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<u>Key Word</u>: Data validation, consistancy of measurements, mass balances, observability, redundancy, large scale systems.

Abstract:

Data reliability is of fundamental importance for process diagnosis, identification and control. Measurements having large, random or biased errors which go undetected lead to poor control of processes. Detection of such errors is therefore very important, but can only be carried out on the basis of a certain knowledge of the process, of its structure, of the location of the data sources (observations), and a certain degree of redundancy. Here we present a method of classifying the variables of steady state linear systems into; observable, unobservable, redundant and no-redundant variables. This classification gives information on the state of the system, the consistancy of the data and leads to a way of validating the observable part of the process. A recurrent estimator is developed on the basis of an estimation of the maximum likelihood. An application of the method to material balance is presented.

1 - Introduction

Data collected from a process is the basis for any evaluation of the performance of the process, of the strategy for its control and in general for any decision to be taken about the process. If the information contains errors, any decision made will lead to poor operation. Data validation is therefore situated between the process measurements aquisition and the decision to be taken.

This validation poses several problems amongst which are the following:

- Process models are non-linear and inaccurate.
- Process models are very large.
- Measuring devices may be defective.
- Measurements are subject to errors.
- Not all variables are measured.

This study is limited to the case of linear systems operating at steady state. Even though this hypothesis seems restrictive this class of system is frequently encountered in industrial applications. In addition the study of the steady state can be considered to be a preliminary to the study of system dynamics.

Process operation models are exact as they are based on mass and energie balances. However measurements and data available are subject to errors wich may be divided into the following two groups:

- random errors are generally taken to be independent, gaussian, with a zero mean value and a "small" variance.
- gross errors are caused by no-random events such as biased instruments, defective transducers, incomplete or imprecise models.

Correct data validation (by making balances) can only be carried out if the parameters have been classified. This allows determination of the redundant and no-redundant measurements, the variables which are not measured and those which can or can not be determinated. Once this classification has been made it is possible to:

- detect gross errors
- diagnose errors
- validate measurements

The complete data validation strategy can be schematized by the block diagram of figure 1.

Before presenting a strategy for data validation we first present some definitions and concepts for linear systems under steady state conditions.

2 - Concepts and definitions

A linear system under steady state condition is defined by :

- A set of constraints (known process model)

$$\mathcal{H} = \{ x \in \mathbb{R}^{V} / Ax - b = 0 \}$$
 (1)

in which A is an $(n \cdot v)$ matrix of coefficients x is the vector of the state

- A measurement vector

$$Z = H x + \varepsilon \tag{2}$$

in which $Z \in R^m$, H is an $(m \cdot v)$ matrix of coefficients and ϵ is a $(n \cdot 1)$ vector of measurement errors.

The system S, described by the pair (H, A), is said to be globally observable if the state x is uniquely determined by the observation Z and the constriants (1).

Observability of linear system under steady state conditions [1], [2], [3]

Observability is independent of measurement errors and is considered on the basis of exact noise free data (ϵ = 0). The system to be considered for observability is:

$$Q \cdot x = d \tag{3}$$

where $a = {H \choose A}$ is the $((m+n) \cdot v)$ observability matrix of the system (1),(2) and $d = {Z \choose b} \in \mathbb{R}^{n+m}$.

a) Partial observability [4]

By analogy whith the dynamic of linear systems the partial observability of linear systems under steady state conditions is defined as follows:

Let
$$\Omega_0 = \{ x \in \mathbb{R}^V / \mathcal{O} x = d \}$$
and $\mathcal{T} : \mathbb{R}^V \longrightarrow \mathbb{E}$ be a linear operator

E is a linear vector space and we wish to determine a neccessary and sufficient conditions under which:

$$\forall (x_{1}, x_{2}) \in \Omega_{0}^{2}, \Upsilon(x_{1}) = \Upsilon(x_{2})$$

$$x_{1} \neq x_{2}$$
(5)

If \Im is a one to one operator, then (5) indicates the uniqueness solution of (3) and therefore the overall observability of the linear system (1), (2).

