Data Reconciliation in Generalized Linear Dynamic Systems

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A generalized linear dynamic model or singular model, for which the standard state space representation and the Kalman filtering cannot be applied, is used to develop a new algorithm to solve the linear dynamic material balance problem. This algorithm is based on the method developed in the steady-state case and leads to a recursive scheme, which is very useful in real-time processing. It reduces the computational problem such as singularities and round-off errors that may occur in complex systems. Convergence conditions are given and verified for the dynamic material balance case.

Introduction

Data reconciliation is of fundamental importance in plant operation due to inaccuracies and uncertainties in the measurements. Most previous works have been limited to the steady-state systems described by linear and bilinear constraints involving unknown parameters (Hlavacek, 1977; Mah, 1981; Tamhane and Mah, 1985; Mah, 1987). In many practical situations, however, the process conditions are continuously undergoing changes, and the steady state is never truly reached.

A quasisteady-state system described by an algebraic model, a measurement equation, and a transition equation defined by a random walk process was treated by Stanley and Mah (1977). It was shown that estimation in this case can be an application of the discrete Kalman filter. Darouach et al. (1988a) have proposed a new algorithm based on Kalman filter and sequential processing developed by additional constraints.

Data reconciliation for linear dynamic systems was treated by Gertler and Almasy (1973). They showed that the dynamic material balance model can be represented by continuous-state space equations or after discretization by a sampled input-output representation. For this representation, Gertler (1979) showed that solving this problem in an optimal way is too complicated to allow a general closed-form solution and a suboptimal approach was presented. Narasimhan and Mah (1988) have extended the formulation of the hypothesis of the GLR (generalized likelihood ratio) method proposed by Willsky and Jones (1974) for the gross error identification in closed-loop dynamic processes decribed by a stochastic linear discrete model. Almasy (1989a,b) presented the dynamic balance equations in state space models form, in which the environmental effects (EE) are described by a random walk process. The data reconciliation in this case are reduced to a discrete Kalman filter as in the quasisteady-state problem.

This article presents a new on-line estimation algorithm for the systems of dynamic material balance equations. The model considered is linear and deterministic with all the variables measured (inputs, outputs, and states). This model can be written in discrete difference equations form $EX_{k+1}=BX_k$, where X_k is the vector formed by all the unknown variables at time instant k. These equations, containing more variables than constraints, cannot be written in a standard state equation form. This model is called a singular or generalized dynamic model (Dai, 1989), because the matrix E is singular and therefore the standard Kalman filter cannot be applied to estimate X_k. Generally this type of model is used to represent dynamical systems described by a set of differential-algebraic equations. These models can be applied to such fast subsystem as exchangers and such slow subsystem as heaters. The dynamics of the fast subsystem can be neglected relative to that of the slow subsystem. Differential algebraic equations are suitable for these processes. A recursive optimal solution in weighted least squares sense is proposed to estimate vector X_k. The convergence conditions are given and verified for the dynamic linear balance equations.

Problem Statement

We consider a linear time-invariant system described by a process network formed by n nodes and v streams. The material balance equations can be written in the following discrete form:

$$W^*_{i+1}=W^*_i+MQ^*_{i+1} \tag{1}$$

where Q^*_{i+1} is the true vector of the flows of dimension v at time instant $(i+1)$, and W^*_i is the true vector of the volumes of dimension n at time instant i. M is the $n \times v$ incidence matrix of full row rank. The element m_{ij} of M denotes the topology of nodes and streams with $m_{ij}=1$ if stream j is an input to node i, and $m_{ij}=-1$ if stream j is an output from node i.

For simplicity, we assume that the balance equations contain only measured variables. The measurements are given by

$$Q_i = Q^*_i + v_i \tag{2}$$

and

$$W_i = W^*_i + w_i \tag{3}$$

where v_i is a $v \times 1$ vector of normally distributed random measurement noise with zero mean and known covariance matrix $V_Q > 0$, and w_i is an $n \times 1$ vector of normally distributed random measurement noise with zero mean and known covariance matrix $V_W > 0$.

Equation 1 can be written

$$-EX^*_{i+1} + B\,X^*_i = 0 \tag{4}$$

where

$$X^*_i = \begin{pmatrix} W^*_i \\ Q^*_i \end{pmatrix},\ E = (I \mid -M) \text{ and } B = (I \mid 0).$$

Also Eq. 2–3 become

$$Z_i = X^*_i + \epsilon_i \tag{5}$$

where

$$Z_i = \begin{pmatrix} W_i \\ Q_i \end{pmatrix} \text{ and } \epsilon_i = \begin{pmatrix} w_i \\ v_i \end{pmatrix}$$

with ϵ_i is a $(n+v) \times 1$ vector of normally distributed random measurement noise with zero mean and known covariance matrix

$$V = \begin{pmatrix} V_W & 0 \\ 0 & V_Q \end{pmatrix} \tag{6}$$

Our aim is to estimate X_i based on the measurement Eq. 5 and the model (Eq. 4).

