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USING SUB-MODELS FOR DYNAMIC DATA RECONCILIATION

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Abstract: The optimal approach for dynamic data reconciliation consists in using a complete and exact process model. Unfortunately, such a model is difficult to obtain in industrial practice. Through an example, several observers based on static, stationary and dynamic sub-models are designed and compared to the optimal approach. The comparisons illustrate that, for the given conditions, static observers generally lead to estimates that are less precise than the measurements. Stationary observers are slightly more precise than static observers but they obviously lack the power of temporal redundancy offered by dynamic models. Deterministic dynamic sub-models, that do not include all physical parameters (thus relatively easy to obtain), which stochastic models are added to, are shown to give good performances.

Keywords: Observers, Singular systems, Measurement noise, Kalman filters, Stochastic modelling.

1. INTRODUCTION

All actions taken to optimize or control a process should be based on the best estimates available for present and past states of the process. Sensors provide measurements of only some of the states and measurement errors are inevitably present. Measurement errors can be gross errors or random measurement noises. Only the later will be addressed in this paper. The objective of data reconciliation is to provide estimates of unmeasured states and to reduce the effects of measurement noise on the measured states. The estimates calculated by data reconciliation must at least satisfy reliable physical constraints such as the equations of mass or energy conservation.

In industry, by far the most popular technique is static data reconciliation which is usually based on static mass conservation as first proposed by Kuehn and Davidson (1961). The main reason for its popularity is certainly that the process modeling is simplified by using only static mass balancing. Several papers have been written on this topic and many references can be found in review papers and books (Crowe, 1996; Romagnoli and Sanchez, 1999; Narasimhan and Jordache, 2000). The fact that applying static data reconciliation on a real-time basis to a dynamic process could be worse than using directly the measurements, as illustrated by Almasy (1990), does not seem to limit the extensive use of this technique in industry. Good results may indeed be expected with static reconciliation for time-averaged data applications such as real-time optimization or metallurgical accounting. However, control applications require dynamic data reconciliation.

On the other hand, although the modeling part is the most difficult task in practice for dynamic data reconciliation, the assumption made by most of the authors is that the exact process model is known. Indeed, the papers are often focused on introducing (Liebman, et al., 1992) or comparing dynamic reconciliation methods (Ramamurthi, et al., 1993). However model mismatch could lead to severely biased estimates (Dochain, 2003). Because of this lack of observer robustness, it is probably better in many practical cases to use a reliable sub-model instead of a complete model with uncertain parameters. The static mass balance is the most popular sub-model but not appropriate for true dynamic applications. Fortunately, other sub-models such as stationary and dynamic sub-models remain very simple while being frequently adequate for dynamic reconciliation.

In their paper, Darouach and Zasadzinski (1991) proposed the use of a generalized Kalman filter for performing dynamic mass balancing. This generalized state space representation and the associated filter and smoother algorithms allow using sub-models for dynamic data reconciliation. They will be extensively used in this paper.

The above process observer is based on the basic lumped dynamic mass conservation equation, without any attempt to model either mixing or material transportation mechanisms or chemical reactions kinetics. Unfortunately, dynamic data reconciliation relying only on this equation usually result in poor filtering ability, and requires the measurement of the process inventories for warranting process observability. Almasy (1990) proposed to use the same dynamic mass conservation equation, while adding the dynamic empirical constraint that species flows behave as random walks. As in the paper by Darouach and Zasadzinski (1991), the mixing and kinetic mechanisms were not addressed in this paper, and the inventory was supposed measured. Furthermore, the problem of tuning the random walk variances is not discussed in the paper. To our knowledge, Stanley and Mah (1977) were the first to introduce the idea of random walks in data reconciliation by coupling them to steady-state conservation equations. A qualitative discussion on how to tune the random walks can be found in their paper.

In this paper, the simulated plant is a continuously stirred tank reactor (CSTR) where only mass balance phenomena are considered. In contrast to most papers, the feed concentration is not supposed to be a deterministic manipulated variable but is defined as a disturbance modeled by a stationary stochastic process. Using the simulated plant, the study objective is to compare thirteen observers based on unbiased sub-models. The benchmark observer is designed from a model identical to the simulator. Four steady-state, four stationary and four dynamic observers are compared to the benchmark. The plant models are of varying complexity including or not including mixing or kinetics information; and adding or not adding empirical stochastic models for stream flow rates modelling.

