Observability and data validation of bilinear systems

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OBSERVABILITY AND DATA VALIDATION OF BILINEAR SYSTEMS

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Abstract . This paper is devoted to data reconciliation by mass balance equilibration of systems described by bilinear equations. It proposes a new approach for their resolution. We particularly insist on a decomposition algorithm which enables the problem of unmeasured variables to be treated. It allows the classification of variables into observable and unobservable, redundant and non redundant, and gives the relations necessary for their determination. Finally, the results of this algorithm are applied to the mass balance equilibration with the use of an iterative method based on hierarchical calculus.

Keywords . Observability; balance equilibration; non-linear systems; error compensation, least squares approximation; hierarchical calculus.

INTRODUCTION

Most processes can be described by material and/or energy balance equations. Generally, available data are conflicting in the sense that they don't verify the mass balance equations. It is then necessary to reconcile these data. One of the principal difficulties in data reconciliation, is the presence of the unmeasured variables. The concepts of observability and redundancy enable the problem to be solved. A steady-state system is said to be observable if its state is uniquely determined from the measurements and the model. A variable is said to be redundant if no loss of observability results from the deletion of its measurement. For linear systems, these notions are now perfectly well known and appropriated procedure have been developed by Vaclavek (1969), Mah (1976) or Darouach (1988). Partial solutions have been found for bilinear systems. The work of Vaclavek and Loucka (1976), who have proposed a structural decomposition method for non-linear systems can notably be cited ; this topic has been also studied by Romagnoli and Stephanopoulos (1980). Based on graph theoretical, Stanley and Mah (1981) have developed an algorithm for non-linear systems which allows the classification of variables, but without giving the equations which lead to their determination. More recently, Crowe (1986) proposes a classification algorithm using projection matrices. Darouach (1986) has formalized the problem of observability of bilinear systems and proposes a decomposition method which reduces the problem of bilinear observability to a sequence of studies of linear systems observability. Finally, Kretsovalis and Mah (1987 and 1988) take into account overall and component mass balances, energy balances, reactions, heat exchanges and stream splitting. The latter method which uses the properties of graph-theoretic proves complex in the case of overall and component mass balance. In that case, we propose, in this paper, a method allowing the classification of the different variables into observable, non observable, redundant and non redundant variables, as well as the equations necessary for their determination. In practice, this problem is often encountered in chemical processes, if only distillation operations are taken into account, or in minerallurgical processes where the separation of different mineral species is proceed.

PROBLEM FORMULATION

Consider the steady state system described by :

- its model :

$$A X + B X^{*}Y = C \qquad (1)$$

where A and B are (n.v) matrices, C a (n.1) vector, and X*Y represent the Hadamard product of X and Y.

If we consider the systems represented by direct graph, which is the case of balances, the model equations are partially decoupled and can be written as :

$$M X = 0 \qquad (2)$$
$$M X^{*}Y = 0 \qquad (3)$$

where M is the incidence matrix of the associated direct graph.

- its measurement equation :

$$Z = H_1 X + H_2 Y + \varepsilon \qquad (4)$$

where H_1 and H_2 are (m.v) matrices, ε a (m.1) measurement errors vector and Z, a (m.1) measurement vector.

In practice, sensors measuring X and Y are different. In fact, the bilinear system class corresponds to systems described by total flowrates and partial flowrates balances ; X is the variable used in total flowrates (massic or volumic) while Y is the variable taken into account in partial flowrates.

Then, the measurement equation (4) reduces to :

$$H_1 X + \varepsilon_1 = Z_1 \qquad (5)$$
$$H_2 Y + \varepsilon_2 = Z_2 \qquad (6)$$

with $\text{rank}(H_1) = m_1$ and $\text{rank}(H_2) = m_2$.

For simplicity, we will consider that the variables X and Y are measured directly. In that case, H_1 and H_2 are identity matrices.

Following these hypothesis and in the case where the measurement errors can be considered as zero mean random variables, the data reconciliation problem consists of determining the estimates $\hat{X}$ and $\hat{Y}$ of the true values X* and Y*, from the measurements X and Y which minimize the criterion :

$$\Phi = \frac{1}{2} \| \hat{X} - X \|^2_{V_X^{-1}} + \frac{1}{2} \| \hat{Y} - Y \|^2_{V_Y^{-1}} \quad (7)$$

subject to $M \hat{X} = 0$

$M \hat{X} * \hat{Y} = 0$

where V_X and V_Y represent the covariance matrices of X and Y.

