Quality-Relevant and Process-Relevant Fault Monitoring with Concurrent Projection to Latent Structures

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A new concurrent projection to latent structures for the monitoring of output-relevant faults that affect the quality and input-relevant process faults is proposed. The input and output data spaces are concurrently projected to five subspaces, a joint input–output subspace that captures covariations between input and output, an output-principal subspace, an output-residual subspace, an input-principal subspace, and an input-residual subspace. Fault detection indices are developed based on the concurrent projection to latent structures (CPLS) partition of subspaces for various fault detection alarms. The proposed CPLS monitoring method offers complete monitoring of faults that happen in the predictable output subspace and the unpredictable output-residual subspace, as well as faults that affect the input spaces and could be incipient for the output. Numerical simulation examples and the Tennessee Eastman challenge problem are used to illustrate the effectiveness of the proposed methods. *AIChE J*, 59: 496–504, 2013
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Introduction

Statistical process monitoring (SPM) based on process variables and quality variables has been developed and applied successfully to many industries over the last two decades. Kresta et al.[1,2] and Wise et al.[3,4] are among the first to apply multivariate statistical methods to process variables and quality variables, which has been studied intensively in multivariate statistical quality control (MSQC).[5] Typically data driven models from principal component analysis (PCA) or partial least squares (PLS) are built to derive process monitoring statistics. In the MSQC literature, however, the main focus is on the monitoring of quality variables, while SPM include process variables in the monitoring scheme to relate potential quality problems to root causes in process variables. Both SPM and MSQC use the same statistics for monitoring, such as the Q statistic and Hotelling's T^2 statistic, although the SPM literature extends the use of multivariate statistics to fault diagnosis[6–12] and reconstruction.[4,8,13] Wise and Gallagher[14] and Qin[15] give a review of the PCA- and PLS-based process monitoring and fault diagnosis methods based on process and quality data collected from normal operations.

Process control systems collect and store huge amount of data on process measurements and product quality measurements. The process variables are usually measured frequently and come with large quantities, whereas quality variables are measured at much lower rates and often come with a significant time delay. When the quality measurements are expensive or difficult to obtain, PCA has been used to monitor abnormal variations in process variables. The majority of process monitoring research and applications belongs to this category. However, when PCA is applied to decompose process data variations, no information from the output quality variables is incorporated. As a consequence, it cannot reveal whether or not a fault detected in process variables is relevant to output quality variables. In fact, feedback controllers are designed to attenuate or reject process disturbances in real time, to make good quality products. Whenever a fault monitoring system detects process faults that do not yield an impact on the product quality, the user of the fault detection system tends to discredit the fault detection system. Alarms like these are referred to as nuisance alarms, which should receive less attention than faults that affect the product quality. On the other hand, PLS has been used to build an input–output relation to infer the quality variables that are hard to measure from easy-to-measure process variables. The input–output PLS relation can be used to monitor the input subspace that is relevant to the output quality and thus give an early indication on whether the quality will be normal by monitoring the input subspaces.

The objective of PLS modeling is to extract the covariation in both process and quality variables and to model the relationship between them.[6,16] Recently, Li et al.[17] develop geometric properties of PLS that are relevant to process monitoring and compared the monitoring policies using different PLS structures. Further, the standard PLS structure has limitations in detecting output-relevant faults by monitoring the PLS scores and detecting output-irrelevant faults

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by monitoring the PLS input residuals. On the one hand, PLS scores that form the T^2 statistic contain variations orthogonal to the output that is irrelevant to the output. On the other hand, PLS does not extract variances in the input space in a descending order unlike PCA. Therefore, the input residuals can still contain large variations, making it inappropriate to be monitored by the Q statistic.

To resolve the above issues, Zhou et al.[18] propose a total PLS (T-PLS) algorithm to decompose the input space into four different subspaces to detect output-relevant faults and output-irrelevant faults. Four fault detection indices are developed to monitor these input subspaces. The T-PLS-based monitoring, however, suffers from two drawbacks. One is that the output-relevant monitoring index only monitors quality variations that are predictable from the process data. In many cases, PLS predicts the output poorly due to lack of excitation in the process data and the existence of large unmeasured process and quality disturbances. This leaves a large portion of the quality variations unpredictable from inputs and thus unmonitored by the T-PLS monitoring method. The other drawback is that the input data space is decomposed unnecessarily into four subspaces, when it can be concisely decomposed into output-relevant and input-relevant variations. In this article, we propose a concurrent PLS (CPLS) algorithm and a set of fault monitoring indices that provide complete monitoring of the output-relevant and input-relevant variations and a concise decomposition of the input space into output-relevant and input-relevant subspaces. Control limits on the fault detection indices are developed based on the results in statistical process monitoring. The CPLS model achieves three objectives: (1) from the standard PLS projection, the scores that are directly relevant to the predictable variations of the output are extracted, which forms the covariation subspace (CVS); (2) the unpredicted output variations are further projected to an output-principal subspace (OPS) and output-residual subspace (ORS) to monitor abnormal variations in these subspaces; and (3) the input variations irrelevant to predicting the output are further projected to an input-principal subspace (IPS) and input-residual subspace (IRS) to monitor abnormal variations in these subspaces.

The remaining part of this article is organized as follows. Fault detection based on PLS models is first reviewed in section "PLS for Process and Quality Monitoring." The CPLS algorithm and associated fault detection indices are developed in section "CPLS for Output-Relevant Input-Relevant Fault Detection." Control limits on the fault detection indices are derived based on multivariate statistics. In section "Synthetic Case Studies," the effectiveness of the proposed methods is illustrated with a few simulation cases. Section "Tennessee Eastman Process Case Studies" gives the application results to the Tennessee Eastman process monitoring problem with the CPLS-based monitoring and compared to PCA-based monitoring. Finally, conclusions are presented in the last section.