2. A CONTINUOUSLY STIRRED TANK REACTOR (CSTR)

A CSTR process is simulated to compare the various observers. Heat balance phenomena are not considered, however this would not impair the validity of the presented qualitative discussions and conclusions. From this simple CSTR model, several sub-models are extracted, leading to a variety of observers.

The chemical reaction taking place in the CSTR is a first order irreversible reaction $A \rightarrow B$. The Euler discretization of the differential mass balance equations leads to:

$$\begin{aligned} D_A(k) &= c_{Ai}(k) - c_{Ai}(k-1) \\ &= -K_0\, c_{Ai}(k-1) + \frac{Q}{V}\left(c_{Af}(k-1) - c_{Ao}(k-1)\right) \end{aligned} \tag{1}$$

$$\begin{aligned} D_B(k) &= c_{Bi}(k) - c_{Bi}(k-1) \\ &= K_0\, c_{Ai}(k-1) - \frac{Q}{V} c_{Bo}(k-1) \end{aligned} \tag{2}$$

where Q is assumed to be constant and perfectly known input and output flowrate; V is the known volume of the tank; c_{Af}, c_{Ai} and c_{Ao} are the variations of concentration of species A around their nominal value respectively in the feed flow, the tank inventory and the output flow; the same notation is used for species B which is not present in the feed (c_{Bi} and c_{Bo}); D_A and D_B are the accumulation rates for species A and B; K_0 is the rate constant of the reaction. Table 1 gives the numerical values of this CSTR simulator.

In addition to mass conservation Equations (1) and (2), perfect mixing is assumed:

$$c_{Ai}(k) = c_{Ao}(k) \tag{3}$$

$$c_{Bi}(k) = c_{Bo}(k) \tag{4}$$

It is straightforward to verify that inserting (3) and (4) into (1) and (2) leads to usual equations for a CSTR. The feed concentration is defined by the following stationary stochastic process:

Table 1. CSTR numerical values

	V	10 L	α	0.9
	Q	2 L/s	σ_ξ^2	0.1
	K_0	1 s^{-1}	σ_{Af}	13.06%
Nominal value	$\overline{C}_{Af}$	5 mol/L	σ_{Ao}	13.32%
	$\overline{C}_{Ao}$	0.833 mol/L	σ_{Bo}	10.81%
	$\overline{C}_{Bo}$	4.167 mol/L		

$$c_{Af}(k) = \frac{\alpha}{1-\alpha Z^{-1}}\xi(k) \qquad (5)$$

where $\xi(k)$ is a zero mean Gaussian white noise of variance σ_ξ^2 that generates variations on the five concentrations. Table 1 lists the standard deviations of these variations (σ_{Af} , σ_{Ao} and σ_{Bo}) expressed in percentage of the corresponding nominal values.

The five measurements are obtained by adding a Gaussian white noise to each concentration. The relative standard deviation of each independent measurement noise is 5% of the corresponding nominal value (thus defining the matrix Σ introduced in Section 3).

Having σ_{Af} , σ_{Ao} and σ_{Bo} larger than the measurement noise standard deviation contributes to obtaining static reconciliation estimates less precise than measurements, as discussed by Almasy (1990). This is a strong incentive for using dynamic data reconciliation.

The objective of the paper is to compare the performances of thirteen observers, using always the same measurement information (the measured values of the five concentrations), while varying the information content in the observer model. The minimum information used is either the steady-state or the dynamic mass conservation constraints. It can be enriched by the information on the reaction kinetics and/or by the information on the mixing properties, and/or by empirical information on the stochastic behaviour of the species flows on the two streams. The observer performances are always compared to the optimal filter based on the complete exact model used for simulation. All the observers are derived using the generalized Kalman filter which is first succinctly described in the next section.

