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On-Line Dynamic Data Reconciliation Incorporating Dynamic Simulation

Rodolfo Téllez-Schmill* William Y. Svrcek† Brent Young‡

*SNC-Lavalin, Inc., rodolfo.tellezschmill@snclavalin.com
†University of Calgary, svrcek@ucalgary.ca
‡University of Auckland, b.young@auckland.ac.nz

On-Line Dynamic Data Reconciliation Incorporating Dynamic Simulation

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Abstract

The formulations for dynamic data reconciliation found in the literature assume that the error minimization problem is solved as a non-linear optimization problem constrained by the material and energy balances in the form of time-dependant non-linear differential equations. In this paper we introduce a new approach or an unconstrained formulation of this problem using a dynamic process simulator or model calculator and its potential application to chemical process control.

1. INTRODUCTION

The main objective of data reconciliation is to estimate the "true" values xi of measured process variables yi by reducing to the extent possible the effect of random or systematic measurement errors, through the minimization of such errors. In reality chemical process are dynamic, and thus a dynamic data reconciliation approach is required if the estimation of time dependant process variables is needed. The formulation of this minimization procedure is stated as a constrained least-squares estimation problem, represented by Equation 1, where the weighted sum of errors by the covariance of the data is minimised subject to constraints represented by Equation 2 (e.g. Narasimhan & Jordache, 2000 and Romagnoli and Sánchez, 2000).

$$\min_{x_i} \sum_{i=1}^{n} \varepsilon_i^T \Psi^{-1} \varepsilon_i \qquad (1)$$

$$\text{s.t. } \dot{x}(t) = f\left(x(t), u(t), t\right) \qquad (2)$$

where ε is the measurement error,

$$\varepsilon_i = y_i - x_i \qquad (3)$$

and Ψ is the covariance matrix of the measured variables *y*. Using this formulation one can adjust a finite number, *n*, of the process measurements, *y*, to obtain values, *x*, which meet the dynamic material and energy balances, Equation 2.

Recent references on dynamic data reconciliation (DDR) (e.g. Zhou, *et al*., 2004) still deal with the resolution of a non-linear problem, such as a continuous stirred tank reactor (CSTR) through the implementation of several strategies to solve the constrained optimization problem. In this article an alternate new formulation is presented to solve the minimization of errors problem, through the use of a process simulator or a model calculator that will transform the constrained optimization problem to an unconstrained minimization problem. In addition, a potential and promising industrial application is provided that improves the performance of a PID controller.

2. NEW FORMULATION

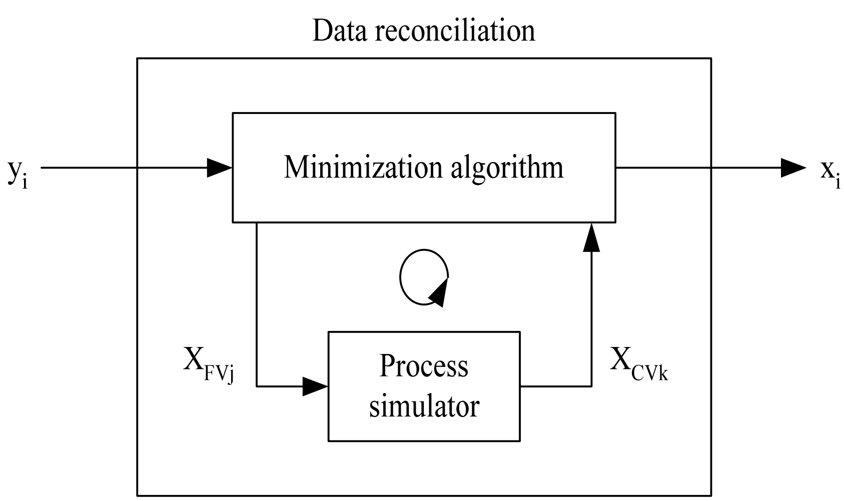
Process simulators or model calculators are designed and built to solve either the steady-state or dynamic material and energy balance equations that represent chemical process unit operations, and embed the thermodynamic calculations needed for these modeling calculations. These tools utilize first principles models, or other types of models derived by other techniques (e.g. Baker, *et al*., 2005) and do always meet the material and energy balance constraints. Hence, the constrained optimization problem formulated by using of Equations 1 and 2 is transformed into an unconstrained optimization problem, Equation 4.

$$\min_{x_j}\left(\sum_{j=1}^{n_{FV}}\varepsilon_j^T\Psi_{FV}^{-1}\varepsilon_j+\sum_{k=1}^{n_{CV}}\varepsilon_k^T\Psi_{CV}^{-1}\varepsilon_k\right) \quad (4)$$

where n_{FV} is the number of free variables, or degrees of freedom in the simulation, and n_{CV} is the number of calculated variables.