Notice that the second constraint can be written as :

$$M \hat{X} * \hat{Y} = (M \otimes \hat{X}) \hat{Y} \quad (8)$$

from the properties of the $\otimes$ product.

The Lagrangian associated to this problem is :

$$L = \Phi + \lambda^T M \hat{X} + \mu^T (M \otimes \hat{X}) \hat{Y} \quad (9)$$

In order to minimize L, it is necessary that :

$$\frac{\partial L}{\partial \hat{X}} = V_X^{-1} (\hat{X} - X) + M^T \lambda + (M \otimes \hat{Y})^T \mu = 0 \quad (10a)$$

$$\frac{\partial L}{\partial \hat{Y}} = V_Y^{-1} (\hat{Y} - Y) + (M \otimes \hat{X})^T \lambda = 0 \quad (10b)$$

$$\frac{\partial L}{\partial \lambda} = M \hat{X} = 0 \quad (10c)$$

$$\frac{\partial L}{\partial \mu} = (M \otimes \hat{X}) \hat{Y} = 0 \quad (10d)$$

HIERARCHICAL SOLUTION

The non-linear system of equations (10) has no analytical solution because the equations are coupled by the X variables (presence of bilinear terms $(M \otimes \hat{X}) \hat{Y}$) ; however the model structure can be used.

From (10a) and (10c) we have :

$$\lambda = (M V_X M^T)^{-1} (M X - M V_X M_Y^T \mu) \quad (11)$$

$$\hat{X} = (I - V_X M^T (M V_X M^T)^{-1} M) (X - V_X M_Y^T \mu) \quad (12)$$

with $M_Y = M \otimes \hat{Y}$. (13)

Likewise, from (10b) and (10d) we obtain :

$$\mu = (M_X V_Y M_X^T)^{-1} M_X Y \quad (14)$$

$$\hat{Y} = (I - V_Y M_X^T (M_X V_Y M_X^T)^{-1} M_X) Y \quad (15)$$

with $M_X = M \otimes \hat{X}$. (16)

Thus, the solution $\hat{X}$, $\hat{Y}$ of the system of equations (10) can be obtained iteratively by a two levels hierarchical structure calculus. The first level calculates λ and $\hat{X}$ from μ initialized to zero, while the second one calculates μ and $\hat{Y}$ from the estimate $\hat{X}$ given by the first level. Then, the scheme of the calculus is the following :

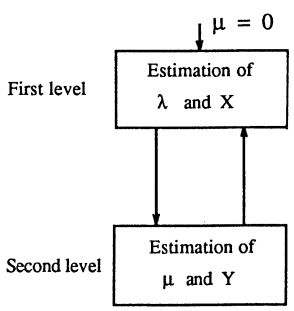

Figure 1 : hierarchical calculus

NECESSITY OF OBSERVABILITY

Generally, all the variable measurements are not available. So it is necessary, in a first step, to classify the different variables by observability and redundancy concepts.

For an illustration, consider the trivial example in figure 2 :

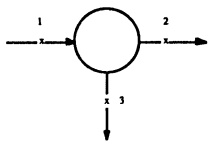

Figure 2 : elementary node

If the streams 1, 2 and 3 are considered completely measured, X_i and Y_i, (i = 1,3) can be reconciled by balance equilibration based on the presented procedure.

If we suppress measurements X_2 and X_3, balance equations are rewritten as :

$$X_1 - \underline{X_2} - \underline{X_3} = 0$$

$$X_1 Y_1 - \underline{X_2} Y_2 - \underline{X_3} Y_3 = 0$$

where the underlining variables are unmeasured.

Solving for $\hat{X}_2$ and $\hat{X}_3$, we find :

$$\hat{X}_2 = X_1 \frac{Y_3 - Y_1}{Y_3 - Y_2} \qquad \hat{X}_3 = X_1 \frac{Y_1 - Y_2}{Y_3 - Y_2}$$

with the condition $Y_3 \neq Y_2$.

This result is very important because it shows that, for bilinear system, observability is a local property which depends upon the values of the measurements.