3. THE GENERALIZED KALMAN FILTER

Since all the state variables are measured in this work, the following generalized state space representation is used to design the observers:

$$E\,x(k) = A\,x(k-1) + w(k) \qquad (6)$$

$$y(k) = x(k) + v(k) \qquad (7)$$

where E is usually a singular matrix and

$$x(k) = \left[c_{Af}(k) \;\; c_{Ai}(k) \;\; c_{Bi}(k) \;\; c_{Ao}(k) \;\; c_{Bo}(k)\right]^{\mathrm{T}} \qquad (8)$$

The covariance matrices W and Σ respectively define the properties of the process noise w and the measurement noise v. The corresponding filtering and smoothing algorithms (Darouach and Zasadzinski, 1991) are:

$$\hat{x}(k+1/k+1) = \Sigma E^T \Omega(k) A\hat{x}(k/k) + \left(I - \Sigma E^T \Omega(k)\, E\right) y(k+1) \qquad (9)$$

$$\hat{x}(j/k+1) = \hat{x}(j/k) + P(j/k)\,A^T \Omega(k)\left(E\,y(k+1) - A\hat{x}(k/k)\right) \qquad (10)$$

$$P(k+1/k+1) = \Sigma - \Sigma E^T \Omega(k) E \Sigma \qquad (11)$$

$$P(j/k+1) = P(j/k)\,A^T \Omega(k) E \Sigma \qquad (12)$$

where $\hat{x}(j/k+1)$ is the estimate of the vector x at time j based on the knowledge of measurements up to time $k+1$ ($j<k+1$).

The matrix $\Omega(k)$ is not defined as in Darouach and Zasadzinski (1991) since a process noise is added to the state Equation (6). It is defined by :

$$\Omega(k) = \left(W + E\Sigma E^T + AP(k/k)A^T\right)^{-1} \qquad (13)$$

4. THE VARIOUS OBSERVERS

Thirteen different observers are designed. Only the observer described in Section 4.1 uses the complete and exact information about the process. In this sense, it defines a benchmark for all other observers that rely on sub-models providing incomplete information about the process. The upper part of Table 2 summarizes the model equations used for each observer.

The mass conservation constraint, which is the minimal information used in the observers is :

$$D_A(k) + D_B(k) = \frac{Q}{V}\left(c_{Af}(k-1) - c_{Ao}(k-1) - c_{Bo}(k-1)\right) \qquad (14)$$

It is obtained by adding (1) and (2) and states that the total number of moles must be conserved. An important practical advantage of this equation is that it does not assume any mechanism for mixing and reaction kinetics.

4.1 Observer based on the complete exact process model

The smoothing obtained by this observer (observer 1 in Table 2) corresponds to the best possible results since it uses the same model as the one being used for process simulation, i.e. (1) to (5). The parameter K_0 is supposed to be exactly known (which is the case for all observers requiring Equations (1) and (2)).Measurement redundancy is provided by the fact that the process is perfectly mixed and that the inventory and output concentrations are independently measured.

The generalized state space representation (6) and (7) for the observer model (1) to (5) is obtained with:

$$E = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & -1 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix} \quad (15)$$

$$A = \begin{bmatrix} \frac{Q}{V} & 1-K_0 & 0 & -\frac{Q}{V} & 0 \\ 0 & K_0 & 1 & 0 & -\frac{Q}{V} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \alpha & 0 & 0 & 0 & 0 \end{bmatrix} \quad (16)$$

$$W = diag([0 \quad 0 \quad 0 \quad 0 \quad 0.081]) \quad (17)$$

One can observe that, in this particular case, the matrix E is non singular. Defining matrices *E, A* and *W* to put the model equations in a form corresponding to the generalized state space representation will be omitted for other observers since the procedure is very similar.

4.2 Steady-state observers

The model equations used by the four static observers are detailed in Table 2 (observers 2.1 to 2.4). The fundamental characteristic of all static observers is that accumulation rates D_A and D_B are set to zero in (1), (2) or (14). The resulting model for each observer can be described by:

$$E\,x(k) = 0 \quad (18)$$

i.e. $A = 0$ and $W = 0$ in (6). Since $A = 0$, the generalised Kalman filter Equations (9) to (13) does not provide smoothing but only filtering, due to the absence of temporal redundancy.

Instantaneous static observers have been considered in this paper and thus horizon-based static observers are not studied.

