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Simultaneous estimation of biases and leaks in process plants

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Abstract

In this paper, a recursive strategy is applied to identify gross errors (biases and leaks) and estimate their magnitude in linear steady state processes. A recursive search scheme is used first to isolate the candidate sources of gross errors and then simultaneous identification/estimation of gross errors is accomplished. A recently proposed equivalency theory is used to correctly assess results. Comparative studies of performance and accuracy of estimation are performed for some process networks when compared to existing techniques. Simulation results show that the proposed approach has higher performance to identify gross errors as well as to estimate their magnitudes. © 1999 Elsevier Science Ltd. All rights reserved.

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1. Introduction

Instrument readings in process plants do not obey basic conservation laws and one has to perform data reconciliation to obtain process variable estimates. Typically, steady state data reconciliation results are corrupted by the presence of biased instruments and leaks, as well as departures from steady state. The latter have been traditionally lumped into variance estimate procedures, while the former are the object of this paper. The accuracy of the data and the quality of the information are related to the algorithm used as well as the sensor network to filter these disturbances appropriately. Therefore, since the onset of the field of data reconciliation in process plants, the issue of detection of gross errors has received central attention. Not only it is desired to have the proper location of gross errors, but it is also advantageous to have an estimate of its size. The former helps instrument maintenance in the case of biases and process monitoring in the case of leaks. The latter constitutes valuable information for production accounting.

There are several statistical tests that have been proposed to perform detection of gross error candidates. The most widely used are the global test (Reilly & Carpani, 1963), the measurement test (Mah & Tamhane, 1982; Crowe, García Campos & Hrymak, 1983), the nodal test (Reilly & Carpani, 1963; Mah, Stanley & Downing, 1976), the generalized likelihood ratio (GLR) (Narasimhan & Mah, 1987), Bonferroni tests (Rollins & Davis, 1992), and the principal component test (PCT) (Tong & Crowe, 1995), among others. Three kinds of strategies have been developed in identifying multiple gross errors: serial elimination (Ripps, 1965; Serth & Hennan, 1986; Rosenberg, Mah & Iordache, 1987) which identifies one gross error at time using some test statistic and eliminates the corresponding measurement until no gross error is detected; serial compensation (Narasimhan & Mah, 1987) which identifies the gross error and its size, compensates the measurement and continues until no error is found; simultaneous or collective compensation (Keller, Dorouach & Karzala, 1994; Kim, Kang, Park & Edgar, 1997; Sánchez & Romagnoli, 1994), which propose the estimation of all gross errors simultaneously. In addition, Bagajewicz and Jiang (1998) proposed a collective compensation strategy for dynamic systems that can be used for steady state cases. Finally the unbiased estima-

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tion technique (UBET) proposed by Rollins and Davis (1992) makes the identification first and then a simultaneous estimation.

Many researchers have evaluated the performance of these approaches. Serial elimination is simple but has the drawback of losing redundancy and not applicable to gross errors which are not directly associated with measurements, for instance leaks (Mah, 1990). Serial compensation is applicable to all types of gross errors and can maintain redundancy during the procedure but its results are completely dependant on the accuracy of estimation for the size of gross errors (Rollins & Davis, 1992).

Serial elimination methods can in principle be used to perform gross error estimation. Once all measurements containing gross errors are eliminated, the resulting ones can be used to calculate the variables corresponding to the eliminated measurements. This strategy may not always be successful, as the variables corresponding to the eliminated measurements can become unobservable. In addition, for those cases where all variables corresponding to eliminated measurements can be calculated, the loss of redundancy deteriorates the precision of the estimates. For this reason, attention is shifting towards methods that are capable of preserving redundancy, such as the serial compensation or simultaneous/collective compensation methods.

This paper builds up on a recently proposed method for simultaneous estimation of gross errors (SEGE) (Sánchez & Romagnoli, 1994; Sánchez, 1996). This strategy was developed for systems with all redundant variables. In the first stage of the procedure, a set of units and measurements suspected of leaks and bias is constructed using the global test. Then all combinations of measurement biases and process leaks from this subset are considered. Gross errors sizes are estimated simultaneously for each combination. In this paper the strategy is extended to consider the case where unmeasured variables are present. In addition, the Gross error equivalency theory recently developed by Bagajewicz and Jiang (1998) is used to identify equivalent sets and avoid singularities present in the original strategy. Comparisons to other methods are also included.

2. Recursive search scheme with simultaneous bias/leak estimation

We first review the SEGE strategy, first proposed by Sánchez and Romagnoli (1994). Consider the measurement model in the absence of gross errors:

$$\mathbf{y} = \mathbf{x} + \boldsymbol{\varepsilon} \tag{1}$$

and its corresponding steady state data reconciliation problem

$$\min\ (\mathbf{y}-\mathbf{x})^{\mathrm{T}}\boldsymbol{\Psi}^{-1}(\mathbf{y}-\mathbf{x})$$

$$s.t.$$

$$\mathbf{A}\mathbf{x} = 0 \tag{2}$$

where $\mathbf{x}$ is the $(z \times 1)$ vector of true values of the variables, $\mathbf{y}$ is the $(z \times 1)$ vector of measurements and $\boldsymbol{\varepsilon}$ is the $(z \times 1)$ vector of random errors. It is assumed that $\boldsymbol{\varepsilon} \approx \mathrm{N}_z(0, \boldsymbol{\Psi})$. $\mathbf{A}$ is the $(m \times z)$ constraint matrix.

In this formulation, all variables are assumed to be measured and redundant. The estimate of $\mathbf{x}$ is given by:

$$\hat{\mathbf{x}} = \mathbf{y} - \boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{A}\mathbf{y} \tag{3}$$

and the variance–covariance matrix of $\hat{\mathbf{x}}$ is a $(z \times z)$ matrix $\boldsymbol{\Sigma}_{\mathbf{c}}$ defined by:

$$\boldsymbol{\Sigma}_{\mathbf{c}} = \boldsymbol{\Psi} - \boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{A}\boldsymbol{\Psi} \tag{4}$$

(Mikhail, 1978; Madron, 1992).

By rearranging terms, Eq. (3) can be rewritten as follows:

$$\hat{\mathbf{x}} = (\boldsymbol{\Psi} - \boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{A}\boldsymbol{\Psi})\boldsymbol{\Psi}^{-1}\mathbf{y} \tag{5}$$

$$\hat{\mathbf{x}} = \boldsymbol{\Sigma}_{\mathbf{c}}\boldsymbol{\Psi}^{-1}\mathbf{y} \tag{6}$$

As it can be seen from Eq. (6), the effect of including a set of constraints is reflected only in matrix $\boldsymbol{\Sigma}_{\mathbf{c}}$. The $(z \times 1)$ vector of measurement adjustments $\hat{\boldsymbol{\varepsilon}}$ is

$$\hat{\boldsymbol{\varepsilon}} = (\mathbf{y} - \hat{\mathbf{x}}) = \boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{A}\mathbf{y} \tag{7}$$

which follows a multivariate normal distribution with zero mean and a $(z \times z)$ variance–covariance matrix $\mathbf{V}$

$$\mathbf{V} = \mathbf{A}^{\mathrm{T}}\boldsymbol{\Psi}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{A}\boldsymbol{\Psi} \tag{8}$$

Furthermore, the objective function value of the least square estimation problem (2), $\mathrm{ofv} = \hat{\boldsymbol{\varepsilon}}^{\mathrm{T}}\boldsymbol{\Psi}^{-1}\hat{\boldsymbol{\varepsilon}}$, has a central chi-square distribution with a number of degrees of freedom equal to the rank of $\mathbf{A}$.

If the presence of gross errors in the proposed measurement and constraint models is investigated, a collective hypothesis statistical test can be initially applied. A statistical test based on the vector of measurement adjustments $\hat{\boldsymbol{\varepsilon}}$ is selected. The null and alternative hypotheses are stated as follows: $\mathrm{H}_0 = \mathrm{E}(\hat{\boldsymbol{\varepsilon}}) = 0$; $\mathrm{H}_1 = \mathrm{E}(\hat{\boldsymbol{\varepsilon}}) \neq 0$. The global test statistic $\hat{\boldsymbol{\varepsilon}}^{\mathrm{T}}\boldsymbol{\Psi}^{-1}\hat{\boldsymbol{\varepsilon}}$ is used to compare both alternatives. Thus an appropriate α level test is to reject H_0 in favor of H_1, iff

$$\hat{\boldsymbol{\varepsilon}}^{\mathrm{T}}\boldsymbol{\Psi}^{-1}\hat{\boldsymbol{\varepsilon}} \geq \chi^2_{g,\alpha} \tag{9}$$

where $\chi^2_{g,\alpha}$ is the upper (100α)th percentile of the χ^2_g with $g = \mathrm{rank}(\mathbf{A})$.

If H_0 is rejected, a subset of equations with gross errors is isolated by the recursive search scheme outlined by Romagnoli (1983), using the global test. From these equations, a list of candidate biases and leaks is constructed. Then, all possible combinations of biases or biases and leaks from this subset are analyzed and included in a model that allows their estimation.

2.1. First stage

The objective of this stage is to isolate a subset of constraints that do not pass the global test. Let us suppose that an initial data reconciliation problem has been resolved using a subset of process constraints $\mathbf{Gx}=0$, where $\mathbf{G}$ is a $(w\times z)$ matrix with $w<m$. The variance–covariance matrix of $\hat{\mathbf{x}}$ for this case is

$$\mathbf{\Sigma_c^{old}}=\mathbf{\Psi}-\mathbf{\Psi G}^{\mathrm{T}}(\mathbf{G\Psi G}^{\mathrm{T}})^{-1}\mathbf{G\Psi} \tag{10}$$

If an equation or a set of equations, represented by a matrix $\mathbf{B_i}$, is added to the set of constraints, then the process model is now represented by

$$\begin{bmatrix}\mathbf{B_i}\\ \mathbf{A}\end{bmatrix}\mathbf{x}=\mathbf{Bx}=0 \tag{11}$$

The variance–covariance matrix of $\hat{\mathbf{x}}$ for the new case is by definition

$$\mathbf{\Sigma_c^{new}}=\mathbf{\Psi}-\mathbf{\Psi B}^{\mathrm{T}}(\mathbf{B\Psi B}^{\mathrm{T}})^{-1}\mathbf{B\Psi} \tag{12}$$

It is desired to express the matrix $\mathbf{\Sigma_c^{new}}$ in terms of the set of added process constraints $\mathbf{B_i}$ and the variance–covariance matrix for the old case $\mathbf{\Sigma_c^{old}}$. This is given by:

$$\mathbf{\Sigma_c^{new}}=\mathbf{\Sigma_c^{old}}-\mathbf{\Sigma_c^{old}B_i^{\mathrm{T}}}(\mathbf{B_i\Sigma_c^{old}B_i^{\mathrm{T}}})^{-1}\mathbf{B_i\Sigma_c^{old}} \tag{13}$$

The derivation of this expression is included in Appendix A. In addition, the vector $\hat{\mathbf{x}}$ for the new case is calculated as

$$\hat{\mathbf{x}}=\mathbf{\Sigma_c^{new}\Psi}^{-1}\mathbf{y} \tag{14}$$

Eqs. (13) and (14) have the advantage that only the reciprocal of the scalar $(\mathbf{B_i\Sigma_c^{old}B_i^{\mathrm{T}}})$ has to be computed in each application of (14) when only one equation is added to the set of process constraints, that is, when matrix $\mathbf{B_i}$ is of dimension $(1\times z)$.

Previous developments are applied to isolate the sources of gross errors for a given set of process constraints. Equations are added one by one to the least square estimation problem of $\mathbf{x}$. After each addition, the objective function of the least square estimation technique is calculated and compared with the critical value τ_c. After incorporating an equation, the following is checked

- If $\mathrm{ofv}>\tau_c$, gross errors are detected, so the last equation is eliminated from the system of equations. All the measurements involved in the constraint and a leak from the corresponding node are added to the list of suspected gross errors.
- If $\mathrm{ofv}=\tau_c$, gross errors are not detected after the addition of the constraint, and the constraint remains in the set.

It is well known that the objective function can also be obtained directly from the vector of equations' residuals $\mathbf{r}$ through the equation: $\mathbf{r}^{\mathrm{T}}\mathbf{J}^{-1}\mathbf{r}$ (Mah, 1990). This requires the calculation of the variance–covariance matrix of the residuals, $\mathbf{J}$, and its inversion, every time a constraint is added. The former method is preferred, as it is less time consuming. Notice that when a matrix $\mathbf{B}$ is formed by addition of an equation $\mathbf{B_i}$ to the system $\mathbf{Gx}=0$, the $(w+1)$ vector of residual is defined as $\mathbf{r_B}=\mathbf{By}$ and its variance–covariance matrix is $\mathbf{J_B}=\mathbf{B\Psi B}^{\mathrm{T}}$ (see Mah, 1990 for details).