Let us consider now that X_2, X_3 and Y_1, Y_2 and Y_3 are known. X_1 can be eliminated from the two mass balance equations ; this operation leads to :

$$\hat{X}_2 (\hat{Y}_1 - \hat{Y}_2) + \hat{X}_3 (\hat{Y}_1 - \hat{Y}_3) = 0$$

Then balance equilibration needs to minimize a quadratic criterion subject to a non-linear equation. Next, the variable $\hat{X}_1$ will be directly deduced from $\hat{X}_1 = \hat{X}_2 + \hat{X}_3$.

Through this elementary example, one can see the difficulties to solve the problem of balance equilibration when all the variables are not measured.

BILINEAR SYSTEMS OBSERVABILITY

Let us consider the bilinear system described by :

$$M X = 0 \quad (17a)$$

$$M X * Y = 0 \quad (17b)$$

The two measurement vectors X and Y can be partitioned into measured and unmeasured parts :

$$X = \begin{bmatrix} X_m \\ X_{\bar{m}} \end{bmatrix} \qquad Y = \begin{bmatrix} Y_m \\ Y_{\bar{m}} \end{bmatrix} \quad (18)$$

These decompositions allow the classification of the variables into four distinct groups. According to the above partition (18), the incidence matrix M is partitionable as well :

$$M = [M_1 \quad M_2 \quad M_3 \quad M_4] \quad (19)$$

Then, the system (17) can be written as :

$$M_1 X_{\bar{m}1} + M_2 X_{\bar{m}2} = - (M_3 X_{m1} + M_4 X_{m2}) = d_1 \quad (20a)$$

$$M_1 X_{\bar{m}1} * Y_{m1} + M_2 X_{\bar{m}2} * Y_{\bar{m}2} + M_3 X_{m1} * Y_{\bar{m}1} = -M_4 X_{m2} * Y_{m2} = d_2 \quad (20b)$$

or in matrix notation :

$$O_{(X_m,Y_m)} \begin{bmatrix} X_{\bar{m}2} \\ X_{\bar{m}1} \\ X_{\bar{m}2} * Y_{\bar{m}2} \\ Y_{\bar{m}1} \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \end{bmatrix} \qquad (21)$$

with

$$O_{(X_m,Y_m)} = \begin{bmatrix} M_2 & M_1 & 0 & 0 \\ 0 & M_1 \otimes Y_{m1} & M_2 & M_3 \otimes X_{m1} \end{bmatrix} \qquad (22)$$

The system will be observable if :

$$\text{rank } O_{(X_m,Y_m)} = \dim \begin{bmatrix} X_{\bar{m}} \\ Y_{\bar{m}} \end{bmatrix} \qquad (23)$$

If the system is not globally observable, a decomposition is necessary. We will demonstrate that the study of observability of bilinear systems can be reduced to a sequential study of observability of linear systems.

For the study of the observability of $X_{\bar{m}1}$, let us introduce two matrices Q and R which allow the elimination of the unmeasured terms $X_{\bar{m}2}$ and $Y_{\bar{m}2}$ in equation (20).

Let us consider Q, an orthogonal matrix such that :

$$Q M_2 = 0 \qquad (24)$$

If we multiply system (20) by Q, we obtain :

$$Q M_1 X_{\bar{m}1} = Q d_1 \qquad (25a)$$

$$(Q M_1 \otimes Y_{m1}) X_{\bar{m}1} + (Q M_3 \otimes X_{m1}) Y_{\bar{m}1} = Q d_2 \qquad (25b)$$

With R, a regular matrix defined by :

$$R Q M_3 = 0 \qquad (26)$$

the system (25) may be transformed to :

$$Q M_1 X_{\bar{m}1} = Q d_1 \qquad (27a)$$

$$(R Q M_1 \otimes Y_{m1}) X_{\bar{m}1} = R Q d_2 \qquad (27b)$$

Four steps are then necessary to study the observability :

a) System (27) enables to extract the observable part of $X_{\bar{m}1}$.

b) Using the already known observable part of $X_{\bar{m}1}$, equation (25) allows to determine the observable part of $Y_{\bar{m}1}$.

c) Observable part of $X_{\bar{m}2}$ is obtained from the knowledge of observable parts of $X_{\bar{m}1}$ and $Y_{\bar{m}1}$, and equation (20a).

d) Similarly, equation (20b) is used to extract the observable part of $Y_{\bar{m}2}$.