The material and energy balance constraints are implicit in the calculation of the calculated variables. The classical data reconciliation constrained optimization problem, represented by Equation 1, becomes a semi-constrained optimization problem. Figure 1 shows schematically how this concept can be applied to data reconciliation.

Figure 1. Data reconciliation scheme



For the solution of the unconstrained optimization problem, several algorithms were tested. It was found the Lavaguard-Mayhem (Fletcher, 2000) optimization

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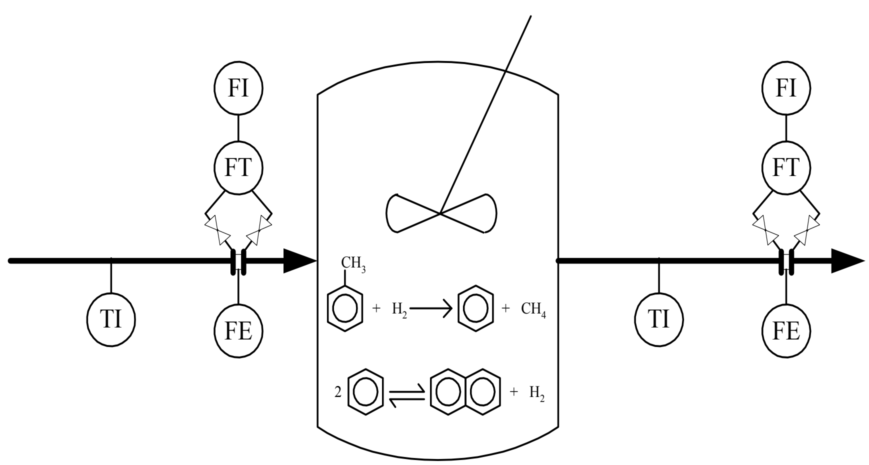
method worked well for this kind of application, and also required a relative limited number of lines of code. However, the disadvantages of using Newton's method are that there is no guarantee that a global minimum/maximum will be found and these methods require a Jacobian (Hessian) at each iteration. Moreover, scaling factors are required to ensure the stability of calculations (Dennis and Schnabel, 1996). Thus the objective function is normalized, in order to attenuate the effect of the magnitude of the different measurement units.

2.1. Steady-state data reconciliation

To illustrate the application of this new formulation, the steady-state data reconciliation of both flow and temperature for the reactor of the HDA plant (Luyben, *et al.,* 1999) is presented. The HDA process reactor is shown in Figure 2, with complete process details being furnished by Luyben *et al.* (1999). Using Aspen-HYSYS® v. 3.2 (Aspen Technology Inc.) measurements of inlet and outlet flow rates and temperatures containing white noise were provided from the simulation. Only free variables are adjusted by the optimization routine, in this case both inlet flow rate and temperature, while both free and calculated variables are used in the objective function. Calculated variables in this case are both outlet flow rate and temperature. Reconciled data were computed using a rigorous steady-sate model of a continuous stirred tank reactor in Excel ® 2000 (Microsoft Corp.). The Aspen-HYSYS simulation acted as a real plant and Excel acted as an on-line dynamic data reconciler.

Figure 2. Chemical reactor of the HDA plant



Figures 3 and 4 show the results of the reconciled data. It is important to note that the trend of the reconciled data depends on the number of free and calculated variables. In this case we have more free variables than calculated ones, and the trend of the former is to follow the nosy data, while the later is closer to the average value. In some sense reconciliation of data "filters" the measurements, opening the door for application is process control as it will be discussed further.

2.2. Dynamic data reconciliation and moving horizon estimator

The dynamic data reconciliation problem will be solved utilizing the moving horizon estimator (MHE), proposed by Abu-el-zeet *et al*., (2002). This estimation problem is defined as a non-linear dynamic optimization problem with a discrete time performance index and a continuous time model with constraints.