4.3 Stationary observers based on the dynamic conservation equation

For these four observers (observers 3.1 to 3.4 in Table 2), the accumulation rates in Equations (1), (2) or (14) are considered as strongly stationary stochastic process instead of being set to zero as for static observers. The resulting models all have the following structure

$$E\,x(k) = w(k) \quad (19)$$

where the covariance matrix W appears as a tuning parameter. The best choice for W is

$$W = E\,X\,E^T \quad (20)$$

where X is the covariance matrix of the generalized state vector x. In practice, calculating (20) is impossible since only the measurements are available (not x). Work is underway to propose practical solutions to this issue. Nevertheless, for fair comparison purposes, W will be calculated using (20). As with static observers, smoothing is not possible, when using only instantaneous observations.

4.4 Observers based only on the dynamic conservation constraint

For setting comparisons to dynamic observers defined in 4.5, a dynamic data reconciliation similar to the one proposed by Darouach and Zasadzinski (1991), i.e. based only on the dynamic conservation Equation (14) (thus $W = 0$), is tested (observer 4 in table 2).

4.5 Dynamic conservation equation with stochastic models for molar flows

These observers are build using the deterministic Equation (14) combined with the following empirical stochastic descriptions of the molar flows:

$$C_{Af}(k) = \beta\, C_{Af}(k-1) + w_2(k) \quad (21)$$

$$C_{Ao}(k)+C_{Bo}(k)=\gamma\left(C_{Ao}(k-1)+C_{Bo}(k-1)\right)+w_3(k) \quad (22)$$

The resulting model again corresponds to (6) with:

$$W = diag([0 \quad W_2 \quad W_3]) \quad (23)$$

The parameters β, γ, W_2 and W_3 have to be determined. Three different cases have been considered (observers 5.1 to 5.3 in Table 2). The first case, inspired by the work of Almasy (1990), assumes random walk behaviours, i.e. $\beta = \gamma = 1$. The second case assumes white noise behaviours, i.e $\beta = \gamma = 0$. For theses two cases, since the parameters β and γ are set, Equations (21) and (22) allow to compute w_2 and w_3 from a set of simulated data, without measurement noise, and therefore to tune W_2 and W_3. The third case uses an identification procedure to estimate β (0.90) and γ (0.94) from the true state signals. The identification residuals provide W_2 (0.081) and W_3 (0.0076). Again, the procedure to obtain the parameter values is based on unavailable true states, but this is an appropriate procedure for the objective to obtain the best possible tuning for each observer.

5. RESULTS AND ANALYSIS

Since the observers are not biased, they can be compared by evaluating the standard deviation of the

relative estimation error (second part of Table 2). For each observer, 2500 samples were simulated.

As already mentioned, it is not surprising that, for this combination of process and instrumentation, steady-state observers are in general worse than measurements. The exception is observer 2.2 which provides good estimates for four variables. This performance is explained by the redundancy provided by the inventory measurements and the perfect mixing constraints. When comparing observers 2.3 and 2.4 to observer 2.2, it can be concluded that in this case no gain is made by adding steady-state kinetic modeling even with the exact knowledge of parameter K_0. Furthermore, all the static observers are unable to increase the precision of the feed concentration probably because its dynamics are too fast to be reconciled in real time with steady state modeling.

Stationary observers produce estimates with better accuracy than measurements, but some variables are significantly less filtered than others. Stationary observer 3.4 which uses the most complete information among the stationary observers gives the best results. This is different from the steady-state observer 2.4 behaviour, because of the adequate tuning of the stationary accumulation rate variances. Nevertheless, the best performance of any stationary observer still remains far from the benchmark, mainly because only instantaneous filtering is possible with stationary observers. To benefit from temporal redundancy and to make smoothing possible, dynamic observers need to be introduced.

The dynamic observer 4 exhibits performances equivalent to those of stationary observers 3.1 and 3.3, because the information contained in the dynamic mass conservation constraint is equivalent to the statistical information on the accumulation rates in the stationary observers. However the dynamic observer 4 is worse than the best stationary observer 3.4 and also worse than 3.2, even if the later ones do not use temporal redundancy. The reason is related to the redundancy created by the perfect mixing constraints.