Finally, the sequence through which the equations are selected does not influence the outcome of stage 1 significantly in practice. Nevertheless, one can make performance simulation studies to select the order that enhances the power.

2.2. Second stage

From the previous stage, a set of measurements and units suspect of being biased or having leaks is obtained. We now present the bias and leak estimation methods.

2.2.1. Estimation of leaks

If one or more leaks are considered, the constraint model for the process is modified to take them into account, as follows

$$\mathbf{Ax}-\mathbf{B_{rp}m_p}=0 \tag{15}$$

The solution of the steady state data reconciliation problem allows the estimation of the size of leaks and process variables

$$\min_{\boldsymbol{\varepsilon},\mathbf{m_p}}\ \boldsymbol{\varepsilon}^{\mathrm{T}}\mathbf{\Psi}^{-1}\boldsymbol{\varepsilon}$$

s.t.

$$\mathbf{A}(\mathbf{y}-\boldsymbol{\varepsilon})-\mathbf{B_{rp}m_p}=0 \tag{16}$$

where $\mathbf{B_{rp}}$ is a $(m\times p)$ matrix with $\mathbf{e_i}$ column vectors indicating leak positions and $\mathbf{m_p}$ is the p dimensional vector of leak magnitudes. The solution to this problem is:

$$\hat{\mathbf{m}}_\mathbf{p}=[\mathbf{B_{rp}^{\mathrm{T}}}(\mathbf{A\Psi A}^{\mathrm{T}})^{-1}\mathbf{B_{rp}}]^{-1}\mathbf{B_{rp}^{\mathrm{T}}}(\mathbf{A\Psi A}^{\mathrm{T}})^{-1}\mathbf{Ay} \tag{17}$$

$$\hat{\boldsymbol{\varepsilon}}=\mathbf{\Psi A}^{\mathrm{T}}(\mathbf{A\Psi A}^{\mathrm{T}})^{-1}[\mathbf{Ay}-\mathbf{B_{rp}}\hat{\mathbf{m}}_\mathbf{p}] \tag{18}$$

$$\hat{\mathbf{x}}=\mathbf{y}-\mathbf{\Psi A}^{\mathrm{T}}(\mathbf{A\Psi A}^{\mathrm{T}})^{-1}[\mathbf{Ay}-\mathbf{B_{rp}}\hat{\mathbf{m}}_\mathbf{p}] \tag{19}$$

2.2.2. Estimation of biases

If one or more measurement biases are proposed, the measurement model is modified as follows

$$\mathbf{y}=\mathbf{x}+\boldsymbol{\varepsilon}\mathbf{B_{rp}m_b} \tag{20}$$

and the following least squares problem results:

$$\min_{\boldsymbol{\varepsilon},\mathbf{m_b}}\ \boldsymbol{\varepsilon}^{\mathrm{T}}\mathbf{\Psi}^{-1}\boldsymbol{\varepsilon}$$

s.t.

$$\mathbf{A}(\mathbf{y}-\boldsymbol{\varepsilon}\mathbf{B_{rb}m_b})=0 \tag{21}$$

where $\mathbf{B_{rb}}$ is a $(z\times s)$ matrix and $\mathbf{e_i}$ the unit column vectors indicating the positions of proposed bias and $\mathbf{m_b}$

is the s dimensional vector of bias magnitudes. The solution is:

$$\hat{\mathbf{m}}_\mathbf{b} = [\mathbf{P}_\mathbf{b}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}\mathbf{P}_\mathbf{b}]^{-1}\mathbf{P}_\mathbf{b}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})\mathbf{A}\mathbf{y} \quad (22)$$

$$\hat{\boldsymbol{\varepsilon}} = \boldsymbol{\Psi}\mathbf{A}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}[\mathbf{A}\mathbf{y} - \mathbf{P}_\mathbf{b}\hat{\mathbf{m}}_\mathbf{b}] \quad (23)$$

$$\hat{\mathbf{x}} = \mathbf{y} - \boldsymbol{\Psi}\mathbf{A}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}[\mathbf{A}\mathbf{y} - \mathbf{P}_\mathbf{b}\hat{\mathbf{m}}_\mathbf{b}] - \mathbf{B}_{\mathbf{rb}}\hat{\mathbf{m}}_\mathbf{b} \quad (24)$$

where $\mathbf{P}_\mathbf{b} = \mathbf{A}\mathbf{B}_{\mathbf{rm}}$.

2.2.3. Estimation of leaks and biases

If leaks and measurement biases combinations are considered, both the measurement model and process constraints model are modified, as Eqs. (15) and (20) indicate. The formulation for the least square problem is as follows:

$$\min_{\boldsymbol{\varepsilon},\mathbf{m}_\mathbf{p},\mathbf{m}_\mathbf{b}} \boldsymbol{\varepsilon}^\mathrm{T}\boldsymbol{\Psi}^{-1}\boldsymbol{\varepsilon}$$

s.t.

$$\mathbf{A}(\mathbf{y} - \boldsymbol{\varepsilon} - \mathbf{B}_{\mathbf{rb}}\mathbf{m}_\mathbf{b}) - \mathbf{B}_{\mathbf{rp}}\mathbf{m}_\mathbf{p} = 0 \quad (25)$$

Which has the following solution:

$$\hat{\boldsymbol{\varepsilon}} = \boldsymbol{\Psi}\mathbf{A}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}[\mathbf{A}\mathbf{y} - \mathbf{P}_\mathbf{b}\hat{\mathbf{m}}_\mathbf{b} - \mathbf{B}_{\mathbf{rp}}\hat{\mathbf{m}}_\mathbf{p}] \quad (26)$$

$$\hat{\mathbf{x}} = \mathbf{y}\text{-}\mathbf{A}^\mathbf{T}(\mathbf{A}\mathbf{A}^\mathbf{T})^{-1}[\mathbf{A}\mathbf{y}\text{-}\mathbf{P}_\mathbf{b}\hat{\mathbf{m}}_\mathbf{b}\text{-}\mathbf{B}_{\mathbf{rp}}\hat{\mathbf{m}}_\mathbf{p}]\text{-}\mathbf{B}_{\mathbf{rb}}\hat{\mathbf{m}}_\mathbf{b} \quad (27)$$

The vectors $\hat{\mathbf{m}}_\mathbf{p}$ and $\hat{\mathbf{m}}_\mathbf{b}$ are now obtained as solution of the following system

$$\begin{bmatrix} \mathbf{A}_\mathbf{b}\mathbf{P}_\mathbf{b} & \mathbf{A}_\mathbf{b}\mathbf{B}_{\mathbf{rp}} \\ \mathbf{C}_\mathbf{p}\mathbf{P}_\mathbf{b} & \mathbf{C}_\mathbf{p}\mathbf{B}_{\mathbf{rp}} \end{bmatrix} \begin{bmatrix} \hat{\mathbf{m}}_\mathbf{b} \\ \hat{\mathbf{m}}_\mathbf{p} \end{bmatrix} = \begin{bmatrix} \mathbf{A}_\mathbf{b}\mathbf{A}\mathbf{y} \\ \mathbf{C}_\mathbf{b}\mathbf{A}\mathbf{y} \end{bmatrix} \quad (28)$$

where $\mathbf{A}_\mathbf{b} = \mathbf{P}_\mathbf{b}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}$ and $\mathbf{C}_\mathbf{p} = \mathbf{B}_{\mathbf{rp}}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}$

When matrices $\mathbf{B}_{\mathbf{rb}}$ and $\mathbf{B}_{\mathbf{rp}}$ are chosen in such a way that the correct locations of the gross errors are picked, these estimators are linear unbiased minimum variance estimators. These assertions are proven in Appendix B. The theoretical variance–covariance matrix for gross error size estimators are also provided in this Appendix. The dynamic counterpart of these estimation models has been presented by Bagajewicz and Jiang (1998).

2.3. Summary of the simultaneous estimation of gross errors method

2.3.1. Initial stage

Apply the global test. If it doesn't fail, then declare no error and stop. Otherwise go to stage one.

2.3.2. Stage one: construction of the gross error candidate list

1. Start with one constraint. Perform the data reconciliation and determine the objective function.
2. Apply the global test. If the test fails (ofv $> \tau_c$) then disregard the constraint, put the measurements involved in the constraint in the candidate bias list and put the node in the candidate leak list.
3. If there are no constraints to add, stop. Otherwise add a new constraint and use Eqs. (13) and (14) to obtain a new set of reconciled values as well as a new objective function value. Go to step 2.

2.3.3. Stage two: identification and estimation of gross errors

From the first stage of the procedure a candidate list of bias and leaks is obtained. In the second stage, combinations of n gross errors from the suspect list are analyzed, beginning with $n = 1$. For each combination of n hypothetical gross errors, the objective function value of the new least square problem is calculated. Each objective function value is a realization of a random variable with chi-square distribution and $(m - n)$ degrees of freedom. All these values are compared with the critical value $\tau_c = \chi^2_{m-n,\alpha}$, that is the $(1 - \alpha)$th quantile of the central chi-square distribution with $(m - n)$ degrees of freedom. If $\tau > \tau_c$ for all combinations then, the procedure is repeated increasing n by one. The procedure stops when $(\tau < \tau_c)$ for one or more combinations and $(n <$ mnh) or $n >$ mnh.

Formally, the second stage is:

1. Set mnh = maximum number of hypothesized gross errors.
2. Set the number of gross errors n to one $(n = 1)$.
3. Take all combinations of n gross errors and run the corresponding reconciliation model (biases only, leaks only, or biases and leaks).
4. Determine which combination of gross errors gives the lowest objective function value.
5. If the global test is satisfied stop. The combination or combinations with the lowest objective function value involve gross errors. Otherwise increase n by one $(n = n + 1)$ and if $(n <$ mnh) go to step 2.

In order to limit the search, one can set a maximum number of gross errors, mnh, as for example a 25% of the maximum possible number of gross errors. Thus reaching this maximum is another criterion to stop.

3. Results of simultaneous estimation of gross errors

A simulation procedure was applied to study the performance of the strategy. The method proposed by Iordache, Mah & Tamhane (1985) was followed. Each result is based on 10 000 simulation trials where the random errors are changed and the magnitudes of gross errors are fixed.

Three performance measures are used: overall power (OP), average number of type I errors (AVTI) and expected fraction of perfect identification (OPF). They are defined as follows:

$$\mathrm{OP} = \frac{\text{No. of gross errors correctly identified}}{\text{No. of gross errors simulated}} \quad (29)$$

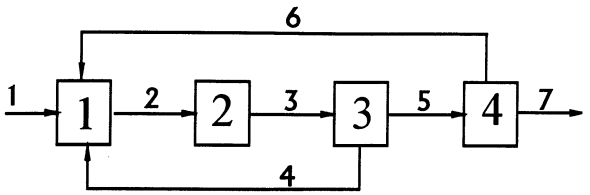

Fig. 1. Flowsheet for Example 1 (Rosenberg et al., 1987).

$$\text{AVTI} = \frac{\text{No. of gross errors } \textit{incorrectly} \text{ identified}}{\text{No. of simulation trials}} \quad (30)$$

$$\text{OPF} = \frac{\text{No. of trials with perfect identification}}{\text{No. of simulation trials}} \quad (31)$$

where a trial is considered perfect if all simulated gross errors are identified in the simulated location.

The two first measures are proposed by Narasimhan and Mah (1987) and the last one by Rollins and Davis (1992).

In order to illustrate the application of SEGE for bias and leaks identification/estimation, the example proposed by Rosenberg et al. (1987) consisting of a recycle system with four units and seven streams is used (Fig. 1).

In this example the true flow rate values are $\mathbf{x} = [5.\ 15.\ 15.\ 5.\ 10.\ 5.\ 5.]$. The flow rate SDs were taken as 2.5% of the true flow rates. Measurement values for each simulation trial were taken as the average of ten random generated values. The GLR and the UBET methods were selected for comparison. In order to compare results on the same basis, the level of significance of each method was chosen such that it gives an AVTI equal to 0.1 under the null hypothesis (Table 1). This common basis of comparison for gross error detection schemes was introduced by Rosenberg et al. (1987). The same confidence level for comparison has been used by different authors too. If a comparison is performed on such basis the conclusions of this paper do not vary.

In the identification part of UBET, the method of pseudonodes proposed by Serth and Hennan (1986) was used and adapted to consider the presence of leaks. In addition, some modifications were performed to the UBET method to improve its performance. When the identification step of UBET selects more candidate gross errors than the number of units (in this case four), some subsets of candidates lead to a singularity of matrix $\mathbf{B}_1$. These combinations are automatically avoided, thus improving UBET's performance. All these issues are discussed by Bagajewicz, Jiang & Sánchez (1999).