Figure 3. Inlet and outlet flow rates

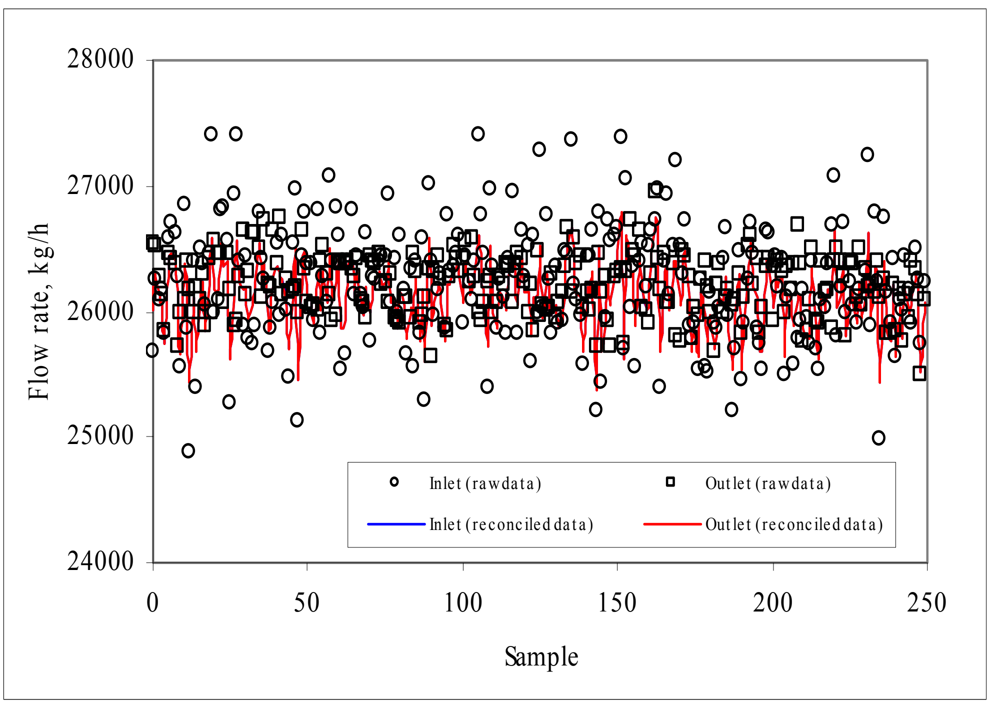
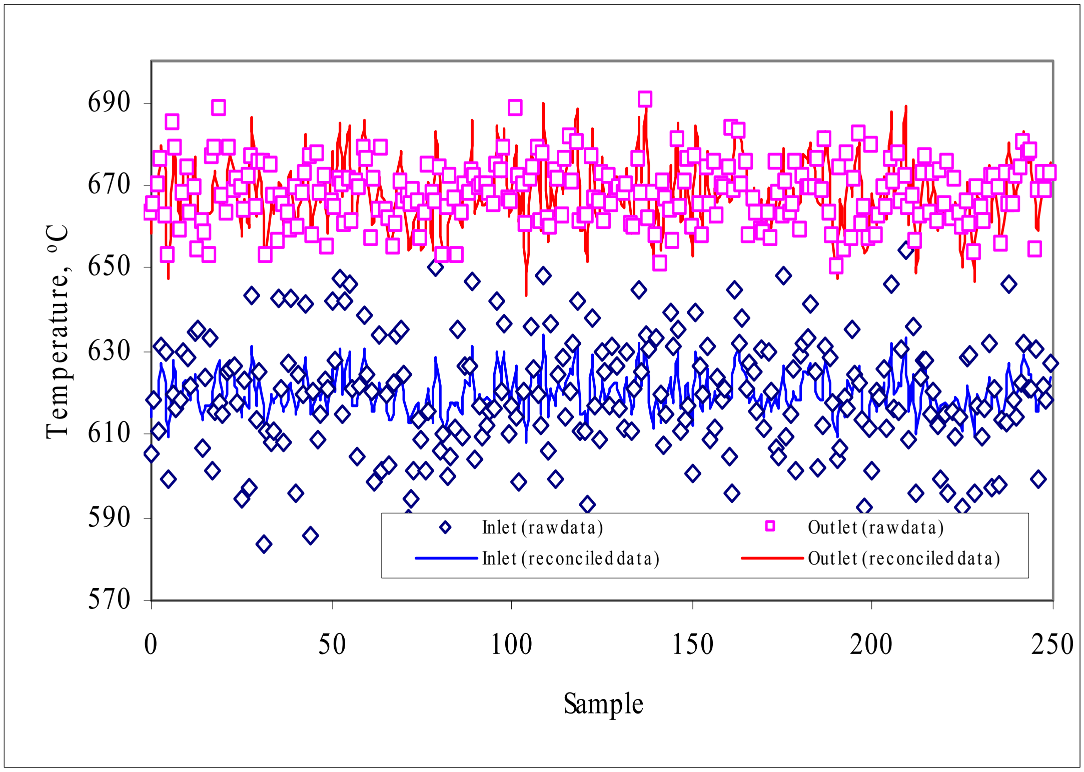