PLS for Process and Quality Monitoring

Collect normal process and quality data and form an input matrix $\mathrm{X} \in \mathbb{R}^{n \times m}$ consisting of n samples with m process variables, and an output matrix $\mathrm{Y} \in \mathbb{R}^{n \times p}$ with p quality variables, PLS scales, and projects $\mathbf{X}$ and $\mathbf{Y}$ to a low-dimensional space defined by a small number of latent variables ($\mathbf{t}_1, \ldots, \mathbf{t}_l$), where l is the number of PLS factors. The scaled and mean-centered $\mathbf{X}$ and $\mathbf{Y}$ are decomposed as follows

$$\begin{cases} \mathbf{X} = \sum_i^l \mathbf{t}_i \mathbf{p}_i^{\mathrm{T}} + \mathbf{E} = \mathbf{T}\mathbf{P}^{\mathrm{T}} + \mathbf{E} \\ \mathbf{Y} = \sum_i^l \mathbf{t}_i \mathbf{q}_i^{\mathrm{T}} + \mathbf{F} = \mathbf{T}\mathbf{Q}^{\mathrm{T}} + \mathbf{F} \end{cases} \tag{1}$$

where $\mathbf{T} = [\mathbf{t}_1, \ldots, \mathbf{t}_l]$ are the latent score vectors, $\mathbf{P} = [\mathbf{p}_1, \ldots, \mathbf{p}_l]$ and $\mathbf{Q} = [\mathbf{q}_1, \ldots, \mathbf{q}_l]$ the loadings for $\mathbf{X}$ and $\mathbf{Y}$, respectively. $\mathbf{E}$ and $\mathbf{F}$ are the PLS residuals corresponding to $\mathbf{X}$ and $\mathbf{Y}$. The number of latent factors l is usually determined by cross-validation that gives the maximum prediction power to the PLS model based on data that are excluded from training data. Detail of PLS algorithms can be found in Refs. 19 and 20. The latent vectors $\mathbf{t}_i$ are computed sequentially from the data so as to maximize the covariance between the deflated input data, $\mathbf{X}_i = \mathbf{X}_{i-1} - \mathbf{t}_{i-1}\mathbf{p}_{i-1}{}^{\mathrm{T}}$; $\mathbf{X}_1 = \mathbf{X}$, and output data $\mathbf{Y}$ for each factor. Weight vectors $\mathbf{w}_i$ are used to calculate the scores $\mathbf{t}_i = \mathbf{X}_i\mathbf{w}_i$.

To represent $\mathbf{t}_i$ in terms of the original data $\mathbf{X}$

$$\mathbf{T} = \mathbf{X}\mathbf{R} \tag{2}$$

where $\mathbf{R} = [\mathbf{r}_1, \ldots, \mathbf{r}_l]$, we have from[20]

$$\mathbf{r}_i = \prod_{j=1}^{i-1} (\mathbf{I}_m - w_j \mathbf{p}_j^{\mathrm{T}}) w_i \tag{3}$$

or $\mathbf{R} = \mathbf{W}(\mathbf{P}^{\mathrm{T}}\mathbf{W})^{-1}$. Matrices $\mathbf{R}$ and $\mathbf{P}$ have the following relation[21]

$$\mathbf{P}^{\mathrm{T}}\mathbf{R} = \mathbf{R}^{T}\mathbf{P} = \mathbf{I}_l \tag{4}$$

To perform process monitoring on a new data sample $\mathbf{x}$ and subsequently $\mathbf{y}$, the PLS model induces an oblique projection on input data space[17]

$$\mathbf{x} = \hat{\mathbf{x}} + \tilde{\mathbf{x}} \tag{5}$$

$$\hat{\mathbf{x}} = \mathbf{P}\mathbf{R}^{\mathrm{T}}\mathbf{x} \in \mathrm{Span}\{\mathbf{P}\} \tag{6}$$

$$\tilde{\mathbf{x}} = (\mathbf{I} - \mathbf{P}\mathbf{R}^{\mathrm{T}})\,\mathbf{x} \in \mathrm{Span}\{\mathbf{R}\}^{\perp} \tag{7}$$

The T^2 and Q statistics are monitored with the following calculations[6,15]

$$\mathbf{t} = \mathbf{R}^{\mathrm{T}}\mathbf{x} \tag{8}$$

$$T^2 = \mathbf{t}^{\mathrm{T}}\Lambda^{-1}\mathbf{t} \leq \frac{l(n^2-1)}{n(n-1)} F_{l,n-l,\alpha} \tag{9}$$

$$Q = \|\tilde{\mathbf{x}}\|^2 = \mathbf{x}^{\mathrm{T}}(\mathbf{I} - \mathbf{P}\mathbf{R}^{\mathrm{T}})\,\mathbf{x} \leq g\chi^2_{h,\alpha} \tag{10}$$

where α defines the confidence level as $(1-\alpha) \times 100\%$. $\Lambda = \frac{1}{n-1}\mathbf{T}^{\mathrm{T}}\mathbf{T}$. $F_{l,n-l}$ is F-distribution with l and $n-l$ degrees of freedom. $\chi_h{}^2$ is the χ^2-distribution with h degrees of freedom. The calculation of g and h is given in Ref. 6

PLS uses the above two indices defined on two subspaces to monitor processes. One is the principal subspace to be monitored by T^2, which is thought to reflect major variations related to $\mathbf{Y}$. The other is the residual subspace to be monitored by Q, which is thought to contain variations unrelated to the output $\mathbf{Y}$. However, the principal subspace projection $\hat{\mathrm{x}}_k$ often contains many factors that include variations orthogonal to $\mathbf{Y}$.

Zhou et al.[18] point out that variations in the PLS principal subspace that are orthogonal to the output are not useful for the monitoring of output-relevant faults. Another issue is that the PLS residual subspace is not necessarily a subspace with minimal variations. Because the PLS objective is to maximize the covariance between **X** and **Y,** it does not extract input variations in a descending order. A later factor can capture more variance in **X** than a preceding factor. Therefore, the residual subspace can contain large variations that are not useful to predict **Y,** and thus it is not appropriate to be monitored using Q. Zhou et al.[18] decompose the residual subspace further with a total projection to latent structures (T-PLS) to resolve these problems.

The T-PLS-based monitoring of Zhou et al.,[18] however, suffers from two severe drawbacks. One is that it only monitors abnormal quality variations that are predictable from the process data. In many cases, the PLS predicted R^2 values are not high. This will leave a large portion of the quality variations unmonitored. The other drawback is that the process data space is decomposed into unnecessarily four subspaces, when it can be concisely decomposed into output-relevant variations and input-relevant variations. In the next section, we propose a CPLS algorithm and related monitoring indices that provide complete monitoring of the output variations and a concise decomposition of the input data space into output-relevant and input-relevant subspaces.

