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USE OF ORTHOGONAL TRANSFORMATIONS IN DATA CLASSIFICATION-RECONCILIATION

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Abstract—In this paper, the use of orthogonal factorizations, more precisely the *Q–R* decomposition, to analyze, decompose and solve the linear and bilinear data reconciliation problem is further investigated. It is shown that the decomposition provides additional insight in identifying structural singularities in the system topology, allowing the problem to decompose into lower dimension sub-problems. Energy balances are explicitly considered. Two examples of application are presented.

1. INTRODUCTION

In the course of daily operation of a chemical plant, it is common practice to adjust the measurements taken from the process, so that random measurement errors can be compensated for. The application of these methods to large-scale complex chemical plants creates problems of very large dimensionality which are difficult to solve. This last feature motivated Václavek (1969) to attempt to reduce the size of the least-squares problem through an elegant classification of the measured and unmeasured process variables for linear systems. Such classification allowed the size reduction of the initial problem and its easier solution. In a later work Václavek and Loucka (1976) covered also the case of bilinear balances.

A similar approach was undertaken by Mah *et al.* (1976) in their attempt to organize the analysis of the process data and to systematize the estimation and measurement correction problem. A simple graph-theoretic procedure for single component flow networks was developed. They later extended the treatment, first to multicomponent flow networks (Kretsovalis and Mah, 1987) and then to the generalized process networks including energy balances and chemical reactions (Kretsovalis and Mah, 1988a, b).

Romagnoli and Stephanopoulos (1980) proposed an equation oriented approach. Solvability of the nodal equations was examined and an output set assignment algorithm (Stadtherr *et al.*, 1974) was employed to classify simultaneously measured and unmeasured variabes.

More recently, a general treatment using projection matrices was proposed by Crowe *et al.* (1983) for linear systems and extended later (Crowe, 1986, 1989) for bilinear systems. Crowe suggested a useful method to decouple the measured variables from the constraint equations, using a projection matrix to eliminate the unmeasured process variables. Orthogonal factorization were first used by Swartz (1989) in the context of successive linearization techniques to eliminate the unmeasured variables from the constraint equations.

In this paper, the use of orthogonal factorizations, more precisely the *Q–R* decomposition, to analyze, decompose and solve the linear and bilinear data reconciliation problem is further investigated. A sequence of simple expressions to be applied in instrumentation analysis and data reconciliation is outlined and they are obtained using sub-products of *Q–R* factorizations. Furthermore, the use of this method, when energy balances are included in the set of process constraints, is also discussed. Results of the application for linear and bilinear systems are provided in terms of two flowsheeting examples, one of them being an existing operating plant.

2. LINEAR CASE

2.1. Problem statement

In the absence of systematic errors, we consider the following measurement model

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

where $\mathbf{x}$ is a $(g \times 1)$ vector of measured variables, $\tilde{\mathbf{x}}$ is a $(g \times 1)$ vector of measured values and ε is a $(g \times 1)$ vector of random errors. The measurement

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errors are assumed to be normally distributed with zero mean and known variance–covariance matrix Ψ_x. A set of m linear balance equations for a steady-state process can be written as:

$$A_1\mathbf{x}+A_2\mathbf{u}=0 \tag{2}$$

where $\mathbf{u}$ is a $(n\times 1)$ vector of unmeasured variables and $A_1(m\times g)$, $A_2(m\times u)$ are matrices of known constants.

In the presence of measurement errors, the balance equations are not satisfied exactly. To compensate for random measurements errors, a general data reconciliation procedure must solve the following least-squares problem:

$$\begin{aligned}\min\quad & (\mathbf{x}-\tilde{\mathbf{x}})^T\Psi_x^{-1}(\mathbf{x}-\tilde{\mathbf{x}}) \\ \text{s.t.}\quad & A_1\mathbf{x}+A_2\mathbf{u}=0.\end{aligned} \tag{3}$$

2.2. Solution using Q–R *factorizations*

Several techniques were proposed to reduce the size of the reconciliation problem by eliminating unmeasured variables (Václavek, 1969; Mah *et al.*, 1976; Romagnoli and Stephanopoulos, 1980). An elegant and useful way of obtaining this decomposition was due to Crowe *et al.* (1983). The method was based on the use of a projection matrix P. It was defined such that pre-multiplying matrix A_2 with P yields:

$$PA_2=0 \tag{4}$$

where the rows of P span the null space of A_2^T, and thus the unmeasured variables are eliminated. The constrained least-squares problem for the overall plant (3) can be replaced now by the equivalent two-problem formulation.

(i) *Least-squares estimation of* $\mathbf{x}$:

$$\begin{aligned}\min\quad & (\mathbf{x}-\tilde{\mathbf{x}})^T\Psi_x^{-1}(\mathbf{x}-\tilde{\mathbf{x}}) \\ \text{s.t.}\quad & G\mathbf{x}=\mathbf{0}.\end{aligned} \tag{5}$$

The solution of this problem is given by:

$$\hat{\mathbf{x}}=\tilde{\mathbf{x}}-\Psi_x G^T(G\Psi_x G^T)^{-1}G\tilde{\mathbf{x}} \tag{6}$$

where $G=P^*A_1$.

(ii) *Estimation of* $\mathbf{u}$ *using* $\hat{\mathbf{x}}$ *and the balance equations*

Both the application of Crowe's matrix projection method and the solution of the reduced least-squares problem can be simplified by using Q–R orthogonal transformations. A brief description of Q–R transformation is included in the Appendix. The application of Q–R factorizations to different stages of the data reconciliation problem (3) follows.

2.2.1. Elimination of unmeasured variables.

By applying software packages for matrix computation, such as MATLAB, the Q–R decomposition of matrix A_2 is easily accomplished. From one code instruction, matrices Q_u, R_u and the permutation matrix Π_u are obtained, such that:

$$A_2\Pi_u=Q_uR_u \tag{7}$$

where Q_u and R_u can be divided into:

$$Q_u=[Q_{u_1}Q_{u_2}] \qquad R_u=\begin{bmatrix}R_{u_2} & R_{u_2}\\ 0 & 0\end{bmatrix} \tag{8}$$

as is indicated in the Appendix, with $r_u=\operatorname{rank}(A_2)=\operatorname{rank}(R_{u_1})$.