Table 1
Confidence level ($1-\alpha$) when no gross error is introduced and AVTI is equal to 0.1

	Leak is assumed impossible	Leak is assumed possible
SEGE	0.90	0.90
UBET	0.84	0.86
GLR	0.875	0.83

Tables 2 and 3 show the results expressed in terms of performance measures for the three methods when one bias is introduced and leaks are not present. As expected, GLR has the highest OP and OPF since GLR test reaches its maximum power when there is only a single bias (Narasimhan & Mah, 1987; Mah & Tamhane, 1982). From Table 3, it can be found that SEGE has the same performance as GLR in the estimation of biases.

Tables 4 and 5 indicate the performance comparison for the three methods when two biases are introduced and leaks are not present. All possible combinations of two measurement biases were simulated. Fixed gross error magnitudes of 7 and 4 SDs were considered for the corresponding flow rates. Table 5 shows that in the majority of the cases GLR exhibits a smaller SD than SEGE. This does not contradict the statement that SEGE is a minimum variance unbiased linear estimator because GLR is not an unbiased estimator, a fact that was proven by Rollins and Davis (1992).

Table 4 has been organized so that successful runs are listed first. The first twelve rows indicate that the identifications have high overall powers (OP). SEGE exhibits a larger fraction of perfect identification runs (OPF) as compared to the other two methods.

There are however failures. Both the SEGE and UBET methods give zero OPF for nine cases as depicted in the last rows of Table 4. In these cases the OPF column indicates the inability of the methods to distinguish the exact location of the gross errors, hence its inability to estimate its size. In addition GLR gives similar results for these cases. For SEGE the minimum value of the objective function is achieved for more than one different combination of gross errors. UBET is also unable to reach numerical results because one of its matrices ($\mathbf{B}_1$) becomes singular. There is one additional case (biases in streams 1 and 5) where UBET is capable of performing an acceptable identification, whereas GLR and SEGE perform poorly. We have no explanation for this anomaly. However, it serves as an indication that the power of a method seems to be location dependent.

In Table 5 bias estimation results are presented. This table includes the cases from Table 4 for which the expected fraction of perfect identification (OPF) is greater than 0.9. Table 5 illustrates that SEGE estimators are the unbiased linear estimators with minimum variance. Similar results can be obtained when leaks are present. These results are included in Tables 6 and 7.

Rollins and Davis made a point illustrating the fact that GLR is a biased estimator. In Table 8 we include

Table 2
Performance results for UBET, GLR and SEGE when one bias is introduced and leaks are not present

Biased stream	SEGE			UBET			GLR		
	AVTI	OP	OPF	AVTI	OP	OPF	AVTI	OP	OPF
1	0.125	0.979	0.896	0.057	0.961	0.908	0.075	0.999	0.926
2	0.099	1.000	0.902	0.096	1.000	0.908	0.075	1.000	0.926
3	0.119	0.977	0.904	0.135	0.983	0.889	0.075	1.000	0.926
4	0.125	0.955	0.880	0.235	0.842	0.773	0.088	0.955	0.916
5	0.110	0.990	0.901	0.109	0.998	0.896	0.075	1.000	0.926
6	0.102	0.995	0.900	0.273	0.909	0.852	0.050	0.996	0.954
7	0.105	0.991	0.904	0.269	0.933	0.864	0.004	0.999	0.999

results presented by Rollins and Davis (1992), corresponding to the process flowsheet in Fig. 1. Two gross errors are simulated of size 7 and 4 SD using $\alpha = 0.05$, sample size = 10, $\mathbf{\Psi} = \mathbf{I}$. As the SD and the variance are large, the table illustrates perfectly the biased nature of GLR. The results for GLR are determined from simulation. For UBET and SEGE, the values for the mean and SDs are the theoretical values.

4. Discussion

The SEGE method proves to be effective in identifying gross errors. It shows also superior performance in estimating their size. However, there are some instances where it fails to achieve a perfect identification. We will discuss each of these cases separately.

4.1. Equivalent gross errors

It only gives a suspicious subset of gross errors and the user is warned that a unique solution is not possible. These instances have been identified as cases when:

- The objective function is equal for different alternatives
- The matrices $[\mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A\Psi A}^{\mathrm{T}})^{-1}\mathbf{B}_{\mathbf{rp}}]$ in (17), $[\mathbf{P}_{\mathbf{b}}^{\mathrm{T}}(\mathbf{A\Psi A}^{\mathrm{T}})^{-1}\mathbf{P}_{\mathbf{b}}]$ in (22), or the system of equations in (28) are singular.

To sort out these difficulties, Sánchez (1996) proposed to add additional information of the process, as for example component or energy balances using fixed values of composition or temperature, in stage 2 of the procedure. Even in such cases, difficulties in choosing the proper set of equations were reported, as sometimes ill-conditioned systems of equations were obtained.

4.2. Unmeasured variables

As presented, SEGE cannot be applied to a system where unobservable variables exist. For example, there may be no redundant node balances and therefore equations would be added one by one without being able to have a successful reconciliation until redundancy is achieved. Thus, even if such approach was undertaken there would be no node to be specifically chosen as suspect of having leaks. Basically, one would be facing the same situation as in the iterative global test method (Rosenberg et al., 1987), where no list of suspects is built when all combinations of biases are investigated.

4.3. Size

The SEGE method makes use of a combinatorial search to increase performance. This creates a problem for large industrial systems, especially those poorly maintained which can show several gross errors at the same time. However, when size is not the issue, the SEGE method can be the method of choice.

4.4. Error identification problems

Other problems of the SEGE strategy are found during the application of stage 1. During the first stage of SEGE, the procedure always points to the last added constraint as a suspect when the global test fails. This may result in poor isolation of gross errors in some cases. Consider for example the process in Fig. 2. The original measurements for each stream are {1, 2, 3, 2, 1, 1, 1, 0.4, 0.6}.

When introducing a leak in node 3 with a size of 0.11, the new measurements are {1, 2, 3, 1.89, 0.89, 1, 1, 0.4, 0.49}. When applying the first stage, the first constraint shows a global test statistics of zero. As the second constraint is added, the global test statistics is still zero. When adding the third constraint, the global test statistical is 4.9873 but less than the corresponding critical value at $\alpha = 0.05$ which is 7.81. When the forth constraint is added, the global test statistical becomes 17.3701 while its critical value is 9.49. SEGE will certainly conclude that node 4, instead of node 3, is a node suspect of a leak. Thus, the true gross error (a leak in node 3) will be obviously missed.

4.5. Conclusions

The cases of equal objective function and singularities can be explained in terms of the theory of equivalent gross errors (Bagajewicz and Jiang, 1998) and provisions to avoid such cases can be made. In the rest of the paper a new version of SEGE, MSEGE is presented. The theory of gross error equivalency is briefly summarized first and the node aggregation strategy is discussed next. Finally, the MSEGE is presented.

5. Equivalency of gross errors

In a recent paper (Bagajewicz and Jiang, 1998) a series of concepts regarding the equivalency of sets of gross errors was presented. We present a brief summary next.

Two sets of gross errors are equivalent when they have the same effect in data reconciliation, that is, when simulating either one, leads to the same value of the objective function. Therefore, the equivalent sets of gross errors are theoretically indistinguishable. In other words, when a set of gross errors is identified, there exists an equal possibility that the true locations of gross errors are in one of its equivalent sets. From the view of graph theory, equivalent sets exist when candidate stream/leaks form a loop in an augmented graph consisting of the original graph representing the flowsheet with the addition of environmental node. This is illustrated next through an example.

Consider the process of Fig. 3 and assume that all streams are measured. As shown in Table 9, a bias of (-2) in S_4 and a bias of $(+1)$ in S_5 (case 1) can be represented by two alternative sets of two gross errors (cases 2 and 3).

5.1. Degenerate cases

The equivalencies above are built in the assumption that the number of gross errors identified is equal to the real number of gross errors. However, there are examples where the actual number of gross errors can be larger than the number of gross errors identified. One such example is shown in Table 10, where a set of two gross errors (case 1) is equivalent to one gross error (case 2). These cases are rare, as they require that the two real gross errors have equal sizes. This poses an additional uncertainty. If a certain number of gross errors are detected, there is a possibility that the actual number of gross errors is larger.

5.2. The concept of perfect identification

As a result of the equivalency of gross errors, the issue of perfect identification of gross errors should be revised. This issue has been raised by Bagajewicz and Jiang (1998), when presenting the equivalency theory, where the concepts of gross error exact detectability and gross error correct detectability were introduced. Exact detectability is possible in principle, only when there are no equivalent sets. Thus the perfect identification performance measure (OPF), as defined by Rollins and Davis should be extended to include equivalent sets. That is, gross error identification should be considered successful if exactly the errors introduced are identified, or an equivalent set is identified. Degenerate cases can also be included in such counting. For example, assume a gross error is introduced in stream S_2 in the flowsheet shown in Fig. 3. Assume now that a certain strategy identifies two equal and opposite sign gross errors in streams S_4 and S_5. This is a degenerate case where two gross errors are exactly equivalent to one gross error. Such a result should not be considered a failure and for this paper it will be considered a success.

6. Modifications to the simultaneous estimation of gross errors strategy to address imperfect identification

The problems experienced by SEGE (and UBET as

Table 3
Biases estimation results for SEGE, UBET and GLR when one bias is introduced and leaks are not present

Biased stream	Sizes	SEGE		UBET		GLR	
		Estimates	SD	Estimates	SD	Estimates	SD
1	0.500	0.501	0.053	0.502	0.056	0.500	0.053
2	1.500	1.501	0.129	1.502	0.135	1.501	0.129
3	1.500	1.500	0.129	1.500	0.138	1.500	0.129
4	0.500	0.504	0.097	0.522	0.116	0.504	0.097
5	1.000	1.000	0.089	1.000	0.100	1.000	0.089
6	0.500	0.499	0.076	0.503	0.090	0.500	0.076
7	0.500	0.500	0.053	0.500	0.086	0.499	0.053

Table 4
Performance results for SEGE, UBET and GLR when two biases are introduced and leaks are not present

Biased stream	SEGE[a]			UBET			GLR		
	AVTI	OP	OPF	AVTI	OP	OPF	AVTI	OP	OPF
1-2	0.008	0.996	0.992	0.066	0.999	0.934	0.167	0.971	0.904
1-3	0.000	1.000	1.000	0.132	0.977	0.915	0.168	0.972	0.903
1-4	0.049	0.974	0.948	0.133	0.932	0.817	0.063	0.973	0.934
1-5	0.615	0.704	0.692	0.134	0.963	0.911	1.950	0.145	0.021
2-5	0.000	0.999	0.999	0.122	0.982	0.914	0.089	0.999	0.911
2-6	0.027	0.987	0.973	0.110	0.980	0.893	0.130	0.966	0.889
2-7	0.002	0.999	0.998	0.303	0.930	0.849	0.057	0.999	0.944
3-5	0.000	1.000	1.000	0.146	0.965	0.924	0.086	1.000	0.913
3-6	0.027	0.987	0.973	0.126	0.972	0.899	0.125	0.967	0.893
3-7	0.001	0.999	0.999	0.163	0.976	0.902	0.054	0.999	0.947
4-7	0.004	0.998	0.996	1.623	0.600	0.520	0.067	0.998	0.936
5-7	0.006	0.997	0.994	0.230	0.946	0.881	0.144	0.996	0.864
1-6	1.000	0.997	1,6,7[a]	0.084	0.966	1,6,7[a]	0.143	0.993	0.868
1-7	1.000	0.997	1,6,7[a]	1.061	0.500	1,6,7[a]	1.074	0.504	0.000
2-3	1.000	0.999	2,3,4[a]	1.077	0.500	2,3,4[a]	1.041	0.997	0.005
2-4	0.948	0.958	2,3,4[a]	0.091	0.944	2,3,4[a]	0.961	0.500	0.000
3-4	0.951	0.960	2,3,4[a]	1.017	0.504	2,3,4[a]	0.964	0.500	0.000
4-5	1.000	0.999	4,5,6[a]	1.083	0.500	4,5,6[a]	0.077	0.999	0.925
4-6	0.999	0.998	4,5,6[a]	0.351	0.875	4,5,6[a]	1.063	0.577	0.002
5-6	0.996	0.977	4,5,6[a]	1.025	0.517	4,5,6[a]	1.026	0.500	0.000
6-7	1.000	1.000	1,6,7[a]	1.050	0.499	1,6,7[a]	0.820	0.886	0.324

[a] At least two of the three locations contain gross errors (Rollins & Davis, 1992).

well as GLR) can now be better explained in the context of the equivalency theory. First, when the objective function has the same value for two sets of suspected gross errors, it is because they are equivalent sets. Consider for example the case when the presence of one gross error is investigated for the flowsheet in Fig. 2. If S_8 or S_9 are flagged by an identification algorithm they will lead to the same result. This effect in the objective function was illustrated in detail by Bagajewicz and Jiang (1998). Second, when all the members of the equivalent sets are included in the suspected list, the matrix used in the bias/leak model is singular. For example, if the presence of two gross errors is investigated and S_8 and S_9 are included simultaneously, the system is singular, because any linear combination of gross errors in these two streams will solve the problem.