However for an arbitrary \mathcal{T} we say that (5) is a condition for partial observability with respect to \mathcal{T} . We may then state the following proposition [4]:

Let P be the operator matrix of ${\mathfrak P}$

The system is partially observable with respect to ${\cal T}$ if and only if

b) Global observability

A linear system under steady state conditions is said to be globally observable when the state x is unique. This correspond to P = I for partial observability and from (6) we may say that :

The system (1), (2) is completly or globally observable if and only if :

If rank θ < rank ($\frac{\theta}{1}$) = v the system described by (1), (2) is not globally observable. In this case as for dynamics systems, the system (1),(2) can be decomposed on the basis of the concept of observability.

c) Decomposition by observability

If rank \mathscr{O} = q < v then there is an (v . v) non singular matrix T such that, for the change of coordinates x = Ty :

$$\overline{a} = a T = (a_1 | 0) = (\frac{H_1}{A_1} | 0)$$
 (8)

where θ_1 is a matrix with q columns and

$$\operatorname{rank} \ \mathcal{O}_1 = \operatorname{rank} \left(\frac{H_1}{A_1} \right) = q \tag{9}$$

In addition, in the new coordinates $y=(\frac{y_1}{y_2})$ in which y_1 corresponds to \mathcal{Q}_1 , the subsystem :

$$Q_1 y_1 = d \tag{10}$$

is observable in \mathbb{R}^q and the remaining subsystem of dimension (v-q) is unobservable.

This result can be shown by orthogonal transformation or decomposition into singular values [5], [6].

d) Redundancy in linear systems under steady state conditions

Definition:

Linear system under steady state conditions (1), (2), is said to be redundant when the data available exceeds the minimum neccessary for a unique determination of the system state.

This definition indicates that measurements are redundant if their suppressions causes no loss of observability. The result for the decomposition by observability can be extended to that of measurements redundancy.

In this case we say that:

The linear steady state system described by the pair (H, A) such that (n+m)>v and rank $(\frac{H}{A})=\mathrm{rank}\ \mathcal{O}=q< v$ (therefore globally unobservable) has a redundancy of r=(n+m-q) and in addition can be decomposed into an observable and an unobservable parts. The observable part can itself be decomposed into redundant and no-redundant parts. These results will be used later in data validation by mass balances.

3 - Data validation

Let us consider a steady state linear system S described by (1),(2) for which we are to estimate its state x.

Hypotheses:

- The system S is globally observable, that is rank $(\frac{H}{A}) = v$.
- ⊢ Rank A = n
- $\dot{\sim}$ The errors ϵ are normally distributed with a zero mean and known covariance matrix V .

Estimator:

With these hypotheses the best estimator, in the sense of the maximum likelihood, is that which maximises the probability density function of the measurements errors subject to the constrainsts (1) of the model.

That is:
$$\min \Phi = \frac{1}{2} || Z - H\hat{x} || \frac{2}{V-1}$$
 (12)

subject to the constrainst $A\hat{x} = b$

The associate lagrangian L is:

$$L = \Phi + \lambda^{T} (A\hat{x} - b)$$
 (13)

where λ is the vector of lagrange parameters of dimension n.

This is stationary when:

$$\begin{cases} \frac{\partial L}{\partial \hat{x}} = -H^T v^{-1} \quad (Z - H\hat{x}) + A^T \lambda = 0 \\ \frac{\partial L}{\partial \lambda} = -A\hat{x} - b = 0 \end{cases}$$
(14)

This system of equations (14) is equivalent to:

$$\begin{cases} (H^{T}v^{-1}H)\hat{x} + A^{T}\lambda = H^{T}v^{-1}Z \qquad (15.1) \\ A\hat{x} = b \qquad (15.2) \end{cases}$$

In general ($H^TV^{-1}H$)⁻¹ does not exist, however as the system is observable, by premultiplying (15.2) by A^T and by adding the result to (15.1), we obtain :

$$R^{-1}\hat{x} + A^{T}\lambda = H^{T}V^{-1}Z + A^{T}b$$
 (16)

where
$$R^{-1} = H^{T}V^{-1}H + A^{T}A$$
 (17)

which can be inverted.