In the same way, the unmeasured process variables can be partitioned into two subsets:

$$\Pi_u^T\mathbf{u}=\begin{bmatrix}\mathbf{u}_{r_u}\\ \mathbf{u}_{n-r_u}\end{bmatrix}. \tag{9}$$

with this notation, the balance equations (2) become:

$$\mathrm{A}_1\mathbf{x}+[Q_{u_1}\quad Q_{u_2}]\begin{bmatrix}R_{u_1} & R_{u_2}\\ 0 & 0\end{bmatrix}\begin{bmatrix}\mathbf{u}_{r_u}\\ \mathbf{u}_{n-r_u}\end{bmatrix}=0. \tag{10}$$

The $Q_{u_2}^T$ matrix is such that its rows span the null space of A_2^T. That is:

$$Q_{u_2}^TA_2=0 \tag{11}$$

so $Q_{u_2}^T$ works as the projection matrix P proposed by Crowe. It differs, however, from P in that the numerical values have no physical significance. Pre-multiplying the system of equations (2) by $Q_{u_2}^T$ the unmeasured variables are eliminated.

Remark 1. In MATLAB, the Q–R decomposition can be easily accomplished through one code instruction. Furthermore, $Q_{u_2}^T$ is obtained as sub-product of Q–$R(A_2)$ without extra computing effort for the user.

2.2.2. Least-squares estimation of x. The following problem must be solved:

$$\begin{aligned}\min\quad & (\mathbf{x}-\tilde{\mathbf{x}})^T\Psi_x^{-1}(\mathbf{x}-\tilde{\mathbf{x}}) \\ \text{s.t.}\quad & G_x\mathbf{x}=0\end{aligned} \tag{12}$$

where

$$G_x=Q_{u_2}^TA_1. \tag{13}$$

Zero columns of G_x correspond to non-redundant measurements; the others belong to redundant measurements as indicated by Crowe *et al.* (1983) and Crowe (1989).

We can solve this constrained problem by the Lagrangian approach; however, using Q–R factorizations, it can be transformed into an unconstrained problem. The constraints equations may be used to solve, functionally, for as many variables as there are constraints. Then an unconstrained least-squares problem is solved to estimate the remaining variables. The procedure is as follows.

(i) Computation of the general solution of the undetermined system ($G_x\mathbf{x}=0$):

A Q–R orthogonal factorization of G_x gives Q_x, R_x, Π_x and allows one to obtain $Q_{x_1}, Q_{x_2}, R_{x_1}, R_{x_2}, \mathbf{x}_{r_x}, \mathbf{x}_{g-r_x}$, such that

$$G_x\Pi_x = Q_xR_x \tag{14}$$

$$Q_x=[Q_{x_1}Q_{x_1}] \qquad R_x=\begin{bmatrix} R_{x_1} & R_{x_2} \\ 0 & 0 \end{bmatrix} \tag{15}$$

$$\Pi_x^T\mathbf{x}=\begin{bmatrix} \mathbf{x}_{r_x} \\ \mathbf{x}_{g-r_x} \end{bmatrix} \tag{16}$$

with $r_x=\text{rank}(R_{x_1})=\text{rank}(G_x)$. The general solution of this problem is:

$$\mathbf{x}_{r_x}=-R_{x_1}^{-1}R_{x_2}\mathbf{x}_{g-r_x} \tag{17}$$

where $\mathbf{x}_{g-r_x}$ is arbitrary.

(ii) Formulation of the unconstrained problem:

Using the previous results, the vector $(\mathbf{x}-\tilde{\mathbf{x}})$ from the objective function is modified, as equation (18) indicates:

$$\begin{aligned}(\mathbf{x}-\tilde{\mathbf{x}}) &= [I_{x_1} \quad I_{x_2}]\begin{bmatrix} \mathbf{x}_{r_x} \\ \mathbf{x}_{g-r_x} \end{bmatrix}-\tilde{\mathbf{x}} \\ &= -I_{x_1}R_{x_1}^{-1}R_{x_2}\mathbf{x}_{g-r_x}+I_{x_2}\mathbf{x}_{g-r_x}-\tilde{\mathbf{x}} \\ &= (I_{x_2}-I_{x_1}R_{x_1}^{-1}R_{x_2})\mathbf{x}_{g-r_x}-\tilde{\mathbf{x}}\end{aligned} \tag{18}$$

where

$$I\Pi_x=[I_{x_1} \quad I_{x_2}] \qquad \tilde{I}=I_{x_2}-I_{x_1}R_{x_1}^{-1}R_{x_2}. \tag{19}$$

I is a $(g\times g)$ identity matrix and $\tilde{I}$ is a $[g\times(g-r_x)]$ matrix with independent columns.

(iii) Estimation of $\mathbf{x}$:

The solution of the unconstrained problem is:

$$\hat{\mathbf{x}}_{g-r_x}=(\tilde{I}^T\Psi_x^{-1}\tilde{I})^{-1}\tilde{I}^T\Psi_x^{-1}\tilde{\mathbf{x}} \tag{20}$$

with the value of $\hat{\mathbf{x}}_{g-r_x}$, one can solve for $\mathbf{x}_{r_x}$ using (17).

Remark 2. The previous approach has two advantages: it avoids the direct use of the constraints into the least-squares estimation and reduces the number of variables to be simultaneously estimated. The process of eliminating part of the variable using the constriants is easily accomplished by means of Q–R factorizations.

2.2.3. Estimation of unmeasured variables. Matrix R_u in the Q–R factorization of the A_2 matrix contains the topological information about the system in terms of the available measurements.

(i) if $\text{rank}(R_u)=r_u=n$, all unmeasured process variables are determinable from the available information.

(ii) if $\text{rank}(R_u)=r_u<n$, then at least $n-r_u+1$ variables cannot be calculated from the available information.

For case (ii), the estimability condition of unmeasured variables can be expressed in terms of Q–R decomposition results of A_2 matrix. The permutation matrix Π_u allows the division of the unmeasured process variables into subsets $\mathbf{u}_{r_u}$ and $\mathbf{u}_{n-r_u}$. The subset $\mathbf{u}_{n-r_u}$ corresponds to $(n-r_u)$ indeterminable unmeasured process variables. Regarding the subset $\mathbf{u}_{r_u}$, some variables can be calculated using only the reconciled measurement values and some depend also on the assumption of the $\mathbf{u}_{n-r_u}$ variables. This result is obtained by pre-multiplying the system equations (10) by Q_u^T and reordering the first r_u equations of system (21) as indicated below:

$$\begin{bmatrix} Q_{u_1}^TA_1 & R_{u_1} & R_{u_2} \\ Q_{u_2}^TA_1 & 0 & 0 \end{bmatrix}\begin{bmatrix} \mathbf{x} \\ \mathbf{u}_{r_u} \\ \mathbf{u}_{n-r_u} \end{bmatrix}=0 \tag{21}$$

$$\mathbf{u}_{r_u}=-R_{u_1}^{-1}Q_{u_1}^TA_1\hat{\mathbf{x}}-R_{u_1}^{-1}R_{u_2}\mathbf{u}_{n-r_u}. \tag{22}$$

To classify variables in subset $\mathbf{u}_{r_u}$, it is necessary to look at the rows of the matrix:

$$R_{IU}=R_{u_1}^{-1}R_{u_2}. \tag{23}$$

The following can be stated:

(i) A variable in subset $\mathbf{u}_{r_u}$ is said to be determinable if the corresponding row in the R_{IU} matrix is zero.