CPLS for Output-Relevant Input-Relevant Fault Detection

Concurrent projection to latent structures

The PLS algorithm extracts the scores **T** to maximize the covariance between **X** and **Y** as shown in Eq. 1. The scores **T** contain variations related to the output **Y** but also contain variations orthogonal to **Y,** which is why orthogonal PLS methods are developed.[22,23] Second, the scores **T** relate only to the predictable portion of **Y**. Therefore, monitoring **T** alone ignores the variations in **Y** that are unpredicted by **X** in the PLS model. To provide a complete monitoring scheme of the quality data and process operation data, a CPLS model is proposed to achieve three objectives: (1) from the standard PLS projection the scores that are directly relevant to the predictable variations of the output are extracted, which forms the CVS; (2) the unpredicted output variations are further projected to an OPS and ORS to monitor abnormal variations in these subspaces; and (3) the input variations irrelevant to predicting the output are further projected to an IPS and IRS to monitor abnormal variations in these subspaces. The CPLS algorithm for multiple input and multiple output data is given as follows.

1. Scale the raw data to zero mean and unit variance to give **X** and **Y.** Perform PLS on **X** and **Y** using Eq. 1 to give **T, Q,** and **R.** The number of PLS factors l is determined by cross-validation.

2. Form the "*predictable output*" $\hat{\mathbf{Y}} = \mathbf{T}\mathbf{Q}^T$ and perform singular value decomposition (SVD)

$$\hat{\mathbf{Y}} = \mathbf{U}_c\mathbf{D}_c\mathbf{V}_c^T \equiv \mathbf{U}_c\mathbf{Q}_c^T \tag{11}$$

where $\mathbf{Q}_c = \mathbf{V}_c\mathbf{D}_c$ includes all l_c nonzero singular values in descending order and the corresponding right singular vectors. As $\mathbf{V}_c$ is orthonormal,

$$\mathbf{U}_c = \hat{\mathbf{Y}}\mathbf{V}_c\mathbf{D}_c^{-1} = \mathbf{X}\mathbf{R}\mathbf{Q}^T\mathbf{V}_c\mathbf{D}_c^{-1} \equiv \mathbf{X}\mathbf{R}_c \tag{12}$$

where $\mathbf{R}_c = \mathbf{R}\mathbf{Q}^{\mathrm{T}}\mathbf{V}_c\mathbf{D}_c^{-1}$.

3. Form the unpredictable output $\tilde{\mathbf{Y}}_c = \mathbf{Y} - \mathbf{U}_c\mathbf{Q}_c^{\mathrm{T}}$ and perform PCA with l_y principal components

$$\tilde{\mathbf{Y}}_c = \mathbf{T}_y\mathbf{P}_y^{\mathrm{T}} + \tilde{\mathbf{Y}} \tag{13}$$

to yield the output-principal scores $\mathbf{T}_y$ and output residuals $\tilde{Y}$.

4. Form the output-irrelevant input by projecting on the orthogonal complement of $\mathrm{Span}\{\mathbf{R}_c\}$, $\tilde{\mathbf{X}}_c = \mathbf{X} - \mathbf{U}_c\mathbf{R}_c^{\dagger}$, *where* $\mathbf{R}_c^{\dagger} = (\mathbf{R}_c^{\mathrm{T}}\mathbf{R}_c)^{-1}\mathbf{R}_c^{\mathrm{T}}$, and perform PCA with l_x principal components

$$\tilde{\mathbf{X}}_c = \mathbf{T}_x\mathbf{P}_x^{\mathrm{T}} + \tilde{\mathbf{X}} \tag{14}$$

to yield the input-principal scores $\mathbf{T}_x$ and input residuals $\tilde{\mathbf{X}}$.

Based on the CPLS algorithm the data matrices **X** and **Y** are decomposed as follows

$$\mathbf{X} = \mathbf{U}_c\mathbf{R}_c^{\dagger} + \mathbf{T}_x\mathbf{P}_x^{\mathrm{T}} + \tilde{\mathbf{X}} \tag{15}$$

$$\mathbf{Y} = \mathbf{U}_c\mathbf{Q}_c^{\mathrm{T}} + \mathbf{T}_y\mathbf{P}_y^{\mathrm{T}} + \tilde{\mathbf{Y}} \tag{16}$$

The CPLS model is characterized by the loadings $\mathbf{R}_c \in \mathbb{R}^{m\times l_c}, \mathbf{P}_x \in \mathbb{R}^{m\times l_x}, \mathbf{Q}_c \in \mathbb{R}^{p\times l_c}, \mathbf{P}_y \in \mathbb{R}^{p\times l_y}$. The scores $\mathbf{U}_c$ represent covariations in **X** that are related to the predictable part $\hat{\mathbf{Y}}$, $\mathbf{T}_x$ represents the variations in **X** that are useless for predicting **Y**, and $\mathbf{T}_y$ represents the variations in **Y** unpredicted by **X**. Let $\mathbf{u}_c^{\mathrm{T}}, \mathbf{x}^{\mathrm{T}}, \mathbf{t}_x^{\mathrm{T}}, \tilde{\mathbf{x}}_c^{\mathrm{T}}, \tilde{\mathbf{x}}^{\mathrm{T}}, \mathbf{y}^{\mathrm{T}}, \mathbf{t}_y^{\mathrm{T}}, \tilde{y}_c^{\mathrm{T}}$, and $\tilde{y}^{\mathrm{T}}$ denote a specific row of $\mathbf{U}_c$, **X**, $\mathbf{T}_x$, $\tilde{\mathbf{X}}_c$, $\tilde{\mathbf{X}}$, **Y**, $\mathbf{T}_y$, $\tilde{\mathbf{Y}}_c$, and $\tilde{\mathbf{Y}}$, respectively. The CPLS model can be written in terms of a single sample as follows

$$\mathbf{x} = \mathbf{R}_c^{\dagger\mathrm{T}}\mathbf{u}_c + \mathbf{P}_x\mathbf{t}_x + \tilde{\mathbf{x}} \tag{17}$$

$$\mathbf{y} = \mathbf{Q}_c\mathbf{u}_c + \mathbf{P}_y\mathbf{t}_y + \tilde{\mathbf{y}} \tag{18}$$