From (16) we have:

$$\hat{x} = R (H^T V^{-1} Z + A^T b - A^T \lambda)$$
 (18)

which replaced in (15.2) gives:

$$\lambda = (ARA^{T})^{-1} ARH^{T}V^{-1}Z + (I - (ARA^{T})^{-1})b$$
 (19)

since rank A = n (hypothesis 2) Finally

$$\hat{x} = P_{R}RH^{T}V^{-1}Z + RA^{T}(ARA^{T})^{-1}b$$
 (20)

with
$$P_{r} = I - RA^{T} (ARA^{T})^{-1} A$$
 (21)

Statistical properties of the estimator

According to hypothesis (3), we have $\epsilon \sim \mathcal{M}(0,V)$ for the measurement errors.

As $Z = Hx + \epsilon$, we deduce that:

$$E(Z) = Hx \tag{22}$$

$$Var(Z) = E(\varepsilon \varepsilon^{T}) = V$$
 (23)

From (21), (22), and (23), we deduce the following properties:

$$E(\hat{x}) = P_{r}RH^{T}V^{-1}Hx + RA^{T}(ARA^{T})^{-1}b$$
 (24)

$$Var(\hat{x}) = P_r R (R^{-1} - AA^T) RP_r^T$$
(25)

Expression (25) can also be written as: $Var(\hat{x}) = P_r R P_r^T - P_r R A^T A R P_r^T$ Since $P_r R A^T = 0$

Then
$$Var(\hat{x}) = P_r R P_r^T = P_r R = \Sigma$$
 (26)

From (21) and (26), the estimate \hat{x} can also be written as:

$$\hat{x} = \Sigma H^T V^{-1} Z + RA^T (ARA^T)^{-1} b$$
 (27)

Supplementary linear constrainsts

Here we consider the estimation of the state variables in linear system under steady state conditions subject to additional linear constrainsts. From knowledge of the estimate without the constrainsts, we establish a recurrence formula which gives a new estimation of the state variables.

Given the globally observable linear system :

$$\begin{cases}
 Hx + \varepsilon = Z \\
 A_1x = b_1
\end{cases}$$
(28)

The estimation of the state of the system is (27):

$$\hat{x}_1 = \Sigma_1 H^T V^{-1} Z + R_1 A_1^T (A_1 R_1 A_1^T)^{-1} b_1$$
 (29)

Where $\Sigma_1 = Var(\hat{x}_1) = P_r R_1$

And

 $R_1 = (H^T V^{-1} H + A_1^T A_1)^{-1}$ (exists since S_1 observable)

$$P_{r1} = I - R_1 A_1^T (A_1 R_1 A_1^T)^{-1} A_1$$

When an additionnal linear constrainst is added, the system S_1 becomes:

$$S_{2} \begin{cases} Hx + \varepsilon = Z \\ A_{1}x = b_{1} \\ A_{2}x = b_{2} \end{cases}$$
 (30)

The problem of estimating the state \mathbf{x} of the system $\mathbf{S_2}$ can then be posed as:

min
$$\Phi = \frac{1}{2} | | Z - H\hat{x}_2 | |_{V-1}^2$$

 \hat{x}_2

subject to the constrainsts:
$$A_1\hat{x}_2 = b_1$$
 (31)
 $A_2\hat{x}_2 = b_2$

The Lagrangian associated with this problem is:

$$L = \Phi + \lambda^{T} (A_{1}\hat{x}_{2} - b_{1}) + \mu^{T} (A_{2}\hat{x}_{2} - b_{2})$$
 (32)