(ii) A variable in subset $\mathbf{u}_{r_u}$ is said indeterminable otherwise.

Remark 3. The classification matrix analysis has been done by Crowe (1989) in terms of the projection matrix P. Here, similar results are obtained in a clearer way using Q–R factorization. In MATLAB, inspection of matrix R_{IU} can be easily accomplished in an automatic way.

3. NON-LINEAR CASE

3.1. Problem statement

Let us now consider a process containing K units denoted by $k=1,\ldots,K$, and J oriented streams $j=1,\ldots J$, with C components $c=1,\ldots C$. Plant topology is represetned by the incidence matrix $\mathbf{L}$, with rows corresponding to units and columns to streams. Then $l_{kj}=$ if stream j enters node k, $l_{kj}=-1$ if stream j leaves mode k, $l_{kj}=0$ otherwise.

The general process constraints are as follows.

Total molar balances:

$$\sum_j l_{kj}F_j+\sum_r\sum_c S_{k,rc}\zeta_{k,rc}=0. \tag{24}$$

Component molar balances:

$$\sum_j l_{kj} F_j m_{jc} + \sum_r S_{k,rc} \zeta_{k,r} = 0. \quad (25)$$

Energy balances:

$$\sum_l l_{kj} F_j h_j + \sum_r H_{k,r} + \mathbf{q}_k = 0. \quad (26)$$

Normalization equations:

$$\sum_c F_j m_{jc} - F_j = 0 \quad (27)$$

where F_j is the total molar flowrate of stream j, $S_{k,rc}$ is the coefficient of the stoichiometric matrix (Crowe *et al.*, 1983) of component c for reaction r in unit k, $\zeta_{k,r}$ is the extent of reaction r in unit k, $m_{j,c}$ is the molar fraction of component c in stream j, h_j represents the specific enthalpy of stream j, $H_{k,r}$ is the total heat of reaction r in unit k and depends on $S_{k,r}$, and $\zeta_{k,r}$, $\mathbf{q}_k$ is the vector of pure energy flows of unit k.

To compensate for random measurements errors, the data reconciliation procedure must solve the following least-squares problem:

$$\min \quad (\mathbf{y} - \tilde{\mathbf{y}})^T \Psi_y^{-1} (\mathbf{y} - \mathbf{y}) \quad (28)$$

$$\text{s.t.} \quad W(\mathbf{y}, \mathbf{z}) = 0$$

where $W(\mathbf{y}, \mathbf{y})$ represents a subset of balances and normalization equations; $\mathbf{y}$ and $\mathbf{z}$ are the vectors of measured and unmeasured variables for bilinear problems.

3.2. *Solution using* Q–R *factorizations*

A scheme for the solution of the bilinear reconciliation problem is proposed by Crowe (1986). In this work, the application of Q–R factorizations within this scheme is analyzed. Furthermore, total flowrates are separately considered from component and enthalpy flowrates and energy balances are explicitly taken into account.

Following Crowe's procedure, the solution to problem (28) can be accomplished in four steps.

3.2.1. Modification of bilinear constraints. The linear terms in $W(\mathbf{y}, \mathbf{z}) = 0$ remain unchanged. Bilienar terms are rewritten using the classification of component and enthalpy flowrates. Component flowrates are divided into three categories depending on the combination of total flow rates and concentration measurements in the stream as shown in Table 1, where M and U indicate measured and unmeasured variables respectively.

Table 1. Categories of component and energy flowrates

Category	F	m/T
1	M	M
2	U	M
3	M/U	U

For energy balances, an expression of specific enthalpy as function of temperature (T) is obtained by using a thermodynamic package, for a stream with constant steady-state simulated values of pressure and composition. Table 1 also represents the categorization of energy flowrates when this approach is applied.

Component/energy balances:

$$B_1 \mathbf{f} + B_2 V \mathbf{d} + B_3 \mathbf{v} = 0. \quad (29)$$

Normalization equations:

$$E_1 \mathbf{f} + E_2 V \mathbf{d} + E_3 \mathbf{v} + E_4 F_M + E_5 F_U = 0 \quad (30)$$

where $\mathbf{f}$ is the vector of component or enthalpy flowrates of Category 1; $\mathbf{d}$ is the vector of measured concentrations and calculated specific enthalpy for component or enthalpy flowrates of Category 2; $\mathbf{v}$ is the vector of component or enthalpy flowrates of Category 3, extent of reaction, unknown pure energy flows, etc; F_M stands for measured total flowrates and F_U for the unmeasured ones; V represents the diagonal matrix of unmeasured total flow rates for component and enthalpy flowrates of Category 2. The number of entries for a stream in V is equal to the number of elements of $\mathbf{d}$ corresponding to this stream.

The measured variable d is replaced by a consistent measured value plus the correction term $\delta_\mathbf{d}$:

$$d = (\tilde{\mathbf{d}} + \delta_\mathbf{d}) \quad (31)$$

and a new variable θ is defined as:

$$\theta = \mathbf{V} \delta_\mathbf{d}. \quad (32)$$

The terms that contain variable d in equations (29) and (30) are replaced by:

$$B_2 V d = B_2 \theta + B_2 V \tilde{\mathbf{d}}$$

$$E_2 V d = E_2 \theta + E_2 V \tilde{\mathbf{d}}. \quad (33)$$

In order to display unmeasured total flow rates for specific flowrates of Category 2 (F_{U_2}) from equations (33), B_4 and E_6 matrices are defined as:

$$B_4(\tilde{\mathbf{d}}) F_{U_2} = B_2 V \tilde{\mathbf{d}}$$

$$E_6(\tilde{\mathbf{d}}) F_{U_2} = E_2 V \tilde{\mathbf{d}}. \quad (34)$$

Each column of B_4 and E_6 contains the sum of the columns of B_2 and E_2 for the stream multiplied by the corresponding consistent concentration or specific enthalpy. To group all unmeasured total flowrates, zero columns are added to B_4 and F_6 if it is necessary. New B_5 and E_7 are obtained such that:

$$B_5(\tilde{\mathbf{d}})F_U = B_2 V\tilde{\mathbf{d}}$$

$$E_7(\tilde{\mathbf{d}})F_U = E_2 V\tilde{\mathbf{d}}. \tag{35}$$

Different linearly independent sets of process constraints can be formulated. One of them may include total mass balances, $C-1$ component balances, energy balances and normalization equations. Another one may contain all component and energy balances and normalization equations. Using previous expressions, the last set can be written as:

$$\begin{bmatrix} O & B_1 & B_2 & B_5 & B_3 \\ E_4 & E_1 & E_2 & E_8 & E_3 \end{bmatrix} \begin{bmatrix} F_M \\ \mathbf{f} \\ \theta \\ F_U \\ \mathbf{v} \end{bmatrix} = 0 \tag{36}$$

where$E_8 = E_7 + E_5$. If we consider the adjustments of total flow rates δ_F and the component and enthalpy flows δ_f, the general reconciliation problem can be stated as:

$$\min\,(\delta_{F_M}^T \Psi_{F_M}^{-1} \delta_{F_M}^T + \delta_f^T \Psi_f^{-1} \delta_f^T + \theta^T \Psi_\theta^{-1} \theta)$$

$$\text{s.t.}\quad [B_{11} \quad B_{22} \quad B_{33}] \begin{bmatrix} \mathbf{t} \\ F_U \\ \mathbf{v} \end{bmatrix} = -\begin{bmatrix} O_1 & B_1 \\ E_4 & E_1 \end{bmatrix} \times \begin{bmatrix} \tilde{F}_M \\ \mathbf{f} \end{bmatrix} = e \tag{37}$$

where

$$\mathbf{t} = \begin{bmatrix} \delta_{F_M} \\ \delta_f \\ \theta \end{bmatrix} \qquad B_{11} = \begin{bmatrix} O_1 & B_1 & B_2 \\ E_4 & E_1 & E_2 \end{bmatrix}$$

$$B_{22} = \begin{bmatrix} B_5 \\ E_8 \end{bmatrix} \qquad B_{33} = \begin{bmatrix} B_3 \\ E_3 \end{bmatrix}$$

Ψ_{F_M}, Ψ_f, Ψ_θ and $\Psi_\mathbf{d}$ are the variance–covariance matrices for F_M, $\mathbf{f}$, θ and $\mathbf{d}$. Ψ_θ is defined as:

$$\Psi_\theta = V \Psi_\mathbf{d} V. \tag{38}$$

Remark 4. By separating total flowrates from component and enthalpy flowrates, clearer expressions for instrumentation analysis and data reconciliation calculations may be obtained.

3.2.2. Elimination of unmeasured variables. These variables are eliminated from the modified constraints using Q–R orthogonal transformations as follows.

(i) A Q–R decomposition of $(m_b \times n_b)$ matrix B_{33} is accomplished, then:

$$B_{33}\Pi_\mathbf{v} = [QB][RB]$$

$$= [QB_1 \quad QB_2] \begin{bmatrix} RB_1 & RB_2 \\ 0 & 0 \end{bmatrix} \tag{39}$$

where, $r_\mathbf{v} = \text{rank}(RB_1)$ and QB_2^T is such that its rows span the null space of B_{33}^T so:

$$QB_2^T B_{33} = 0. \tag{40}$$

(ii) Equation (37) is multiplied by QB_2^T so the unmeasured variables $\mathbf{v}$ are eliminated and the process constraints are defined as:

$$QB_2^T B_{11} t + QB_2^T B_{22} F_U = QB_2^T e. \tag{41}$$

(iii) A new $(m_d \times n_d)$ matrix D is defined and equation (41) is rewritten as:

$$QB_2^T B_{11} t + D F_U = QB_2^T e. \tag{42}$$

(iv) A Q–R orthogonal trnsformation is performed on matrix D:

$$D\Pi_{F_U} = [QD][RD]$$

$$= [QD_1 \quad QD_2] \begin{bmatrix} RD_1 & QD_2 \\ 0 & 0 \end{bmatrix} \tag{43}$$

where $r_f = \text{rank}(RD_1)$ and QD_2^T is such that its rows span the null space of D^T, then the process constraints can be reduced to:

$$QD_2^T QB_2^T B_{11} t = QD_2^T QB_2^T e. \tag{44}$$

3.2.3. Estimation of measured variables and unmeasured total flow rates.

After eliminating unmeasured variables, the reconciliation of measured variables and the estimation of unmeasured total flow rates are accomplished by an iterative procedure:

Step 1:

Using an estimation of unmeasured total flow rates, Ψ_θ is evaluated. The following linear reconciliation problem needs to be solved:

$$\min \quad \mathbf{t}^T \Psi_t^{-1} \mathbf{t} \tag{45}$$

$$\text{s.t.} \quad G_t \mathbf{t} = b$$

where

$$G_t = QD_2^T QB_2^T B_{11}$$

$$b = QD_2^T QB_2^T e \tag{46}$$

with solution given by

$$\hat{\mathbf{t}} = \Psi_t G_t^T (G_t \Psi_t G_t^T)^{-1} b. \tag{47}$$

When the Q–R decomposition of G_t is applied to estimate $\hat{\mathbf{t}}$, the calculation has the same advantages as indicated for the Linear Case.

Step 2:

The estimation of unmeasured total flow rates is done by using the Q–R orthogonal decomposition of matrix D. Equation (42) can be written as:

$$QB_2^T B_{11}\hat{t} + [QD_1 \quad QD_2] \times \begin{bmatrix} RD_1 & RD_2 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} F_{U_{rf}} \\ \hline F_{U_{N_d-rf}} \end{bmatrix} = QB_2^T e \quad (48)$$

where

$$\begin{bmatrix} F_{U_{rf}} \\ F_{U_{n_d-rf}} \end{bmatrix} = \Pi_{F_U}^T F_U. \quad (49)$$

The subset $F_{U_{n_d-rf}}$ corresponds to the indeterminable total flow rates. Regarding the subset $F_{U_{rf}}$ nothing can be said, since some of these variables can be calulated directly from the measurements and some depends on $F_{U_{n_d-rf}}$. Further information to classify variables in subset $F_{U_{rf}}$ can be obtained pre-multiplying equation (48) by QD^T and writing the vector $\mathbf{F}_{U_{rf}}$ in terms of the other variables:

$$\mathbf{F}_{U_{rf}} = RD_1^{-1}QD_1^T QB_2^T e - RD_1^{-1}QD_1^T QB_2^T B_{11}\mathbf{t} - \mathrm{RD}_1^{-1}\mathrm{RD}_2 \mathrm{F}_{\mathrm{U}_{n_d-rf}}. \quad (50)$$

Notice that if the last term in the RHS of equation (50) is zero, all the $\mathbf{F}_{U_{rf}}$ can be calculated from the available information. In order to classify the variables in $\mathbf{F}_{U_{rf}}$ a matrix R_{IF} is defined as:

$$R_{IF} = RD_1^{-1}RD_2 \quad (51)$$

and the following can be stated:

(i) a variable in subset $\mathbf{F}_{U_{rf}}$ is determinable if the corresponding row in R_{IF} is zero;
(ii) a variable in subset $\mathbf{F}_{U_{rf}}$ is indeterminable otherwise.