Figure 4. Inlet and outlet temperatures



The moving horizon estimation problem consists of the minimization of a weighting function L, Equation 5, which in fact is a variation of Equation 1.

$$\min_{x_0} J = \sum_{i=0}^{nh-1} L\big(z(t_0 + i\Delta t), y(t_0 + i\Delta t), i\big) \tag{5}$$

$$\text{s.t} \quad \dot{x}(t) = f\big(x(t), u(t), t\big) \tag{6}$$

$$x(t_0) = x_0 \tag{7}$$

$$z(t) = C\big(x(t), u(t), t\big) \tag{8}$$

where $\boldsymbol{x(t)}$ is the state vector of process variables, nh is the most recent time at which data is available, t_0 is the initial time, t is the current time and Δt is the sampling time interval. $u(t)$ is the degrees of freedom vector (manipulated variables) that guarantee feasible operation, z in Equation 8 is the vector of model outputs, and t_0 is the initial time of the dynamic process.

3. PROCESS CONTROL APPLICATION

A number of authors (e.g. Abu-el-zeet, *et al*., 2002 and Zhu, *et al*., 2004) have discussed process control applications that contain dynamic data reconciliation, in particular advanced control strategies, such a model predictive control (MPC). In this paper one potential application of dynamic data reconciliation is the filtering of control signals, particularly the filtering of noise for the derivative action of controllers. This application is of interest to industry and its implementation is easier and less costly than MPC applications. The idea here is to use an on-line dynamic data reconciliation routine that not only reconciles data for inventory requirements, but also does data filtering for a distributed control system (DCS), since the derivative action of a PID controller amplifies the noise in a noisy signal (Marlin, 2000 and Svrcek, *et al.,* 2000). In order to tackle this problem, instead of using conventional filters, reconciled data can be utilised as filtered data for the DCS or other process monitoring systems, e.g. real time optimisation (RTO), as shown in Figure 5. To implement this application, sampling time is an issue. The sampling time depends on how fast the control loop must be and the processing time of the data reconciliation routine. To be effective the sampling times in the range of 100 ms for flow and pressure controllers are required, which often creates application issues. For temperature loops, sampling times are in the range of 10 to 20 seconds. In this situation dynamic data reconciliation is attractive. Note, similar slow response loops are also good candidates for this application.

A non-linear dynamic case study of a tube and shell heat exchanger was used to test this new approach, Figure 6. The hot stream is liquid benzene entering at 140^{o}C, flowing on the shell side of the heat exchanger at a rate of 100 kg/h and leaving at 48^{o}C. The coolant is water at 20^{o}C. The heat exchanger shell volume is 0.4 m^3 and tubes volume is 0.3 m^3. An Aspen-HYSYS® simulation was again utilised as a surrogate plant, and Excel® 2000 (Microsoft Corp.) as the on-line dynamic data reconciler . The idea here is to control the outlet temperature of the hot stream by manipulating the flow rate of the cooling water stream using a standard PID digital controller. Comparison with a Kalman filter (e.g. Grewal & Andrews, 2001) is presented in order to show the advantages of MHE and the new solution formulation versus established techniques that have been applied for nearly forty years for dynamic data reconciliation. Process control applications of Kalman filtering and dynamic data reconciliation are found in the open literature (e.g. Musulin, *et al*., 2005 and Vachhani, *et al.*, 2005).