This is stationary when:

$$\frac{\partial L}{\partial \hat{x}_{2}} = -H^{T}V^{-1}(Z - H\hat{x}_{2}) + A_{1}^{T}\lambda + A_{2}^{T}\mu = 0$$

$$\frac{\partial L}{\partial \lambda} = A_{1}\hat{x}_{2} - b_{1} = 0$$

$$\frac{\partial L}{\partial \mu} = A_{2}\hat{x}_{2} - b_{2} = 0$$
(33)

Which can also be written as:

$$\begin{cases} (H^{T}v^{-1}H) \hat{x}_{2} + A_{1}^{T}\lambda + A_{2}^{T}\mu &= H^{T}v^{-1}Z \\ A_{1}\hat{x}_{2} &= b_{1} \\ A_{2}\hat{x}_{2} &= b_{2} \end{cases}$$
(34.1)
$$(34.2) (34)$$

$$(34.3)$$

Using expression (27) the solution of the system (34.1), (34.2) leads to :

$$\hat{x}_{2} = \Sigma_{1} H^{T} V^{-1} Z + R_{1} A_{1}^{T} (A_{1} R_{1} A_{1}^{T}) b_{1} - \Sigma_{1} A_{2}^{T} \mu$$
(35)

where $\Sigma_1 = (I - R_1 A_1^T (A_1 R_1 A_1^T)^{-1} A_1) R_1$

From expression (35) and (34.3) we obtain:

$$\mu = (A_2 \Sigma_1 A_2^T)^{-1} (A_2 \Sigma_1 H^T V^{-1} Z + A_2 R_1 A_1^T (A_1 R_1 A_1^T)) b_1 - b_2$$
 (36)

and
$$\hat{x}_2 = (I - \Sigma_1 A_2^T (A_2 \Sigma_1 A_2^T)^{-1} A_2) \hat{x}_1 + \Sigma_1 A_2^T (A_2 \Sigma_1 A_2^T)^{-1} b_2$$
 (37)

in which \hat{x}_1 is expressed by (29).

Statistical properties of the estimations \hat{x}_1 and \hat{x}_2

We have :

$$E(\hat{x}_1) = \Sigma_1 H^T V^{-1} H x + R_1 A_1^T (A_1 R_1 A_1^T)^{-1} b_1$$
 (38)

and
$$Var(\hat{x}_1) = \Sigma_1$$
 (39)

From which, using (37), we deduce the following:

$$E(\hat{x}_{2}) = (I - \Sigma_{1}A_{2}^{T} (A_{2}\Sigma_{1}A_{2}^{T})^{-1} A_{2}) E(\hat{x}_{1}) + \Sigma_{1}A_{2}^{T} (A_{2}\Sigma_{1}A_{2}^{T})^{-1} b_{2}$$
(40)

$$Var(\hat{x}_2) = \Sigma_2 = \Sigma_1 - \Sigma_1 A_2^T (A_2 \Sigma_1 A_2^T)^{-1} A_2 \Sigma_1$$
 (41)

Generalisation

More generally, if we call \hat{x}_k the estimation and Σ_k the variance of the estimation in presence of the constrainst $A_k\hat{x} = b_k$, the changes in the estimation and in its variance can be explicited in terms of the additional constrainst $A_{k+1}\hat{x} = b_{k+1}$.

$$\hat{x}_{k+1} = (I - Z_k A_{k+1}^T (A_{k+1} \Sigma_k A_{k+1}^T)^{-1} A_{k+1}) \hat{x}_k + \Sigma_k A_{k+1}^T (A_{k+1} \Sigma_k A_{k+1}^T)^{-1} b_{k+1}$$
(42)

$$Var(\hat{x}_{k+1}) = \sum_{k+1} - \sum_{k} - \sum_{k} A_{k+1}^{T} (A_{k+1} \sum_{k} A_{k+1}^{T})^{-1} A_{k+1} \sum_{k} (43)$$

This recurrence formula is especially useful if the matrix A_{k+1} reduces to a row vector. In this case, calculation of Σ_{k+1} and consequently x_{k+1} only requires the inversion of a scalar.