or

$$\tilde{\mathbf{x}}_c = \mathbf{x} - \mathbf{R}_c^{\dagger\mathrm{T}}\mathbf{u}_c = \mathbf{P}_x\mathbf{t}_x + \tilde{\mathbf{x}} \tag{19}$$

$$\tilde{\mathbf{y}}_c = \mathbf{y} - \mathbf{Q}_c\mathbf{u}_c = \mathbf{P}_y\mathbf{t}_y + \tilde{\mathbf{y}} \tag{20}$$

where

$$\mathbf{u}_c = \mathbf{R}_c^{\mathrm{T}}\mathbf{x} \tag{21}$$

$$\mathbf{t}_x = \mathbf{P}_x^{\mathrm{T}}\tilde{\mathbf{x}}_c \tag{22}$$

$$\mathbf{t}_y = \mathbf{P}_y^{\mathrm{T}}\tilde{\mathbf{y}}_c \tag{23}$$

and

$$\tilde{\mathbf{x}} = (\mathbf{I} - \mathbf{P}_x\mathbf{P}_x^{\mathrm{T}})\,\tilde{\mathbf{x}}_c \tag{24}$$

$$\tilde{\mathbf{y}} = (\mathbf{I} - \mathbf{P}_y\mathbf{P}_y^{\mathrm{T}})\,\tilde{\mathbf{y}}_c \tag{25}$$

Equations 21–25 give all the principal and residual variations that are either output relevant or input relevant.

CPLS-based fault monitoring

From the CPLS model given in the previous subsection, it is straightforward to design fault monitoring indices. It is clear that all the output and input variations are defined in Eqs. 21–25. The output-relevant scores in Eq. 21 can be calculated from the input data alone, and, thus, it can be monitored before the output data are obtained. The input-relevant variations and residuals are captured in Eqs. 22 and 24, respectively, which should be monitoring for abnormal process conditions. Although these variations may not have impact on the output variables, it is undesirable to leave these variations unmonitored as they may lead to subsequent performance loss in the process operation. These variations can be monitored, as soon as the input data are obtained. Furthermore, the unpredicted output variations and residuals in Eqs. 23 and 25 must also be monitored, which is an essential task of multivariate quality monitoring.[5,24]

The output-relevant scores (12) are orthonormalized and hence each element of $\mathbf{u}_c$ is zero mean with variance $\frac{1}{n-1}$. Therefore, it can be monitored with the following T^2 statistic

$$T_c^2 = (n-1)\,\mathbf{u}_c^{\mathrm{T}}\mathbf{u}_c = (n-1)\,\mathbf{x}^{\mathrm{T}}\mathbf{R}_c\mathbf{R}_c^{\mathrm{T}}\mathbf{x} \tag{26}$$

The input-relevant scores (22) and residuals (24) can be monitored by the following T^2 statistic and Q-statistic,[1,5] respectively

$$T_x^2 = \mathbf{t}_x^{\mathrm{T}}\Lambda_x^{-1}\mathbf{t}_x = \tilde{\mathbf{x}}_c^{\mathrm{T}}\mathbf{P}_x\Lambda_x^{-1}\mathbf{P}_x^{\mathrm{T}}\tilde{\mathbf{x}}_c \tag{27}$$

$$Q_x = \|\tilde{\mathbf{x}}\|^2 = \tilde{\mathbf{x}}_c^{\mathrm{T}}(\mathbf{I} - \mathbf{P}_x\mathbf{P}_x^{\mathrm{T}})\,\tilde{\mathbf{x}}_c \tag{28}$$

where $(\mathbf{I}-\mathbf{P}_x\mathbf{P}_x^T)^2 = \mathbf{I}-\mathbf{P}_x\mathbf{P}_x^T$ is used and $\Lambda_x = \frac{1}{n-1}\mathbf{T}_x^T\mathbf{T}_x = \mathrm{diag}\{\lambda_{x,1}, \lambda_{x,2}, \cdots, \lambda_{x,l_x}\}$ are the variances of the principal components.

The unpredicted output scores (23) and residuals (25) can be monitored by the following T^2 statistic and Q-statistic, respectively

$$T_y^2 = \mathbf{t}_y^{\mathrm{T}}\Lambda_y^{-1}\mathbf{t}_y = \tilde{\mathbf{y}}_c^{\mathrm{T}}\mathbf{P}_y\Lambda_y^{-1}\mathbf{P}_y^{\mathrm{T}}\tilde{\mathbf{y}}_c \tag{29}$$

$$Q_y = \|\tilde{\mathbf{y}}\|^2 = \tilde{\mathbf{y}}_c^{\mathrm{T}}(\mathbf{I} - \mathbf{P}_y\mathbf{P}_y^{\mathrm{T}})\,\tilde{\mathbf{y}}_c \tag{30}$$

where $\Lambda_y = \frac{1}{n-1}\mathbf{T}_y^{\mathrm{T}}\mathbf{T}_y = \mathrm{diag}\{\lambda_{y,1,\lambda_{y,2},\cdots,\lambda_{y,l_y}}\}$ are the variances of the principal components.

To perform monitoring based on the above indices, control limits should be calculated from the statistics of the normal data. As the covariation, input-relevant, and output-relevant scores are all orthogonal due to the use of SVD, the control limits can be calculated the same way as those used in PCA-based monitoring[15] or in Eqs. 9 and 10. If n is large enough, the T^2 and Q indices approximately follow χ^2 distributions.[25] The monitoring procedure should check the covariation scores first, which is summarized as follows.

1. If $T_c^2 > \tau_{c,\alpha}^2 = \chi_{l_c,\alpha}^2$, an output-relevant fault is detected with $(1 - \alpha)$ confidence based on the new input measurement **x.**
2. If $Q_x > \delta_{x,\alpha}^2 = g_x\chi_{hx,\alpha}^2$, a potentially output-relevant fault is detected with $(1 - \alpha)$ confidence based on the new input measurement **x**.
3. If $T_x^2 > \tau_{x,\alpha}^2 = \chi_{l_x,\alpha}^2$, an output-irrelevant but input-relevant fault is detected with $(1 - \alpha)$ confidence based on the new input measurement **x.**
4. When the output measurement **y** is available, If $T_y^2 > \tau_{y,\alpha}^2 = \chi_{l_y,\alpha}^2$ and/or $Q_y > \delta_{y,\alpha}^2 = g_y\chi_{h_y,\alpha}^2$, an output-relevant fault unpredictable from the input is detected with $(1 - \alpha)$ confidence.