These sequential operations can be applied directly on the observability matrix. If M_{22} is the biggest regular part of M_2, the system (21) can be rewritten as :

$$O_1 \begin{bmatrix} X_{\bar{m}21} \\ X_{\bar{m}22} \\ X_{\bar{m}1} \\ X_{\bar{m}21} * Y_{\bar{m}21} \\ X_{\bar{m}22} * Y_{\bar{m}22} \\ Y_{\bar{m}1} \end{bmatrix} = \begin{bmatrix} d_{11} \\ d_{12} \\ d_{21} \\ d_{22} \end{bmatrix} \qquad (28)$$

with

$$O_1 = \begin{bmatrix} M_{21} & M_{22} & M_{11} & 0 & 0 & 0 \\ M_{23} & M_{24} & M_{12} & 0 & 0 & 0 \\ 0 & 0 & M_{11} \otimes Y_{m1} & M_{21} & M_{22} & M_{31} \otimes X_{m1} \\ 0 & 0 & M_{12} \otimes Y_{m1} & M_{23} & M_{24} & M_{32} \otimes X_{m1} \end{bmatrix}$$

Let us define the regular matrix T_1 by :

$$T_1 = \begin{bmatrix} M_{22}^{-1} & 0 & 0 & 0 \\ -M_{24}^{-1} M_{22}^{-1} & I & 0 & 0 \\ 0 & 0 & M_{22}^{-1} & 0 \\ 0 & 0 & -M_{24}^{-1} M_{22}^{-1} & I \end{bmatrix} \qquad (29)$$

Multiply equation (28) by T_1 ; we obtain :

$$O_2 \begin{bmatrix} X_{\bar{m}21} \\ X_{\bar{m}22} \\ X_{\bar{m}1} \\ X_{\bar{m}21} * Y_{\bar{m}21} \\ X_{\bar{m}22} * Y_{\bar{m}22} \\ Y_{\bar{m}1} \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix} \qquad (30)$$

with

$$O_2 = \begin{bmatrix} A_1 & I & A_2 & 0 & 0 & 0 \\ 0 & 0 & A_3 & 0 & 0 & 0 \\ 0 & 0 & A_2 \otimes Y_{m1} & A_1 & I & B_1 \otimes X_{m1} \\ 0 & 0 & A_3 \otimes Y_{m1} & 0 & 0 & B_2 \otimes X_{m1} \end{bmatrix}$$

$$A_1 = M_{22}^{-1} M_{21} \ , \ A_2 = M_{22}^{-1} M_{11} \ , \ A_3 = M_{12} - M_{24} M_{22}^{-1} M_{11}$$

$$B_1 = M_{22}^{-1} M_{31} \ , \ B_2 = M_{32} - M_{24} M_{22}^{-1} M_{31}$$

$$b_1 = M_{22}^{-1} d_{11} \ , \ b_2 = d_{12} - M_{24} M_{22}^{-1} d_{11}$$

$$b_3 = M_{22}^{-1} d_{21} \ , \ b_4 = d_{22} - M_{24} M_{22}^{-1} d_{21}$$

Finally, adequate permutations of rows and columns in matrix O_2 express the system (30) as :

$$O_3 \begin{bmatrix} X_{\bar{m}1} \\ Y_{\bar{m}1} \\ X_{\bar{m}21} \\ X_{\bar{m}22} \\ X_{\bar{m}21} * Y_{\bar{m}21} \\ X_{\bar{m}22} * Y_{\bar{m}22} \end{bmatrix} = \begin{bmatrix} b_2 \\ b_4 \\ b_1 \\ b_3 \end{bmatrix} \qquad (31)$$

with

$$O_3 = \begin{bmatrix} A_3 & 0 & 0 & 0 & 0 & 0 \\ A_3 \otimes Y_{m1} & B_2 \otimes X_{m1} & 0 & 0 & 0 & 0 \\ A_2 & 0 & A_1 & I & 0 & 0 \\ A_2 \otimes Y_{m1} & B_1 \otimes X_{m1} & 0 & 0 & A_1 & I \end{bmatrix}$$

At this step, it is clear that the first two "rows" of system (31) are the same as those of system described by (25).