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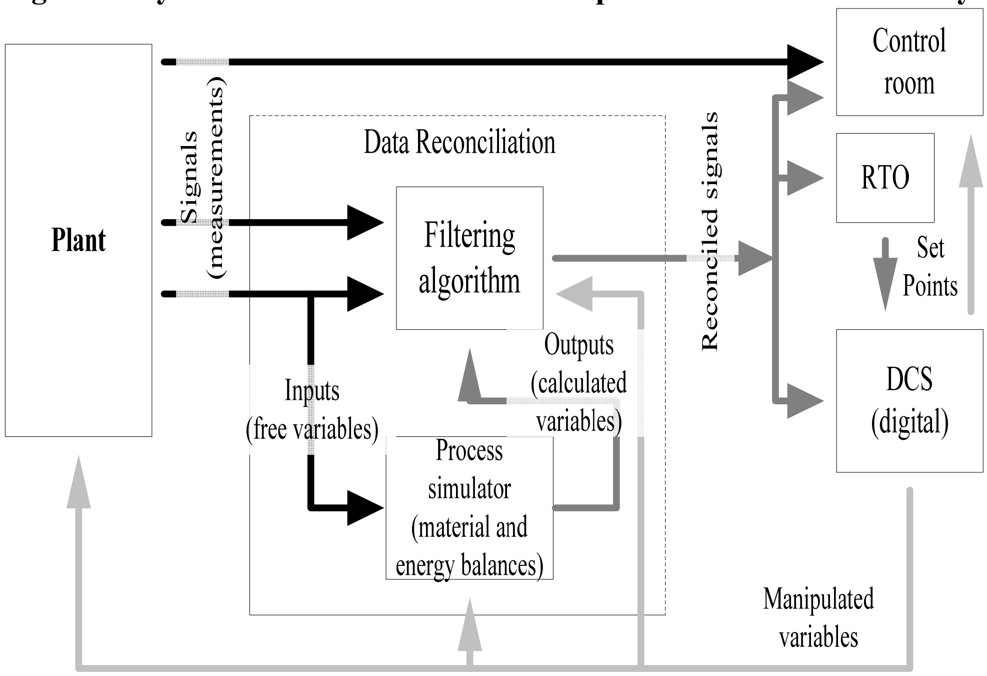
Figure 5. Dynamic data reconciliation on top of a distributed control system



Material and energy balances differential equations in the time domain were transformed to difference equations by using the fourth order Runge-Kutta method. Reconciliation of raw data was performed by solving Equations 5 to 8, using the new proposed formulation and the appropriate initial values x_0 of both free variables and calculated variables, for each measurement made at each time $t_0 + i\Delta T$. Since the free variables and calculated variables are available, the free variables are used in the optimization routine and the calculated variables are used in the objective function.

Several scenarios are provided that consist of a set point change in the aromatics outlet temperature, from 48°C to 60°C, when no noise is present and therefore no data reconciliation is required and when the signal is noisy and no data reconciliation is applied. Figure 7 provides a comparison of the performance for a set point change in the temperature control for these two scenarios.

Other two scenarios were studied, when Kalman filtering is used and when MHE filtering is utilised. Figure 8 shows the behaviour of the manipulated variable for the same set of temperature set point changes.

Figure 6. Dynamic case of a tube and shell heat exchanger

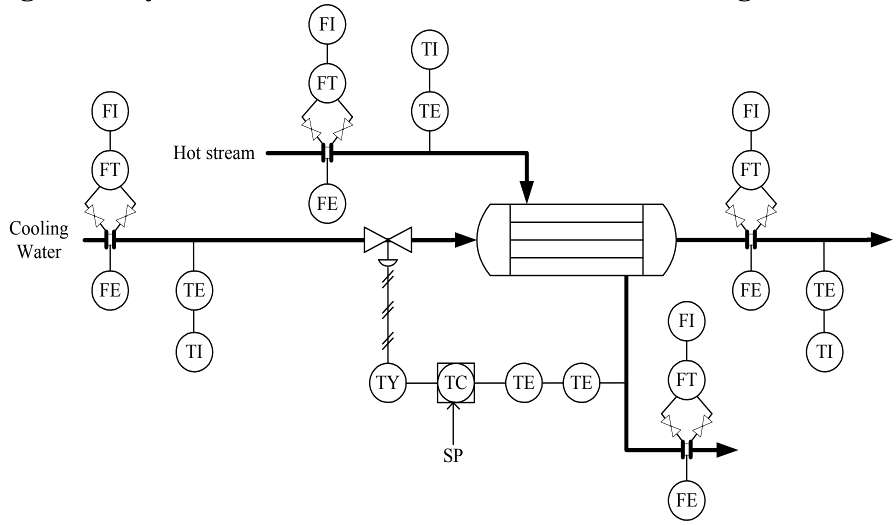


Figure 7. Outlet temperature response to a set point change, PID controller with no data reconciliation.