Derivation of the Estimation Algorithm

Here we consider the problem of estimating the vector X_i at time instants $i = 1, 2, \ldots, k+1$. From Eqs. 4 and 5 we can collect the $(k+1)$ measurements and the k constraints as follows:

$$Z = X^* + \epsilon \tag{7a}$$

$$\Phi_k\, X^* = 0 \tag{7b}$$

where $Z = (Z_i)$, $X^* = (X^*_i)$, $\epsilon = (\epsilon_i)$ for $i = 1$ to $k+1$ and

$$\Phi_k = \begin{pmatrix} B\text{-}E\,0 & \ldots & 0 \\ 0\; BE\,0 & \ldots & 0 \\ \cdots & \cdots & \cdots \\ 0 & \ldots & 0\,B\text{-}E \end{pmatrix} = \begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \vdots \\ \varphi_k \end{pmatrix}$$

Now with these notations, dynamic data reconciliation problem can be formulated as in the steady-state case, that is, the minimization of

$$J = \frac{1}{2}(\hat{X} - Z)^T\, V^{-1}\, (\hat{X} - Z) \tag{8a}$$

subject to the constraint

$$\Phi_k\, \hat{X} = 0 \tag{8b}$$

The solution of this problem is given by:

$$\hat{X} = PZ \tag{9}$$

where P is the projection matrix

$$P = I - V\Phi_k^T(\Phi_k\, V\, \Phi_k^T)^{-1}\,\Phi_k \tag{10}$$

From Eqs. 9–10 we can see that the computational volume increases with a number of observations, which leads to several numerical problems such as round-off errors and singularities. To avoid these, a recursive solution based on the sequential method developed for the steady-state case (Darouach et al., 1988b) can be proposed. Matrix Φ_k is partitioned as follows:

$$\Phi_k = \begin{pmatrix} \Phi_{k-1} \\ \varphi_k \end{pmatrix} \tag{11}$$

where the $nx\,[(k+1)(v+n)]$ matrix φ_k is the kth block of n rows of matrix Φ_k given by

$$\varphi_k = (0 \mid 0 \ldots 0 \mid B \mid -E) \tag{12}$$

Matrix Φ_k is a full row rank matrix, if matrix pencil $(sE - B)$, where s is a complex variable, is of full row rank (Gantmacher, 1959). We can apply the result of Appendix A to obtain the following algorithm.

The estimates $\hat{X}_{j/k+1}$ of the vector X_j at time instant j based on the knowledge of measurements up to time $k+1$ $(j < k+1)$ is given by

$$\hat{X}_{j/k+1} = \hat{X}_{j/k} + \Sigma_{jk}^k B^T \Omega_k (EZ_{k+1} - B\hat{X}_{k/k}) \tag{13a}$$

$$\hat{X}_{k+1/k+1} = VE^T\Omega_k B\hat{X}_{k/k} + (I - VE^T\Omega_k E)\,Z_{k+1} \tag{13b}$$

and its covariance matrices are

$$\Sigma_{j(k+1)}^{k+1} = \Sigma_{jk}^k B^T \Omega_k\, EV \quad \text{for } j < k+1 \tag{14a}$$

$$\Sigma_{(k+1)(k+1)}^{k+1} = V - VE^T\,\Omega_k\, EV \tag{14b}$$

where

$$\Omega_k = (B\Sigma_{kk}^k B^T + EVE^T)^{-1} \qquad (14c)$$

with the initial conditions $\hat{X}_{1/1} = Z_1$ and $\Sigma_{11}^1 = V > 0$.

The recursive expressions of Eqs. 13 and 14 constitute a generalized algorithm of the Kalman filter in the absence of process noise and represent a systematic approach to real-time linear filtering (Eq. 13b) and smoothing (Eq. 13a) with a well-established optimality criterion. Standard Kalman filter can be obtained from Eqs. 13–14 with $E = I$.

Equations 13 and 14 are obtained only under the assumption that matrix pencil $(sE - B)$ is of full row rank. The model (Eq. 4) is general; since E may be singular, it can include algebraic equations.

Before turning to the application of the above algorithm to the initial problem described by Eqs. 1–3, we can analyze its asymptotic properties and give sufficient conditions for its convergence.

Convergence Analysis of the Algorithm

The stability properties of the filter given by Eqs. 13–14 are considered here since the filter's stability is important from both practical and theoretical points of view. Stability refers to the behavior of estimates given by Eqs. 13.

From Eq. 13b we can see that the state transition matrix of the filter is $\Psi_k = VE^T\Omega_k B$, which is a function of sequence Ω_k. From Eq. 13a, the new estimate $\hat{X}_{j/k+1}$ is given by the prior estimate $\hat{X}_{j/k}$ plus an appropriately weighted measurement residual $(EZ_{k+1} - B\hat{X}_{k/k})$. If sequence Σ_{jk}^k converges to zero when k increases, then there is no significant change in the new estimate. This implies that the filter memory is limited, and the estimate can be calculated only on the fixed number of measurements.

It is easy to see that expression 14a can be rewritten as a system of $(n+v) \times (n+v)$ matrix difference equation:

$$Y_{k+1} = \Psi_k \, Y_k \qquad (15)$$

where

$$Y_k^T = \Sigma_{jk}^k \text{ and } \Psi_k = V E^T \Omega_k B.$$

This shows that the stability of the filter (Eq. 13b) implies the convergence of sequence Σ_{jk}^k to zero when k increases. This stability is given by the following theorem (Willems, 1970).

Theorem 1

For the matrix Ψ_k bounded, the null solution of Eq. 15 is uniformly asymptotically-stable, if and only if there exists a nonstationary, decreasing, positive-definite Lyapunov function whose difference along the solution of Eq. 15 is given by a decreasing, negative-definite, nonstationary quadratic form.