The values for g_x, h_x, g_y, and h_y are derived in Appendix A.

Alternatively to Step (4), a combined index can be used to monitor the quality output faults unpredicted from the input, which combines Q_y and T_y^2 as follows

$$\varphi_y = \frac{Q_y}{\delta_{y,\alpha}^2} + \frac{T_y^2}{\tau_{y,\alpha}^2} = \tilde{\mathbf{y}}_c^{\mathrm{T}}\Phi_y\tilde{\mathbf{y}}_c \tag{31}$$

where

$$\Phi_y = \frac{\mathbf{P}_y\Lambda_y^{-1}\mathbf{P}_y^{\mathrm{T}}}{\tau_{y,\alpha}^2} + \frac{\mathbf{I} - \mathbf{P}_y\mathbf{P}_y^{\mathrm{T}}}{\delta_{y,\alpha}^2} \tag{32}$$

Using the approximate distribution in Ref. 25 to calculate the control limit of the combined index with a confidence level γ, an output-relevant fault unpredicted from input is detected by φ_y if

$$\varphi_y > \zeta_\varphi^2 = g_\varphi\chi_{h\varphi,\gamma}^2 \tag{33}$$

where

$$g_\varphi = \frac{tr(S_y\Phi_y)^2}{tr(S_y\Phi_y)} \tag{34}$$

$$h_\varphi = \frac{[tr(S_y\Phi_y)]^2}{tr(S_y\Phi_y)^2} \tag{35}$$

and $\mathbf{S}_y = \frac{1}{n-1}\tilde{\mathbf{Y}}_c^{\mathrm{T}}\tilde{\mathbf{Y}}_c$ is the sample covariance of $\tilde{\mathbf{y}}_c$.

In summary, the CPLS-based process monitoring performs quality-relevant monitoring using the T_c^2 index that is output relevant and the Q_x index that is potentially output relevant, as soon as the input data are measured. It also monitors the unpredictable part of the quality variation using the φ_y index after the output data are available. In addition, the input-relevant T_x^2 index that is monitored as soon as the input data are measured. Alarms from this index are output irrelevant and should receive less attention than those output-relevant alarms.

When PCA is used for process monitoring, all relevant process variables should be included to detect process faults. On the other hand, when PLS is used for quality prediction (or inferential sensor), only output-relevant process variables should be included (i.e., including irrelevant process variables tends decrease model quality). It appears that using CPLS for monitoring is in between PCA and PLS in terms of variable selection. One should include all relevant process variables for process monitoring and for quality monitoring in the CPLS model. Variables or subspaces that show irrelevance to the output will be separated from those that are and monitored with a different index, T_x^2.

Synthetic Case Studies

In this section, we use synthetic simulations to create a number of representing fault scenarios to demonstrate the effectiveness of CPLS in terms of detecting quality-relevant and input-relevant faults. The advantages of the CPLS-based monitoring over other existing methods are pointed out using the simulation cases.

Table 1. PLS Matrices, l = 4

R				P				Q^T	
0.4807	−0.2526	0.0805	0.7374	0.4784	−0.3020	−0.0474	0.7211	0.5322	0.5263
0.4190	0.5147	−0.0461	−0.3894	0.4180	0.5430	0.0949	−0.4554	0.1291	−0.1193
0.4579	0.5003	−0.4788	0.1700	0.4637	0.4265	−0.4580	0.2273	0.0985	0.4687
0.5251	−0.2289	0.7303	−0.1813	0.5134	−0.1108	0.7074	−0.2393	0.0935	0.0206
0.3286	−0.6072	−0.5007	−0.5113	0.3438	−0.6679	−0.5439	−0.4085		

The simulated numerical example without faults is as follows.[18]

$$\begin{cases} \mathbf{x}_k = \mathbf{A}\mathbf{z}_k + \mathbf{e}_k \\ \mathbf{y}_k = \mathbf{C}\mathbf{x}_k + \mathbf{v}_k \end{cases} \tag{36}$$

where $\mathbf{z_k} \in \mathbb{R}^3 \sim \mathbf{U}([\mathbf{0},\mathbf{1}]), \mathbf{A} = \begin{bmatrix} 1 & 3 & 4 & 4 & 0 \\ 3 & 0 & 1 & 4 & 1 \\ 1 & 1 & 3 & 0 & 0 \end{bmatrix}^T$,

$\mathbf{C} = \begin{bmatrix} \mathbf{2} & \mathbf{2} & \mathbf{1} & \mathbf{1} & \mathbf{0} \\ \mathbf{3} & \mathbf{1} & \mathbf{0} & \mathbf{4} & \mathbf{0} \end{bmatrix}, \mathbf{e_k} \in \mathbb{R}^5 \sim \mathbf{N}(\mathbf{0}, \mathbf{0.2^2}), \mathbf{v_k} \in \mathrm{x}_\mathbf{k}^*$ and $\mathbb{R}^2 \sim N(0, 0.1^2)$. $\mathbf{U}([0, 1])$ means the uniform distribution in the interval [0,1].

We use 100 samples under normal conditions to derive a PLS model on (**X, Y**). The PLS factors number l = 4 is determined by 10-fold cross-validation. The PLS matrices are listed in Table 1.

A fault is added in the following form in the input space

$$\mathbf{x}_k = \mathbf{x}_k^* + \Xi_x f_x \tag{37}$$

or in the output space

$$\mathbf{y}_k = \mathbf{y}_k^* + \Xi_y f_y \tag{38}$$

where Ξ_x and Ξ_y are the fault-free values, T_c^2, T_y^2, T_x^2 are the orthonormal fault direction matrices or vectors, and f_x and f_y are the respective fault magnitudes.

Fault scenarios, with 100 faulty samples each produced by Eq. 37 or 38, are used to perform the fault detection under various faulty cases. In the figures presented later in this section, the first 100 samples are normal samples, and the last 100 samples are faulty samples for each scenario. From the CPLS training results, we end up with p = 2 and l_y = 2, so that Q_y is null. Therefore, four indices T_c^2, T_y^2, T_x^2 and Q_x are shown in the following results.