Therefore, the SEGE can be modified as follows:

1. If a set to be investigated in stage 2 is equivalent to a set previously considered, the set is ignored, as the result is known.
2. If a set to be investigated in stage 2 is included in any loop of the augmented graph, the set is ignored. It is known it will be singular, as it cannot capture the number of gross errors targeted.
3. All equivalent sets are identified at the end of the application of the algorithm.

7. Modification to the simultaneous estimation of gross errors strategy to address the presence of unmeasured variables

As it was described above, SEGE cannot be applied to a system where unobservable variables exist. For example, there may be no redundant node balances and therefore equations would be added one by one without being able to have a successful reconciliation until redundancy is achieved. Thus, even if such approach was undertaken there would be no node to be specifically chosen as suspect of having leaks.

When unmeasured variables are present, the least square estimation problem is defined by the following equation:

$$\min\ (\mathbf{y}-\mathbf{x})^{\mathrm{T}}\boldsymbol{\Psi}^{-1}(\mathbf{y}-\mathbf{x})$$

$$s.t.$$

$$\mathbf{Ax}+\mathbf{Cu}=0 \tag{32}$$

where $\mathbf{u}$ represents the unmeasured variables.

Several methods have been suggested to transform this model into one that only contains redundant measured variables. Among the most popular methods, the following can be mentioned: reduced balance scheme (Václavek, 1969), matrix projection (Crowe et al., 1983), QR decomposition (Swartz, 1989; Sánchez & Romagnoli, 1996) and matrix co-optation

(Madron, 1992). In all cases, a so-called canonical matrix $\mathbf{A_R}$ is obtained, such that the problem can be expressed as follows:

$$\min(\mathbf{y}-\mathbf{x})^{\mathrm{T}}\boldsymbol{\Psi}^{-1}(\mathbf{y}-\mathbf{x})$$

s.t.

$$\mathbf{A_R}\mathbf{x}=0$$

Depending on the method of choice, matrix $\mathbf{A_R}$ may not represent balances around nodes, but rather a linear combination of nodes. Take for example the flowsheet of Fig. 4.

The incidence matrix for this system is:

$$\mathbf{A}=\begin{array}{c} \begin{array}{cccc} S_1 & S_2 & S_3 & S_4 \end{array} \\ \begin{bmatrix} 1 & -1 & & \\ & 1 & -1 & \\ & & 1 & -1 \end{bmatrix} \end{array}$$

Assume for example that stream S_2 is unmeasured. Thus, $\mathbf{A_R}$, obtained by applying co-optation (Madron, 1992) is

$$\mathbf{A_R}=\begin{array}{c} \begin{array}{ccc} S_1 & S_3 & S_4 \end{array} \\ \begin{bmatrix} 1 & -1 & \\ 1 & & -1 \end{bmatrix} \end{array}$$

which contains a balance around nodes U_1 and U_2 and a balance around the whole system.

One could in principle apply stage 1 of SEGE to this system. However, if after applying the second constraint (row 2), the global test fails, then there is uncertainty as of what are the nodes that should be added to the candidate leak list. For the case of co-optation, the form of matrix $\mathbf{A_R}$ depends on the order in which the process of column rearrangement and Gauss–Jordan elimination takes place.

Thus, to be able to construct a proper list of candidate leaks without including an excessive number of units, the node aggregation strategy of Václavek (1969) is applied. This aggregation strategy is:

1. Identify each unmeasured stream
2. If the stream is not an inlet or outlet stream, merge the two nodes that this stream is connecting into one pseudonode. This can be performed in matrix **C**, by identifying the two rows were the entries are 1 and -1 for this stream. Add the first row to the second and eliminate the first row and the corresponding column.
3. If the stream is an inlet or outlet stream to the flowsheet, eliminate the node connected to this stream. In matrix **C**, this can be performed by identifying the row that has a 1 (inlet) or a -1 (outlet) for the corresponding stream. The identified row is eliminated. In addition, all columns with zero entries should be eliminated.

This process gives rise to a matrix of redundant measurements that contains pseudonodes resulting from the simple aggregation of nodes connected by unmeasured streams. Thus, each balance represented by this matrix constitutes a balance that contains the minimum possible of candidate leaks.

Table 5
Biases estimation results for SEGE,UBET and GLR when leaks are not present

Biased stream	Sizes	SEGE		UBET		GLR	
		Estimates	SD	Estimates	SD	Estimates	SD
1–2	0.875	0.876	0.053	0.875	0.056	0.805	0.052
	1.500	1.503	0.127	1.499	0.144	1.474	0.126
1–3	0.875	0.876	0.053	0.876	0.056	0.805	0.052
	1.500	1.501	0.129	1.499	0.143	1.475	0.126
1–4	0.875	0.876	0.054	0.874	0.056	0.925	0.053
	0.500	0.505	0.099	0.515	0.118	0.487	0.095
2–5	2.625	2.625	0.130	2.626	0.135	2.404	0.128
	1.000	0.999	0.091	1.000	0.095	0.973	0.089
2–6	2.625	2.627	0.137	2.626	0.144	2.330	0.128
	0.500	0.503	0.082	0.501	0.092	0.439	0.071
2–7	2.625	2.625	0.129	2.623	0.153	2.478	0.128
	0.500	0.499	0.053	0.501	0.110	0.491	0.052
3–5	2.625	2.626	0.131	2.624	0.142	2.405	0.129
	1.000	0.998	0.091	1.000	0.105	0.973	0.089
3–6	2.625	2.628	0.138	2.625	0.146	2.331	0.129
	0.500	0.503	0.082	0.501	0.092	0.444	0.071
3–7	2.625	2.626	0.130	2.626	0.145	2.478	0.129
	0.5	0.499	0.053	0.500	0.056	0.492	0.053
4–7	0.875	0.875	0.103	0.925	0.121	0.895	0.168
	0.5	0.499	0.054	0.478	0.081	0.554	0.087
5–7	1.750	1.748	0.092	1.754	0.134	1.552	0.090
	0.5	0.499	0.054	0.501	0.056	0.47	0.051

Table 6
Performance results for SEGE, UBET and GLR when two gross errors are introduced and leaks are present[a]

Gross errors	SEGE			UBET			GLR		
	AVTI	OP	OPF	AVTI	OP	OPF	AVTI	OP	OPF
L2, B4	0.014	0.993	0.990	0.168	0.961	0.900	0.025	0.996	0.979
L2, B5	0.000	0.999	0.999	0.213	0.952	0.891	1.380	0.837	0.000
L2, B6	0.007	0.996	0.993	0.154	0.969	0.917	0.058	0.999	0.944
L2, B7	0.020	0.990	0.980	0.162	0.951	0.928	1.897	0.872	0.000
L3, B2	0.038	0.981	0.981	0.327	0.921	0.831	0.974	0.999	0.077
L3, B6	0.003	0.999	0.999	0.202	0.963	0.892	0.216	0.937	0.925

[a] L*n* means a leak in node *n* and B*n* means a bias in stream *n*.

8. Modification to the simultaneous estimation of gross errors strategy to address improper suspected constraint

To address the problem of identifying the wrong source of a gross error, the following modification is suggested.

Before applying stage 1 of SEGE, obtain the global test statistics for each constraint. During the first stage of SEGE, when the global test fails, the constraint with the largest GT (instead of the latest added constraint) is considered as a suspect.

9. Summary of the modified simultaneous estimation of gross errors method

9.1. Preparation stage: obtain a redundant system

1. Take all inlet/outlet unmeasured streams. Delete the node to which they are connected. Eliminate the other inlet/outlet streams connected to that node.
2. Take all the remaining unmeasured streams and merge the nodes they connect into single pseudonodes.

9.2. Stage one: construction of the gross error candidate list

1. Calculate global test (GT) statistic for each node.
2. Start with one constraint. Perform the data reconciliation and determine the objective function.
3. Apply the global test. If the test fails ($ofv > \tau_c$) then disregard the constraint and put the node with the largest GT in the candidate leak list. If this node is already in the list, put the node with the second largest GT in the candidate leak list and so on. Put the measurements involved in the constraint in the candidate bias list. A leak from a pseudonode should be considered as a leak coming equivalently from any participating node.
4. If there are no constraints to add, stop. Otherwise add a new constraint and use (Eqs. (13) and (14)) to obtain a new set of reconciled values and a new objective function value. Go to step 2.

9.3. Stage two: identification and estimation of gross errors

1. Set the number of gross errors n to one ($n = 1$)
2. Take all combinations of n gross errors.
3. If the set chosen is equivalent to a set already analyzed, skip the set.
4. If the set contain a loop in the augmented graph, then skip the set.
5. Run the corresponding reconciliation model (biases only, leaks only, or biases and leaks).
6. Determine which combination of gross errors gives the lowest objective function.
7. If the global test is satisfied, go to step 8. Otherwise increase n ($n = n + 1$) and go to step 2.
8. Determine all sets equivalent to the set identified.

Similar modifications have been made to UBET and GLR. Details of these are given in Bagajewicz et al., 1999.

10. Results of modified simultaneous estimation of gross errors, MUBET and MGLR

With the aid of equivalency theory we can now extend the definition of OPF to include all trials which identify the perfect set, equivalent sets and degenerate sets as successful trials. We call this new measure overall performance of equivalent identification (OPFE)

$$\text{OPFE} = \frac{\text{No. of trials with successful identification}}{\text{No. of simulation trials}} \tag{34}$$

Using this new measure, the MSEGE strategy achieves a significant increase in the identification performance for the last nine cases of Table 4. Also the modified method gets a better performance when gross errors in streams 1 and 5 of the same flowsheet are simulated.

These results are included in Table 11, which has to be compared with Table 4.

As mentioned, the MSEGE strategy can be applied to a system with unmeasured streams. Table 12 illustrates some cases of Fig. 1.

Results shown in this table correspond to cases where the random errors have been removed and the true values with the biases or leaks are used.

11. Conclusions

A three-step procedure for gross bias/leaks errors was developed as an extension of an existing efficient two step strategy. The method was compared to existing approaches. The preparation stage of the procedure allows the determination of a redundant system matrix that leads to a minimum number of suspected leaks. The first stage of the developed procedure allows a good isolation of gross errors sources, reducing thus the size of the combinatorial search. The second stage allows an effective identification and rather accurate estimation of both biases and leaks. The theory of gross error equivalency is used to avoid singularities and to identify all possible alternatives of gross errors.

