Reformulation of data reconciliation problem with unknown-but-bounded errors.

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Abstract
In this paper, a new formulation of the problem of mass and energy balance equilibration in the case of unknown-but-bounded errors is proposed. The bounds of the errors are specified both over a measurement noise and the balance equations. Both bounds are mainly motivated by experimental considerations upon the measurement precision; with a more general interpretation they can be considered as parameters that the user has to adjust in order to make possible the reconciliation. The method is particularly suitable for linear models but has been extended to non linear ones. Simulations provide results that may be favourably compared with those of classical reconciliation methods involving maximum likelihood estimation based on statistical knowledge of the measurement errors.
1. Introduction

The problem of obtaining reliable estimates of process variables from measurements (data validation) and the related problem of detecting and isolating gross errors has been well studied. Historically speaking, likely due to measurement availability, static redundancy equations have been first utilised in the mineral processing and the chemical industries. The first studies (Ripps, 1962, Vaclavek, 1969, Smith et al., 1973) were concerned with data reconciliation using the now classical technique of equilibration of production's balances. In the following stages this data reconciliation principle has been generalized to processes which are described by algebraic equations either linear in the case of total flowrates (Crowe et al., 1983) or non linear in the case of chemical concentrations (Sood et al., 1979, Crowe, 1986).

At the same time, data reconciliation went into use for more general applications than establishing statistically coherent balances. It was then applied to more fundamental problems such as: detection, localisation and estimation of gross errors (Narasimhan et al., 1989, Ragot et al., 1990), diagnosis and observability of systems (Kretsovalis et al., 1988, Crowe 1989), optimization of sensors location (Maquin et al., 1987, 1996) and study of the reliability of a measurement system (Turbatte et al., 1991). Specific work concerning the numerical regularisation of the estimation technique using projection matrix has been studied (Kelly, 1998).

Most approaches to data reconciliation ensure that the estimates of process variables satisfy the material and energy balances either in their linear or non linear form. The second important point is that reconciliation is only possible if we have redundancy equation i.e. equations containing only redundant variables. Let us recall here that a measured variable is called redundant if it can be calculated from the remaining measured variables. As previously mentioned, this redundancy generally leads to a discrepancy
between the equations and the data which have to be reconciled; so it provides a check on
the reliability of a given set of measurements. At last, it seems relevant to validate and
adjust the measurements taking into account the degree of precision of each measurement
and key physical laws. Most of the methods used techniques based upon statistical
considerations, where the noise affecting the records is often characterized by the mean
and the covariance of an amplitude probability function. Maximising the likelihood
function issued from this probability function allows to express the estimation of the true
data. A survey of the methods used in data reconciliation can be found in (Crowe, 1996).
In 1996, Crowe investigated another formulation of the problem of data reconciliation by
using the concept of information entropy ; that allows to deduce probability distributions
of the data by taking into account bounds on the data and/or variance-covariance matrix of
the data.

As mentioned above, most previous investigators have used statistical criteria such as least
squares as the criteria for calculating the best estimates of process variables. However, the
results provided by such estimators are valid under the following restrictive conditions :

- the nature of the measurement noise has to be known
- the model of the process has to be perfectly known.

It can be a difficult task to estimate the validity of such assumptions and in a certain
number of applications, it is obvious that both conditions are not fully respected.
Therefore, it becomes very hazardous and mathematically not correct to reconcile operation
data with regard to an uncertain model without taking this fact into account. Some attempts
in this direction have been already published (Mandel et al., 1998), (Maquin et al., 2000).
An alternative method is proposed here which do not use any hypothesis about the noise
distribution. The only information needed about the noise is the value of its bounds. As
the process model may be inaccurate, it is not necessary that the estimate exactly verify the
model ; it is only desired that the model residual belong to a given interval. Indeed our
strategy is based on interval constraint satisfaction both for the variable estimations and the
model residuals. On an historical point of view, the paper of Himelblau (1985) is
probably one of the first which gives the formulation of such data rectification principles.
This idea has been confirmed in (Kyriakopoulos et al., 1996) and in (Harjumar et al.,
1993). In fact, the proposed method was based on a least square estimates subject to
inequality constraint. More recently (Dovi et al., 1999) generalize the fundamental method
of data reconciliation developed by Crowe (1996) to allow for the presence of censored
measurements. In his paper published in 2001, Soderstrom suggest a reconciliation
method which also uses inequality constraints for the determination of the bias within a
mixed integer optimization framework.
Here our strategy involves inequality on the estimates and on the residuals on balance
equations and may be considered as an alternative of this idea. Moreover, the probability
distribution of the measurement errors is not used and only bounds on these errors are
considered which is, may be, less restrictive. The aim of this presentation is to provide
elements necessary to the implementation of a procedure using this type of formalisation
based on inequality constraints.