Application to mass balances

The case of mass balances corresponds to a system represented by a directed graph. Its arcs represent the process streams and its nodes represent the unit operations (tanks, flotation cells, reactors, etc ...). With this system, we associate an (n . v) incidence matrix A defined by:

$$A = (a_{ij})$$

 $a_{ij} = 1$ if the flow j enters in the unit i,

= -1 if the flow j leaves the unit i,

= 0 if the unit i has no connection with the flow j.

and rank A = n

We will limit this discussion to overall mass balances, so that only mass flow rates are considered. Furthermore measurements are direct, as its is generally the case in practice.

The system (1), (2) becomes:

- Overall mass balance :

$$A x = 0 (44)$$

- Measurement equation:

$$Z = (I \mid 0) x + \varepsilon \tag{45}$$

In this, I is the (m . m) identity matrix.

Partitionning x by components of $(I \mid 0)$ gives:

$$x = \begin{bmatrix} x_m \\ x_{\overline{m}} \end{bmatrix} \qquad \text{with} \qquad \qquad \dim x_m = m$$

$$\dim x_{\overline{m}} = \overline{m}$$

According to the same criterion for classification, the incidence matrix is partitioned in the form :

$$A = (A_m \mid A_m)$$

with $\dim A_m = n \cdot m$ and $\dim A_m = n \cdot (v - m)$

After these partitionings, equation (44) becomes:

$$A_{m}x_{m} + A_{m}x_{m} = 0 (46)$$

 $A_{m} x_{m} = -A_{m} x_{m} \tag{47}$

The observability of the system (44), (46) is determined from that of system (47). The procedure (8) used previously can be applied to (47) as, if r is the rank of $A_{\rm m}$, there then exist orthogonal transformations S and T such that :

$$A_{\overline{m}} = S \begin{bmatrix} R & O \\ O & O \end{bmatrix} T \tag{48}$$

where R is an upper triangular matrix of rank r,

S and T are (n . m) and (v . v) orthogonal matrices.

This very general procedure will not be used for the particular case of mass balances as the structure of the incident matrices is sparse, only containing +1's and -1's, and where a echelon form transformation is more suitable. Thus if r is the rank of block $A_{\overline{m}}$, a permutation of the rows and columns of $A_{\overline{m}}$ allows the regular part of $A_{\overline{m}+12}$ to be isolated.

As $A = \frac{1}{m}$ is regular an equivalent form (echelon form) is:

Finally by linear combination, A is also equivalent to:

Examination of this matrix allows the observability and the redundancy of all the variables to be explicited:

- Block 4 concerns the equations of redundancy as it only includes measured variables. The corresponding incidence matrix is:

$$A_r = A_{m2} - A_{m22} - A_{m12} - A_{m1}$$

- If block 2 contains rows of zeros then rows of the same rank in block 3 give the indices of the unmeasured variables which can be determined.
- The measured variables, which can not be estimated correspond to the indice of columns of block 4 composed of all zero elements.
- The decision variables of the global observability are the no zero elements of block 2.

The procedure using these results to validate data by mass balance can be schematized by figure 2.

This diagram demonstrates the decomposition of the initial problem (47),(48) into two smaller sub-problems which can be solved sequentially.

First sub-problem

$$\min \phi = \frac{1}{2} \left| \left| Z - \hat{x}_{m} \right| \right|_{V}^{2}$$

$$\hat{x}_{m}$$
subject to
$$A_{r} \hat{x}_{m} = 0$$
(52)

is solved in a recurrent fashion using the procedure (28)-(46). Taking into account that H = I and b = 0 we obtain:

$$\hat{x}_{m} = (I - VA_{r}^{T} (A_{r}VA_{r}^{T})^{-1} A_{r}) Z$$
 (53)

and

$$Var(\hat{x}_m) = V - VA_r^T (A_rVA_r^T)^{-1}A_rV$$

$$= \hat{V}_m$$
(54)