At this point the vector $\mathbf{F}_U$ can be divided into:

$$\mathbf{F}_U = \begin{bmatrix} \mathbf{F}_{U_d} \\ \mathbf{F}_{U_i} \end{bmatrix} \quad (52)$$

where $\mathbf{F}_{U_d}$ is the f_e-dimensional vector of determinable total flowrates ($f_e < r_f$); $\mathbf{F}_{U_i}$ is the $(n_d - f_e)$-dimensional vector of indeterminable total flowrates; $\mathbf{F}_{U_d}$ contains the f_e variables in subset $\mathbf{F}_{U_{rf}}$ which satisfy condition (i) while $\mathbf{F}_{u_i}$ includes the variables in subset $\mathbf{F}_{U_{rf}}$ which satisfy condition (ii) plus the variables in subset $\mathbf{F}_{U_{n_d-rf}}$.

After updating the value of determinable total folw rates, the procedure is re-initiated until convergence is achieved.

Remark 5. If total flowrates are separated from component and energy flowrates, Crowe's specifications for the calculation of total flowrates corrections are not necessary.

2.3.4. Estimation of vector $\mathbf{v}$. In order to estimate the unmeasured variables contained in v, the matrix B_{22} is divided in two parts by column permutation. The first f_e columns correspond to the determinable total flow rates and the $(n_d - f_e)$ remaining ones belong to indeterminable total flowrates.

$$B_{22} = [B_{2d} \quad B_{2i}]. \quad (53)$$

Using the Q–R decomposition of matrix B_{33}, the set of constraints (37) is rewwritten as:

$$B_{11}\hat{\mathbf{t}} + B_{2d}F_{U_d} + B_{2i}F_{U_i} + [QB_1 \quad QB_2] \times \begin{bmatrix} RB_1 & RB_2 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{v}_{r_v} \\ \mathbf{v}_{n_b-r_v} \end{bmatrix} = e \quad (54)$$

where

$$\Pi_v^T \mathbf{v} = \begin{bmatrix} \mathbf{v}_{r_v} \\ \mathbf{v}_{n_b-r_v} \end{bmatrix}. \quad (55)$$

The subset $\mathbf{v}_{n_b-r_v}$ corresponds to the indeterminable variables in $\mathbf{v}$. For the classification of variables in subset v_{r_v}, additional information can be obtained by expressing $\mathbf{v}_{r_v}$ in terms of the other variables:

$$\mathbf{v}_{r_v} = RB_1^{-1}QB_1^T e - RB_1^{-1}QB_1^T B_{11}\hat{\mathbf{t}} - RB_1^{-1}QB_1^T B_{2d}F_{U_d} - RB_1^{-1}QB_1^T B_{2i}F_{U_i} - RB_1^{-1}RB_2\mathbf{v}_{n_b-r_v}. \quad (56)$$

The first three terms of the previous equation are known, so if the last ones are zero, all the variables in $\mathbf{v}_{r_v}$ can be evaluated using the available information. In order to classify the variables in $\mathbf{v}_{r_v}$, two new matrices are defined:

$$R_{IV} = RB_1^{-1}RB_2 \quad (57)$$

$$R_{IF_i} = RB_1^{-1}QB_1^T B_{2i} \quad (58)$$

and the following can be stated:

(i) a variable in subset $\mathbf{v}_{r_v}$ is determinable if the corresponding rows of R_{IV} and R_{IF_i} are zero;
(ii) a variable in subset v_{r_v} is indeterminable otherwise.

At this time, the vector $\mathbf{v}$ can be divided into:

$$\mathbf{v} = \begin{pmatrix} \mathbf{v}_d \\ \mathbf{v}_i \end{pmatrix} \quad (59)$$

where $\mathbf{v}_d$ is the $\mathbf{v}_e$-dimensional vector of determinable variables in v ($\mathbf{v}_e \le r_v$); $\mathbf{v}_i$ is the $(n_b - \mathbf{v}_e)$-dimensional vector of indeterminable variables in v; $\mathbf{v}_d$ contains the $\mathbf{v}_e$ variables in subset $\mathbf{v}_{r_v}$ which satisfy condition (i) while $\mathbf{v}_i$ includes the variables in subset $\mathbf{v}_{r_v}$ which satisfy condition (ii) plus the variables in subset $\mathbf{v}_{n_b-r_v}$.

After the calculation of the elements in v_d, unmeasured concentrations and temperatures which correspond to component and enthalpy flows in $\mathbf{v}_d$

are determinable if the total flowrate of the stream is measured or determinable. Otherwise, they are indeterminable. The inclusion of intensiive process constraints can change the classification but it is not on the scope of this paper.

3.3. *Further discussion on energy balances*

Through the above discussion, simplified expressions of streamspecific enthapy as function of temperature are used. They have to be updated during process operation to consider changes in steady-state compositions.

The application of a more precise expression for enthalpy, at least, as a function of temperature and composition requires a new categorization of enthalpy flowrates. They can be divided into three categories depending on the combination of total flowrates, composition and temperature measurements, as indicated in Table 2.

The problem arises for the last measurement combination. It is due to the difficulty of adjusting temperatue measurement values for streams which compositions are unmeasured or partially measured. In this context, the temperature of a stream j may be adjusted only for the following conditions:

— all component molar fractions are unmeasured;

— rule of mixing: $h_j = \sum m_{jc} h_{jc}$;

— h_{jc} is approximated as a linear function of temperature for the steady-state operation range.

The following solution scheme can be implemented:

(i) estimation of unmeasured total flowrates and unmeasured species flowrates for streams with unmeasured temperatures;
(ii) simultaneous elimination of unmeasured variables. A two-stage procedure of decomposition does not give advantages because measurements are involved in Category 3 flowrates;
(iii) Least-squares adjustment of measurements;
(iv) estimation of unmeasured variables;
(v) iteration until convergence is achieved.

Hence, factorization methods can be only applied to solve particluar cases of data reconciliation when energy balances are considered. Other equation oriented techniques, such as PLADAT (Sánchez *et al.*, 1992), can be used to tackle the general problem.