In section two, we recall the principle of reconciliation of measures based on a model and a
measurement system and we give an alternative approach to solve this classical problem
based on the respect of inequality constraints set by the user. Then, in section three we
propose an extension of the technique for non linear systems. Section four is devoted to
numerical results and discussion.

2. Data reconciliation. The linear case
A linear system (under steady-state conditions) can be described, in the fault-free case, by
the following relations:

\[ \text{a model equation : } Mx^* = 0, \ x^* \in \mathbb{R}^n, \ M \in \mathbb{R}^{m \times n} \quad (1a) \]
\[ \text{a measurement equation : } z = x^* + \epsilon, \ z \in \mathbb{R}^n \quad (1b) \]
where \( x^* \) is the vector of process variables, \( z \) the vector of measurements, \( M \) the \( m \times n \) matrix of model equations (without loss of generality, it is supposed of full row rank), and \( e \) is a vector of errors due to measurement noise.

The estimation or data reconciliation problem of system (1) involves finding a set of adjustments such that the adjusted values verify the model equation (1a) with a given level of satisfaction.

In the context of unknown-but-bounded error, the noise \( e \) is assumed to verify a relation of the form:

\[
\| e \| \leq e
\]  

(2a)

where \( e \) is a known bound. Consequently, the \( \hat{x} \) estimations are subjected to the constraints:

\[
\| z - \hat{x} \| \leq e
\]  

(2b)

In the context of an approximate model, bounds on balance equations can be imposed; thus, we are looking to adjust the estimated \( \hat{x} \) such as:

\[
\| M\hat{x} \| \leq r
\]  

(2c)

where the bound \( r \) is chosen by the user and may be also fixed to zero if it is desired to exactly verify the balance equations. In this alternative approach for data reconciliation, it is thus desired to correct the raw data with bounds (2b) and to satisfy approximately the model equation with a bounded residual (2c). We can say that for the user, it is a natural way to reconcile the data. Indeed the user has a certain knowledge about the quality of the measures; he has also information concerning the precision of the model. Consequently, he can define a maximal value for the correction of each variable and a kind of satisfaction level of the process equations. It should be noticed that the first point of view has already been taken into account in the literature, see for example (Harikumar et al., 1993) and (Narasimhan et al., 1993).

Thus, summarising, the problem of data reconciliation may be turned into the following constraints:

\[
\| z - \hat{x} \| \leq e \\
\| M\hat{x} \| \leq r
\]  

(3)

In a more sophisticated situation, the bounds can be expanded according to upper and lower bounds corresponding to asymmetrical corrections and satisfaction levels of the constraints:

\[
\| e \| \leq z - \hat{x} \| \leq e \\
\| r \| \leq M\hat{x} \| \leq r
\]  

(4)

For numerical solution, the system (4) is expressed using only simple inequalities:

\[
\begin{bmatrix}
\| \hat{x} + z \| \\
\| \hat{x} \| \\
\| M\hat{x} \|
\end{bmatrix}
\leq
\begin{bmatrix}
\| \hat{x} + e \| \\
\| \hat{x} \| \\
\| M\hat{x} + e \|
\end{bmatrix}
\leq
\begin{bmatrix}
\| z \| \\
\| z + e \| \\
\| z + e \|
\end{bmatrix}
\leq
\begin{bmatrix}
0 \\
0 \\
0
\end{bmatrix}
\]  

(5)
The bounds \( \varepsilon \) and \( \bar{\varepsilon} \) will be chosen as a function of empirical knowledge concerning the state of the process and particularly the probable variation domain of the different variables. As these bounds express the amplitude of the corrections applied to the measures, they can be indexed on an estimation of the precision of these measures. The bounds \( r \) and \( \bar{r} \) are linked to the degree of satisfaction of the balance constraints and depend on the relative importance given to the different balance equations.