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Appendix A

In this appendix, the derivation of Eq. (13) is performed. First consider the difference between Eqs. (12) and (10)

$$\begin{aligned}\boldsymbol{\Sigma}_c^{new}-\boldsymbol{\Sigma}_c^{old}&=(\boldsymbol{\Psi}-\boldsymbol{\Psi}\mathbf{B}^T(\mathbf{B}\boldsymbol{\Psi}\mathbf{B}^T)^{-1}\mathbf{B}\boldsymbol{\Psi})\\&\quad-(\boldsymbol{\Psi}-\boldsymbol{\Psi}\mathbf{G}^T(\mathbf{G}\boldsymbol{\Psi}\mathbf{G}^T)^{-1}\mathbf{G}\boldsymbol{\Psi})\\\boldsymbol{\Sigma}_c^{new}-\boldsymbol{\Sigma}_c^{old}&=\boldsymbol{\Psi}\mathbf{G}^T(\mathbf{G}\boldsymbol{\Psi}\mathbf{G}^T)^{-1}\mathbf{G}\boldsymbol{\Psi}-\boldsymbol{\Psi}\mathbf{B}^T(\mathbf{B}\boldsymbol{\Psi}\mathbf{B}^T)^{-1}\mathbf{B}\boldsymbol{\Psi}\end{aligned}\tag{A-1}$$

The product $\mathbf{B}^T(\mathbf{B}\boldsymbol{\Psi}\mathbf{B}^T)^{-1}\mathbf{B}$ can be expressed as a function of matrix $\mathbf{G}$ and $\mathbf{B}_i$ as follows

$$\begin{aligned}\mathbf{B}^T(\mathbf{B}\boldsymbol{\Psi}\mathbf{B}^T)^{-1}\mathbf{B}&=\begin{bmatrix}\mathbf{B}_i^T & \mathbf{G}^T\end{bmatrix}\begin{bmatrix}\mathbf{B}_i\boldsymbol{\Psi}\mathbf{B}_i^T & \mathbf{B}_i\boldsymbol{\Psi}\mathbf{G}^T\\ \mathbf{G}\boldsymbol{\Psi}\mathbf{B}_i^T & \mathbf{G}\boldsymbol{\Psi}\mathbf{G}^T\end{bmatrix}^{-1}\begin{bmatrix}\mathbf{B}_i\\ \mathbf{G}\end{bmatrix}\\&=\begin{bmatrix}\mathbf{B}_i^T & \mathbf{G}^T\end{bmatrix}\begin{bmatrix}\mathbf{C}_{11} & \mathbf{C}_{12}\\ \mathbf{C}_{21} & \mathbf{C}_{22}\end{bmatrix}\begin{bmatrix}\mathbf{B}_i\\ \mathbf{G}\end{bmatrix}\\&=[(\mathbf{B}_i^T\mathbf{C}_{11}+\mathbf{G}^T\mathbf{C}_{21})(\mathbf{B}_i^T\mathbf{C}_{12}+\mathbf{G}^T\mathbf{C}_{22})]\\&\quad\times\begin{bmatrix}\mathbf{B}_i\\ \mathbf{G}\end{bmatrix}\\&=\mathbf{B}_i^T\mathbf{C}_{11}\mathbf{B}_i+\mathbf{G}^T\mathbf{C}_{21}\mathbf{B}_i+\mathbf{B}_i^T\mathbf{C}_{12}\mathbf{G}\\&\quad+\mathbf{G}^T\mathbf{C}_{22}\mathbf{G}\end{aligned}$$

where:

$$\begin{aligned}\mathbf{C}_{11}&=[\mathbf{B}_i\boldsymbol{\Psi}\mathbf{B}_i^T-\mathbf{B}_i\boldsymbol{\Psi}\mathbf{G}^T(\mathbf{G}\boldsymbol{\Psi}\mathbf{G}^T)^{-1}\mathbf{G}\boldsymbol{\Psi}\mathbf{B}_i^T]^{-1}\\&=[\mathbf{B}_i(\boldsymbol{\Psi}-\boldsymbol{\Psi}\mathbf{G}^T(\mathbf{G}\boldsymbol{\Psi}\mathbf{G}^T)^{-1}\mathbf{G}\boldsymbol{\Psi})\mathbf{B}_i^T]^{-1}=[\mathbf{B}_i\boldsymbol{\Sigma}_c^{old}\mathbf{B}_i^T]^{-1}\\\mathbf{C}_{12}&=-\mathbf{C}_{11}\mathbf{B}_i\boldsymbol{\Psi}\mathbf{G}^T(\mathbf{G}\boldsymbol{\Psi}\mathbf{G}^T)^{-1}\\\mathbf{C}_{21}&=-(\mathbf{G}\boldsymbol{\Psi}\mathbf{G}^T)^{-1}\mathbf{G}\boldsymbol{\Psi}\mathbf{B}_i^T\mathbf{C}_{11}\\\mathbf{C}_{22}&=(\mathbf{G}\boldsymbol{\Psi}\mathbf{G}^T)^{-1}\\&\quad+(\mathbf{G}\boldsymbol{\Psi}\mathbf{G}^T)^{-1}\mathbf{G}\boldsymbol{\Psi}\mathbf{B}_i^T\mathbf{C}_{11}\mathbf{B}_i\boldsymbol{\Psi}\mathbf{G}^T(\mathbf{G}\boldsymbol{\Psi}\mathbf{G}^T)^{-1}\end{aligned}$$

The elements of $\mathbf{C}$ are obtained using the partitioned matrix inverse (Noble, 1969).

Replacing the expression obtained into Eq. (A-1) one obtains:

$$\begin{aligned}\boldsymbol{\Sigma}_c^{new}&=\boldsymbol{\Sigma}_c^{old}-\boldsymbol{\Psi}\mathbf{B}_i^T[\mathbf{B}_i\boldsymbol{\Sigma}_c^{old}\mathbf{B}_i^T]^{-1}\mathbf{B}_i\boldsymbol{\Psi}\\&\quad+\boldsymbol{\Psi}\mathbf{G}^T(\mathbf{G}\boldsymbol{\Psi}\mathbf{G}^T)^{-1}\mathbf{G}\boldsymbol{\Psi}\mathbf{B}_i^T[\mathbf{B}_i\boldsymbol{\Sigma}_c^{old}\mathbf{B}_i^T]^{-1}\mathbf{B}_i\boldsymbol{\Psi}\end{aligned}$$

Table 7
Gross error estimation for SEGE, UBET and GLR when two gross errors are introduced and leaks are present

Gross errors	Sizes	SEGE		UBET		GLR	
		Estimates	SD	Estimates	SD	Estimates	SD
L2, B4	1.8	1.800	0.051	1.801	0.147	1.779	0.051
	0.625	0.626	0.099	0.628	0.127	0.622	0.100
L2, B5	1.8	1.801	0.054	1.807	0.151	1.578	0.004
	1.25	1.250	0.093	1.246	0.093	0.885	0.021
L2, B6	1.8	1.801	0.052	1.801	0.129	1.879	0.051
	0.625	0.625	0.077	0.625	0.091	0.600	0.074
L2, B7	1.8	1.801	0.082	1.801	0.136	/	/
	0.625	0.626	0.085	0.625	0.093	/	/
L3, B2	1.25	1.250	0.052	1.240	0.119	1.400	0.049
	1.875	1.879	0.130	1.902	0.141	1.683	0.105
L3, B6	1.25	1.251	0.051	1.251	0.130	1.273	0.051
	0.625	0.625	0.076	0.625	0.091	0.618	0.073

Table 8
Comparison of estimation performance

Biased stream	Sizes	SEGE		UBET		GLR	
		Estimates	SD	Estimates	SD	Estimates	SD
1–2	7	7	0.4031	7	0.6325	6.69	0.5089
	4	4	0.4031	4	0.4472	3.98	0.3996
1–3	7	7	0.4031	7	0.6325	6.69	0.5095
	4	4	0.4031	4	0.4472	3.98	0.4045
1–4	7	7	0.4082	7	0.7071	7.61	0.7340
	4	4	0.4655	4	0.5477	3.87	0.4720
1–5	7	7	0.4140	7	0.6325	6.08	1.0092
	4	4	0.4309	4	0.5477	3.76	0.4726
2–5	7	7	0.4140	7	0.4472	6.08	1.0062
	4	4	0.4309	4	0.5477	3.76	0.4736
2–6	7	7	0.4082	7	0.4472	6.38	0.7338
	4	4	0.4655	4	0.5477	3.87	0.4741
2–7	7	7	0.4031	7	0.4472	6.69	0.5046
	4	4	0.4031	4	0.5477	3.98	0.4031
3–5	7	7	0.4140	7	0.4472	6.08	1.0037
	4	4	0.4309	4	0.5477	3.76	0.4714
3–6	7	7	0.4082	7	0.5477	6.39	0.7346
	4	4	0.4655	4	0.5477	3.87	0.4789
3–7	7	7	0.4031	7	0.5477	6.69	0.5073
	4	4	0.4031	4	0.5477	3.98	0.4029
4–7	7	7	0.4655	7	0.4472	7.80	0.9210
	4	4	0.4082	4	0.5477	3.87	0.4167
5–7	7	7	0.4309	7	0.4472	6.00	1.0830
	4	4	0.4140	4	[a]	[a]	[a]

[a] Not published.

$$+\boldsymbol{\Psi}\mathbf{B}_i^T[\mathbf{B}_i\boldsymbol{\Sigma}_c^{old}\mathbf{B}_i^T]^{-1}\mathbf{B}_i\boldsymbol{\Psi}\mathbf{G}^T(\mathbf{G}\boldsymbol{\Psi}\mathbf{G}^T)^{-1}\mathbf{G}\boldsymbol{\Psi}$$
$$-\boldsymbol{\Psi}\mathbf{G}^T(\mathbf{G}\boldsymbol{\Psi}\mathbf{G}^T)^{-1}\mathbf{G}\boldsymbol{\Psi}\mathbf{B}_i^T[\mathbf{B}_i\boldsymbol{\Sigma}_c^{old}\mathbf{B}_i^T]^{-1}\mathbf{B}_i\boldsymbol{\Psi}\mathbf{G}^T(\mathbf{G}\boldsymbol{\Psi}\mathbf{G}^T)^{-1}$$
$$\times\mathbf{G}\boldsymbol{\Psi}$$

$$\boldsymbol{\Sigma}_c^{new}=\boldsymbol{\Sigma}_c^{old}-\boldsymbol{\Psi}\mathbf{B}_i^T[\mathbf{B}_i\boldsymbol{\Sigma}_c^{old}\mathbf{B}_i^T]^{-1}$$
$$\times\mathbf{B}_i[\boldsymbol{\Psi}-\boldsymbol{\Psi}\mathbf{G}^T(\mathbf{G}\boldsymbol{\Psi}\mathbf{G}^T)^{-1}\mathbf{G}\boldsymbol{\Psi}]$$
$$+\boldsymbol{\Psi}\mathbf{G}^T(\mathbf{G}\boldsymbol{\Psi}\mathbf{G}^T)^{-1}\mathbf{G}\boldsymbol{\Psi}\mathbf{B}_i^T[\mathbf{B}_i\boldsymbol{\Sigma}_c^{old}\mathbf{B}_i^T]^{-1}$$
$$\times\mathbf{B}_i[\boldsymbol{\Psi}-\boldsymbol{\Psi}\mathbf{G}^T(\mathbf{G}\boldsymbol{\Psi}\mathbf{G}^T)^{-1}\mathbf{G}\boldsymbol{\Psi}]$$

$$\boldsymbol{\Sigma}_c^{new}=\boldsymbol{\Sigma}_c^{old}-\boldsymbol{\Psi}\mathbf{B}_i^T[\mathbf{B}_i\boldsymbol{\Sigma}_c^{old}\mathbf{B}_i^T]^{-1}\mathbf{B}_i\boldsymbol{\Sigma}_c^{old}$$
$$+\boldsymbol{\Psi}\mathbf{G}(\mathbf{G}\boldsymbol{\Psi}\mathbf{G}^T)^{-1}\mathbf{G}\boldsymbol{\Psi}\mathbf{B}_i^T[\mathbf{B}_i\boldsymbol{\Sigma}_c^{old}\mathbf{B}_i^T]^{-1}\mathbf{B}_i\boldsymbol{\Sigma}_c^{old}$$

$$\boldsymbol{\Sigma}_c^{new}=\boldsymbol{\Sigma}_c^{old}-[\boldsymbol{\Psi}-\boldsymbol{\Psi}\mathbf{G}^T(\mathbf{G}\boldsymbol{\Psi}\mathbf{G}^T)^{-1}\mathbf{G}\boldsymbol{\Psi}]\mathbf{B}_i^T[\mathbf{B}_i\boldsymbol{\Sigma}_c^{old}\mathbf{B}_i^T]^{-1}$$
$$\times\mathbf{B}_i\boldsymbol{\Sigma}_c^{old}$$

$$\boldsymbol{\Sigma}_c^{new}=\boldsymbol{\Sigma}_c^{old}-\boldsymbol{\Sigma}_c^{old}\mathbf{B}_i^T[\mathbf{B}_i\boldsymbol{\Sigma}_c^{old}\mathbf{B}_i^T]^{-1}\mathbf{B}_i\boldsymbol{\Sigma}_c^{old}$$

Q.E.D

Appendix B

(A) When $\mathbf{B}_{rp}$ is chosen in such a way that the correct location of the gross error is picked, then the estimates obtained from problem (16) are unbiased.

Proof: Consider the constraint model (B-1), and the measurement model (B-2)

$$\mathbf{Ax}-\mathbf{B}_{rp}\mathbf{m}_p=0 \tag{B-1}$$

$$\mathbf{y}=\mathbf{x}+\boldsymbol{\varepsilon} \tag{B-2}$$

By applying the constraint model, vector $\mathbf{m}_p$ may be calculated in terms of $\mathbf{x}$ as follows:

$$\mathbf{B}_{rp}\mathbf{m}_p=\mathbf{Ax} \tag{B-3}$$

Premultiplying both members of (B-3) by $\mathbf{B}_{rp}^T(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^T)^{-1}$, the following expression is obtained

$$\mathbf{B}_{rp}^T(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^T)^{-1}\mathbf{B}_{rp}\mathbf{m}_p=\mathbf{B}_{rp}^T(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^T)^{-1}\mathbf{Ax} \tag{B-4}$$

from which we evaluate $\mathbf{m}_p$ in terms of $\mathbf{x}$

$$\mathbf{m}_p=(\mathbf{B}_{rp}^T(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^T)^{-1}\mathbf{B}_{rp})^{-1}\mathbf{B}_{rp}^T(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^T)^{-1}\mathbf{Ax} \tag{B-5}$$

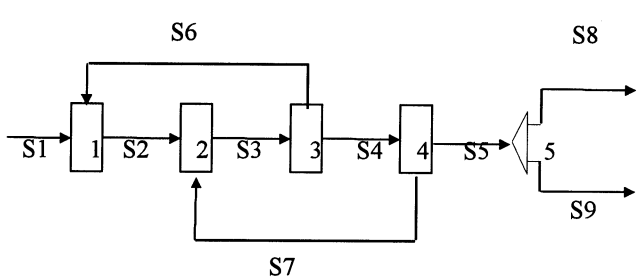

Fig. 2. Flowsheet for example 2.