To study this stability, we must first study the asymptotic properties of sequences Ω_k or Σ_{kk}^k. From Eqs. 14b and 14c we have the following recursive equation:

$$\Sigma_{(k+1)(k+1)}^{k+1} = V - VE^T \, (B\Sigma_{kk}^k B^T + EVE^T)^{-1} \, EV \qquad (16)$$

To simplify this we adopt the following notation:

$$\Sigma_{kk}^k = V_k \qquad (17)$$

Then Eq. 16 becomes

$$V_{k+1} = V - VE^T \, (BV_k B^T + EVE^T)^{-1} EV \qquad (18)$$

If matrices E and B are of full row rank (Zasadzinski, 1990) by using the inversion lemma, we obtain

$$V_{k+1} = D + FV_kF^T - FV_kB^T \, (BV_kB^T + R)^{-1} BV_kF^T \qquad (19)$$

with $F = VE^T \, (EVE^T)^{-1} \, B$, $R = EVE^T$, and $D = V - VE^T \, (EVE^T)^{-1} \, EV$, and where R is a positive definite matrix and D is a semipositive definite matrix.

Equation 19 is the standard form of the Riccati equation (Caines, 1988). The study of the asymptotic properties of sequences Σ_{kk}^k or Ω_k is reduced to the study of the convergence of the Riccati equation (Eq. 19). We can give the following theorem (Caines, 1988).

Theorem 2

Let (B,F) be detectable and let (F,S) be stabilizable where S is any square-root matrix of D. Given any symmetric-positive condition $V_0 > 0$, the sequence of solutions $\{V_k$, k is the positive integer$\}$ generated by Eq. 19 converges to the unique symmetric semipositive solution Y to the algebraic Riccati equation

$$Y = D + FYF^T - FYB^T \, (BYB^T + R)^{-1} \, BYF^T \qquad (20)$$

In the case of the controllable (F,S), Y is strictly positive.

The proof of this theorem is given by Caines (1988). The conditions for detectability and stabilizability are summarized in Appendix B.

If the conditions of convergence of Eq. 19 are verified, the sequence Ω_k generated by Eq. 14c converges to the unique solution Ω given by

$$\Omega = (BYB^T + EVE^T)^{-1} \qquad (21)$$

where Y is the solution of Eq. 20. The convergence of sequence Ω_k from theorem 2 guarantees that the state transition matrix of state space equation (Eq. 13b) is bounded.

Application to Data Reconciliation

We now turn to the data reconciliation problem described by Eqs. 1, 2 and 3, which corresponds to matrices $E = (I \mid -M)$ and $B = (I \mid 0)$. In this case, the rank condition, rank $(sE - A) = n$, is always verified. The algorithm (Eqs. 13–14) with E and B replaced by their values becomes

$$\hat{X}_{j/k+1} = \begin{pmatrix} \hat{W}_{j/k+1} \\ \hat{Q}_{j/k+1} \end{pmatrix}$$

$$= \begin{pmatrix} \hat{W}_{j/k} \\ \hat{Q}_{j/k} \end{pmatrix} + \Sigma_{jk}^k \begin{pmatrix} \Omega_k W_{k+1} - \Omega_k M Q_{k+1} - \Omega_k \hat{W}_{k/k} \\ 0 \end{pmatrix} \qquad (22a)$$

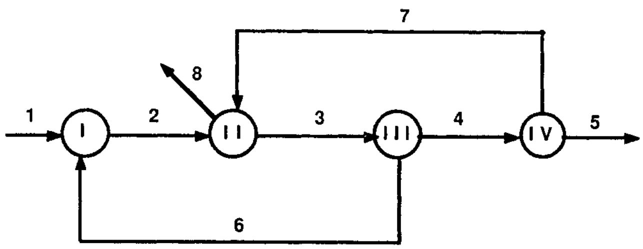

Figure 1. Process network.

$$\hat{X}_{k+1/k+1} = \begin{pmatrix} \hat{W}_{k+1/k+1} \\ \hat{Q}_{k+1/k+1} \end{pmatrix} =$$

$$\begin{pmatrix} (I - V_W\Omega_k) W_{k+1} + V_W\Omega_k M Q_{k+1} + V_W \Omega_k \hat{W}_{k/k} \\ (I - V_Q M^T \Omega_k M) Q_{k+1} + V_Q M^T \Omega_k W_{k+1} - V_Q M^T \Omega_k \hat{W}_{k/k} \end{pmatrix} \quad (22b)$$

$$\Sigma^{k+1}_{j(k+1)} = \Sigma^k_{jk} \begin{pmatrix} \Omega_k V_W & -\Omega_k M V_Q \\ 0 & 0 \end{pmatrix} \quad (23a)$$

$$\Sigma^{k+1}_{(k+1)(k+1)} = \begin{pmatrix} V_W - V_W \Omega_k V_W & V_W \Omega_k M V_Q \\ V_Q M^T \Omega_k V_W & V_Q - V_Q M^T \Omega_k M V_Q \end{pmatrix} \quad (23b)$$

$$\Omega_k = (\Sigma^k_W + V_W + M V_Q M^T)^{-1} \quad (23c)$$

with

$$\Sigma^k_{kk} = \begin{pmatrix} \Sigma^k_W & \Sigma^k_{QW} \\ \Sigma^k_{WQ} & \Sigma^k_Q \end{pmatrix}$$

where Σ^k_Q is the variance matrix of the estimate $\hat{Q}_{k/k}$, Σ^k_W is the variance matrix of $\hat{W}_{k/k}$ and Σ^k_{QW} is the cross-covariance matrix of $\hat{Q}_{k/k}$ and $\hat{W}_{k/k}$.