Thus, the data reconciliation problem is to find estimates that satisfy the constraints \( (5) \). It should be noted that when the bound \( r \) is set to zero that force the balance equation to be perfectly respected. Due to the nature of the problem (i.e. the presence of inequality constraints), it is clear that the estimates can no longer be obtained analytically. Moreover there is no guarantee that the estimates will be unbiased or will have the minimum variance. However, there are many tools to solve a system of linear inequalities and all of them are referred to LMI concept (Boyd, 1994); the reader may refer to a summary explanation given in annex concerning the LMI solving.

Generally speaking, for technical and/or financial reasons a process cannot be completely instrumented and thus some variables are not measured. This point can easily be taken into account, in the problem of balance formulation, by means of a matrix \( C \) (of dimension \( p.n \)) of measurement selection. The observability analysis that is required by the presence of unmeasured variables is not explained here, but the reader can consult the reference (Ragot, 1990), for more details. The problem of the reconciliation of measurements is then expressed by the set of inequalities:

\[
\begin{align*}
C\hat{x} + z \begin{bmatrix} 0 \\
-\varepsilon 
\end{bmatrix} & \geq 0 \\
z + C\hat{x} + \varepsilon \begin{bmatrix} 0 \\
0
\end{bmatrix} & \leq 0 \\
M\hat{x} \begin{bmatrix} 0 \\
0
\end{bmatrix} & \leq 0 \\
M\hat{x} + \xi \begin{bmatrix} 0 \\
0
\end{bmatrix} & \geq 0
\end{align*}
\]  

(6)

where \( z \in \mathbb{R}^p \), \( \varepsilon \in \mathbb{R}^n \). Indeed, LMI system \( (6) \) is a straightforward generalisation of system \( (5) \).

For the problem in which all the variables are measured \( (5) \), a reduction of the number of inequality constraints is observed, as corrective terms may be calculated for measured variables only. Another way of proceeding consists in keeping the set of equations \( (5) \) and in relaxing the constraints related to the unmeasured variables. Thus, if for instance the variable \( k \) isn’t measured, a “large” threshold is chosen for the element of row \( k \) of the vector \( \bar{\varepsilon} \), a “small” threshold for the element of same row of vector \( \varepsilon \) and the missing measurement may be replaced arbitrarily by 0; from a practical point of view, that is equivalent to not enforcing any proximity between the \( k \) th variable and its measurement (since it doesn’t exist!).

3. Data reconciliation. The non linear case

We now consider the more general case where both model and measurement system are non linear and described by:

\[
\begin{align*}
f(x^*) = 0, \quad f \in \mathbb{R}^m \\
z = h(x^*) + \begin{bmatrix} 0 \end{bmatrix}, \quad h \in \mathbb{R}^p
\end{align*}
\]  

(7)

This general description includes the case where the device measurement is linear, i.e. where \( h \) reduces to identity. Thus, according to the previous strategy, the data reconciliation problem is to find estimates \( \hat{x} \) that satisfy the bounds on process variables. Thus generalising system \( (6) \), the state estimation has to verify the inequality constraints:
By re-adopting the principle of linear balance reconciliation, we propose linearizing the equations of balances and using the LMI technique to resolve the system thus produced. At the outset, to apply this algorithm, it is necessary to have an initial estimation $\hat{x}^{(0)}$ of the variables; for the measured variables, the measurements provide appropriate initial values, and for the unmeasured variables, the user will be guided in his choice by the a priori knowledge he may have of the process. At step $i$ linearizing the constraint functions $f$ and $h$ around a previous solution $\hat{x}_i$ gives:

$$
\tilde{f}(x) = f_i + F_i x \\
\tilde{h}(x) = h_i + H_i x
$$

(9a)

with the definitions:

$$
F_i = \left. \frac{\partial f}{\partial x} \right|_{x = \hat{x}_i} \\
f_i = f(\hat{x}_i) \\
F_i = \left. \frac{\partial h}{\partial x} \right|_{x = \hat{x}_i} \\
h_i = h(\hat{x}_i)
$$

(9b)

