REFERENCES

Alhéritière, C., Thornhill, N. F., Fraser, S., and Knight, M. J. (1998) Cost benefit analysis of refinery process data: Case study. Computers & Chemical Engineering, 22(Suppl. 1), S1031-S1034.

Bagajewicz, M. (2004a) On the Definition of Software Accuracy in Redundant Measurements Systems. Submitted to AIChE Journal.

Bagajewicz, M. (2004b) Value of Accuracy in Linear Systems. Submitted to AIChE Journal.

Bagajewicz, M., and Rollins, D. (2004) On the Consistency of the Measurement and GLR test for Gross Error Detection. Submitted to Computers & Chemical Engineering.

Bagajewicz, M., Markowski, M., and Budek, A. (2003) Economic Value of Precision in the Monitoring of Linear Systems. Submitted to AIChE Journal.

Bagajewicz, M. (2000). A Brief Review of Recent Developments in Data Reconciliation and Gross Error Detection/Estimation. Latin American Applied Research, 30(4), 335-342.

Bagajewicz, M. and Sánchez, M. (2000) Reallocation and upgrade of instrumentation in process plants. Computers & Chemical Engineering, 24(8), 1945-1959.

Bagajewicz, M., Jiang, Q. and Sanchez, M. (1999) Removing Singularities and Assessing Uncertainties in Two Efficient Gross Error Collective Compensation Methods. Chemical Engineering Communication, 178, 1-20.

Bagajewicz, M. and Jiang, Q. (1998) Gross Error Modeling and Detection in Plant Linear Dynamic Reconciliation. Computers & Chemical Engineering, 22 (12), 1789-1810.

Christiansen, L.J., Olsen, N.B., Carstensen, J.H., and Schrøder, M. (1997) Performance evaluation of catalytic processes. Computers & Chemical Engineering, 21(Suppl. 1), S1179-S1184.

Chiari, M., Bussani, G., Grottoli, M.G., and Pierucci S. (1997) On-line data reconciliation and optimisation: Refinery applications. Computers & Chemical Engineering, 21(Suppl. 1), S1185-S1190.

Crowe, C.M., Hrymak, A. and Campos, Y.A.G. (1983) Reconciliation of Process Flow Rates by Matrix Projection. I. The Linear Case. AIChE Journal, *29*, 881-888.

Dempf, D. and List, T. (1998) On-line data reconciliation in chemical plants. Computers & Chemical Engineering, 22(Suppl. 1), S1023-S1025.

Evans, M. and Swartz, T., (2000) Approximating integrals via Monte Carlo and deterministic methods. Oxford: Oxford University Press.

Iordache, C., Mah, R. and Tamhane, A. (1985) Performance Studies of the Measurement Test for Detection of Gross Errors in Process Data. AIChE Journal, 31, 1187-1201.

Jiang, Q. and Bagajewicz, M. (1999) On a Strategy of Serial Identification with Collective Compensation for Multiple Gross Error Estimation in Linear Steady-State Reconciliation. Industrial & Engineering Chemistry Research, 38 (5), 2119 -2128.

Jiang, Q., Sánchez, M., and Bagajewicz, M. (1999) On The Performance of Principal Component Analysis in Multiple Gross Error Identification. Industrial & Engineering Chemistry Research, 38(5), 2005-2012 .

Kim, I., Kang, M.S., Park, S. and Edgar, T. (1997) Robust Data Reconciliation and Gross Error Detection: The Modified MIMT using NLP. Computers & Chemical Engineering, 21, 775-782.

Lee, M.H., Lee, S.J., Han, C., Chang, K.S., Kim, S.H. and You, S.H., (1998) Hierarchical on-line data reconciliation and optimization for an industrial utility plant. Computers & Chemical Engineering, 22(Suppl. 1), S247-S254.

Lu, Z. and Zhang, D. (2003) On importance sampling Monte Carlo approach to uncertainty analysis for flow and transport in porous media. Advances in Water Resources, 26(11), 1177-1188.