This gives motivation for using the additional modeling Equations (21) and (22) which are empirical equations that remain to be tuned. Observer 5.1 is indeed doing significantly better than observer 4 because the random walk assumption is a reasonable approximation of the autocorrelated behaviours of the output and input signals. Observer 5.2 is not significantly better than observer 4, because the white noise assumption ignores the temporal correlation of the flowrates variations. Observer 5.3 is a little more precise than observer 5.1. This small improvement is explained by a better selection of β and γ, which are slightly smaller than one, the value used for random walks.

6. CONCLUSION

Several sub-models of the same process were proposed to design steady-state, stationary and dynamic data reconciliation algorithms.

Steady-state observers may produce estimation errors which are larger than measurement errors. This is the consequence of neglecting process dynamics, when the process variable variance due to dynamics is larger than the variance induced by measurement errors, a case that was simulated in the present study. Unfortunately, this is the usual industrial situation, thus precluding the use of such algorithms for real time data reconciliation, although it seems to be an increasingly popular approach in industry.

Stationary observers, which allow mass accumulation rates to statistically deviate from zero, are an efficient alternative to steady-state observers for real time data reconciliation. They produce estimates that are more reliable than measured values, while requiring only a rough estimate of the accumulation rate variances. Although they are noticeably less efficient than filters based on full process models, they are simple to build and tune.

Dynamic observers, based on the minimal dynamic information consisting of the mass conservation constraints (observer 4), are not significantly better than stationary observers, because of the low level of information redundancy. However they are better than steady-state observers forcing static mass conservation (observer 2.1).

The dynamic filter can be improved by adding empirical information to the dynamic mass balance constraint, such as stochastic models of time evolution of flow characteristics evolution. The empirical models can be identified from the experimental data, or simply assumed to be random walks.

The stationary or dynamic proposed observers are all significantly less precise than the optimal observer using the full phenomenological model of the process (observer 1). However, great care must be taken if considering the design of an observer based on a complete dynamic model, since biases may result from badly identified model parameters. The main advantage of the proposed observers is a modeling effort that is considerably less important. This advantage becomes even more important in real applications where several units, such as the one presented in this paper, are present in the plants. Indeed, the observers are mainly based on conservation equations defined by few or no parameters, combined with stochastic modeling that may be tuned from experiments.

The present work was limited to linear systems in the Kalman filtering framework. Similar conclusions could probably be drawn for nonlinear dynamic data reconciliation based on nonlinear programming.

Table 2. The observers and their performances

		Benchmark	Steady-state				Stationary				Dynamic			
		1	2.1	2.2	2.3	2.4	3.1	3.2	3.3	3.4	4	5.1	5.2	5.3
Observation model	A, B species balance - Equations (1) and (2)	X			X*	X*			X**	X**				
	Mixing – Equations (3) and (4)	X		X		X		X		X				
	Mole conservation - Equation (14)		X*	X*			X**	X**			X	X	X	X
	Feed generator – Equation (5)	X										X	X	X
	Stochastic flows – Equations (21) and (22)											X	X	X
Relative estimation error	A feed	2.23	5.82	6.60	5.15	5.66	4.46	4.31	3.97	4.07	4.72	3.30	4.53	3.30
	A inventory	2.63	4.99	3.54	5.19	4.56	4.96	3.52	4.17	3.14	4.91	4.90	4.85	4.90
	B inventory	0.89	5.03	3.95	5.01	5.53	5.06	3.35	4.91	3.25	2.12	1.96	2.10	1.95
	A output	2.63	5.18	3.54	4.92	4.57	4.99	3.52	5.08	3.14	5.05	4.92	4.95	4.92
	B output	0.88	5.52	3.95	6.10	5.53	4.53	3.35	4.33	3.25	4.87	2.38	4.50	2.35
	Sum of relative variances***	20.37	141.38	99.83	139.98	134.88	115.52	65.80	101.81	57.41	100.10	68.61	93.21	68.43

* Accumulation rates D_A and/or D_B are set to zero.
** Accumulation rates D_A and/or D_B are described by a zero mean stochastic processes.
***The measurement relative estimation error is 5.00 % for each variable, and leads to a sum of relative variances of 125.

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