The data reconciliation problem defined by (8) can be replaced by the problem:

$$
H_i \hat{x} + h_i \bar{z} + e \bar{z} \preceq 0 \\
F_i \hat{x} + f_i \bar{r} \preceq 0 \\
F_i \hat{x} + f_i \bar{r} \preceq 0
$$

(10)

which corresponds to the analysis of a set of linear inequalities. Thus an iterative algorithm can be easily constructed for solving the non linear data reconciliation problem as follows:

E1: set $i = 0$, select an initial value for $\hat{x}_i$ (for the measured variables, their corresponding values may be used as initial values for the estimates). If measurements are given with an interval representation, the initial value may be chosen belonging to this interval.

E2: compute the gradients of the functions $f$ and $h$ (9b) linearise the model equation around solution at step $i$ (9a)

E3: collect all the constraints of the estimation problem (10)

E4: using a LMI routine, solve the linear matrix inequations, and set $\hat{x}_{i+1} = \hat{x}$

E5: test for convergence of the solution by analysing the series $\hat{x}$. stop the procedure or $i \geq i + 1$ and go to step E2.

4. Examples
First example
Consider the following academic model depending on six variables (with $a = 5.5254$):

\[
\begin{align*}
1 \cdot x_2 + x_5 & = a = 0 \\
\exp(x_1) + \exp(x_2) & = 1 = 0 \\
x_1 x_5 & = 0 \\
x_2 x_3 & = 0 \\
2 \cdot x_3 & = 0 \\
2 \cdot x_5 & = x_1 / x_4 = x_6 = 0
\end{align*}
\]  

The measurement function (eq. 5) is $h = I_6$ (identity matrix of dimension 6), i.e. all the variables are measured. The reconciliation technique has been applied with the bounds $\bar{r} = [r] = 10^{[3.5]}$. The table 1 presents the results with data obtained from the simulated process (11). The upper and lower bounds of the measurements are given in rows 2 and 3; they have been reasonably fixed by the user according to his knowledge upon the precision of the measurements. A better perception of the measurements may be obtained by considering the centre (row 4) and the radius of the measurement interval (row 5). These values give an idea of the mean measurement values and their dispersion. The estimations are given by the 6th row. The reconciliation has been solved by using the iterative scheme of section 3 with initial estimation equal to the centres of the measurement intervals. Only twelve iterations has been performed to satisfy all the constraints. The 7th line of table 1 gives the correction ratio obtained by dividing the magnitude of the correction (difference between the centre of the measurement interval and the estimate) by the centre of the measurement interval; the magnitude of these ratios are reasonably small and therefore, roughly speaking, there are no abnormal data. In other situations, a gross magnitude of a ratio may be used to detect and localise gross errors or bias in the raw data (Narasimhan et al., 1989). All the mass balances (eq. 11) computed with the reconciled values are close to zero with a precision of $3 \cdot 10^{-6}$ which perfectly agrees with the selected bounds $\bar{r}$ and $\bar{r}$.

The second part of the table relates the results obtained when applying a classical non-linear least square procedure. For that, we have considered as measurements those obtained by taking the centres of the measurement interval; for sake of simplicity, the weighting factors $w$ have been chosen proportional to the normalised dispersions $z_r / z_c$. (row 5 of the first part of table 1) The two estimates (LMI and LS) are in the same vicinity and the corrective ratios have comparable magnitudes; however, it would be hazardous to go further in this comparison due the very different concepts of the approaches.