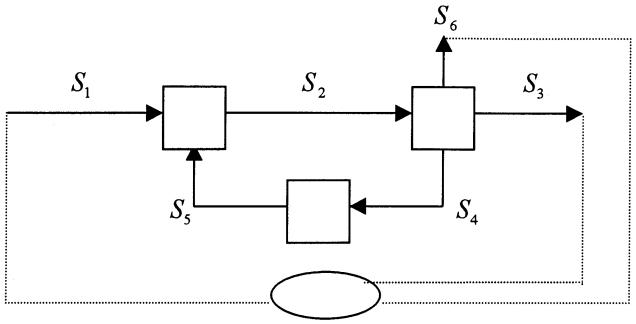

Fig. 3. Illustration of gross error equivalency.

The least squares estimate of $\mathbf{m_p}$ (Eq. (17)) is

$$\hat{\mathbf{m}}_\mathbf{p} = [\mathbf{B}_{\mathbf{rp}}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}\mathbf{B}_{\mathbf{rp}}]^{-1}\mathbf{B}_{\mathbf{rp}}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}\mathbf{A}\mathbf{y} \quad \text{(B-6)}$$

and its expected value is:

$$\mathrm{E}(\hat{\mathbf{m}}_\mathbf{p}) = [\mathbf{B}_{\mathbf{rp}}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}\mathbf{B}_{\mathbf{rp}}]^{-1}\mathbf{B}_{\mathbf{rp}}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}\mathbf{A}\mathrm{E}(\mathbf{y}) \quad \text{(B-7)}$$

Considering $\boldsymbol{\varepsilon} \approx \mathrm{N}_z(0, \boldsymbol{\Psi})$, then $\mathrm{E}(\mathbf{y}) = \mathbf{x}$, therefore

$$\mathrm{E}(\hat{\mathbf{m}}_\mathbf{p}) = [\mathbf{B}_{\mathbf{rp}}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}\mathbf{B}_{\mathbf{rp}}]^{-1}\mathbf{B}_{\mathbf{rp}}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}\mathbf{A}\mathbf{x} \quad \text{(B-8)}$$

From (B-8) and (B-5),

$$\mathrm{E}(\hat{\mathbf{m}}_\mathbf{p}) = \mathbf{m}_\mathbf{p} \quad \text{(B-9)}$$

Thus, $\hat{\mathbf{m}}_\mathbf{p}$ is an unbiased estimator of $\mathbf{m_p}$. In turn, the least squares estimate of $\mathbf{x}$ (Eq. (19)) is

$$\hat{\mathbf{x}} = \mathbf{y} - \boldsymbol{\Psi}\mathbf{A}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}[\mathbf{A}\mathbf{y} - \mathbf{B}_{\mathbf{rp}}\hat{\mathbf{m}}_\mathbf{p}] \quad \text{(B-10)}$$

and its expected value is:

$$\mathrm{E}(\hat{\mathbf{x}}) = \mathrm{E}(\mathbf{y}) - \boldsymbol{\Psi}\mathbf{A}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}\mathbf{A}\mathrm{E}(\mathbf{y}) + \boldsymbol{\Psi}\mathbf{A}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}\mathbf{B}_{\mathbf{rp}}\mathrm{E}(\hat{\mathbf{m}}_\mathbf{p}) \quad \text{(B-11)}$$

Considering $\mathrm{E}(\mathbf{y}) = \mathbf{x}$ and $\mathrm{E}(\hat{\mathbf{m}}_\mathbf{p}) = \mathbf{m}_\mathbf{p}$, as it was previously shown, we obtain:

$$\mathrm{E}(\hat{\mathbf{x}}) = \mathbf{x} - \boldsymbol{\Psi}\mathbf{A}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}\mathbf{A}\mathbf{x} + \boldsymbol{\Psi}\mathbf{A}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}\mathbf{B}_{\mathbf{rp}}\mathbf{m}_\mathbf{p} \quad \text{(B-12)}$$

$$\mathrm{E}(\hat{\mathbf{x}}) = \mathbf{x} - \boldsymbol{\Psi}\mathbf{A}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}(\mathbf{A}\mathbf{x} - \mathbf{B}_{\mathbf{rp}}\mathbf{m}_\mathbf{p}) \quad \text{(B13)}$$

By applying the constraint model (B-1) in (B-13),

$$\mathrm{E}(\hat{\mathbf{x}}) = \mathbf{x}$$

Thus, $\hat{\mathbf{x}}$ is an unbiased estimator of $\mathbf{x}$.
Q.E.D.

(B) When $\mathbf{B}_{\mathbf{rm}}$ is chosen in such a way that the correct location of the gross error is picked, then the estimates obtained from problem (21) are unbiased.

Proof: Consider the constraint model (B-13), and the measurement model (B-15)

$$\mathbf{A}\mathbf{x} = 0 \quad \text{(B-14)}$$

$$\mathbf{y} = \mathbf{x} + \boldsymbol{\varepsilon} + \mathbf{B}_{\mathbf{rm}}\mathbf{m}_\mathbf{b} \quad \text{(B-15)}$$

Considering $\boldsymbol{\varepsilon} \approx \mathrm{N}_z(0, \boldsymbol{\Psi})$, then $\mathrm{E}(\mathbf{y}) = \mathbf{x} + \mathbf{B}_{\mathbf{rm}}\mathbf{m}_\mathbf{b}$.

The least squares estimate of $\mathbf{m_b}$ (Eq. (22)) is

$$\hat{\mathbf{m}}_\mathbf{b} = [\mathbf{P}_\mathbf{b}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}\mathbf{P}_\mathbf{b}]^{-1}\mathbf{P}_\mathbf{b}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}\mathbf{A}\mathbf{y} \quad \text{(B-16)}$$

and its expected value is:

$$\mathrm{E}(\hat{\mathbf{m}}_\mathbf{b}) = [\mathbf{P}_\mathbf{b}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}\mathbf{P}_\mathbf{b}]^{-1}\mathbf{P}_\mathbf{b}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}\mathbf{A}\mathrm{E}(\mathbf{y}) \quad \text{(B-17)}$$

$$\mathrm{E}(\hat{\mathbf{m}}_\mathbf{b}) = [\mathbf{P}_\mathbf{b}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}\mathbf{P}_\mathbf{b}]^{-1}\mathbf{P}_\mathbf{b}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}\mathbf{A}(\mathbf{x} + \mathbf{B}_{\mathbf{rb}}\mathbf{m}_\mathbf{b}) \quad \text{(B-18)}$$

Introducing (B-13) in (B-18), the following expressions are obtained

$$\mathrm{E}(\hat{\mathbf{m}}_\mathbf{b}) = [\mathbf{P}_\mathbf{b}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}\mathbf{P}_\mathbf{b}]^{-1}\mathbf{P}_\mathbf{b}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}\mathbf{P}_\mathbf{b}\mathbf{m}_\mathbf{b} \quad \text{(B-19)}$$

$$\mathrm{E}(\hat{\mathbf{m}}_\mathbf{b}) = \mathbf{m}_\mathbf{b} \quad \text{(B-20)}$$

Thus, $\hat{\mathbf{m}}_\mathbf{b}$ is an unbiased estimator of $\mathbf{m_b}$. In turn, the least squares estimate of $\mathbf{x}$ (Eq. (24)) is

$$\hat{\mathbf{x}} = \mathbf{y} - \boldsymbol{\Psi}\mathbf{A}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}[\mathbf{A}\mathbf{y} - \mathbf{P}_\mathbf{b}\hat{\mathbf{m}}_\mathbf{b}] - \mathbf{B}_{\mathbf{rb}}\hat{\mathbf{m}}_\mathbf{b} \quad \text{(B-21)}$$

and its expected value is:

$$\mathrm{E}(\hat{\mathbf{x}}) = \mathrm{E}(\mathbf{y}) - \boldsymbol{\Psi}\mathbf{A}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}[\mathbf{A}\mathrm{E}(\mathbf{y}) - \mathbf{P}_\mathbf{b}\mathrm{E}(\hat{\mathbf{m}}_\mathbf{b})] - \mathbf{B}_{\mathbf{rb}}\mathrm{E}(\hat{\mathbf{m}}_\mathbf{b}) \quad \text{(B-22)}$$

Considering $\mathrm{E}(\mathbf{y}) = \mathbf{x} + \mathbf{B}_{\mathbf{rm}}\mathbf{m}_\mathbf{b}$ and $\mathrm{E}(\hat{\mathbf{m}}_\mathbf{b}) = \mathbf{m}_\mathbf{b}$, as was previously shown

$$\mathrm{E}(\hat{\mathbf{x}}) = \mathbf{x} + \mathbf{B}_{\mathbf{rm}}\mathbf{m}_\mathbf{b} - \boldsymbol{\Psi}\mathbf{A}^\mathrm{T}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^\mathrm{T})^{-1}[\mathbf{A}(\mathbf{x} + \mathbf{B}_{\mathbf{rm}}\mathbf{m}_\mathbf{b}) - \mathbf{P}_\mathbf{b}\mathbf{m}_\mathbf{b}] - \mathbf{B}_{\mathbf{rb}}\mathbf{m}_\mathbf{b} \quad \text{(B-23)}$$

Table 9
Illustration of Equivalent Sets in $\{S_2, S_4, S_5\}$ of Fig. 3

	S_1	S_2	S_3	S_4	S_5	S_6	
Measurement		12	18	10	4	7	2
Case 1 (bias in S_4, S_5)	Reconciled data	12	18	10	6	6	2
	Estimated biases				−2	1	
Case 2 (bias in S_2,S_4)	Reconciled data	12	19	10	7	7	2
	Estimated biases		−1		−3		
Case 3 (bias in S_2,S_5)	Reconciled data	12	16	10	4	4	2
	Estimated biases		2			3	

Table 10
Illustration of degenerate cases in $\{S_2, S_4, S_5\}$ of Fig. 3

		S_1	S_2	S_3	S_4	S_5	S_6
Measurement		12	18	10	7	7	2
Case 1 (bias in S_4, S_5)	Reconciled data	12	18	10	6	6	2
	Estimated biases				1	1	
Case 2 (bias in S_2)	Reconciled data	12	19	10	7	7	2
	Estimated biases		−1				

$$\mathrm{E}(\hat{\mathbf{x}}) = \mathbf{x} + \mathbf{B}_{\mathbf{rm}}\mathbf{m}_{\mathbf{b}} - \boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}[\mathbf{A}\mathbf{x} + \mathbf{P}_{\mathbf{b}}\mathbf{m}_{\mathbf{b}} - \mathbf{P}_{\mathbf{b}}\mathbf{m}_{\mathbf{b}}] - \mathbf{B}_{\mathbf{rb}}\mathbf{m}_{\mathbf{b}} \quad \text{(B-24)}$$

$$\mathrm{E}(\hat{\mathbf{x}}) = \mathbf{x}$$

Thus, $\hat{\mathbf{x}}$ is an unbiased estimator of $\mathbf{x}$.
Q.E.D.

(C) When $\mathbf{B}_{\mathbf{rp}}$ and $\mathbf{B}_{\mathbf{rm}}$ are chosen in such a way that the correct location of the gross error is picked, then the estimates. The estimates obtained from problem (25) are unbiased.