Table 2. Categories of enthalpy flowrates

Category	F	T	m
1	M	M	M
2	U	M	M
3	M/U	U	M
3	M/U	M	U

4. EXAMPLES

4.1. *Example 1—Linear Case: application to a section of an ethylene plant*

This sector of the Olefin plant includes the ethylene refrigeration and compression to C_2 splitter sections. A simplified node diagram of the process is given in Fig. 1. Cracked gases coming out from the gas compressor enter the pre-cooling and drying sections. The cooled, cracked streams enter the de-ethaniser colums (nodes 3 and 4) where C_3 and higher hydrocarbons are separated as bottom product. The top product of unit 3, consisting of C_2 and lower hydrocarbons (C_2H_6, C_2H_4, C_2H_2, CH_4, H_2, etc.) enters the acetylene hydrogenation reactor where acetylene is hydrogenated to ethylene. The hydrogenated gaseous stream enters the cold section, where it is passed through a number of heat exchangers and separators. A portion of liquid stream from unit 10 is used as the recycle stream. Hydrogen is separated as a gaseous stream in unit 12. The liquid streams from separators 7–11 enter the de-methaniser column (unit 13). The top product of this column is methane, which is sent to fuel gas stream via cold section and drying/pre-cooling section. The bottom product enters the C_2 splitter column (unit 15) as a feed. The top product of this column is cooled and compressed and subsequently stored as ethylene product. The bottom product of the C_2 splitter column is ethane, which is sent back to the cracking furnace as feed stock through the pre-cooling section.

The Q–R factorization is applied to adjust measured flowrates of the whole sector, such that mass balances are satisfied. The section has 31 units and 63 process variables of which only 29 are measured. From the analysis arises that:

(a) there are eight redundant equations containing all the 29 measured variables;
(b) first the unmeasured flowrates can be divided into:

$$\mathbf{u}_r = [3\ 5\ 10\ 24\ 34\ 35\ 36\ 38\ 39\ 40\ 41\ 42\ 44\ 45\ 48\ 49\ 50\ 51\ 54\ 55\ 56\ 59\ 61]$$

$$\mathbf{u}_{n-r} = [4\ 6\ 11\ 43\ 47\ 52\ 57\ 58\ 60\ 62\ 63].$$

Furthermore, from the inspection of the R_{IU} matrix, the flowrates of streams 24, 34–36 and 49 are determinable.

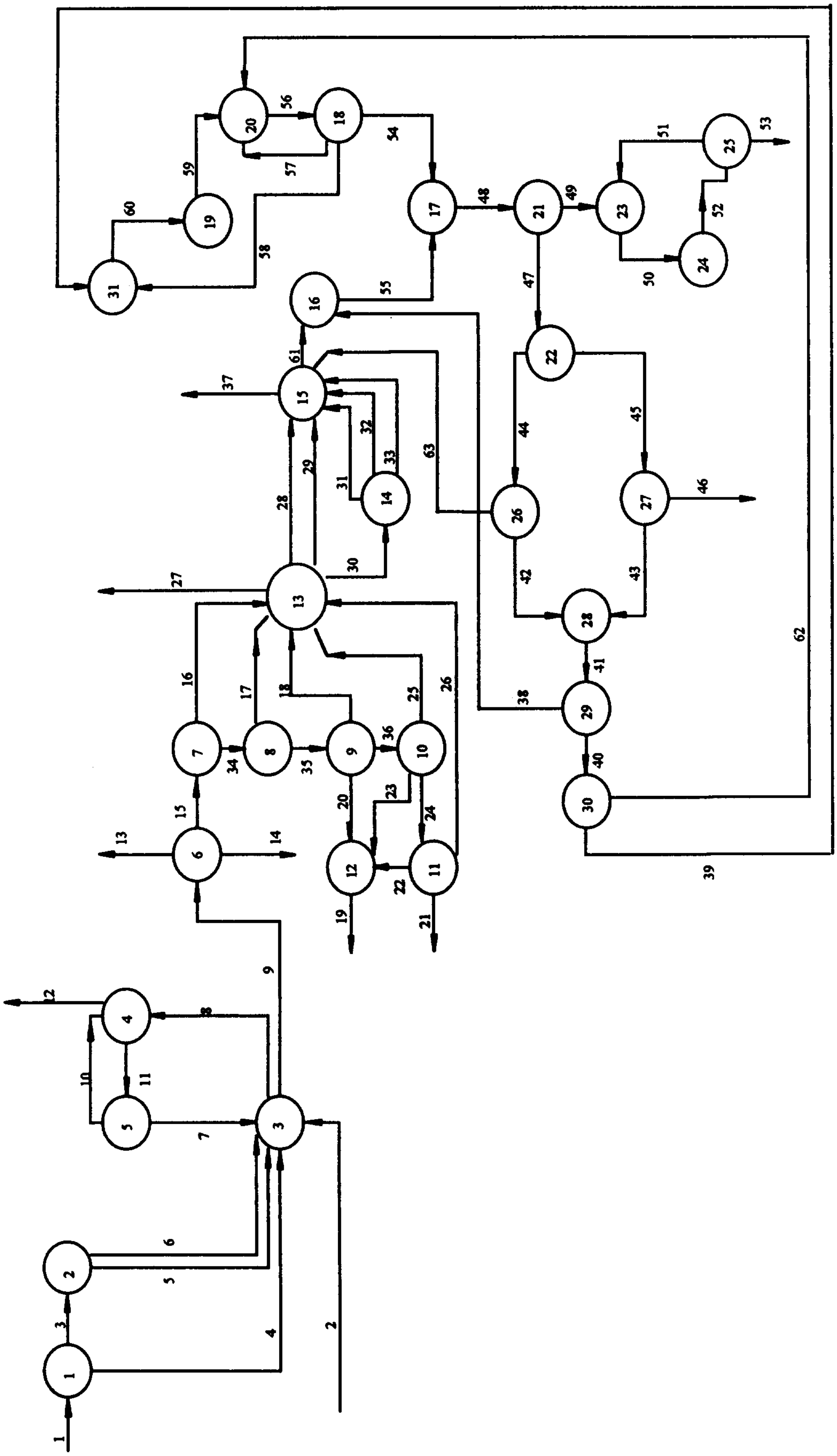

Fig. 1. Simplified node diagram of a section of an olefine plant.

Table 3. Data and results for Example 1

Stream	Variances	Measured values	Reconciled values
1	10.87	70.49	70.105
2	0.2030	7.103	7.096
7	2.624	13.04	11.980
8	0.3970	35.38	35.540
9	5.76	53.21	53.641
12	0.922	23.90	23.560
13	0.608	0.00	−0.024
14	5.76	0.0765	−0.150
15	0.23	54.59	53.816
16	1.44	12.78	11.934
17	0.7060	23.42	23.005
18	0.017	0.2378	0.229
19	0.13	8.657	8.618
20	0.09	5.087	5.413
21	0.014	1.74	1.787
22	0.0002	0.0255	0.026
23	0.018	3.113	3.178
25	0.09	5.407	5.354
26	0.014	2.898	2.889
27	0.36	11.83	13.239
28	0.563	8.197	8.907
29	0.023	1.364	1.393
30	1.103	20.94	19.872
31	0.008	1.051	1.069
32	0.397	12.58	13.465
33	0.152	4.999	5.338
37	0.09	5.73	5.969
46	0.13	4.25	4.595
53	1.232	16.34	19.608

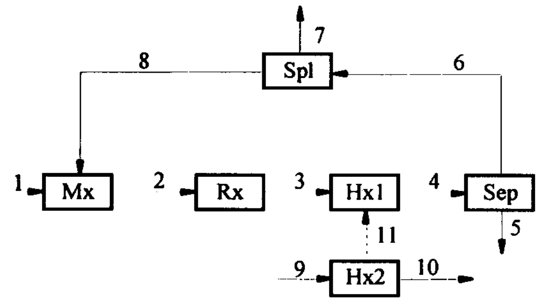

Fig. 2. Simplified amonia plant.