<table>
<thead>
<tr>
<th>Variable</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Meas. lower bound $z_\ell$</td>
<td>0.67</td>
<td>5.35</td>
<td>4.42</td>
<td>1.54</td>
<td>0.62</td>
<td>18.01</td>
</tr>
<tr>
<td>Meas. upper bound $\bar{z}$</td>
<td>0.91</td>
<td>7.23</td>
<td>5.98</td>
<td>2.08</td>
<td>0.84</td>
<td>24.37</td>
</tr>
<tr>
<td>Interval centre $z_c = (\bar{z} + z_\ell) / 2$</td>
<td>0.79</td>
<td>6.29</td>
<td>5.2</td>
<td>1.81</td>
<td>0.73</td>
<td>21.19</td>
</tr>
<tr>
<td>Interval radius $z_r = (\bar{z} - z_\ell) / 2$</td>
<td>0.112</td>
<td>0.94</td>
<td>0.78</td>
<td>0.27</td>
<td>0.11</td>
<td>3.18</td>
</tr>
<tr>
<td>Estimation $\hat{x}$</td>
<td>0.768</td>
<td>6.215</td>
<td>5.325</td>
<td>1.599</td>
<td>0.751</td>
<td>21.78</td>
</tr>
<tr>
<td>Cor. ratio $100</td>
<td>\hat{x} \cdot z_c / z_c$</td>
<td>2.4</td>
<td>1.2</td>
<td>2.4</td>
<td>11.7</td>
<td>2.6</td>
</tr>
<tr>
<td>weight $w = z_r / z_c$</td>
<td>0.15</td>
<td>0.15</td>
<td>0.15</td>
<td>0.15</td>
<td>0.15</td>
<td>0.15</td>
</tr>
<tr>
<td>LS Estimation</td>
<td>0.742</td>
<td>6.468</td>
<td>5.73</td>
<td>1.620</td>
<td>0.728</td>
<td>24.39</td>
</tr>
<tr>
<td>Cor. ration</td>
<td>5.3</td>
<td>2.3</td>
<td>2.5</td>
<td>12.5</td>
<td>0.4</td>
<td>0.1</td>
</tr>
</tbody>
</table>

Table 1. Measures and estimations (LMI and LS)

Second example
This test problem consists of a continuous stirred tank reactor (CSTR) with a second order exothermic reaction and heat removal by a coil or jacket. A mathematical modelling of the CSTR has been developed based on the principle of mass and energy conservation equations (Smith et al., 1985). This example has been used by many authors in the technical literature and constitutes a kind of benchmark for parameter estimation, state estimation, diagnosis and control. The feed is characterized by the rate $F$ ($m^3 / s$), the concentration of the reactant $C_i$ (kgmole / $m^3$) and the temperature $T_i$ ($^\circ C$). The output is characterized by analogous quantities $F$, $C$ and $T$. For the coolant, $F_c$ ($m^3 / s$) and $T_{ci}$ ($^\circ C$) denote the rate and the temperature while for the output the same quantities are noted $F_c$ and $T_c$. Here, we only consider the system under steady-state condition:

\[
\begin{align*}
0 &= \frac{F}{V}(C_i - C) - kC^2 \\
0 &= \frac{F}{V}(T_i - T) - \frac{H}{Vc_p}kC^2 - \frac{U}{Vc_p}T - kT_c \\
0 &= \frac{UA}{Vc_p}c_{pc}((T - T_c) - \frac{F_c}{Vc}(T_c - T_{ci})) \\
k &= k_0 \exp \left(-\frac{E_0}{R(K + T)}\right)
\end{align*}
\]  

(12)

Table 2 lists the values of the parameters used in the model.

<table>
<thead>
<tr>
<th>$V$</th>
<th>7.08 $m^3$</th>
<th>$c_p$</th>
<th>1.815 $10^5$ J/kg.C</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_c$</td>
<td>1.82 $m^3$</td>
<td>$f_{pc}$</td>
<td>4184 J/kg.C</td>
</tr>
<tr>
<td>$A$</td>
<td>5.40 $m^2$</td>
<td>$l$</td>
<td>19.2 kg/$m^3$</td>
</tr>
<tr>
<td>$U$</td>
<td>3550 J/s.$m^2$.C</td>
<td>$l_c$</td>
<td>1000 kg/$m^3$</td>
</tr>
<tr>
<td>$K$</td>
<td>273.16 C</td>
<td>$k_0$</td>
<td>0.0744 $m^3/s$.kgmole</td>
</tr>
<tr>
<td>$R$</td>
<td>8314.39 J/kgmole</td>
<td>$E_0$</td>
<td>818 000 J/kgmole</td>
</tr>
<tr>
<td>$H$</td>
<td>$[\bar{9}.86 \ 10^7$ J/kgmole</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 2. Parameter’s values