Fault occurs in CVS only

To generate a fault that happens in the covariation space only, we choose Ξ_x to be the first column of $\mathbf{R}_c$ and normalize it to unit norm, thus the fault occurs in CVS only. The fault detection indices are shown in Figure 1. The result indicates that only $T_c{}^2$ detects the fault, whereas other fault detection indices are not affected by the fault. This result implies that the fault detected in the input space by T_c^2 is output-relevant fault. As shown in Figure 2, this fault does affect both outputs.

Fault occurs in IPS only

Let Ξ_x be the first column of $\mathbf{P}_x$, and thus the fault occurs in IPS only. The fault detection indices are shown in Figure 3. As shown in Figure 4, this fault does not affect either output y. The result indicates that T_x^2 detects the input-relevant fault, but it is not output relevant. A PCA-based monitoring method that monitors variability in the input space would signal this fault as an alarm, but it is not be able to indicate that this fault is irrelevant to the output.

Fault occurs in OPS only

Let Ξ_y be the first column of $\mathbf{P}_y$, thus the fault occurs in OPS only. To see if this fault will affect the output quality, we calculate the fault detection indices as shown in Figure 5.

The result indicates that, although the fault happens only in the residual space of the input data, T_y^2 detects the fault as output relevant that is unpredictable from the input.

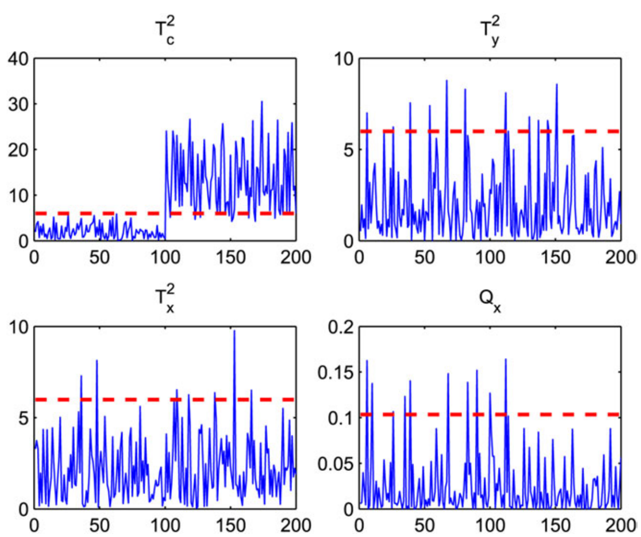

Figure 1. Fault detection indices when fault occurs in CVS only, f_x = 4.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

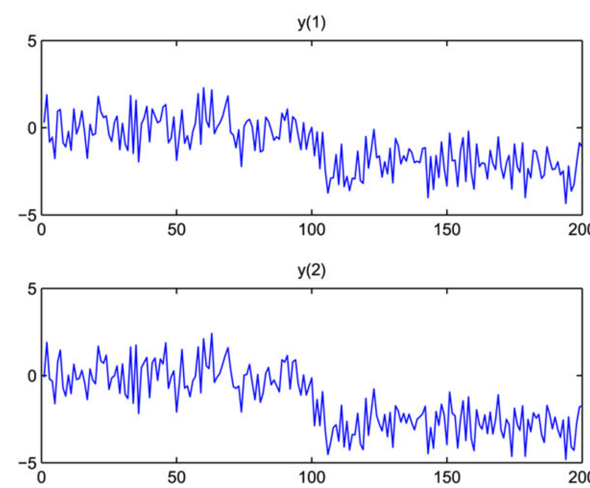

Figure 2. When a fault occurs in CVS only, both outputs are affected.

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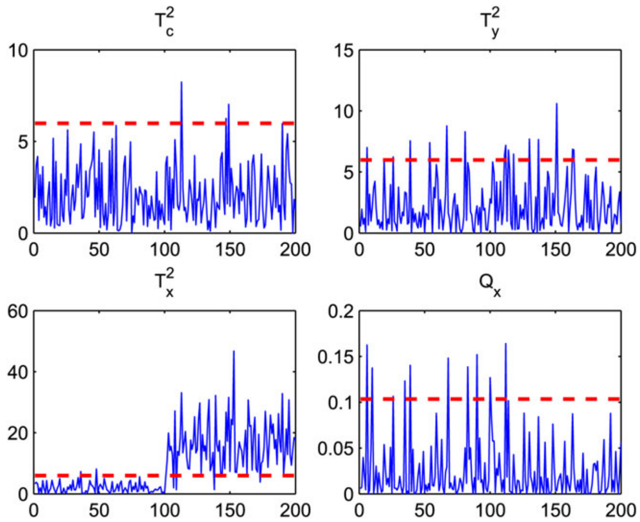

Figure 3. Fault detection indices when fault occurs in IPS only, f_x = 4.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

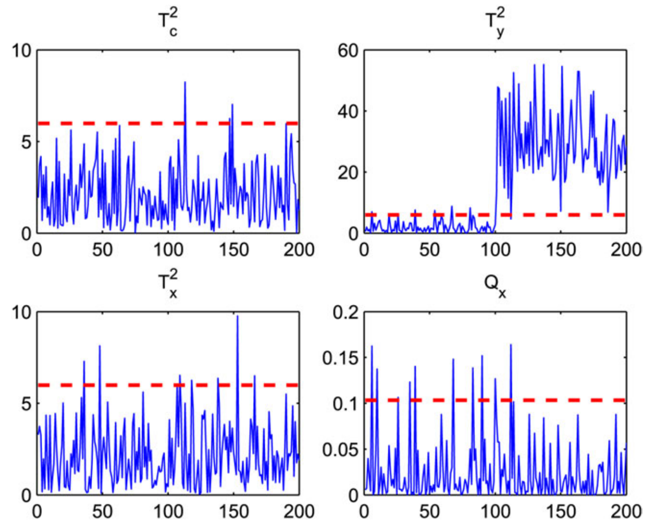

Figure 5. Fault occurs in OPS only, f_y = 0.1.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Fault occurs in IRS only

From Eqs. 19, 21, and 24, it can be shown that

$$\tilde{\mathbf{x}} = \left(\mathbf{I} - \mathbf{P}_x\mathbf{P}_x^{\mathrm{T}}\right)\left(\mathbf{I} - \mathbf{R}_c\mathbf{R}_c^{\dagger}\right)\mathbf{x} \tag{39}$$

Therefore, the basis vectors of IRS would be the left singular vectors of $(\mathbf{I} - \mathbf{P}_x\mathbf{P}_x^{\mathrm{T}})(\mathbf{I} - \mathbf{R}_c\mathbf{R}_c^{\dagger})$ related to nonzero singular values.