According to the convergence conditions given by theorem 2, first we must calculate matrices F and D given by

$$F = VE^T\ (EVE^T)^{-1}\ B \quad (24)$$

and

$$D = V - VE^T\ (EVE^T)^{-1}\ EV \quad (25)$$

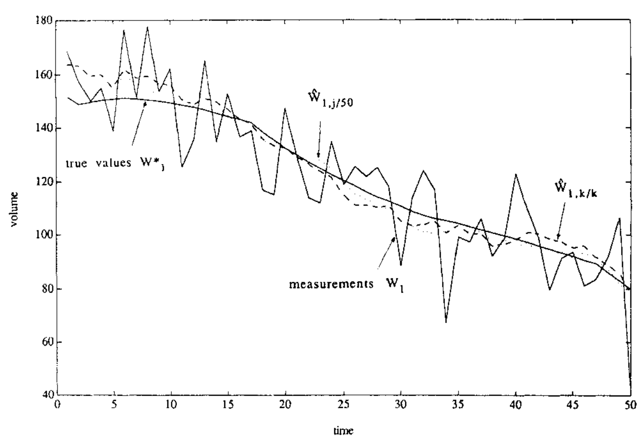

Figure 2. True, measured and estimated values of W_1.

Using Eqs. 1 and 4 in Eqs. 24 and 25 gives

$$F = \begin{pmatrix} F_1 & 0 \\ F_2 & 0 \end{pmatrix}$$

where

$$F_1 = V_W (V_W + M V_Q M^T)^{-1}$$

and

$$F_2 = -V_Q M^T (V_W + M V_Q M^T)^{-1}$$

and

$$D = \begin{pmatrix} D_1 & D_2 \\ D_2^T & D_3 \end{pmatrix}$$

where

$$D_1 = V_W - V_W (V_W + M V_Q M^T)^{-1} V_W$$

$$D_2 = V_W (V_W + M V_Q M^T)^{-1} M V_Q$$

$$D_3 = V_Q - V_Q M^T (V_W + M V_Q M^T)^{-1} M V_Q$$

The pair (B,F) is given by

$$(B,F) = \left[\begin{pmatrix} I | 0 \end{pmatrix},\ \begin{pmatrix} F_1 & 0 \\ F_2 & 0 \end{pmatrix} \right]$$

and we have

$$(F^T,\ B^T) = \left[\begin{pmatrix} F_1^T & F_2^T \\ 0 & 0 \end{pmatrix},\ \begin{pmatrix} I \\ 0 \end{pmatrix} \right] \quad (26)$$

In Appendix C, we prove that (F,S) is stabilizable and (B,F) detectable, with S being any square root matrix of D. Consequently, the convergence of sequence Σ^k_{kk} is proved for the system described by Eqs. 1, 2 and 3.

From Eqs. 13b and 15, theorem 1 reduces the stability of the filter and the convergence of sequence Σ^k_{jk} to the following conditions:

1. Ψ_k must be bounded.
2. There exists a Lyapunov function.

These conditions are always verified, see Appendix D.

Numerical Example

As an application example of the algorithm, let us consider the system represented by the process network of Figure 1. This system is formed by eight streams and four nodes. Its incidence matrix is given by

$$M = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 1 & -1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 & -1 & 0 \end{pmatrix}$$

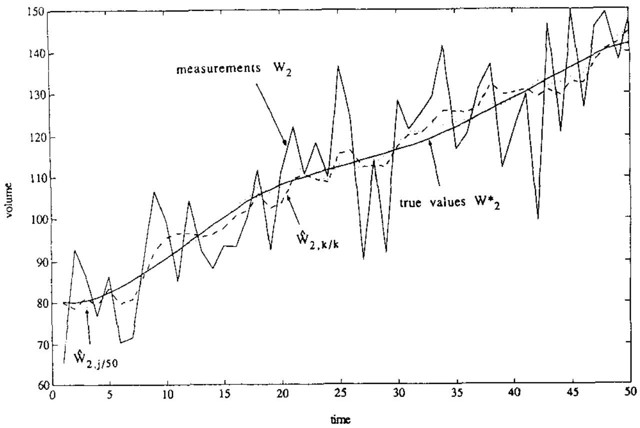

Figure 3. True, measured and estimated values of W_2.

The measurement data were generated from the true values that obey the balance relations with an addition of normally distributed random noises, with variances V_W and V_Q of measurement errors on W and Q, respectively

$$V_W = \begin{pmatrix} 225 & 0 & 0 & 0 \\ 0 & 144 & 0 & 0 \\ 0 & 0 & 324 & 0 \\ 0 & 0 & 0 & 484 \end{pmatrix}$$

$$V_Q = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1.96 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.21 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.49 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.36 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.16 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.09 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.25 \end{bmatrix}$$

The true, measured and estimated values of volumes W_1, W_2, W_3 and W_4 of nodes 1, 2, 3 and 4 are shown in Figures 2, 3, 4 and 5, respectively.