The columns 3 and 5 of table 3 respectively contain the lower and upper bounds for the measurements, which have been used for the computation of the estimations (column 4). As the process has been simulated, the true values are available and indicated in column 2. All the constraints concerning the magnitudes of the corrections are fulfilled and the three balance equations are closed to zero with a precision of $10^{-5}$ (table 4). It is somewhat difficult to analyse the inconstancy and/or the consistency of the raw data through the balance residuals. Indeed we have to keep in mind the magnitudes of the different terms allowing to calculate these residuals. It is important to note that residuals are computed as an algebraic sum of several quantities ; if one of these quantities is negligible in regard to the others, then a bad data in this quantity will have a very small effect on the residual. For example we observe that the second mass balance equation in (12) is the algebraic sum of three quantities ; table 5 reveals that these three quantities have comparable magnitudes and consequently no particular problem of sensitivity occurs in this example. Moreover, the magnitudes of the different terms are significatively greater than the residual.
(-0.0062, table 4) ; thus the later one may be considered as small suggesting the absence of gross errors in the data.

<table>
<thead>
<tr>
<th>True values</th>
<th>Meas. Lower bound</th>
<th>Estimation</th>
<th>Meas. Upper bound</th>
<th>Cor. ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>$F_c$</td>
<td>0.0073</td>
<td>0.00723</td>
<td>0.008</td>
<td>3.6</td>
</tr>
<tr>
<td>$F$</td>
<td>0.0075</td>
<td>0.00992</td>
<td>0.012</td>
<td>-4.5</td>
</tr>
<tr>
<td>$C_i$</td>
<td>2.88</td>
<td>2.5744</td>
<td>3.0</td>
<td>0</td>
</tr>
<tr>
<td>$C$</td>
<td>1.13</td>
<td>1.1645</td>
<td>1.25</td>
<td>0.9</td>
</tr>
<tr>
<td>$T_i$</td>
<td>66.075</td>
<td>63.7390</td>
<td>70</td>
<td>1.9</td>
</tr>
<tr>
<td>$T_{ci}$</td>
<td>27.00</td>
<td>29.3692</td>
<td>30</td>
<td>-17.4</td>
</tr>
<tr>
<td>$T_c$</td>
<td>50.50</td>
<td>45.6308</td>
<td>55</td>
<td>8.7</td>
</tr>
<tr>
<td>$T$</td>
<td>88.00</td>
<td>89.4017</td>
<td>92</td>
<td>-0.5</td>
</tr>
</tbody>
</table>

Table 3. Measurements and estimations

<table>
<thead>
<tr>
<th>Balance residuals with interval centre</th>
<th>Res. 1</th>
<th>Res. 2</th>
<th>Res. 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Before equilibration</td>
<td>-0.0001</td>
<td>&lt;10$^{-5}$</td>
<td>&lt;10$^{-5}$</td>
</tr>
<tr>
<td>After equilibration</td>
<td>-0.0062</td>
<td>&lt;10$^{-5}$</td>
<td>&lt;10$^{-5}$</td>
</tr>
</tbody>
</table>

Table 4. Balance residuals before and after reconciliation

$$2 \frac{F}{V}(T_i \parallel T) = [0.0360, 0.0559, 0.0199]$$

Table 5. Contribution of the different terms of the second residual equation

To analyse the results, table 6 exhibits the influence of the modification of some bounds on the reconciliation. The same example is used on which two simulations have been performed. The left part of the table 6 relates the case where the interval on the temperatures ($T_i$, $T_{ci}$) have been reduced by 3 °C, whereas the right part of the table shows a very large increase of the temperature interval $T$ (one may also consider that a large interval may represent the absence of measurement).

The comparison of the estimations (tables 5 and 6) shows (on this example) that the sensitivity in respect to the length of an interval is low; in particular the suppression of a measurement by increasing the corresponding interval, with the restriction that the system remains observable, do not set any problem of estimation.

It is however clear that, on a general point of view, the characteristics of an interval (centre and length) may influence the estimation. If, for a particular measurement the corresponding interval is fully away of the true data, the LMI system becomes inconsistent, i.e. no solution exist. For example taking the interval measurement $T = [100, 120]$ do not allow the existence of a solution. This remark may be used intensively if it desired to detect and isolate gross errors affecting the measurements.
Another point to analyse is the convergence of the LMI resolution. It is well known that results obtained by LMI solvers are dependant on the starting point. For the given example, but the conclusion yields only for this example, the estimations are weakly influenced by this starting point. The estimations collected in table 7 have been obtained with three different starting points. The first columns recall the name of the estimated variables. The second column gives the estimated variables when the procedure is initialized with the lower bound of the measurement interval (see table 3, 3rd column). The two last columns gather the estimations obtained when the initialization respectively uses the centre and the upper bound of the measurement interval. Thus, it can be concluded, according to this example and also to many others, that the state estimation is not very sensitive to the choice of the starting point.