Meyer, M., Koehret, B., and Enjalbert, M. (1993) Data reconciliation on multicomponent network process. Computers & Chemical Engineering, 17(8), 807-817.

Mah, R.S.H. (1990) Chemical Process Structures and Information Flows. Stoneham, MA: Butterworths.

Mah, R.S.H. and Tamhane, A.C. (1982) Detection of Gross Errors in Process Data. AIChE Journal, 28, 828-830.

Mori, Y. and Kato, T. (2003). Multinormal integrals by importance sampling for series system reliability. Structural Safety, 25(4), 363-378.

Narasimhan, S., and Jordache, C. (2000) Data Reconciliation & Gross Error Detection: An Intelligent Use of Process Data. Houston, Texas: Gulf Publishing.

Narasimhan, S. and Mah, R. (1987) Generalized Likelihood Ratio Method for Gross Error Identification. AIChE Journal, 33, 1514-1521.

Pierucci, S., Brandani, P., Ranzi, E., and Sogaro, A. (1996) An industrial application of an on-line data reconciliation and optimization problem. Computers & Chemical Engineering, 20(Suppl. 2), S1539-S1544.

Rollins, D. and Davis, J. (1992) Unbiased Estimation of Gross Errors in Process Measurements. AIChE Journal, 38(4), 563-572.

Sánchez, M., Romagnoli, J., Jiang, Q., and Bagajewicz, M. (1999) Simultaneous Estimation of Biases and Leaks in Process Plants. Computers and Chemical Engineering, 23(7), 841-858.

Soderstrom, T.A., Himmelblau, D.M., and Edgar, T.F. (2001) A mixed integer optimization approach for simultaneous data reconciliation and identification of measurement bias. Control Engineering Practice, 9(8), 869-876.

Serth, R. and Heenan, W. (1986) Gross Error Detection and Data Reconciliation in Steam Metering Systems. AIChE Journal, 32, 733-742.

Tong, H. and Crowe, C. (1995) Detection of Gross Errors in Data Reconciliation by Principal Component Analysis. AIChE Journal, 41, 1712-1722.

Tjoa, I.B., and Biegler, L.T. (1991) Simultaneous strategies for data reconciliation and gross error detection of nonlinear systems. Computers and Chemical Engineering, 15(10), 679–690.

APPENDIX

This appendix shows proof for $W_{i1i1} > W'_{i1i1}$; where W' is the updated matrix W after a redundant measurement has been eliminated and W_{i1i1} and W'_{i1i1} are diagonal elements of matrices W, W'. The expression $W_{i1i1} > W'_{i1i1}$ is equivalent to the expression $W^{+}_{i1i1} > W_{i1i1}$; where W^{+} is the updated matrix W after a redundant measurement has been added. We aim at showing that $W^{+}_{i1i1} > W_{i1i1}$.

The matrix W is given by:

$$W = A^T(ASA^T)^{-1}A$$

The matrix W is given by:

$$W^{+} = \left[A^{+}\right]^T (A^{+}S^{+}\left[A^{+}\right]^T)^{-1} A^{+}$$

where A^{+}, S^{+} are the updated matrices A (constraint matrix) and S (covariance matrix of measurements) after a redundant measurement has been added.

We obtain the new constraint matrix A^{+} corresponding to the system to which a redundant measurement is added by simply adding one constraint relating this new measurement with some other redundant measurements in the system:

We write A^{+} at form:

$$A^{+} = \begin{pmatrix} \begin{bmatrix} A \\ n \times m \end{bmatrix} & \begin{bmatrix} 0 \\ n \times 1 \end{bmatrix} \\ \left[B_i, 1xm\right] & \delta \end{pmatrix}$$

where vector $[B_i, \delta] = [1 \times (m+1)]$ is the last row corresponding to the new constraint relating the new redundant measurement with some other redundant measurements in the systems; vector $[0, \delta] = [(n+1) \times 1]$ is the last column corresponding to the new redundant measurement (δ can take value of 1 or -1).