As previously, the biggest regular part, B_{22} can be extracted from B_2. Then the system (31) can be rewritten as follow:

$$O_4 \begin{bmatrix} X_{\bar{m}1} \\ Y_{\bar{m}11} \\ Y_{\bar{m}12} \\ X_{\bar{m}21} \\ X_{\bar{m}22} \\ X_{\bar{m}21} * Y_{\bar{m}21} \\ X_{\bar{m}22} * Y_{\bar{m}22} \end{bmatrix} = \begin{bmatrix} b_2 \\ b_{41} \\ b_{42} \\ b_1 \\ b_3 \end{bmatrix} \qquad (32)$$

with

$$O_4 = \begin{bmatrix} A_3 & 0 & 0 & 0 & 0 & 0 & 0 \\ A_{31}\otimes Y_{m1} & B_{21}\otimes X_{m1} & B_{22}\otimes X_{m1} & 0 & 0 & 0 & 0 \\ A_{32}\otimes Y_{m1} & B_{23}\otimes X_{m1} & B_{24}\otimes X_{m1} & 0 & 0 & 0 & 0 \\ A_2 & 0 & 0 & A_1 & I & 0 & 0 \\ A_2\otimes Y_{m1} & B_{11}\otimes X_{m1} & B_{12}\otimes X_{m1} & 0 & 0 & A_1 & I \end{bmatrix}$$

The final form (33)

$$O_5 \begin{bmatrix} X_{\bar{m}1} \\ Y_{\bar{m}11} \\ Y_{\bar{m}12} \\ X_{\bar{m}21} \\ X_{\bar{m}22} \\ X_{\bar{m}21} * Y_{\bar{m}21} \\ X_{\bar{m}22} * Y_{\bar{m}22} \end{bmatrix} = \begin{bmatrix} b_2 \\ c_2 \\ c_1 \\ b_1 \\ b_3 \end{bmatrix} \qquad (33)$$

is obtained by multiplying (32) by the regular matrix T_2, and the permutation of "rows" 2 and 3 of the result matrix :

$$T_2 = \begin{bmatrix} I & 0 & 0 & 0 & 0 \\ 0 & B_{22}^{-1} & 0 & 0 & 0 \\ 0 & -B_{24}^{-1}B_{22}^{-1} & I & 0 & 0 \\ 0 & 0 & 0 & I & 0 \\ 0 & 0 & 0 & 0 & I \end{bmatrix} \qquad (34)$$

with

$$O_5 = \begin{bmatrix} A_3 & 0 & 0 & 0 & 0 & 0 & 0 \\ C_2\otimes Y_{m1} & 0 & 0 & 0 & 0 & 0 & 0 \\ C_1\otimes Y_{m1} & C_3\otimes X_{m1} & I\otimes X_{m1} & 0 & 0 & 0 & 0 \\ A_2 & 0 & 0 & A_1 & I & 0 & 0 \\ A_2\otimes Y_{m1} & B_{11}\otimes X_{m1} & B_{12}\otimes X_{m1} & 0 & 0 & A_1 & I \end{bmatrix}$$

$$C_1 = B_{22}^{-1}A_{31}\ ,\ C_2 = A_{32} - B_{24}B_{22}^{-1}A_{31}\ ,\ C_3 = B_{22}^{-1}B_{21}$$

$$c_1 = B_{22}^{-1}c_{41}\ ,\ c_2 = b_{42} - B_{24}B_{22}^{-1}b_{41}$$

Notice that the first two "rows" of this system correspond to equation (27), thus they allow the study of the observability of $X_{\bar{m}1}$ which leads to the classification into observable and non observable parts, redundant and non redundant parts. The other "rows" of system (34) can be only used to deduce unmeasured variables.

ESTIMATION OF REDUNDANT VARIABLES

Generally speaking, the balance equations for the redundant variables, can always be written as :

$$A\,X = 0$$
$$(B \otimes Y)\,S\,X = 0$$

with A, of dimension $n_a.v_a$, such as :

$$A = \begin{array}{|c|c|c|} \hline O & C & \\ \hline B & O & \\ \hline \end{array}$$