<table>
<thead>
<tr>
<th></th>
<th>lower bound</th>
<th>interval centre</th>
<th>upper bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>( F_c )</td>
<td>0.00723</td>
<td>0.00723</td>
<td>0.00723</td>
</tr>
<tr>
<td>( F )</td>
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<td>0.00992</td>
<td>0.00992</td>
</tr>
<tr>
<td>( C_i )</td>
<td>2.5744</td>
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<tr>
<td>( C )</td>
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<td>1.1646</td>
<td>1.1646</td>
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<tr>
<td>( T_i )</td>
<td>63.7386</td>
<td>63.7377</td>
<td>63.7383</td>
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<tr>
<td>( T_{ci} )</td>
<td>29.3701</td>
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<tr>
<td>( T_c )</td>
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<tr>
<td>( T )</td>
<td>89.40192</td>
<td>89.4019</td>
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</tr>
</tbody>
</table>

Table 7. Sensibility in respect to the starting point

Discussion

As explained in the introduction, the LMI approach gives the guarantee that the state estimation perfectly respects the model constraints and the measurement intervals. Indeed, the method may furnish all the admissible solutions satisfying these constraints; however, the numerical resolution of the LMI is often reduced in giving one solution, for example those corresponding to the interior point (see annexe). It would be more interesting to enumerate all the admissible solutions, those satisfying all the LMI. This is a tedious task and the obtained result would be not very convenient for the user.

Let us illustrate the latter point with a toy example. Consider the reconciliation problem:

\[
\begin{align*}
  x_1 & - x_2 - x_3 = 0 \\
  x_1 & \in [12, 14] \\
  x_2 & \in [4, 6] \\
  x_3 & \in [7, 9]
\end{align*}
\]

According to the LMI reconciliation approach, the state estimates are defined as a set of constraints:

\[
\begin{align*}
  x_1 & \in [10, 15] \\
  x_2 & \in [12, 14] \\
  x_3 & \in [4, 6] \\
  x_4 & \in [7, 9]
\end{align*}
\]

Direct application of the interior approach gives the following (and trivial) results:

\[
\begin{align*}
  \hat{x}_1 & = 13 \\
  \hat{x}_2 & = 5 \\
  \hat{x}_3 & = 8
\end{align*}
\]
On figure (1a) the solution is given in the plan \((x_2, x_3)\). We have indicate the domain in which the solution lies (defined by eq. 13 and corresponding to the intersection of 3 strips) and the LMI interior point (eq. 14). On one hand it is clear that the interior point does not reflect the set of admissible solution; on the other hand, the whole set of admissible solutions expressed by (13) is not very easy to use. A compromise would be to approximate the whole set of solution (eq. 13) by independent constraints. The reader will verify that the following solution respects all the constraints and fits for use:

\[
\hat{x}_2 \in [4.5, 5.5] \\
\hat{x}_3 \in [7.5, 8.5]
\]

On figure 1b, this set of solution is thus defined by a box (in grey color) in the plan \((x_2, x_3)\). For each solution inside this box, \(\hat{x}_1\) may be easily defined by direct substitution \(\hat{x}_1 = \hat{x}_2 + \hat{x}_3\).

Summarizing, the point we have discuss on this toy example highlight the fact the reconciliation problem when analysed with a LMI approach may produce a set of admissible solutions. Moreover these solutions may be described under a convenient form (independent intervals). The previous discussion may be the starting point of an enlarging reflexion about the problem of data reconciliation.

5. Conclusion

The exposed technique represents an interesting alternative to the classical technique of data reconciliation using the principle of the likelihood function maximisation based on the distribution of the measurement errors. It requires very few theoretic hypotheses for its implementation and is essentially based on a semi-empirical knowledge relative to the variable plausible confidence domains as well as the definition of a satisfaction threshold for the different balances, that is depending on the confidence that is placed in them.