To show the convergence of the algorithm, the evolution of

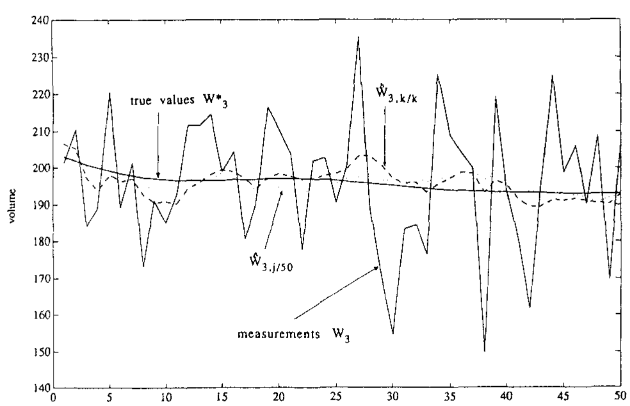

Figure 4. True, measured and estimated values of W_3.

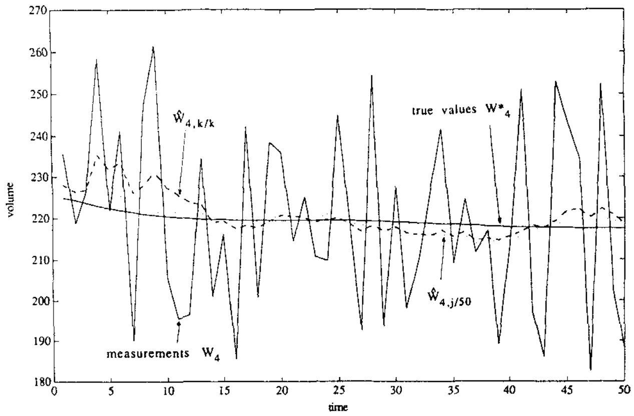

Figure 5. True, measured and estimated values of W_4.

the norm $\|\Sigma_{kk}^k\|$ (the largest singular value) is plotted in Figure 6. This norm converges to a constant value 29.09. Convergence conditions of theorem 2 are verified since pair (F,S) is stabilizable and controllable and pair (B,F) is detectable. Indeed, if we take matrix K_{13} in Eq. C4 as

$$K_{13} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

spectral radius of matrix $(F-SK)$ is less than one (C-3).

Once sequence Σ_{kk}^k has converged, the estimation algorithm is then reduced to Eqs. 22 and 23a.

Figure 7 shows the evolution of the norm $\|\Sigma_{jk}^k\|$ (the largest singular value) for $j=1$, 10, 20, 30, and 40. We can see the parallel evolution of norms $\|\Sigma_{jk}^k\|$.

In addition to update the past estimates at time instant j in the presence of measurements at time instant k ($k>j$), we can use a moving window for Eq. 22a.

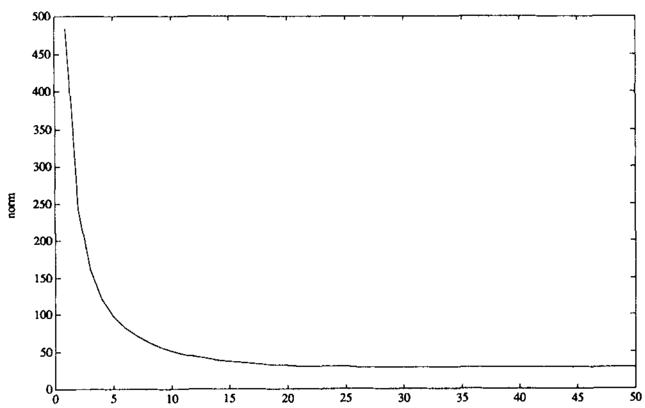

Figure 6. Evolution of the norm $\|\Sigma_{kk}^k\|$.

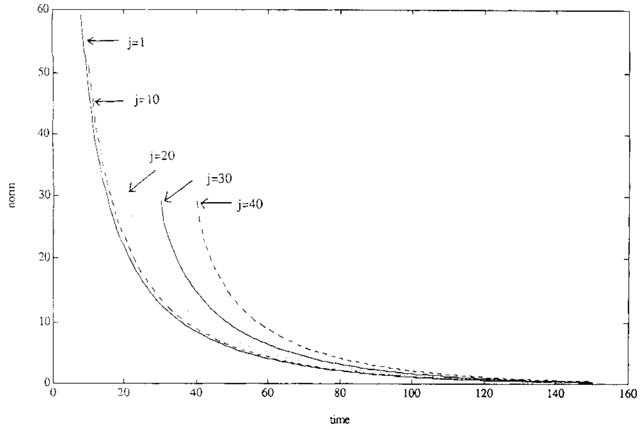

Figure 7. Evolution of the norm $\|\Sigma_{jk}^{k}\|$ for $j = 1, 10, 20, 30$, and 40.

Conclusions

We have shown that the dynamic material balance equation (Eq. 1) can be represented by a generalized dynamic model (Eq. 4). This formulation is used to develop a new method for solving the data reconciliation problem. The obtained recursive estimates include filtering (Eqs. 13b and 14b) and smoothing (Eqs. 13a and 14a), and represent a systematic approach to real-time processing. Only deterministic systems with uncertain measurements have been considered. The convergence of this method has been proved in the dynamic data reconciliation case.

Differential-algebraic equations are usually met in chemical processes and constitute a class of singular systems. The algorithm presented can be applied to these systems.