Category $X_{\bar{m}1}Y_{m1}$ $X_{m2}Y_{m2}$ $X_{m1}Y_{\bar{m}1}$

B, of dimension $n_b.v_b$,

and S, a selection matrix partitioned as :

$$S = [I \mid 0]$$

The least squares estimation problem of true values is reduced to find the minimum with regard to $\hat{X}$ et $\hat{Y}$ of the criterion :

$$\Phi = \frac{1}{2}\,\|H\hat{X} - X\|^2_{V_X^{-1}} + \frac{1}{2}\,\|\hat{Y} - Y\|^2_{V_Y^{-1}} \qquad (35)$$

subject to $A\hat{X} = 0$
$(B \otimes Y)\,S\,X = 0$

where H is the matrix of measurement function partitioned as H = [0 | I],

X and Y are the measurement vectors of respective dimensions m and v_b,

$\hat{X}$ et $\hat{Y}$, the estimation vectors of dimensions v_a and v_b,

The associated Lagrangian is :

$$L = \Phi + \lambda^T A\hat{X} + \mu^T (B \otimes \hat{Y})\,S\,\hat{X} \qquad (36)$$

The stationary conditions of first order required that :

$$\frac{\partial L}{\partial \hat{X}} = H^T V_X^{-1}(H\hat{X} - X) + A^T\lambda + S^T(B\otimes\hat{Y})^T\mu = 0 \quad (37a)$$

$$\frac{\partial L}{\partial \hat{Y}} = V_Y^{-1}(\hat{Y} - Y) + (B\otimes S\,\hat{X})^T\lambda = 0 \quad (37b)$$

$$\frac{\partial L}{\partial \lambda} = A\,\hat{X} = 0 \quad (37c)$$

$$\frac{\partial L}{\partial \mu} = (B\otimes\hat{Y})\,S\,\hat{X} = 0 \quad (37d)$$

In order to simplify the notations, let :

$$N_X = B \otimes S\,\hat{X} \qquad (38)$$
$$N_Y = B \otimes \hat{Y} \qquad (39)$$

The following calculus allow to determine the estimation $\hat{X}$; multiply equation (37c) by A^T :

$$A^T A\,X = 0 \qquad (40)$$

then (37d) by $S^T N_Y^T$:

$$S^T N_Y^T\ N_X\,\hat{Y} = 0 \qquad (41)$$

Substituting (38) and (39) in (41), we get :

$$S^T N_Y^T\ N_Y\,S\,\hat{X} = 0 \qquad (42)$$

By adding equations (40), (41) et (37a), we obtain :

$$G^{-1}\,\hat{X} = H^T V_X^{-1} X - A^T\lambda - S^T N_Y^T\mu \qquad (43)$$

with $G^{-1} = H^T V_X^{-1} H + A^T A + S^T N_Y^T\ N_Y\,S$ (44)

Notice that G matrix is always regular because of the global observability of the system.

Thus, the estimation $\hat{X}$ can be written as :

$$\hat{X} = (I - G\,A^T(A\,G\,A^T)^{-1}A)\,G\,\bar{X}$$
with $\bar{X} = H^T V_X^{-1} X - S^T N_Y^T\mu$ (45)

Therefore, from equations (37b) et (37d) we have :

$$\hat{Y} = (I - V_Y N_X^T(N_X\,V_Y\,N_X^T)^{-1}N_X)\,Y \qquad (46)$$

$$\mu = (N_X\,V_Y\,N_X^T)^{-1}N_X\,Y \qquad (47)$$

In order to simplify the numerical calculus, we use the diagonal matrices Λ_{S_X} and Λ_Y formed with $S\,\hat{X}$ and $\hat{Y}$ vectors.

From (37b) we have :

$$B^T \mu = \Lambda_{S_X}^{-1} V_Y^{-1} (\hat{Y} - Y) \qquad (48)$$

Then $\overline{X}$ vector can be written as a function of X, Y et $\hat{Y}$:

$$\overline{X} = H^T V_X^{-1} X - S^T \Lambda_Y \Lambda_{S_X}^{-1} V_Y^{-1} (\hat{Y} - Y) \qquad (49)$$

Then the estimation $\hat{Y}$ becomes :

$$\hat{Y} = \Lambda_{S_X} [\Gamma - \Gamma B^T (B \Gamma B^T)^{-1} B \Gamma]^{-1} \Lambda_{S_X}^{-1} V_Y^{-1} Y$$

with $\Gamma = \Lambda_{S_X} V_Y \Lambda_{S_X}$ (50)

Finally, the solution is obtained through a direct iteration algorithm :

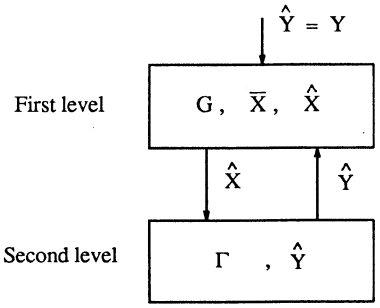

Figure 3 : estimation algorithm

The first level estimates $\hat{X}$ after calculating G and $\overline{X}$ as a function of the estimation $\hat{Y}$, initialized to Y.