We have shown that the classical problems of material balance equilibration can be solved: total balances, partial balances, balances with missing measures. Various extensions can be envisaged. The first concerns the development of a reconciliation method using simultaneously the precise knowledge (structurally exact balances equations), the imprecise knowledge (balances expressed by inequalities constraints), the distribution functions of the errors (when they are available) and the inequality constraints on the correction rate (when the probability distribution functions are unknown). The second extension concerns the integration of fuzzy models or constraints under the form of...
propositions (for instance: the flow rate of a given stream of the process is “large”) or under the form of rules composed of premises and consequences (for instance: if the flow rate of a given stream of the process is “small” then the concentration of the corresponding flow is “high”). That would allow the whole available knowledge on a process to be used with their respective weights.

Last of all, it will be interesting to examine the case of dynamic systems. A priori, by making an abstraction of the problems associated with the calculation time, the technique proposed can be applied because it suffices to express at any given moment the set of constraints (on the rates of correction and on the degree to which the balances must be satisfied) and to find the solution which verifies them. Studies of this extension are currently under way.

Annex : Linear Matrix Inequality
A linear matrix inequality takes the form:

$$F(x) = F_0 + \sum_{i=1}^{m} x_i F_i > 0$$

(A1)

where $x \in \mathbb{R}^m$, $F_i \in \mathbb{R}^{n \times n}$, $m$ is the set of all real vectors of length $m$ and $n \times n$ is the set of all real $n \times n$ matrices. The symmetric matrices $F_i = F_i^T$, $i = 0 \ldots m$, are fixed and $x$ is the variable. The matrix $F(x)$ is an affine function of the elements of $x$ and is a positive definite matrix, that is $z^T F(x) z > 0$, $z \neq 0$, $z \in \mathbb{R}^n$.

The LMI (A1) is equivalent to $n$ polynomial inequalities.

Solving LMIs means to say if the problem is feasible and, if it is, to compute a feasible point. There are many algorithms to solve the LMI problem (Boyd, 1994) and among them the ellipsoid algorithm. May be, this is not the more efficient one, but it is very simple to apply.

The idea is the following. First we start with an ellipsoid $E^{(0)}$ that is guaranteed to contain the optimal point. Then we compute a cutting plane (that passes through the centre $x^{(0)}$ of $E^{(0)}$) in order to better localise the optimal point.

In order to determine this cutting plane, let us note that if $x^{(0)}$ satisfy the LMI (A1), there exists a non zero $u$ such that

$$u^T F(x^{(0)}) u > 0$$

(A2)

Define $g$ by

$$g_i = u^T F_i u$$

(A3)

for $i = 1 \ldots m$. Then for any $z$ satisfying

$$g^T (z \otimes x^{(0)}) < 0$$

(A4)

we have:
\[ u^T F(z)u = u^T F(x^{(0)})u + u^T \left( F(z) \bigwedge_1^m F(x^{(0)}) \right) u \]
\[ = u^T F(x^{(0)})u + u^T \bigwedge_1^m \left( z_i \bigwedge_1^{x_i^{(0)}} \right) F(z) \]

From (A3), one deduce:
\[
u^T F(z)u = u^T F(x^{(0)})u + \bigwedge_1^m \left( z_i \bigwedge_1^{x_i^{(0)}} \right) g_i \tag{A5}\]

From (A2) and (A4) we deduce that \( u^T F(z)u > 0 \). It follows that every feasible point lies in the half space \( \left\{ z \mid g^T \left( z \bigwedge_{x^{(0)}} \right) < 0 \right\} \) i.e. the vector \( g \) defines a cutting plane for the LMI problem at the point \( x \).

We then know that the sliced half-ellipsoid
\[ E^{(0)} \bigwedge \left\{ z \mid g^T \left( z \bigwedge_{x^{(0)}} \right) < 0 \right\} \]
contains the optimal point. We compute the ellipsoid \( E^{(1)} \) of minimum volume that contains this slice half-ellipsoid; \( E^{(1)} \) is guaranteed to contain the optimal point. The process is the repeated.

References


D.L. Ripps (1962). Adjustment of experimental data. Chemical Engineering Progress, 58 (10), p. 120.