The new covariance matrix of measurements is:

$$S^{+} = \begin{pmatrix} \begin{bmatrix} S \\ m \times m \end{bmatrix} & \begin{bmatrix} 0 \\ m \times 1 \end{bmatrix} \\ \left[0, 1 \times m\right] & s_i \end{pmatrix}$$ (we assume S & S^{+} are diagonal matrices)

where m, n are the (old) number of redundant measurements and the (old) number of constraints, respectively.

Then:

$$\left(A^+S^+\left[A^+\right]^T\right)^{-1} = \begin{pmatrix} \begin{bmatrix} ASA^T \\ n\,x\,n \end{bmatrix} & \begin{bmatrix} ASB_i^T \\ n\,x\,1 \end{bmatrix} \\ \left[B_iSA^T, 1\,x\,n\right] & B_iSB_i^T + s_i\delta^2 \end{pmatrix}^{-1} = \begin{pmatrix} P & Q \\ R & S \end{pmatrix}^{-1}$$

$$= \begin{bmatrix} X & -P^{-1}QY \\ -YRP^{-1} & Y \end{bmatrix}$$

where:

$$Y = (S - RP^{-1}Q)^{-1}$$
$$X = P^{-1} + P^{-1}QYRP^{-1}$$

(formula taken from Noble, B. and Daniel, J.W. 1988 Applied linear algebra 3rd edition, p.41, Prentice Hall).

In this case S and Y are scalars.

Then:

$$\left[A^+\right]^T (A^+S^+\left[A^+\right]^T)^{-1} A^+$$

$$= \begin{pmatrix} \left[A^T\right] & \left[B_i^T\right] \\ [0] & \delta \end{pmatrix} \begin{pmatrix} [X] & \left[-P^{-1}QY\right] \\ \left[-YRP^{-1}\right] & Y \end{pmatrix} \begin{pmatrix} [A] & [0] \\ [B_i] & \delta \end{pmatrix}$$

$$= \begin{pmatrix} \left[\left[A^TX\right] + \left[B_i^T[-YRP^{-1}]\right]\right] & \left[\left[A^T[-P^{-1}QY]\right] + \mathrm{Y}\left[B_i^T\right]\right] \\ \delta\,x\left[-YRP^{-1}\right] & \delta Y \end{pmatrix} x \begin{pmatrix} [A] & [0] \\ [B_i] & \delta \end{pmatrix}$$

$$= \begin{pmatrix} \left[\left(\left[A^TX\right] + \left[B_i^T[-YRP^{-1}]\right]\right)[A] + \left(\left[A^T[-P^{-1}QY]\right] + Y\left[B_i^T\right]\right)[B_i]\right] & \delta\left[\left[A^T[-P^{-1}QY]\right] + Y\left[B_i^T\right]\right] \\ \left[\delta\left[-YRP^{-1}\right][A] + \delta Y[B_i]\right] & \delta^2 Y \end{pmatrix}$$

We concentrate only on diagonal elements of matrix $W^+ = \left[A^+\right]^T (A^+S^+\left[A^+\right]^T)^{-1} A^+$ and matrix $W = A^T(ASA^T)^{-1}A$

Consider:

$$\left[\left(\left[A^TX\right] + \left[B_i^T[-YRP^{-1}]\right]\right)[A] + \left(\left[A^T[-P^{-1}QY]\right] + Y\left[B_i^T\right]\right)[B_i]\right]$$

$$= \left[A^TXA\right] + \left[B_i^T[-YRP^{-1}]A\right] + \left[A^T[-P^{-1}QY]B_i\right] + Y\left[B_i^TB_i\right]$$

Now we have:

$Y = (S - RP^{-1}Q)^{-1}$ (a scalar) > 0 because matrix $(ASA^T)^{-1}$ or $(A^+S^+\left[A^+\right]^T)^{-1}$ is positive definite (Bagajewicz, M., and Rollins, D. (2004). On the Consistency of the Measurement and GLR test for Gross Error Detection. Submitted to Computers & Chemical Engineering.)