The second level estimates $\hat{Y}$ after calculating Γ as a function of $\hat{X}$ which is produced by the upper level.

Notice that the calculus in each level are relatively reduced, due to the particularly forms of equations (45) and (50). This allows the usage of recurrence formula for matrix inversion which degenerates into computing the reciprocal of scalars (Maquin 1987).

The calculus is stopped when all the derivatives of the Lagrangian are kept below a given threshold.

ILLUSTRATIVE EXAMPLE

As an example of the application of the algorithm, let us consider the simplified flow sheet of a grinding-classification process.

A network representation of the system consisting of 6 nodes and 12 streams is shown in figure 4.

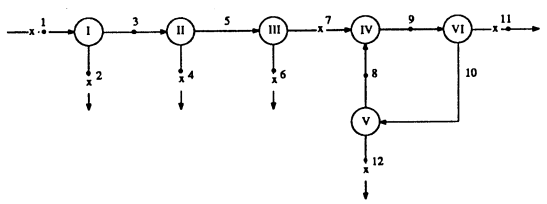

Figure 4 : flow sheet of a grinding-classification process

The measurements location of massic flow rates are indicated by x ; those of concentration of the three different components are indicated by •.We consider here, that when the composition of certains streams is measured, it is measured for all components.

System (33) can be described by the following matrix :

$$\left[\begin{array}{c|c} O_5 & \begin{matrix} b_2 \\ c_2 \\ c_1 \\ b_1 \\ b_3 \end{matrix} \end{array}\right] \qquad (51)$$

According to the measurements location of our example, this matrix is expressed as :

3	8	9	7	5	10	5	10	7	1	4	11	2	6	12
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	-1	-1	-1
-1	.	.	1	.	.	.	.	.	.	1	.	.	1	.
-1	.	.	.	1	.	.	.	.	.	1	.	.	.	.
.	.	-1	.	.	1	.	.	.	.	.	1	.	.	.
-1	.	.	.	.	.	1	.	.	.	1	.	.	.	.
.	.	-1	.	.	.	.	1	.	.	.	1	.	.	.

Remarks : To simplify the notation, only the structural matrices have been written (C_2 for $C_2 \otimes Y_{m1}$ as example). Notice that, for this example, C_3 and A_1 matrices doesn't exist.

After examination of this matrix, we conclude that this network is globally observable.

The system of redundancy equations can be written as :

$$X_1 - X_2 - X_4 - X_6 - X_7 = 0$$

$$X_3 - X_4 - X_6 - X_{11} - X_{12} = 0$$
$$X_3Y_3 - X_4Y_4 - X_6Y_6 - X_{11}Y_{11} - X_{12}Y_{12} = 0$$

$$X_1 - X_2 - X_4 - X_6 - X_{11} - X_{12} = 0$$
$$X_1Y_1 - X_2Y_2 - X_4Y_4 - X_6Y_6 - X_{11}Y_{11} - X_{12}Y_{12} = 0$$

$$X_8 - X_9 + X_{11} + X_{12} = 0$$
$$X_8Y_8 - X_9Y_9 + X_{11}Y_{11} + X_{12}Y_{12} = 0$$

The table 5 gives the different raw measured data and their accuracy.

	Massic flowrate		Concentration 1		Concentration 2		Concentration 3	
Stream	Measure	Accuracy	Measure	Accuracy	Measure	Accuracy	Measure	Accuracy
1	2219	15 %	0,62	5 %	2,02	5 %	28,69	5 %
2	221	5 %	0,54	2 %	2,16	2 %	23,30	2 %
3	-	-	0,61	5 %	1,98	5 %	29,33	5 %
4	557	5 %	1,69	2 %	4,63	2 %	37,62	2 %
5	-	-	-	-	-	-	-	-
6	170	5 %	0,61	2 %	3,93	2 %	35,01	2 %
7	1170	5 %	-	-	-	-	-	-
8	-	-	0,20	2 %	0,74	3 %	41,36	2 %
9	-	-	0,14	2 %	0,58	3 %	29,06	2 %
10	-	-	-	-	-	-	-	-
11	677	20 %	0,08	2 %	0,28	3 %	5,53	2 %
12	490	5 %	0,18	2 %	0,93	2 %	50,51	1 %

Table 5 : the measurements

Table 6 summarizes the results obtained after the reconciliation. For each estimation, an adjustment ratio has been computed such that :

$$\text{adjustment ratio} = \frac{\text{estimation - measurement}}{\text{measurement}}$$

The comparison of this adjustment ratio with the accuracy (in per cent) allows to appreciate the quality of the measurements.