Measurement values, variances and reconciled values for the measured flowrates are included in Table 3.

4.2. Example 2—Nonlinear Case: a simplified ammonia plant

The process flowsheet is shown in Fig. 2. Measured variables for this process are presented in Table 4. Simulation values for process variables are obtained from SEPSIM Manual (Andersen *et al.*, 1991). It is considered that all components (N_2, H_2, Ar and NH_3) are present in all streams except the feed.

Table 4. Measured variables for Example 2

Measurements	Stream numbers
Total flowrate	3 5 6
Composition of N_2	1 2 3 6 7 8
Composition of H_2	4
Composition of Ar	4
Composition of NH_3	2 3 5
Temperature	1 3 4 5 6 7 8 9

The set of process constraints includes: component and energy balances and normalization equations. Equality of concentrations and temperatures of the splitter streams are not taken into account in this particular example. Expressions of stream enthalpy as function of temperature are obtained using thermodynamic packages for simulated values of presion and composition. These expressions have to be updated to consider changes in steady state. After modification of bilinear terms, vectors $\mathbf{F}_M$, $\mathbf{f}$, $\mathbf{F}_U$, $\boldsymbol{\theta}$ and $\mathbf{v}$ are:

$$\mathbf{F}_M^T = [F_3\,F_5\,F_6]$$

$$\mathbf{F}_u^T = [F_1\,F_2\,F_4\,F_7\,F_8\,F_9\,F_{10}]\ldots$$

$$\mathbf{f}^T = [f_{3,1}\,f_{3,4}\,fh_3\,fh_5\,f_{6,1}\,fh_6\,f_{5,4}]$$

$$\theta^T = [\theta_{1,1}\,\theta h_1\,\theta_{2,1}\,\theta_{4,2}\,\theta_{4,3}\;\theta h_4\,\theta_{7,1}\;\theta h_7\,\theta_{8,1}\,\theta_8\,\theta h_9\,\theta_{2,4}]$$

$$\mathbf{v} = [\nu_{1,2}\,\nu_{1,3}\,\nu_{2,2}\,\nu_{2,3}\,\nu h_2\,\nu_{3,2}\,\nu_{3,3}\,\nu_{4,1}\;\nu_{4,4}\,\nu_{6,2}\,\nu_{6,3}\;\nu_{7,2}\,\nu_{7,3}\,\nu_{8,2}\,\nu_{8,3}\,\nu h_{10}\;\nu h_{11}\,\zeta\nu_{5,1}\,\nu_{5,2}\,\nu_{5,3}\,\nu_{6,4}\,\nu_{8,4}\,\nu_{7,4}\,H_r]$$

where $f_{j,n}$ and fh_j are Category 1 component and enthalpy flowrates, $\theta_{j,n}$ and θh_j stand for adjustments of Category 2 component and enthalpy flowrates, $\nu_{j,n}$ and νh are Category 3 component and enthalpy flowrates.

For variable classification and data reconciliation the following procedure is applied:

(a) Matrices QB_1, QB_2, RB_1, RB_2, Π_v and vectors $\mathbf{v}_{r_v}$ and $\mathbf{v}_{nb-r_v}$ are obtained by the Q–R decomposition of matrix B_{33}.

(b) After calculating matrix D, a Q–R orthogonal decomposition of D gives QD_1, QD_2, RD_1, RD_2, Π_d matrices and $\mathbf{F}u_{r_d}$, $\mathbf{F}u_{nd-r_d}$ vectors. R_{IF} inspection allows to classify unmeasured total flowrates in:

$$\mathbf{F}_{Ud}^T = [F_1\,F_2\,F_4\,F_7\,F_8]$$

$$\mathbf{F}_{U_i}^T = [F_9\,F_{10}].$$

(c) B_{2i}, R_{IV} and R_{IF_i} are obtained. The inspection of the last two matrices is used to classify unmeasured variables in υ:

$$\mathbf{v}_d = [\zeta\nu_{2,3}\,\nu_{4,1}\,\nu_{8,4}\,\nu_{3,2}\,\nu_{4,4}\,\nu_{3,3}\,q_{11}\,\nu_{2,2}\;\nu_{5,1}\,\nu_{6,4}\,\nu h_2\,\nu_{7,4}\,H_r]$$

$$\mathbf{v}_i = [\nu_{6,2}\,\nu_{6,3}\,\nu_{8,2}\,\nu_{1,3}\,\nu_{7,3}\,\nu_{8,3}\,\nu_{5,2}\,\nu h_{10}\,\nu_{1,2}].$$

(d) Matrix G_t is calculated and measurement classification is accomplished. Non redundant

Table 5. Measured and reconciled values for Example 2 (F = [mol kg/h] − T = [K])

Variable	Mes. value	Rec. value	Variable	Mes. value	Rec. value
F_3	174.616	172.720	T_1	701.4	701.4
F_5	25.52	25.1423	$c(2,1)$	0.2419	0.2389
F_6	147.263	147.577	$c(4,2)$	0.5821	0.5726
$c(3,1)$	0.1880	0.1957	$c(4,3)$	0.0172	0.01749
$c(3,4)$	0.2126	0.2144	T_4	270.5	269.16
T_3	700.1	698.3	$c(7,1)$	0.2308	0.2306
T_5	272.7	270.7	T_7	267.1	266.7
$c(6,1)$	0.2299	0.2305	$c(8,1)$	0.2265	0.2304
T_6	267.1	266.6	T_8	272.5	272.0
$c(5,4)$	0.9853	0.9856	T_9	282.0	282.0
$c(1,1)$	0.2504	0.2504	$c(2,4)$	0.0359	0.0368

Table 6. Estimated values of unmeasured determinable variables for Example 2 F = [mol kg/h]; v = [Mol kg/h]; vh_j, q, Q = [MJ/h]

Variable	Estimation	Variable	Estimation	Variable	Estimation
F_1	101.608	$v(4,1)$	33.801	$v(5,1)$	0.0002
F_2	202.491	$v(8,4)$	7.267	$v(6,4)$	12.2569
F_4	172.720	$v(3,2)$	98.910	vh_2	2853.141
F_7	46.694	$v(4,4)$	37.039	$v(7,4)$	4.989
F_g	100.882	$v(3,3)$	2.969	Hr	915.220
ξ	14.885	q_{11}	2989.72		
$v(2,3)$	2.969	$v(2,2)$	143.566		

measurements are T_3, $c(5,4)$, $c(1,1)$, T_1 and T_9. The remaining measurements are redundant.