Let Ξ_x be a basis vector of IRS, so that the fault occurs in IRS only. The fault detection indices are shown in Figure 6. The result in Q_x successfully detects the fault in the input-residual subspace, and subsequently T_y^2 indicates that the fault is output relevant. This is that case where the normally unexcited input-residual space can contain output-relevant faults.

Tennessee Eastman Process Case Studies

The Tennessee Eastman Process[26] is used to evaluate the effectiveness of the proposed CPLS method. The whole process is composed of five unit operations, including a chemical reactor, condenser, compressor, vapor/liquid separator, and stripper. The process has four reactants A, C, D, and E and an inert B, and the process produces two products G and H along with a byproduct F. The detailed description of the Tennessee Eastman Process can be found in Downs and Vogel.[26] The control strategy applied to the process is described in Lyman and Georgakis.[27] The simulation data were downloaded from Professor Richard D. Braatz's website.

Both CPLS-based monitoring and PCA-based monitoring are performed. For CPLS, the input variables are XMEAS(1–36) and XMV(1–11), where XMEAS(1–36) are the process measurements, and XMV(1–11) are the manipulated variables; the output variables are XMEAS(37–41), where XMEAS(37–41) are the quality measurements. For PCA, the variables are XMEAS(1–36) and XMV(1–11). (The XMEAS and XMV notations are from Downs and Vogel.[26])

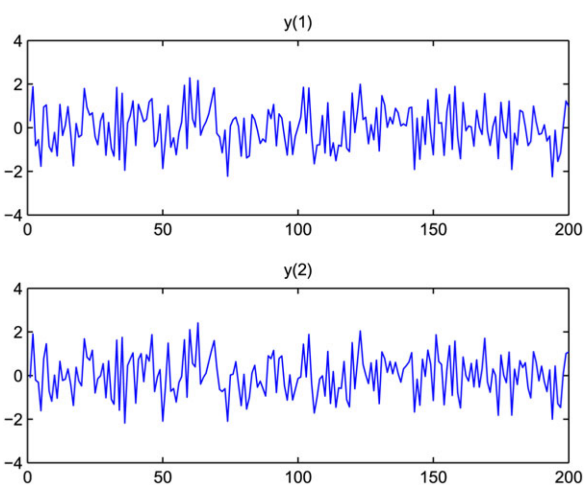

Figure 4. When fault occurs in IPS only, *y* is not affected.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

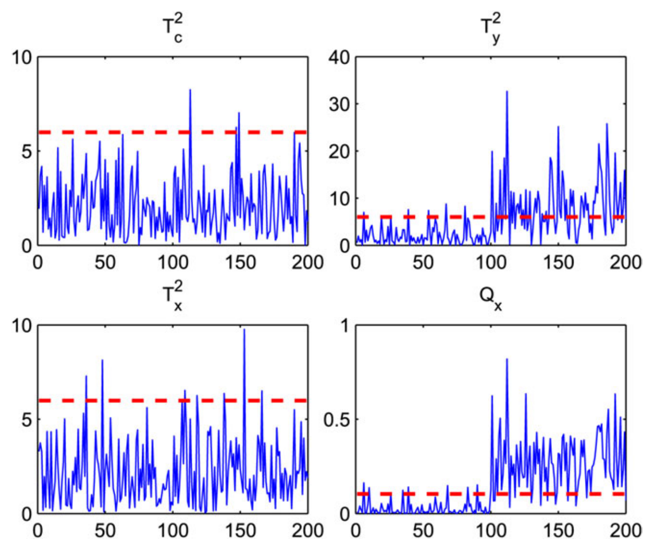

Figure 6. Fault occurs in IRS only, f_x = 0.5.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

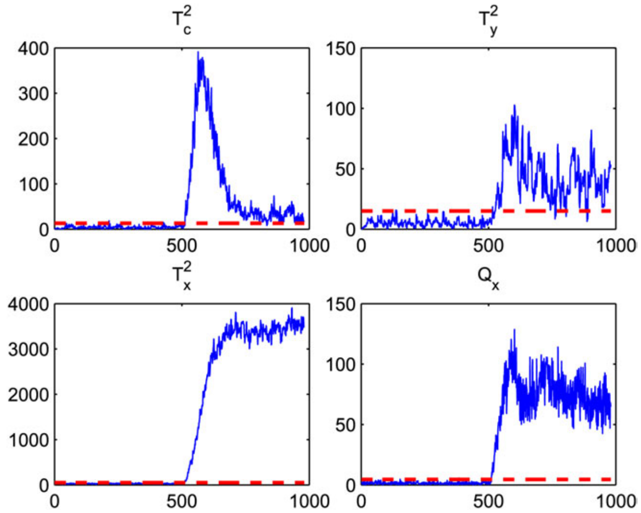

Figure 7. CPLS-based monitoring result for a step change in B composition.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

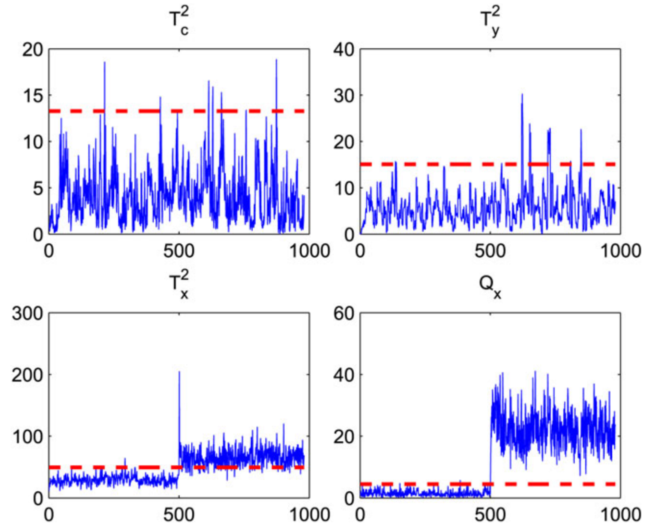

Figure 9. CPLS-based monitoring result for a step change in reactor cooling water inlet temperature.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

In the figures presented in this section, the first 500 samples are normal data, and the last 480 samples are faulty data. The PLS factor $l = 4$ is determined by 10-fold cross-validation. From the CPLS training, we have $p = 5$ and $l_y = 5$, thus Q_y is null that does not need to be monitored. A 99% control limit is used for both CPLS and PCA. Three faulty scenarios are reported as follows.