$$-YRP^{-1} = -Y\left[B_iSA^T\right]\left[ASA^T\right]^{-1}$$

$$-P^{-1}QY = -\left[ASA^T\right]^{-1}\left[ASB_i^T\right]Y = -Y\left[ASA^T\right]^{-1}\left[ASB_i^T\right]$$

$$X = P^{-1} + P^{-1}QYRP^{-1} = \left[ASA^T\right]^{-1} + \left[ASA^T\right]^{-1}\left[ASB_i^T\right]Y\left[B_iSA^T\right]\left[ASA^T\right]^{-1}$$

$$= \left[ASA^T\right]^{-1} + Y\left[ASA^T\right]^{-1}\left[ASB_i^T\right]\left[B_iSA^T\right]\left[ASA^T\right]^{-1}$$

Therefore:

$$\left[B_i^T\right]\left[-YRP^{-1}\right][A] = \left[B_i^T\right]\left[-Y\left[B_iSA^T\right]\left[ASA^T\right]^{-1}\right][A]$$

$$= -Y\left[B_i^T\right]\left[\left[B_iSA^T\right]\left[ASA^T\right]^{-1}\right][A] = -YB_i^TB_iS\left[A^T\right]\left[ASA^T\right]^{-1}[A]$$

$$\left[A^T\right]\left[-P^{-1}QY\right][B_i] = \left[A^T\right]\left[-Y\left[ASA^T\right]^{-1}\left[ASB_i^T\right]\right][B_i]$$

$$= -Y\left[A^T\right]\left[ASA^T\right]^{-1}\left[ASB_i^T\right][B_i] = -Y\left[A^T\right]\left[ASA^T\right]^{-1}[A]SB_i^TB_i$$

Then:

$$\left[A^TXA\right] + \left[B_i^T[-YRP^{-1}]A\right] + \left[A^T[-P^{-1}QY]B_i\right] + Y\left[B_i^TB_i\right]$$

$$= \left[A^T\right]\left(\left[ASA^T\right]^{-1} + Y\left[ASA^T\right]^{-1}\left[ASB_i^T\right]\left[B_iSA^T\right]\left[ASA^T\right]^{-1}\right)[A]$$

$$-YB_i^TB_iS\left[A^T\right]\left[ASA^T\right]^{-1}[A] - Y\left[A^T\right]\left[ASA^T\right]^{-1}[A]SB_i^TB_i + Y\left[B_i^TB_i\right]$$

$$= \left[A^T\right]\left[ASA^T\right]^{-1}[A] + Y\left[A^T\right]\left[ASA^T\right]^{-1}\left[ASB_i^T\right]\left[B_iSA^T\right]\left[ASA^T\right]^{-1}[A]$$

$$-YB_i^TB_iS\left[A^T\right]\left[ASA^T\right]^{-1}[A] - Y\left[A^T\right]\left[ASA^T\right]^{-1}[A]SB_i^TB_i + Y\left[B_i^TB_i\right]$$

$$= \left[A^T\right]\left[ASA^T\right]^{-1}[A] + Y\left[A^T\right]\left[ASA^T\right]^{-1}[A]\left[SB_i^TB_iS\right]\left[A^T\right]\left[ASA^T\right]^{-1}[A]$$

$$-YB_i^TB_iS\left[A^T\right]\left[ASA^T\right]^{-1}[A] - Y\left[A^T\right]\left[ASA^T\right]^{-1}[A]SB_i^TB_i + Y\left[B_i^TB_i\right]$$

Now

$$\left[A^T\right]\left[ASA^T\right]^{-1}[A]\left[SB_i^TB_iS\right]\left[A^T\right]\left[ASA^T\right]^{-1}[A]$$

$$= WS(B_i^TB_i)SW = WSBSW$$

where $B = B_i^TB_i$

(since $W = A^T(ASA^T)^{-1}A$)

Diagonal elements B_{ii} of matrix $\boldsymbol{B}$ (m x m) are b_i^2 where b_i are elements of the vector $\boldsymbol{B_i}$ (1 x m). Matrix $\boldsymbol{B}$ is also a symmetric matrix whose element $B_{ij} = B_{ji} = b_i b_j$ (b_i, b_j are elements of the vector $\boldsymbol{B_i}$ and can be 0, +1 or -1).