(e) An iterative procedure is performed to adjust measurements and to estimate unmeasured determinable total flowrates. Measured and reconciled values for this example are displayed in Table 5.

(f) Then the estimation of determinable variables in v is done. In Table 6 the estimated values of unmeasured determinable variables are presented.

5. CONCLUSIONS

In this work, the application of Q–R factorization to analyze, decompose and solve the linear and bilinear reconciliation problem is discussed in the context of Crowe's projection scheme.

The proposed approach has several computational advantages when compared with respect to the conventional approaches. Furthermore, it allows straightforward implementation within the MATLAB environment.

The separation of total flowrates from component and enthalpy flowrates has two important advantages:

(a) There is a notational convenience. It allows to obtain more clear expressions for instrumentation analysis and data reconciliation which are not explicitly included in previous works. The expressions are written in terms of subproducts of Q–R factorizations.

(b) The use of assumptions for total flowrate adjustment is avoided.

Results of the application for linear and bilinear systems were provided in terms of two flowsheeting examples, one of them being an existing operating plant.

NOMENCLATURE

Linear Case

$\mathbf{x}$ = Vector of measured variables ($g \times 1$)
A_1 = Matrix for measured variables ($m \times g$)
P = Projection matrix
G_x = Matrix equation (13) [$(m - r_u) \times g$]
$[Q_u, R_u, \Pi_u] = QR(A_2)$
r_u = Rank (R_{u_1})
$\mathbf{u}_{r_u}, \mathbf{u}_{n-r_u}$ = Partitions of $\mathbf{u}$
I_{x_1}, I_{x_2} = Partitions of I for $\mathbf{x}_{r_x}, \mathbf{x}_{g-r_x}$
$\bar{\mathbf{I}}$ = [Matrix equation (19) [$g \times (g - r_x)$]
$\mathbf{u}$ = Vector of unmeasured variables (n × 1)
A_2 = Matrix for unmeasured variables ($m \times n$)
$G = PA_1$
I = Identity matrix
$[Q_x, R_x, \Pi_x] = QR(G_x)$
r_x = Rank(R_{x_1})
$\mathbf{x}_{r_x}, \mathbf{x}_{g-r_x}$ = Partitions of $\mathbf{x}$
R_{IU} = Matrix equation (23) [$r_u \times (n - r_u)$]

Non-linear Case

K = Number of units
k = Unit index
J = Number of streams
j = Stream index
F = Molar total flowrate
S = Stoichiometrix matrix
r = Index of reaction
m = Molar fractions
h = Specific enthalpy
B_i = Matrices for comp./enthapy balances
f = Specific flowrates in Category 1

d = M molar fractions and sp. enthalpy
υ = Specific flowrates in Category 3
V = Diagonal matrix of $\mathbf{F}_{U_2}$
E_i = Matrices for normalization equations
$\mathbf{F}_{U_{rf}}, \mathbf{F}_{U_{nd-rf}}$ = Partitions of $\mathbf{F}_U$
$D = QB_2^T B_{22}$
C = Number of components
c = Comp. index
L = Incidence matrix
l = Incident matrix index
H = Total heat of reaction
q = Pure energy flow
y = Measured variables
z = Unmeasured variables
T = Temperature
$\mathbf{t}, \mathbf{w}, \mathbf{e}$ = Vectors equation (37)
B_{ii} = Matrices equation (37)
$ii = 1, 3$
O = Zero matrix
$[QB, RB, \Pi_\upsilon] = QR(B_{33})$
$[QD, RD, \Pi_d] = QR(D)$
Gt, b = Equation (46)
$\mathbf{v}_{r_v}, \mathbf{v}_{nb-r_v}$ = Partitions of υ
R_{IF}, R_{IV}, R_{IF_i} = Inspection matrices

Greek letters

ε = Vector of random errors
Ψ_i = Variance–covariance matrix of i
ζ = Vector of extents of reaction
δ_i = Correction of i
θ = Vector equation (32)

Superscripts

$\sim$ = With measured values
$\wedge$ = With reconciled values

Subscripts

M, U = Measured or unmeasured variable
d, i = Determinable or indeterminable variable

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APPENDIX

Let A be a given $m \times n$ matrix with $m \geqslant m$ and n linearly independent columns. Then there exists a $m \times m$ unitary matrix Q and a $m \times n$ matrix R, such that $A = QR$, where:

$$R = \begin{bmatrix} R_1 \\ 0 \end{bmatrix} \text{ and } R_1 \text{ is an upper trianglular matrix.}$$

If A is rank-deficient, then at least one diagonal entry in R_1 is zero.

Let us examine why the Q–R factorization approach can fial in the case when $\mathrm{rant}(A) = r < n$.

The mission of any orthogonalization method is to compute an orthonormal basis for the range of A, $R(A)$. Indeed, if $R(A) = R(Q_1)$ where $Q_1 = [q_1, \ldots, q_r]$ has orthonormal columns then $A = Q_1 N$ for some $N \in \Re^{r \times n}$. Unfortunately, if $r < n$, then the Q–R factorization does not necessarily produce an orthonomral basis for $R(A)$. However, the Q–R decomposition can be modified in a simple way so as to produce an orthonormal basis for A's range. The modified algorithm computes the factorization:

$$A\Pi = [Q_1 \;\; Q_2] \begin{bmatrix} R_{11} & R_{12} \\ 0 & 0 \end{bmatrix}$$

where Q_1, Q_2, R_{11} and R_{12} are matrices of dimension $(m \times r)$, $[m \times (m-r)]$, $(r \times r)$ and $[r \times (n-r)]$ respectively, Π is a permutation matrix and R_{11} is upper trinagular. If:

$$A\Pi = [a_{c_1}, \ldots, a_{c_n}] \quad \text{and} \quad Q = [q_1, \ldots, q_m]$$

then for $k = 1, \ldots, n$ we have:

$$a_{ck} = \sum_{i=1}^{\min\{r,k\}} r_{ik} q_i \in \mathrm{span}\{q_1, \ldots, q_r\}.$$

Also, it follows that for any vector satisfying $Ax = b$, then:

$$\Pi^T x = \begin{bmatrix} \mathbf{y} \\ \mathbf{z} \end{bmatrix} \quad \text{and} \quad Q^T b = \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix}$$

where $\mathbf{y}$ and $\mathbf{c}$ are r-dimensional vectors, $\mathbf{z}$ is an $(n-r)$-dimensional vector and $\mathbf{d}$ is an $(m-r)$-dimensional vector.