	Massic flowrate		Concentration 1		Concentration 2		Concentration 3	
Stream	Estimation	Adjust. ratio	Estimation	Adjust. ratio	Estimation	Adjust. ratio	Estimation	Adjust. ratio
1	2106	-5,1 %	0,65	4,2 %	2,14	6,1 %	29,75	3,7 %
2	220	-0,4 %	0,54	0,0 %	2,16	-0,1 %	23,29	-0,1 %
3	1885	-	0,66	8,0 %	2,14	8,1 %	30,51	4,0 %
4	600	7,7 %	1,66	-1,7 %	4,56	-1,6 %	37,44	-0,5 %
5	1286	-	0,19	-	1,01	-	27,27	-
6	171	0,5 %	0,61	-0,2 %	3,92	-0,4 %	34,97	-0,1 %
7	1115	-4,7 %	0,13	-	0,57	-	26,09	-
8	250	-	0,20	0,0 %	0,73	-0,8 %	41,42	0,1 %
9	1364	-	0,14	0,0 %	0,60	3,6 %	28,89	-0,6 %
10	759	-	0,19	-	0,86	-	47,51	-
11	605	-10,6 %	0,08	0,0 %	0,28	-1,1 %	5,53	0,0 %
12	510	4,1 %	0,18	-0,6 %	0,92	-1,2 %	50,49	0,0 %

Table 6 : the estimations

CONCLUSION

Observability and redundancy are basic information in designing process performance monitoring systems. The principal objective of this investigation is to provide a computational tool to obtain the classification of all variables and the system of equations which allows their determination. The matricial operations used are very simple and a computer code can be implemented very easily. Then a direct iteration algorithm is proposed to solve the problem of equilibration. The usage of recurrence formula for matrix inversion also allows the estimation algorithm to be computationaly efficient.

REFERENCES

Crowe, C.M., (1986). Reconciliation of process flow rates by matrix projection. AIChE Journal, 32, 616-623.

Darouach, M., (1986). Observabilité et validation des données de systèmes de grandes dimensions. Application à l'équilibrage des bilans de mesures. Thèse d'état de l'Université de Nancy I, juin 1986, France.

Darouach, M., J., Ragot, J., Fayolle and D., Maquin, (1988). Data validation in large scale steady state linear systems. 12th World Congress on Scientific Computation IMACS, Paris, july 18-22.

Kretsovalis, A., and R.S.H., Mah, (1987). Observability and redundancy classification in multicomponent process networks. AIChE Journal, 33, 70-82.

Kretsovalis, A., and R.S.H., Mah, (1988). Observability and redundancy classification in generalized process networks. 1- Theorems. Comput. Chem. Engng., 12, 671-687.

Mah, R.S.H., G.M., Stanley, and D.M., Downing, (1976). Reconciliation and rectification of process flow and inventory data. Ind. Eng. Chem. Process. Des. Dev., 15, 175-183.

Maquin, D., (1987). Observabilité, diagnostic et validation de données des procédés industriels. Thèse de Doctorat de l'Université de Nancy I, novembre 1987, France.

Romagnoli, J.A., and G., Stephanopoulos, (1980). On the rectification of measurement errors for complex chemical plants. Chem. Eng. Sci., 35, 1067-1081.

Stanley, G.M., and R.S.H., Mah, (1981). Observability and redundancy classification in process networks. Chem. Eng. Sci., 36, 1941-1954.

Vaclavek, V., (1979). A note to the problem of adjustment of material balance of chemical reactor. Coll. czech. chem. commun., 34, 2662-2673.

Vaclavek, V., and M., Loucka, (1976). Selection of measurements necessary to achieve multicomposant mass balance in chemical plant. Chem. Eng. Sci., 31, 2, 1199-1205.