Then:

$$\left[A^T\right]\left[ASA^T\right]^{-1}[A] + Y\left[A^T\right]\left[ASA^T\right]^{-1}[A]\left[SB_i^T B_i S\right]\left[A^T\right]\left[ASA^T\right]^{-1}[A]$$
$$-YB_i^T B_i S\left[A^T\right]\left[ASA^T\right]^{-1}[A] - Y\left[A^T\right]\left[ASA^T\right]^{-1}[A]SB_i^T B_i + Y\left[B_i^T B_i\right]$$
$$= \left[A^T\right]\left[ASA^T\right]^{-1}[A] + Y(WSBSW - BSW - WSB + B) = W + Y(WSBSW - BSW - WSB + B)$$

We have $Y > 0$. Therefore if diagonal elements of the matrix $\boldsymbol{WSBSW - BSW - WSB + B}$ are positive then we have: $W^+_{i1i1} > W_{i1i1}$ because $W^+_{i1i1} = W_{i1i1} + Y$x*Diagonal elements ii* of matrix $\boldsymbol{WSBSW - BSW - WSB + B}$.

If we assume that $\boldsymbol{S}$ & $\boldsymbol{S^+}$ are diagonal matrices, then *diagonal element 11* of matrix $\boldsymbol{WSBSW}$ is given by:

$$\begin{aligned}(WSBSW)_{11} = \sum_j (WSB)_{1j}(SW)_{j1} &= (W_{11}S_{11}B_{11} + W_{12}S_{22}B_{21} + \ldots + W_{1m}S_{mm}B_{m1})S_{11}W_{11} \\ &+ (W_{11}S_{11}B_{12} + W_{12}S_{22}B_{22} + \ldots + W_{1m}S_{mm}B_{m2})S_{22}W_{21} \\ &+ \ldots\ldots\ldots \\ &+ (W_{11}S_{11}B_{1m} + W_{12}S_{22}B_{2m} + \ldots + W_{1m}S_{mm}B_{mm})S_{mm}W_{m1}\end{aligned}$$

Because matrix $\boldsymbol{B}$ is a symmetric matrix whose elements $B_{ij} = B_{ji} = b_i b_j$, we have:

$$\begin{aligned}(WSBSW)_{11} &= (W_{11}S_{11}b_1 + W_{12}S_{22}b_2 + \ldots + W_{1m}S_{mm}b_m)b_1S_{11}W_{11} \\ &+ (W_{11}S_{11}b_1 + W_{12}S_{22}b_2 + \ldots + W_{1m}S_{mm}b_m)b_2S_{22}W_{21} \\ &+ \ldots\ldots\ldots \\ &+ (W_{11}S_{11}b_1 + W_{12}S_{22}b_2 + \ldots + W_{1m}S_{mm}b_m)b_mS_{mm}W_{m1} \\ &= (W_{11}S_{11}b_1 + W_{12}S_{22}b_2 + \ldots + W_{1m}S_{mm}b_m)(b_1S_{11}W_{11} + b_2S_{22}W_{21} + \ldots + b_mS_{mm}W_{m1})\end{aligned}$$

It can be easily verified that matrix $\boldsymbol{W}$ is symmetric (since $\boldsymbol{ASA^T}$ is symmetric, therefore $(\boldsymbol{ASA^T})^{-1}$ is also symmetric, thus $W = A^T(ASA^T)^{-1}A$ is a symmetric matrix), in other words: $W_{ij} = W_{ji}$