Notation

B, E = constraint matrices in generalized dynamic system, Eq. 4
C, C_1 = matrices in Appendix D, Eq. D7
D = matrix, Eq. 19
D_1, D_2, D_3 = submatrices of D
F = matrix, Eq. 19
F_1, F_2 = submatrices of F
I = identity matrix
J = quadratic criterion
$K, K_1, K_2, K_{11}, \ldots K_{14}$ = matrices in Appendix C
M = incidence matrix
m_{ij} = element (i,j) of incidence matrix M
n = number of constraints or nodes
P, P_k = projection matrices
Q_i = vector of flow measurements at time instant i
Q_i^* = vector of true flow values at time instant i
$\hat{Q}_{j/k}$ = vector of flow estimates at time instant j given the measurements up to k
R = matrix, Eq. 19
S = square root of matrix D
S_1, S_2, S_3 = submatrices of S in Appendix C
V = covariance matrix of measurement errors
$V_k = \Sigma_{kk}^{k}$
V_Q = covariance matrix of measurement errors on flows Q
V_W = covariance matrix of measurement errors on volumes W
v = number of flows
v_i = vector of measurement errors on Q_i
W_i = vector of volume measurements at time instant i
W_i^* = vector of true values of volumes at time instant i
$\hat{W}_{j/k}$ = vector of volume estimates at time instant j given the measurements up to k
w_i = vector of measurement errors on W_i
X^* = vector of true values of unknown variables from time instant 1 to $(k+1)$, Eq. 7
$\hat{X}$ = vector of unknown variable estimates from time instant 1 to $(k+1)$, Eq. 9
X_i^* = vector of true values of unknown variables at time instant i
$\hat{X}_{j/k}$ = vector of unknown variable estimates at time instant j given the measurements up to k
Y = matrix V_k when sequence (Eq. 20) has converged
$Y_k = (\Sigma_{jk}^{k})^T$
Z = vector of measurements from time instant 1 to $(k+1)$, Eq. 7
Z_i = vector of measurements at time instant i

Greek letters

ϵ = vector of measurement errors from time instant 1 to $(k+1)$, Eq. 7
$\vartheta(.)$ = Lyapunov function in Appendix D
ϵ_i = vector of measurement errors at time instant i
Σ_k = covariance matrix in Appendix A, Eq. A5
Σ_{ij}^{k} = block (i,j) of Σ_k
Σ_Q^k = covariance of Q_k
Σ_W^k = covariance matrix of W_k
$\Sigma_{WQ}^k, \Sigma_{QW}^k$ = cross-covariance matrices between Q_k and W_k
Φ_k = constraint matrix, Eq. 7
φ_k = kth block of n rows of Φ_k
Ψ_k = transition matrix, Eq. 15
Ω = matrix Ω_k at the convergence
Ω_k = matrix, Eq. 14

Other symbols

$\rho(.)$ = spectral radius of matrix
Det(.) = determinant of matrix
$\|.\|$ = norm of matrix (largest singular value)
(.,.) = pair of matrices
rank(.) = rank of matrix

Literature Cited

Almasy, G. A., "Sensor Validation on the Basis of Linear Submodels," *AIPAC-IFAC Conf.*, Nancy, France (1989).
Almasy, G. A., *Principles of Dynamic Balancing,* (1989).
Caines, P. E., *Linear Stochastic Systems,* Wiley, New York (1988).
Dai, L., "Singular Control Systems," *Lecture Notes on Control and Info. Sci.*, **118**, Springer-Verlag (1989).
Darouach, M., D. Mehdi, and C. Humbert, "Validation des Mesures des Systèmes Quasistatiques Linéaires," *Int. Conf. on Computer, Method and Water Resources,* RABAT, Maroc (1988).
Darouach, M., J. Ragot, J. Fayolle, and D. Maquin, "Data Validation in Large-Scale Steady-State Linear Systems,' *World Cong. on Scientific Computation,* IMACS-IFAC, Paris (1988).
Gantmacher, F. R., *The Theory of Matrices,* Chelsea (1959).
Gertler, J., and G. A. Almasy, "Balance Calculation through Dynamic System Modeling," *Automatica,* **9**, 79 (1973).
Gertler, J., "A Constrained Minimum Variance Input-Output Estimator for Linear Dynamic Systems," *Automatica,* **15**, 353 (1979).
Hlavacek, V., "Analysis of a Complex Plant: Steady State and Transient Behaviour," *Computer in Chem. Eng.*, **1**, 75 (1977).
Horn, R. A., and C. R. Johnson, *Matrix Analysis,* Cambridge University Press (1985).

Mah, R. S. H., "Design and Analysis of Process Performance Monitoring Systems," *Proc. Engineering Foundation Conf. on Chemical Process Control,* **2**, 525, New York (1981).
Mah, R. S. H., "Data Screening," *Foundation of Computer-Aided Process Operations,* G. V. Reiklaitis and H. D. Spriggs, eds., Elsevier, New York (1987).
Mahmoud, M. S., and M. G. Singh, *Discrete Systems: Analysis, Control and Optimization,* Springer Verlag, New York (1984).
Narasimhan, S. and R. S. H. Mah, "Generalized Likelihood Ratios for Gross Error Identification in Dynamic Processes," *AIChE J.,* **34**, 1321 (1988).
Stanley, G. M., and R. S. H. Mah, "Estimation of Flows and Temperatures in Process Networks," *AIChE J.,* **23**, 642 (1977).
Tamhane, A. C., and R. S. H. Mah, "Data Reconciliation and Gross Error Detection in Chemical Process Network," *Technometrics,* **27**, 409 (1985).
Willems, J. L., *Stability Theory of Dynamical Systems,* Wiley, New York (1970).
Willsky, A. S., and H. L. Jones, "A Generalized Likelihood Ratio Approach to the State Estimation in Linear Systems Subject to Abrupt Changes," *Proc. IEEE Conf. Decision and Control,* 846 (1974).
Zasadzinski, M., "Contribution à l'Estimation de l'Etat des Systèmes Singuliers: Application à la Validation de Données des Systèmes Dynamiques Linéaires," Thèse de Doctorat, Université de Nancy I, France (1990).