thus

$$\hat{x}_{m} = \hat{v}_{m} v^{-1} Z \tag{54}$$

In practice A_r is partitioned in the form :

$$A_{r} = \begin{pmatrix} A_{i} \\ A_{i+1} \end{pmatrix}$$

The estimated state for the system described by \mathbf{A}_{i} is :

$$\hat{x}_{i} = \hat{v}_{i} v^{-1} Z$$

$$\hat{v}_{i} = Var(\hat{x}_{i})$$
(56)

with

Adding the constrainst corresponding to the matrix A_{i+1} , we obtain the new estimation given by :

$$\hat{x}_{i+1} = \hat{v}_{i+1} v^{-1} z \tag{57}$$

with

$$\hat{V}_{i+1} = Var(\hat{x}_{i+1})$$

$$\hat{V}_{i+1} = \hat{V}_{i} - \hat{V}_{i} A_{i+1}^{T} (A_{i+1} \hat{V}_{i} A_{i+1}^{T})^{-1} A_{i+1} \hat{V}_{i}$$
(58)

and

$$\hat{V}_{i} = V - V A_{i}^{T} (A_{i} V A_{i}^{T})^{-1} A_{i} V$$
 (59)

In this case when the partitioning is performed according to the nodes of the system, each block A_i becomes a row vector of v elements. Matrix \hat{V}_m can therefore be calculated in n iterations each of which only requires the inversion of a scalar.

We apply (58) for i=1,n with
$$\hat{V}_0 = V$$
 and $\hat{V}_{n+1} = \hat{V}_m$

Second sub-problem

Once the level 1 validation is completed the estimation of the observable part of the unmeasured variables is made by direct deduction from the estimate variables of the first level and the relationships corresponding to the rows of the elements in the matrix $A = 1 \ m = 12 \ m = 11$.

Conclusion

The method of data validation presented here takes into account the topology of a process (its structure) and the data which is available (the measurements made, their location and their precision). It involves decomposing the problem of validation in two smaller sub-problems. In the case of large scale systems a recurrence formula provides an estimation of the redundant variables.

There are a great number of practical applications of this method. Particular mention may be made of the diagnosis of industrial systems in which the process configuration and the location of the measurement points change with time. The extension to the case of bi-linear systems will be treated in a later study.

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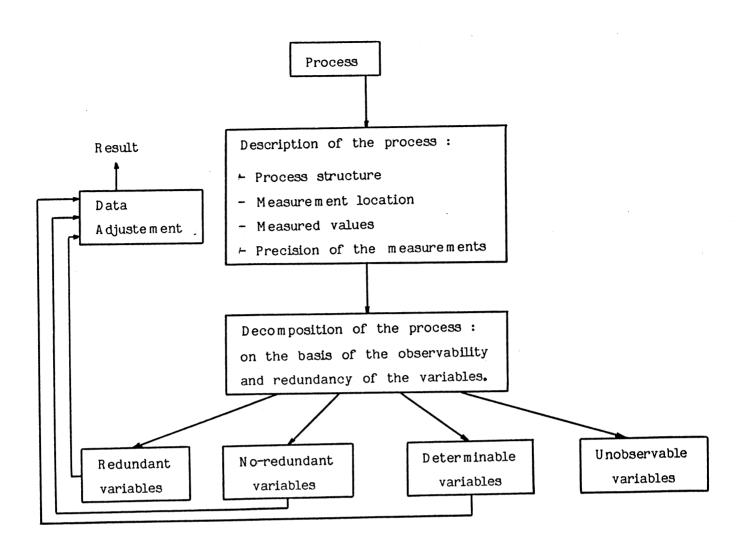


Figure 1: General strategy for data adjustement.