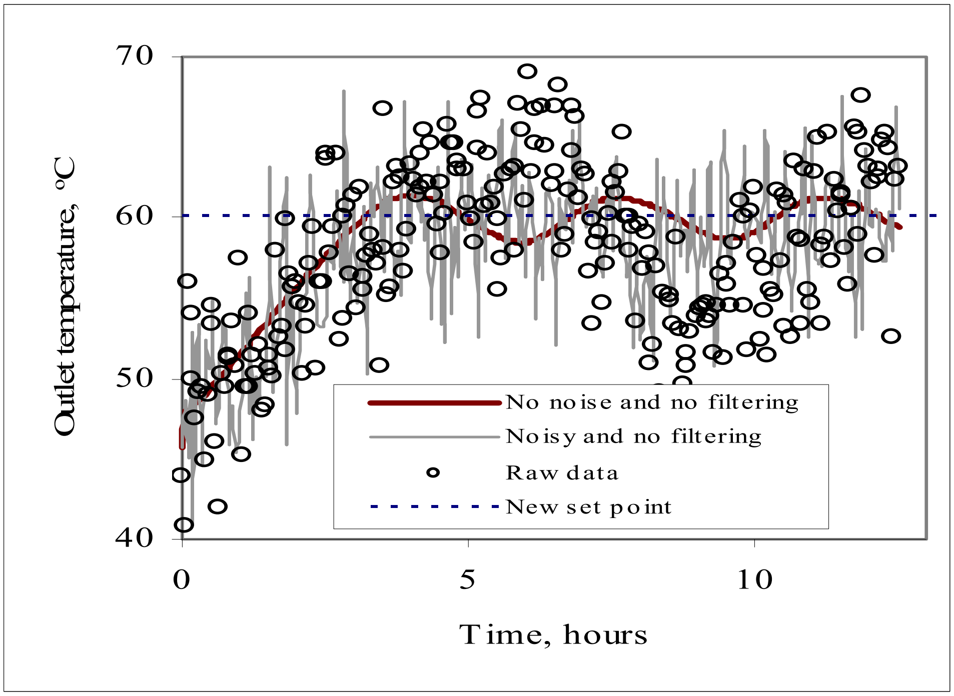


Figure 8. Outlet temperature response to a set point change, PID controller with data reconciliation