Proof: Consider the constraint model (B-26), and the measurement model (B-27)

$$\mathbf{A}\mathbf{x} - \mathbf{B}_{\mathbf{rp}}\mathbf{m}_{\mathbf{p}} = 0 \quad \text{(B-26)}$$

$$\mathbf{y} = \mathbf{x} + \boldsymbol{\varepsilon} + \mathbf{B}_{\mathbf{rm}}\mathbf{m}_{\mathbf{b}} \quad \text{(B-27)}$$

The vectors $\mathbf{m}_{\mathbf{p}}$ and $\mathbf{m}_{\mathbf{b}}$ are computed by solving the following system of equation:

$$\begin{bmatrix}\mathbf{m}_{\mathbf{b}}\\ \mathbf{m}_{\mathbf{p}}\end{bmatrix} = \begin{bmatrix}\mathbf{P}_{\mathbf{b}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{P}_{\mathbf{b}} & \mathbf{P}_{\mathbf{b}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{B}_{\mathbf{rp}}\\ \mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{P}_{\mathbf{b}} & \mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{B}_{\mathbf{rp}}\end{bmatrix}^{-1} \times \begin{bmatrix}\mathbf{P}_{\mathbf{b}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{A}\mathbf{y}\\ \mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{A}\mathbf{y}\end{bmatrix} \quad \text{(B-28)}$$

where the elements of the inverse matrix, called **C,** are (Noble, 1969):

$$\mathbf{C} = \begin{bmatrix}\mathbf{P}_{\mathbf{b}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{P}_{\mathbf{b}} & \mathbf{P}_{\mathbf{b}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{B}_{\mathbf{rp}}\\ \mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{P}_{\mathbf{b}} & \mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{B}_{\mathbf{rp}}\end{bmatrix}^{-1} = \begin{bmatrix}\mathbf{C}_{11} & \mathbf{C}_{12}\\ \mathbf{C}_{21} & \mathbf{C}_{22}\end{bmatrix} \quad \text{(B-29)}$$

$$\mathbf{C}_{11} = [\mathbf{P}_{\mathbf{b}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{P}_{\mathbf{b}} - \mathbf{P}_{\mathbf{b}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{B}_{\mathbf{rp}}\{\mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{B}_{\mathbf{rp}}\}^{-1} \times \mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{P}_{\mathbf{b}}]^{-1}$$

$$\mathbf{C}_{12} = -\mathbf{C}_{11}\mathbf{P}_{\mathbf{b}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{B}_{\mathbf{rp}}\{\mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{B}_{\mathbf{rp}}\}^{-1}$$

$$\mathbf{C}_{21} = -\{\mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{B}_{\mathbf{rp}}\}^{-1}\mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{P}_{\mathbf{b}}\mathbf{C}_{11}$$

$$\mathbf{C}_{22} = \{\mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{B}_{\mathbf{rp}}\}^{-1} - \{\mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{B}_{\mathbf{rp}}\}^{-1}\mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{P}_{\mathbf{b}}\mathbf{C}_{12} \quad \text{(B-30)}$$

The least squares estimate of $\mathbf{m}_{\mathbf{b}}$ is

$$\hat{\mathbf{m}}_{\mathbf{b}} = \mathbf{C}_{11}\mathbf{P}_{\mathbf{b}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{A}\mathbf{y} + \mathbf{C}_{12}\mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{A}\mathbf{y} \quad \text{(B-31)}$$

and then, the expected value of $\hat{\mathbf{m}}_{\mathbf{b}}$ is:

$$\mathrm{E}(\hat{\mathbf{m}}_{\mathbf{b}}) = \mathbf{C}_{11}\mathbf{P}_{\mathbf{b}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{A}\mathrm{E}(\mathbf{y}) + \mathbf{C}_{12}\mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{A}\mathrm{E}(\mathbf{y}) \quad \text{(B-32)}$$

$$\mathrm{E}(\hat{\mathbf{m}}_{\mathbf{b}}) = \mathbf{C}_{11}\mathbf{P}_{\mathbf{b}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{A}(\mathbf{x} + \mathbf{B}_{\mathbf{rm}}\mathbf{m}_{\mathbf{b}}) + \mathbf{C}_{12}\mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{A}(\mathbf{x} + \mathbf{B}_{\mathbf{rm}}\mathbf{m}_{\mathbf{b}}) \quad \text{(B-33)}$$

Replacing $\mathbf{C}_{12}$ in (B-33), the expected value of $\hat{\mathbf{m}}_{\mathbf{b}}$ is

$$\mathrm{E}(\hat{\mathbf{m}}_{\mathbf{b}}) = \mathbf{C}_{11}\mathbf{P}_{\mathbf{b}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}[\mathbf{A}\mathbf{x} - \mathbf{B}_{\mathbf{rp}}\mathbf{m}_{\mathbf{p}}] + \mathbf{C}_{11}\mathbf{P}_{\mathbf{b}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{P}_{\mathbf{b}}\mathbf{m}_{\mathbf{b}} - \mathbf{C}_{11}\mathbf{P}_{\mathbf{b}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{B}_{\mathbf{rp}}\{\mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{B}_{\mathbf{rp}}\}^{-1} \times \mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{P}_{\mathbf{b}}\mathbf{m}_{\mathbf{b}} \quad \text{(B-34)}$$

$$\mathrm{E}(\hat{\mathbf{m}}_{\mathbf{b}}) = \mathbf{C}_{11}[\mathbf{P}_{\mathbf{b}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{P}_{\mathbf{b}} - \mathbf{P}_{\mathbf{b}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{B}_{\mathbf{rp}}\{\mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{B}_{\mathbf{rp}}\}^{-1} \times \mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{P}_{\mathbf{b}}]\mathbf{m}_{\mathbf{b}} \quad \text{(B-35)}$$

$$\mathrm{E}(\hat{\mathbf{m}}_{\mathbf{b}}) = \mathbf{C}_{11}\mathbf{C}_{11}^{-1}\mathbf{m}_{\mathbf{b}} = \mathbf{m}_{\mathbf{b}} \quad \text{(B-36)}$$

Thus, $\hat{\mathbf{m}}_{\mathbf{b}}$ is an unbiased estimator of $\mathbf{m}_{\mathbf{b}}$. In turn, the least squares estimate of $\mathbf{m}_{\mathbf{p}}$ is

$$\hat{\mathbf{m}}_{\mathbf{p}} = \mathbf{C}_{21}\mathbf{P}_{\mathbf{b}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{A}\mathbf{y} + \mathbf{C}_{22}\mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{A}\mathbf{y} \quad \text{(B-37)}$$

Then, the expected value of $\hat{\mathbf{m}}_{\mathbf{p}}$ is given by

$$\mathrm{E}(\hat{\mathbf{m}}_{\mathbf{p}}) = \mathbf{C}_{21}\mathbf{P}_{\mathbf{b}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{A}\mathrm{E}(\mathbf{y}) + \mathbf{C}_{22}\mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{A}\mathrm{E}(\mathbf{y}) \quad \text{(B-38)}$$

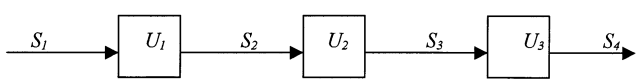

Fig. 4. Linear flowsheet.

Table 11
OPFE results for MSEGE, MUBET and MGLR

Biased stream	OPFE		
	MSEGE	MUBET	MGLR
1–6	0.998	0.923	0.961
1–7	0.994	0.901	0.891
6–7	1.000	0.956	0.354
2–3	1.000	0.980	0.998
2–4	0.876	0.836	0.865
3–4	0.873	0.939	0.866
4–5	1.000	0.949	0.925
4–6	0.995	0.914	0.898
5–6	0.949	0.923	0.906
1–5	0.882	0.919	0.027

$$E(\hat{\mathbf{m}}_p) = \mathbf{C}_{21}\mathbf{P}_b^T(\mathbf{A}\Psi\mathbf{A}^T)^{-1}\mathbf{A}(\mathbf{x}+\mathbf{B}_{rm}\mathbf{m}_b) + \mathbf{C}_{22}\mathbf{B}_{rp}^T(\mathbf{A}\Psi\mathbf{A}^T)^{-1}\mathbf{A}(\mathbf{x}+\mathbf{B}_{rm}\mathbf{m}_b) \quad \text{(B-39)}$$

Replacing $\mathbf{C}_{21}$ and $\mathbf{C}_{22}$ in (B-39), and using (B-26):

$$\begin{aligned} E(\hat{\mathbf{m}}_p) = & -\{\mathbf{B}_{rp}^T(\mathbf{A}\Psi\mathbf{A}^T)^{-1}\mathbf{B}_{rp}\}^{-1}\mathbf{B}_{rp}^T(\mathbf{A}\Psi\mathbf{A}^T)^{-1} \\ & \times \mathbf{P}_b\mathbf{C}_{11}\mathbf{P}_b^T(\mathbf{A}\Psi\mathbf{A}^T)^{-1}[\mathbf{A}\mathbf{x}-\mathbf{B}_{rp}\mathbf{m}_p]+\mathbf{m}_p \\ & -\{\mathbf{B}_{rp}^T(\mathbf{A}\Psi\mathbf{A}^T)^{-1}\mathbf{B}_{rp}\}^{-1}\mathbf{B}_{rp}^T(\mathbf{A}\Psi\mathbf{A}^T)^{-1} \\ & \times \mathbf{P}_b\mathbf{C}_{11}\mathbf{C}_{11}^{-1}\mathbf{m}_b \\ & +\{\mathbf{B}_{rp}^T(\mathbf{A}\Psi\mathbf{A}^T)^{-1}\mathbf{B}_{rp}\}^{-1}\mathbf{B}_{rp}^T(\mathbf{A}\Psi\mathbf{A}^T)^{-1}\mathbf{P}_b\mathbf{m}_b \end{aligned} \quad \text{(B-40)}$$

or

$$E(\hat{\mathbf{m}}_p) = \mathbf{m}_p \quad \text{(B-41)}$$

Thus, $\hat{\mathbf{m}}_p$ is an unbiased estimator of $\mathbf{m}_p$. In turn, the least square estimator of $\hat{\mathbf{x}}$ is:

$$\hat{\mathbf{x}} = \mathbf{y} - \Psi\mathbf{A}^T(\mathbf{A}\Psi\mathbf{A}^T)^{-1}[\mathbf{A}\mathbf{y}-\mathbf{P}_b\hat{\mathbf{m}}_b-\mathbf{B}_{rp}\hat{\mathbf{m}}_p]-\mathbf{B}_{rm}\hat{\mathbf{m}}_b \quad \text{(B-42)}$$

and the expected value of $\hat{\mathbf{x}}$ is given by

$$E(\hat{\mathbf{x}}) = E(\mathbf{y}) - \Psi\mathbf{A}^T(\mathbf{A}\Psi\mathbf{A}^T)^{-1} \times [\mathbf{A}E(\mathbf{y})-\mathbf{P}_bE(\hat{\mathbf{m}}_b)-\mathbf{B}_{rp}E(\hat{\mathbf{m}}_p)]-\mathbf{B}_{rm}E(\hat{\mathbf{m}}_b) \quad \text{(B-43)}$$

$$\begin{aligned} E(\hat{\mathbf{x}}) = & \mathbf{x}+\mathbf{B}_{rm}\mathbf{m}_b \\ & -\Psi\mathbf{A}^T(\mathbf{A}\Psi\mathbf{A}^T)^{-1}[\mathbf{A}(\mathbf{x}+\mathbf{B}_{rm}\mathbf{m}_b)-\mathbf{P}_b\mathbf{m}_b-\mathbf{B}_{rp}\mathbf{m}_p] \\ & -\mathbf{B}_{rm}\mathbf{m}_b \end{aligned} \quad \text{(B-44)}$$

$$E(\hat{\mathbf{x}}) = \mathbf{x}-\Psi\mathbf{A}^T(\mathbf{A}\Psi\mathbf{A}^T)^{-1} \times [\mathbf{A}\mathbf{x}-\mathbf{B}_{rp}\mathbf{m}_p+\mathbf{A}\mathbf{B}_{rm}\mathbf{m}_b-\mathbf{P}_b\mathbf{m}_b] \quad \text{(B-45)}$$

$$E(\hat{\mathbf{x}}) = \mathbf{x}-\Psi\mathbf{A}^T(\mathbf{A}\Psi\mathbf{A}^T)^{-1}[\mathbf{P}_b\mathbf{m}_b-\mathbf{P}_b\mathbf{m}_b] = \mathbf{x} \quad \text{(B-46)}$$

$$E(\hat{\mathbf{x}}) = \mathbf{x} \quad \text{(B-47)}$$

Thus, $\hat{\mathbf{x}}$ is an unbiased estimator of $\mathbf{x}$.
Q.E.D.