Appendix A

We consider the problem (Eq. 8) with definitions 11 and 12, and we call $\hat{X}_k$ the estimate and Σ_k its variance in the presence of the constraint $\Phi_k \hat{X}_k = 0$. From the steady-state sequential method obtained by additional linear constraints (Darouach et al., 1988b), we prove that the new estimate $\hat{X}_{k+1}$ and its variance Σ_{k+1} can be established in term of the additional constraint $\varphi_k \hat{X}_{k+1} = 0$, and we obtain the following results:

$$\hat{X}_{k+1} = P_{k+1}\, \hat{X}_k \tag{A1}$$

$$\Sigma_{k+1} = P_{k+1}\, \Sigma_k \tag{A2}$$

with

$$P_{k+1} = I - \Sigma_k\, \varphi_k^T\, \Omega_k\, \varphi_k \tag{A3}$$

and

$$\Omega_k = (\varphi_k\, \Sigma_k\, \varphi_k^T)^{-1} \tag{A4}$$

The covariance matrix Σ_k can be written as:

$$\Sigma_k = \begin{pmatrix} \Sigma_{11}^k & .. & \Sigma_{1k}^k & 0 \\ .. & .. & .. & .. \\ \Sigma_{k1}^k & .. & \Sigma_{kk}^k & 0 \\ 0 & .. & 0 & V \end{pmatrix} \tag{A5}$$

where Σ_{ij}^k is the element in the (i,j) block of dimension $(n+v)\times(n+v)$. After some manipulations, using Eqs. 12 and A1 to A5, one obtains

$$\Omega_k^{-1} = B\Sigma_{kk}^k B^T + EVE^T \tag{A6}$$

and

$$P_{k+1} = \begin{pmatrix} I & 0 & . & 0 & -\Sigma_{1k}^k B^T \Omega_k B & \Sigma_{1k}^k B^T \Omega_k E \\ . & . & . & . & . & . \\ 0 & . & 0 & I & -\Sigma_{(k-1)k}^k B^T \Omega_k B & \Sigma_{(k-1)k}^k B^T \Omega_k E \\ 0 & . & . & 0 & I - \Sigma_{kk}^k B^T \Omega_k B & \Sigma_{kk}^k \Omega_k B^T E \\ 0 & . & . & 0 & VE^T \Omega_k B & I - VE^T \Omega_k E \end{pmatrix} \tag{A7}$$

Equation A7 requires only the kth block column of the matrix Σ_k. From Eq. A7, the $(k+1)$th block column of covariance matrix Σ_{k+1} is given by:

$$\begin{pmatrix} \Sigma_{1(k+1)}^{k+1} \\ \vdots \\ \Sigma_{k(k+1)}^{k+1} \\ \Sigma_{(k+1)(k+1)}^{k+1} \end{pmatrix} = \begin{pmatrix} \Sigma_{1k}^k B^T \Omega_k EV \\ \vdots \\ \Sigma_{kk}^k B^T \Omega_k EV \\ V - VE^T \Omega_k EV \end{pmatrix} \tag{A8}$$

The estimate $\hat{X}_{k+1}$ is given in term of $\hat{X}_k$ by:

$$\hat{X}_{k+1} = \begin{pmatrix} \hat{X}_{1/k+1} \\ \vdots \\ \hat{X}_{k/k+1} \\ \hat{X}_{k+1/k+1} \end{pmatrix} = P_{k+1} \begin{pmatrix} \hat{X}_k \\ Z_{k+1} \end{pmatrix} = P_{k+1} \begin{pmatrix} \hat{X}_{1/k} \\ \vdots \\ \hat{X}_{k/k} \\ Z_{k+1} \end{pmatrix} \tag{A9}$$

which can be written as:

$$\begin{pmatrix} \hat{X}_{1/k+1} \\ \vdots \\ \hat{X}_{k/k+1} \\ \hat{X}_{k+1/k+1} \end{pmatrix} = \begin{pmatrix} \hat{X}_{1/k} - \Sigma_{1k}^k B^T \Omega_k (B\hat{X}_{k/k} - EZ_{k+1}) \\ \vdots \\ \hat{X}_{k/k} - \Sigma_{kk}^k B^T \Omega_k (B\hat{X}_{k/k} - EZ_{k+1}) \\ Z_{k+1} + VE^T \Omega_k (B\hat{X}_{k/k} - EZ_{k+1}) \end{pmatrix} \tag{A10}$$

Appendix B

For the detectability and stabilizability (Mahmoud and Singh, 1984) let us consider the linear discrete-time system:

$$x_{k+1} = Ax_k + Bu_k \tag{B1}$$

$$z_k = Cx_k \tag{B2}$$

Definition 1

Let A be a $n\times n$ matrix and B a $n\times m$ matrix. If there exists a $m\times n$ matrix, K such as the eigenvalues of $(A-BK)$ lies within the unit circle, and (A,B) is said to be stabilizable.

As for observability and controllability, there is a duality between detectability and stabilizability. (C,A) is detectable if (A^T,C^T) is stabilizable, clearly, (A,B)-controllable implies (A,B)-stabilizable and (C,A)-observable implies (C,A)-detectable. This also offers the following definitions.

Definition 2

The system (Eqs. B1-B2) is said to be stabilizable if all the uncontrollable modes have eigenvalues strictly inside the unit circle.