Therefore:

$$\begin{aligned}(WSBSW)_{11} &= (W_{11}S_{11}b_1 + W_{12}S_{22}b_2 + \ldots + W_{1m}S_{mm}b_m)(b_1S_{11}W_{11} + b_2S_{22}W_{21} + \ldots + b_mS_{mm}W_{m1}) \\ &= (W_{11}S_{11}b_1 + W_{12}S_{22}b_2 + \ldots + W_{1m}S_{mm}b_m)^2\end{aligned}$$

Diagonal element 11 of matrix $\boldsymbol{WSB}$ is given by:

$$(\boldsymbol{WSB})_{11} = \sum_j (\boldsymbol{WS})_{1j} \boldsymbol{B}_{j1} = W_{11}S_{11}B_{11} + W_{12}S_{22}B_{21} + ...W_{1m}S_{mm}B_{m1}$$
$$= (W_{11}S_{11}b_1b_1 + W_{12}S_{22}b_2b_1 + ...W_{1m}S_{mm}b_mb_1)$$
$$= b_1(W_{11}S_{11}b_1 + W_{12}S_{22}b_2 + ...W_{1m}S_{mm}b_m)$$

Diagonal element 11 of matrix ***BSW*** is given by:

$$(\boldsymbol{BSW})_{11} = \sum_j (\boldsymbol{B})_{1j}(\boldsymbol{SW})_{j1} = B_{11}S_{11}W_{11} + B_{12}S_{22}W_{21} + ...B_{1m}S_{mm}W_{m1}$$
$$= b_1b_1S_{11}W_{11} + b_1b_2S_{22}W_{21} + ...b_1b_mS_{mm}W_{m1}$$
$$= b_1(b_1S_{11}W_{11} + b_2S_{22}W_{21} + ...b_mS_{mm}W_{m1})$$
$$= b_1(W_{11}S_{11}b_1 + W_{12}S_{22}b_2 + ...W_{1m}S_{mm}b_m)$$

Diagonal elements B_{11} of matrix $\boldsymbol{B}$ is b_1^2

Therefore, the *diagonal element 11* of matrix $\boldsymbol{WSBSW} - \boldsymbol{BSW} - \boldsymbol{WSB} + \boldsymbol{B}$ is given by:

$$(W_{11}S_{11}b_1 + W_{12}S_{22}b_2 + ...W_{1m}S_{mm}b_m)^2 - b_1(W_{11}S_{11}b_1 + W_{12}S_{22}b_2 + ...W_{1m}S_{mm}b_m)$$
$$- b_1(W_{11}S_{11}b_1 + W_{12}S_{22}b_2 + ...W_{1m}S_{mm}b_m) + b_1^2$$
$$= (W_{11}S_{11}b_1 + W_{12}S_{22}b_2 + ...W_{1m}S_{mm}b_m)^2 - 2b_1(W_{11}S_{11}b_1 + W_{12}S_{22}b_2 + ...W_{1m}S_{mm}b_m) + b_1^2$$
$$= \left[(W_{11}S_{11}b_1 + W_{12}S_{22}b_2 + ...W_{1m}S_{mm}b_m) - b_1\right]^2 \geq 0$$

In general, the *diagonal element ii* of matrix $\boldsymbol{WSBSW} - \boldsymbol{BSW} - \boldsymbol{WSB} + \boldsymbol{B}$ is:

$$\left[(W_{i1}S_{11}b_1 + W_{i2}S_{22}b_2 + .. + W_{ii}S_{ii}b_i + ... + W_{im}S_{mm}b_m) - b_i\right]^2 \geq 0$$

And the updated W_{ii} is:

$$W_{ii}^+ = W_{ii} + Y\left[(W_{i1}S_{11}b_1 + W_{i2}S_{22}b_2 + .. + W_{ii}S_{ii}b_i + ... + W_{im}S_{mm}b_m) - b_i\right]^2 \geq W_{ii}$$

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