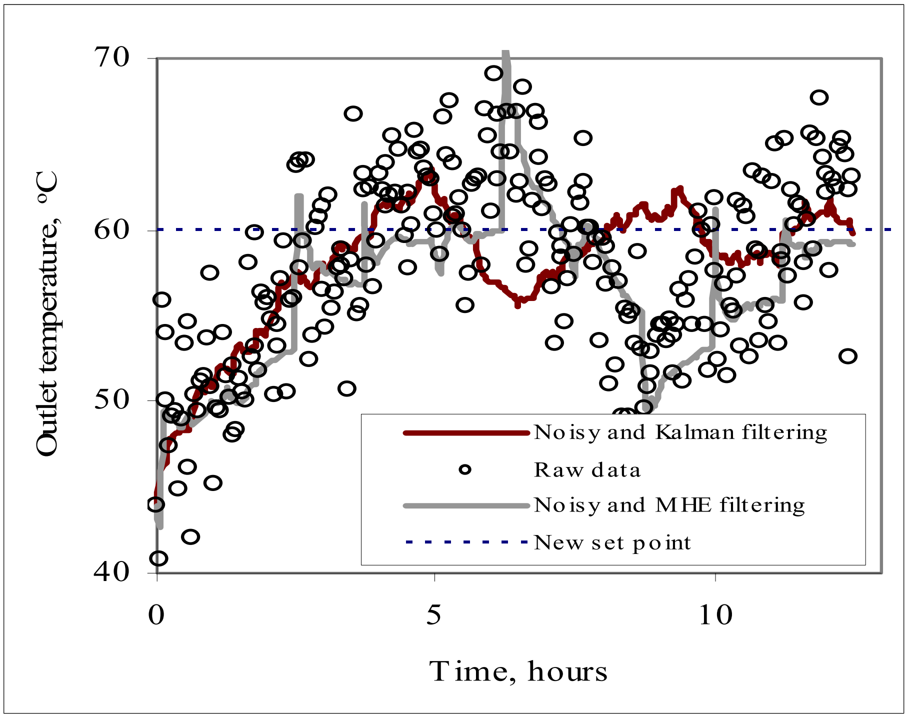


Figure 9. Manipulated variable response to a set point change.

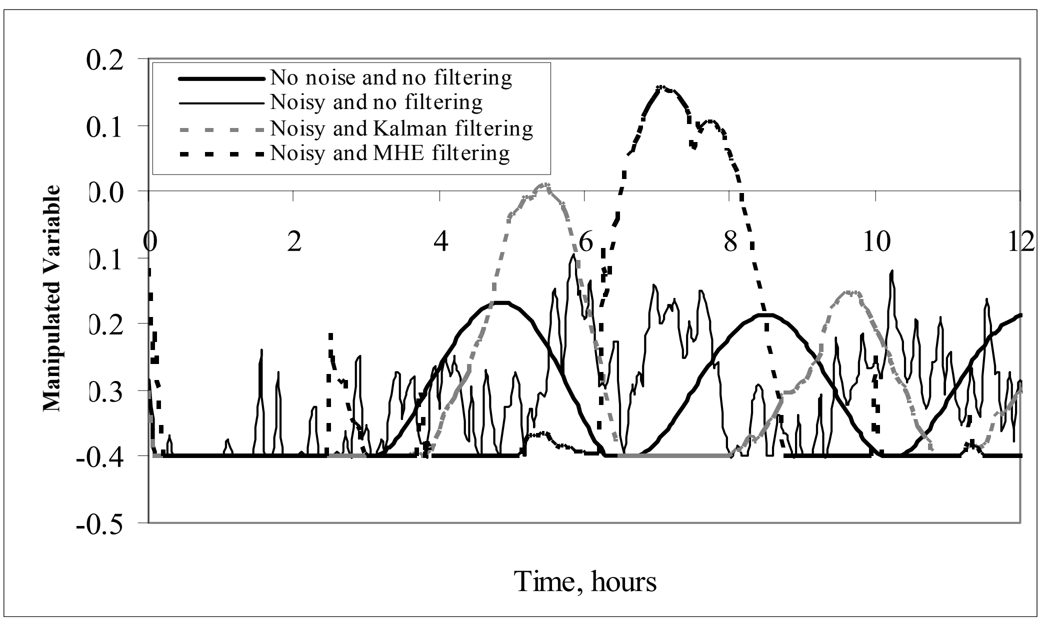


Figure 7 does indeed show the PID controller without filtering amplifies the noise. In Figure 8 the Kalman filtering technique shows an improvement, although some noise is observed, but its amplitude is not as large as the case with no filtering. MHE shows some noise as well, and the overshoots are due to the prediction horizon, which in this case is 2 hours. The new approach can be improved by determining how the values in the previous prediction horizon affect the performance of the MHE filtering. Figure 9 shows the behaviour of the manipulated variable. It is interesting to note that Kalman and MHE filtering show a smooth variation of the manipulated variable, which is useful from an operational perspective, however there is a maximum variation in both cases when the process variable crosses the set point and the controller is struggling to settle the process variable. Again, MHE filtering does overshoot when changing the prediction horizon.

4. CONCLUSIONS

It was shown that the use of a process simulator or a surrogate model a process can be successfully utilised in dynamic data reconciliation and effective transforms a constrained optimization problem into an unconstrained optimization problem. This approach results in standard unconstrained optimization algorithms with relatively fewer code lines and less computational effort and time being utilised.

The filtering of plant data is a very promising application for process control, particularly for those control loops for which the sampling time is long enough to allow computations before taking any control action on the process. The dynamic behaviour of manipulated variables is improved when noise is mitigated, and it permits utilising the full advantage of the derivative action of PID controllers.

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