(D) Covariance matrix of gross error size estimates

(D-1) *Leaks*

The least squares estimate of vector $\hat{\mathbf{m}}_p$ is given by Eq. (B-6)

$$\hat{\mathbf{m}}_p = [\mathbf{B}_{rp}^T(\mathbf{A}\Psi\mathbf{A}^T)^{-1}\mathbf{B}_{rp}]^{-1}\mathbf{B}_{rp}^T(\mathbf{A}\Psi\mathbf{A}^T)^{-1}\mathbf{A}\mathbf{y} = \mathbf{Z}_1\mathbf{A}\mathbf{y}$$

Therefore, its variance–covariance matrix is:

$$\mathbf{H}_p = \mathbf{Z}_1\mathbf{A}\Psi\mathbf{A}^T\mathbf{Z}_1^T \quad \text{(B-48)}$$

where $\mathbf{Z}_1 = [\mathbf{B}_{rp}^T(\mathbf{A}\Psi\mathbf{A}^T)^{-1}\mathbf{B}_{rp}]^{-1}\mathbf{B}_{rp}^T(\mathbf{A}\Psi\mathbf{A}^T)^{-1}$.

(D-2) *Biases*

The least squares estimate of vector $\hat{\mathbf{m}}_b$ is given by Eq. (B-16)

$$\hat{\mathbf{m}}_b = [\mathbf{P}_b^T(\mathbf{A}\Psi\mathbf{A}^T)^{-1}\mathbf{P}_b]^{-1}\mathbf{P}_b^T(\mathbf{A}\Psi\mathbf{A}^T)^{-1}\mathbf{A}\mathbf{y} = \mathbf{Z}_2\mathbf{A}\mathbf{y}$$

Therefore, its variance–covariance matrix is:

$$\mathbf{H}_b = \mathbf{Z}_2\mathbf{A}\Psi\mathbf{A}^T\mathbf{Z}_2^T \quad \text{(B-49)}$$

where $\mathbf{Z}_2 = [\mathbf{P}_b^T(\mathbf{A}\Psi\mathbf{A}^T)^{-1}\mathbf{P}_b]^{-1}\mathbf{P}_b^T(\mathbf{A}\Psi\mathbf{A}^T)^{-1}$.

(D-3) *Biases and leaks*

The least squares estimates of vector $\hat{\mathbf{m}}_b$ and $\hat{\mathbf{m}}_p$ are given by Eqs. (B-31) and (B-37), respectively

$$\hat{\mathbf{m}}_b = \mathbf{C}_{11}\mathbf{P}_b^T(\mathbf{A}\Psi\mathbf{A}^T)^{-1}\mathbf{A}\mathbf{y}+\mathbf{C}_{12}\mathbf{B}_{rp}^T(\mathbf{A}\Psi\mathbf{A}^T)^{-1}\mathbf{A}\mathbf{y} = \mathbf{Z}_3\mathbf{A}\mathbf{y}$$

$$\hat{\mathbf{m}}_p = \mathbf{C}_{21}\mathbf{P}_b^T(\mathbf{A}\Psi\mathbf{A}^T)^{-1}\mathbf{A}\mathbf{y}+\mathbf{C}_{22}\mathbf{B}_{rp}^T(\mathbf{A}\Psi\mathbf{A}^T)^{-1}\mathbf{A}\mathbf{y} = \mathbf{Z}_4\mathbf{A}\mathbf{y}$$

Table 12
MSEGE results when there are unmeasured streams

Unmeasured stream	Introduced gross errors		Identified gross errors		Equivalent sets to (1)
	Location	Size	Location (1)	Size	
Stream 3	Biases in stream 1	0.875	Bias in stream 1	0.875	{Leak in node 1}
Stream 3	Biases in stream 2, 5	2.0, 1.0	Biases in stream 2, 6	1.0, −1.0	{Biases in stream 2, 5} {biases in stream 4, 5} {biases in stream 4, 6} {biases in stream 5, 6}
Stream 3	Leak in node 2	1.0	Leak in node 3	1.0	{Leak in node 2}

Therefore, the variance–covariance matrix for this case is:

$$\mathbf{H_b} = \mathbf{Z}_3\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}}\mathbf{Z}_3^{\mathrm{T}} \tag{B-50}$$

$$\mathbf{H_p} = \mathbf{Z}_4\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}}\mathbf{Z}_4^{\mathrm{T}} \tag{B-51}$$

where:

$$\mathbf{Z}_3 = \mathbf{C}_{11}\mathbf{P}_{\mathbf{b}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1} + \mathbf{C}_{12}\mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1} \text{ and}$$

$$\mathbf{Z}_4 = \mathbf{C}_{21}\mathbf{P}_{\mathbf{b}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1} + \mathbf{C}_{22}\mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}$$

(E) When $\mathbf{B_{rp}}$ and $\mathbf{B_{rm}}$ are chosen in such a way that the correct location of the gross error is picked, then the estimators of leaks and biases are minimum linear variance estimators.

A minimum variance estimator T is defined by $Var(T_i) \leq Var(P_i)$, where P is any other estimator. In our case we are restricting the proof to linear estimators. The proof follows the same line of arguments as the Gauss–Markov theorem (Kshirsagar, 1983).

Proof: (1) *Leaks*

Let us consider $\hat{m}_i = \mathbf{e_i}\mathbf{L}\mathbf{y}$ is the ith estimator of gross errors sizes. Since it is unbiased, $\mathrm{E}(\hat{m}_i) = \mathbf{e_i}\mathbf{L}\mathrm{E}(\mathbf{y}) = m_i$, where m_i represents its true value. Furthermore $\mathbf{L} = \mathbf{S}^{-1}\mathbf{X}$, where $\mathbf{S} = [\mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{B_{rp}}]$ and $\mathbf{X} = \mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{A}$ thus $\mathbf{X}\boldsymbol{\Psi}\mathbf{X}^{\mathrm{T}} = \mathbf{S}$.

Let us consider that $\hat{m}_i^* = \mathbf{e_i}\mathbf{L}^*\mathbf{y}$ is another unbiased estimator of m_i, then $\mathrm{E}(\hat{m}_i^*) = \mathbf{e_i}\mathbf{L}^*\mathrm{E}(\mathbf{y}) = \mathbf{e_i}\mathbf{L}\mathrm{E}(\mathbf{y}) = m_i$, which implies $\mathbf{e_i}\mathbf{L}^* = \mathbf{e_i}\mathbf{L}$. Finally, observe that

$$\mathbf{e_i}\mathbf{L}^*\mathbf{y} = (\mathbf{e_i}\mathbf{L}^*\mathbf{y} - \mathbf{e_i}\mathbf{L}\mathbf{y}) + \mathbf{e_i}\mathbf{L}\mathbf{y} \tag{B-52}$$

and therefore,

$$V(\mathbf{e_i}\mathbf{L}^*\mathbf{y}) = V(\mathbf{e_i}\mathbf{L}^*\mathbf{y} - \mathbf{e_i}\mathbf{L}\mathbf{y}) + V(\mathbf{e_i}\mathbf{L}\mathbf{y}) + 2Cov(\mathbf{e_i}\mathbf{L}^*\mathbf{y} - \mathbf{e_i}\mathbf{L}\mathbf{y}; \mathbf{e_i}\mathbf{L}\mathbf{y}) \tag{B-53}$$

We will show now that the last term in the previous equation is zero

$$\begin{aligned} Cov(\mathbf{e_i}\mathbf{L}^*\mathbf{y} - \mathbf{e_i}\mathbf{L}\mathbf{y}; \mathbf{e_i}\mathbf{L}\mathbf{y}) &= Cov\{(\mathbf{e_i}\mathbf{L}^* - \mathbf{e_i}\mathbf{L})\mathbf{y}; \mathbf{e_i}\mathbf{L}\mathbf{y}\} \\ &= (\mathbf{e_i}\mathbf{L}^* - \mathbf{e_i}\mathbf{L})\boldsymbol{\Psi}\mathbf{L}^{\mathrm{T}}\mathbf{e_i}^{\mathrm{T}} \\ &= (\mathbf{e_i}\mathbf{L}^* - \mathbf{e_i}\mathbf{L})\boldsymbol{\Psi}\mathbf{X}^{\mathrm{T}}(\mathbf{S}^{-1})^{\mathrm{T}}\mathbf{e_i}^{\mathrm{T}} \\ &= (\mathbf{e_i}\mathbf{L}^* - \mathbf{e_i}\mathbf{L})\boldsymbol{\Psi}\mathbf{X}^{\mathrm{T}}\mathbf{S}^{-1}\mathbf{e_i}^{\mathrm{T}} \\ &= (\mathbf{e_i}\mathbf{L}^*\boldsymbol{\Psi}\mathbf{X}^{\mathrm{T}} - \mathbf{e_i}\mathbf{S}^{-1}\mathbf{X}\boldsymbol{\Psi}\mathbf{X}^{\mathrm{T}}) \\ &\quad \times \mathbf{S}^{-1}\mathbf{e_i}^{\mathrm{T}} \\ &= (\mathbf{e_i}\mathbf{L}\boldsymbol{\Psi}\mathbf{X}^{\mathrm{T}} - \mathbf{e_i}\mathbf{S}^{-1}\mathbf{S})\mathbf{S}^{-1}\mathbf{e_i}^{\mathrm{T}} \\ &= (\mathbf{e_i}\mathbf{S}^{-1}\mathbf{X}\boldsymbol{\Psi}\mathbf{X}^{\mathrm{T}} - \mathbf{e_i})\mathbf{S}^{-1}\mathbf{e_i}^{\mathrm{T}} \\ &= (\mathbf{e_i} - \mathbf{e_i})\mathbf{S}^{-1}\mathbf{e_i}^{\mathrm{T}} = 0 \end{aligned} \tag{B-54}$$

Thus, since the variance of a variable is non-negative, we obtain,

$$V(\mathbf{e_i}\mathbf{L}^*\mathbf{y}) > V(\mathbf{e_i}\mathbf{L}\mathbf{y}).$$

(2) *Biases*

The proof is the same as in the case of leaks, but using instead the following matrices: $\mathbf{S} = [\mathbf{P}_{\mathbf{b}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{P_b}]$ and $\mathbf{X} = \mathbf{P}_{\mathbf{b}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{A}$.

(3) *Biases and leaks*

The proof is the same as in the case of leaks, but using the following matrices:

$$\mathbf{S} = \begin{bmatrix} \mathbf{P}_{\mathbf{b}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{P_b} & \mathbf{P}_{\mathbf{b}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{B_{rp}} \\ \mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{P_b} & \mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{B_{rp}} \end{bmatrix}$$

$$\mathbf{X} = \begin{bmatrix} \mathbf{P}_{\mathbf{b}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{A} \\ \mathbf{B}_{\mathbf{rp}}^{\mathrm{T}}(\mathbf{A}\boldsymbol{\Psi}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{A} \end{bmatrix}.$$

Appendix C

Notation

$\mathbf{A}$	$(m \times z)$ balance matrix
$\mathbf{A_R}$	reduced balance matrix
AVTI	average number of type I errors
$\mathbf{B}$	matrix defined by Eq. (11)
$\mathbf{B_i}$	row vector corresponding to a balance constraint
$\mathbf{B_{rp}}$	$(m \times p)$ matrix with $\mathbf{e_i}$ column vectors indicating leak positions
$\mathbf{B_{rm}}$	$(z \times s)$ matrix with $\mathbf{e_i}$ column vectors indicating the positions of hypothesized biases
$\mathbf{C}$	balance matrix for unmeasured variables
$\mathbf{e_i}$	vector with unit in the ith place and zero elsewhere
g	rank of $\mathbf{A}$
$\mathbf{G}$	balance matrix for a previous data reconciliation problem
$\mathbf{J}$	variance–covariance matrix of $\mathbf{r}$
$\mathbf{m_b}$	s-dimensional vector of bias magnitudes
$\mathbf{m_p}$	p-dimensional vector of leak magnitudes
n	number of hypothesized gross errors
mnh	maximum number of hypothesized gross errors
ofv	least square objective function value
OP	Overall power
OPF	expected fraction of correct identification
p	number of leaks
$\mathbf{r}$	equations' residuals

s	number of bias
U_i	unit i
$\mathbf{V}$	variance–covariance matrix of $\hat{\boldsymbol{\varepsilon}}$
$\mathbf{x}$	vector of true values of variables
$\hat{\mathbf{x}}$	vector of the estimates of $\mathbf{x}$
$\mathbf{y}$	vector of measurements
$\mathbf{u}$	unmeasured variables
w	number of rows of matrix $\mathbf{G}$
z	number of variables

Greek symbols

$\boldsymbol{\varepsilon}$	vector of random measurement errors
$\hat{\boldsymbol{\varepsilon}}$	vector of measurement adjustments
τ_c	critical value for the test statistic
$\boldsymbol{\Psi}$	measurement error variance–covariance matrix
$\boldsymbol{\Sigma}_c$	variance–covariance matrix of $\hat{\mathbf{x}}$
$\boldsymbol{\Sigma}_c^{old}$	$\boldsymbol{\Sigma}_c$ for a solved problem
$\boldsymbol{\Sigma}_c^{new}$	$\boldsymbol{\Sigma}_c$ for a new problem
α	significance level of the test
χ^2	chi-square distribution

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