outliers on C_{b1}, data reconciliation disabled.

Objective: combined (regulate C_{b1} at 0.060 while maximizing C_{b2}).

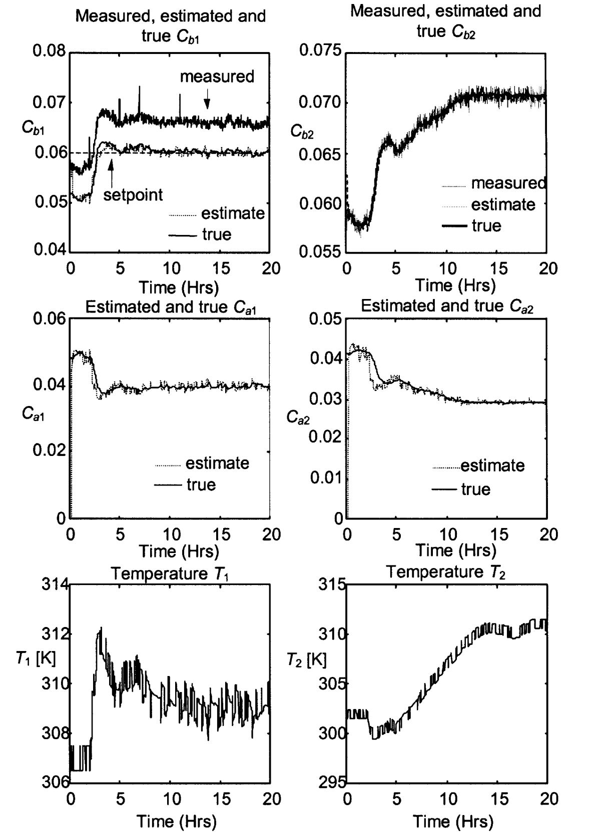

Figure 9. Measured, estimated and true C_{b1} and C_{b2}, estimated and true C_{a1} and C_{a2}, trends of manipulated variables T_1 and T_2, bias and outliers on C_{b1}, data reconciliation enabled.

Objective: combined (regulate C_{b1} at 0.060 while maximizing C_{b2}).

regulate measurement C_{b1} at a value of 0.060 while trying to maximize the product C_{b2}. Figures 8 and 9 show the case when this objective function is used. Figure 8 shows the case where data reconciliation is not employed. It can be observed that while C_{b2} is maximized, the controller fails to regulate the measurement C_{b1} at its set point because temperature T_1 reached an upper limit constraint (312.5 K). However, Figure 9, in which data reconciliation is enabled, shows the fact that C_{b1} is closely following the set point while the controller attempts to maximize C_{b2}.

Conclusions

Dynamic data reconciliation techniques have been combined with a model-based predictive control scheme and the utility of the approach has been successfully demonstrated using a simulation case study consisting of two coupled chemical reactors under model predictive control. It has been shown that the overall performance of the model-based predictive controller improves considerably when the data is first reconciled prior to being fed to the controller. The scheme effectively compensates measurement data contaminated by systematic bias and outliers. Research continues on applying the described dynamic data reconciliation technique to further case studies.

Acknowledgments

This work is supported by the United Kingdom Engineering and Physical Research Council, Grant No. GR/L64478.

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Manuscript received Nov. 22, 2000, and revision received Aug. 8, 2001.