Definition 3

The system (Eqs. B1-B2) is said to be detectable if all the unobservable modes have eigenvalues strictly inside the unit circle.

If this system is transformed into the following form:

$$Y_{k+1}=\begin{pmatrix}A_1 & A_2\\ 0 & A_4\end{pmatrix}Y_k+\begin{pmatrix}B_1\\ 0\end{pmatrix}U_k \tag{B3}$$

we can state that the linear time-invariant system (Eq. B1) is stabilizable, if and only if the pair (A_1,B_1) is completely reachable and all the eigenvalues of the matrix A_4 have moduli strictly less than one.

Appendix C

From Appendix B, the detectability of (B,F) is given by the stabilizability of (F^T,B^T) and can be reduced to the reachability of the pair (F_1^T,I), which can be verified by:

$$\text{rank}\ (I|F_1^T|F_1^{2T}|\ldots)=n \tag{C1}$$

Now let S be any square root matrix of D

$$S=\begin{pmatrix}S_1 & S_2\\ S_2^T & S_3\end{pmatrix} \tag{C2}$$

The stabilizability of the pair (F,S) can be verified by the existence of the matrix K such that the eigenvalues of $(F-SK)$ lie within the unit circle.

Consider the matrix $K=S^TK_1$, then the matrix $(F-SK)$ can be written as:

$$F-SK=F-DK_1 \tag{C3}$$

For

$$K_1=\begin{pmatrix}K_{11} & K_{12}\\ K_{13} & K_{14}\end{pmatrix},$$

the matrix $(F-DK_1)$ is given by:

$$F-DK_1=\begin{pmatrix}F_1-D_1K_{11}-D_2K_{13} & 0\\ F_2-D_2^TK_{11}-D_3K_{13} & 0\end{pmatrix} \tag{C4}$$

for $K_{12}=K_{14}=0$.

The eigenvalues of $(F-DK_1)$ are the solutions of the equation:

$$\text{Det}\ [\lambda I-(F-DK_1)]=\text{Det}(\lambda I)$$

$$\text{Det}[\lambda I-(F_1-D_1K_{11}-D_2K_{13})]=0 \tag{C5}$$

The matrix $D_1=V_W-V_W(V_W+MV_QM^T)^{-1}V_W=V_W(V_W+MV_QM^T)^{-1}(MV_QM^T)$ is nonsingular.

If we take $K_{11}=-D_1^{-1}D_2K_{13}$, Eq. C5 becomes

$$\text{Det}(\lambda I)\text{Det}(\lambda I-F_1)=0 \tag{C6}$$

The stabilizability condition is reduced to spectral radius of F_1 which must be less than one. This condition can be written as:

$$\rho(F_1)=\rho[V_W(V_W+MV_QM^T)^{-1}]<1 \tag{C7}$$

which is verified (Horn and Johnson, 1985, p. 471), since

$$V_W+MV_QM^T>V_W \tag{C8}$$

Consequently, the convergence of the recurrence (Eq. 23b) is proved for the system described by Eq. 1.

Appendix D

The state transition matrix Ψ_k can be written as:

$$\Psi_k=VE^T\,\Omega_k\,B=\begin{pmatrix}V_W\Omega_k & 0\\ -V_QM^T\Omega_k & 0\end{pmatrix} \tag{D1}$$

Its spectral radius is given by the one of $(V_W\Omega_k)$. From Eq. 14c we have

$$V_W\Omega_k=V_W(\Sigma_W^k+V_W+MV_QM^T)^{-1} \tag{D2}$$

Since Σ_W^k is a positive definite matrix we have

$$\Sigma_W^k+V_W+MV_QM^T>V_W \tag{D3}$$

which yields to the condition $\rho(\Omega_kV_W)<1$ as in Eq. C7. Thus, $\rho(\Psi_k)<1$ and Ψ_k is bounded.

To complete the proof of the stability, we consider the following Lyapunov function:

$$\vartheta(x_k)=x_k^T\,V^{-1}\,x_k \tag{D4}$$

and we shall prove that $[\vartheta(x_{k+1})-\vartheta(x_k)]$ is negative. This difference is given by

$$\vartheta(x_{k+1}) - \vartheta(x_k) = x_{k+1}^T V^{-1} x_{k+1} - x_k^T V^{-1} x_k$$

$$= x_k^T[\Psi_k^T V^{-1} \Psi_k - V^{-1}] x_k$$

$$= x_k^T C x_k \qquad \text{(D5)}$$

and we must prove that

$$C = [\Psi_k^T V^{-1} \Psi_k - V^{-1}] \qquad \text{(D6)}$$

is a negative definite matrix. Substituting Eq. D1 into Eq. D6 we obtain

$$C = \begin{pmatrix} C_1 & 0 \\ 0 & -V_Q^{-1} \end{pmatrix} \qquad \text{(D7)}$$

where

$$C_1 = \Omega_k [V_W + MV_Q M^T - \Omega_k^{-1} V_W^{-1} \Omega_k^{-1}] \Omega_k \qquad \text{(D8)}$$

From the expression of Ω_k^{-1} (Eq. 23c), we have

$$\Omega_k^{-1} V_W^{-1} \Omega_k^{-1} = V_W + MV_Q M^T + G \qquad \text{(D9)}$$

where G is a symmetric positive definite matrix. Substituting Eq. D9 into Eq. D8 gives $C_1 < 0$ and matrix C is negative-definite.

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