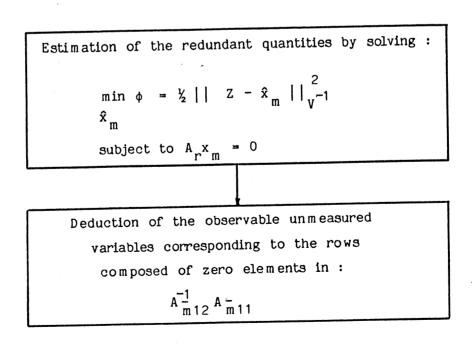


Figure 2 : Schematic diagram of the procedure for data validation by linear mass balances

The cicuit considered in this example is described by the flowsheet of figure 3, it consists of 19 nodes and 32 streams. The measurements location of the flow rates are indicated by x. The results of the data validation are sumarized in tables (1-2)

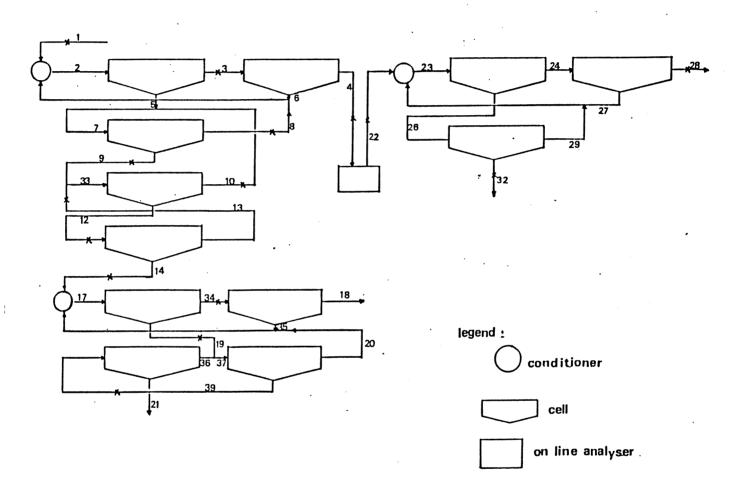


Figure 3 : Flotation circuit

	 HEASURED		 UNMEASURED	
 BTREAH	 ESTIMADLE	UNESTI- -MARLE	DETER- -MINABLE 	
1 6 8 2 2 3 3 5 4 1 10 17 7 9 1 13 3 3 1 1 1 1 1 1 1 1 1 1 1 1 1 1	X 	X 	X	

Table 1: Result of variables classification

1	!	!	!	ESTIMATED
I STREAM	I MEASUREMENTS	! ESTIMATIONS	STANDART !	STANDART
1	İ	!	DEVIATION !	DEVIATION
!	 			
1 1	1 4.683	4.595	0.234	0.096
16	1	2.242	1	0.322
18 !	0.531	0.531 l	0.027	0.027
12 1	' L	7.368	1	0.310
13 !	6.166	6.166	0.308	0.308
15 !		1.202	!	0.036
14 1	4.000 !	3.924 !	0.200	0.074
! 10 !	0.300	0.295	0.015	0.014
17 !		1.497	!	0.037
19 1	0.917	0.966	0.046 !	0.026
! 13 !	0.264	0.271 !	0.013	0.013
1 33 1	!	1.237 !		0.028
1 12 1	1.050	0.912	0.053	0.026
! 14 !	0.652 !	0.671	0.033 !	0.024
1 35	1	. !	. !	• !
1. 20	!	!	!	احمم
1 17	!	1.115		0.042
! 19	0.756	0.756	0.038	0.038
! 34	0.359	0.359	0.018	0.018
18	0.550	0.550	0.028	0.028
1 21 1	1	1	1	1
i 36	i	İ	ļ	. !
1 37 🖟 1	f	1	1	
1 22 1	3.700	3.924	0.185 !	0.094 1
l 27	1	.!.	!	. !
1 29	1		!	. !
23	!	· · · · · · · · · · · · · · · · · · ·	!	!
24 !	!	· •	!	1
26	!	!	0.450	0.007
28 !	3.000 !	2.932	0.150	0.097 1
32 !	1.000	0.992	0.050	0.048

Table 2: Flotation mass balance results