Scenario 1: Step disturbance in B composition

This faulty case is IDV(2) in Downs and Vogel.[26] A step change occurs in the B composition of the stripper inlet stream. The process monitoring results for CPLS and PCA methods are shown in Figures 7 and 8, respectively. All the four indices in the CPLS method and the two indices in PCA method successfully detect the fault. For CPLS, T_c^2 reduces toward normal values after the step change occurs, while the input-relevant variability index T_x^2 remains at a high value. This indicates that quality variables tend to return to normal, because the feedback controllers in the process are working to reduce the effect of the fault. In the PCA monitoring results, the effect of the feedback on quality changes cannot be observed. Therefore, CPLS is better than PCA in that it successfully detects the quality changes.

Scenario 2: Step disturbance in reactor cooling water inlet temperature

The faulty case is IDV(4) in Downs and Vogel.[26] A step change occurs in reactor cooling water inlet temperature. The process monitoring results for CPLS and PCA methods are shown in Figures 9 and 10, respectively.

Because the reactor temperature is controlled through a cascade controller, this disturbance does not affect the product quality. For CPLS, T_c^2 shows that the fault is quality

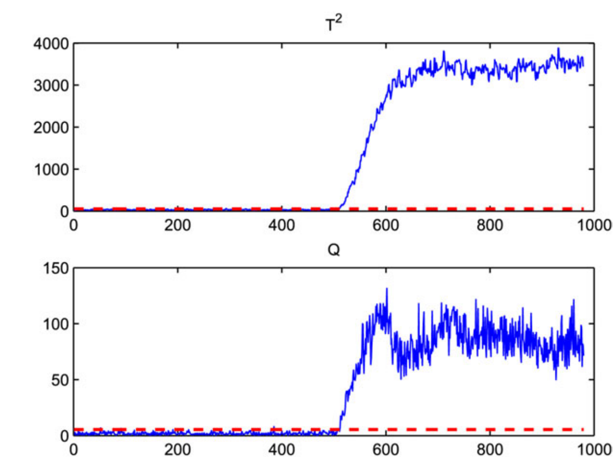

Figure 8. PCA-based monitoring result for a step change in B composition.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

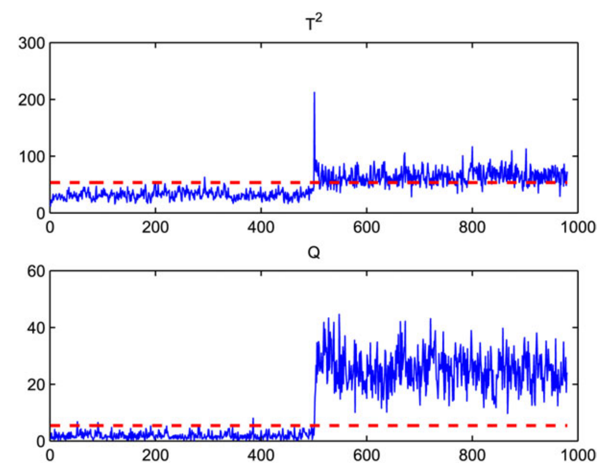

Figure 10. PCA-based monitoring result for a step change in reactor cooling water inlet temperature.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

irrelevant, T_x^2 and Q_x detect the fault in the IPS and IRS. The fault detection rates of them are 96.46% and 100%, respectively. For PCA, both T^2 and Q detect the fault. However, PCA-based monitoring cannot indicate that this disturbance is quality-irreverent. Existing work in the literature that reports high detection rates for this fault at best gives nuisance alarms. In this example, CPLS shows its superior performance over PCA in filtering out the quality-irrelevant fault.

Scenario 3: Step disturbance in condenser cooling water inlet temperature

The faulty case is IDV(5) in Downs and Vogel.[26] A step change occurs in condenser cooling water inlet temperature. The process monitoring results for CPLS and PCA methods are shown in Figures 11 and 12, respectively. It could be seen that CPLS detects the fault in all the four subspaces. The results of CPLS and PCA show similar patterns that the process tends to return to normal after Sample 700.

Conclusions

In this article, we propose a new CPLS algorithm for the monitoring of output-relevant faults and input-relevant faults. The input and output data are concurrently projected to five subspaces. Process fault detection indices are developed based on the five subspaces for various types of fault detection alarms. This method gives a complete monitoring of faults that happen in the predictable output subspace and the unpredictable output-residual subspace, as well as faults that affect the input spaces and could be incipient for the output. In the numerical simulation examples, four different fault scenarios are simulated to demonstrate that proposed methods correctly and effectively detect the various faulty cases. The application results to the Tennessee Eastman process monitoring problem show that the CPLS-based monitoring effectively detects faults that are output relevant and faults that output irrelevant, thus avoiding nuisance alarms due to disturbances that are effectively attenuated by the feedback controllers. A future

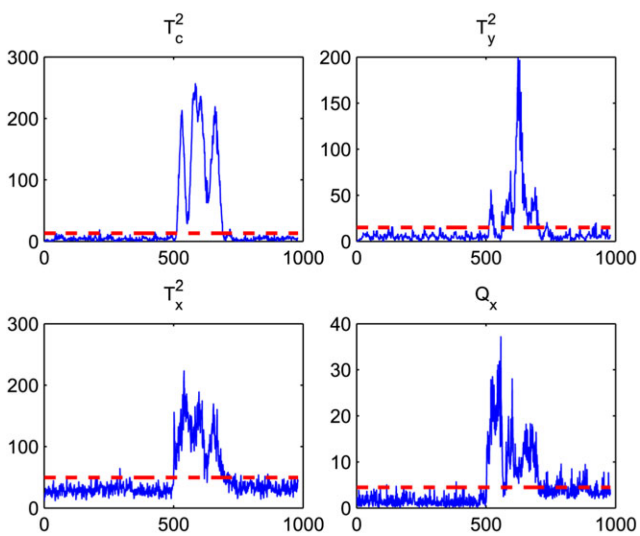

Figure 11. CPLS-based monitoring result for a step change in condenser cooling water inlet temperature.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

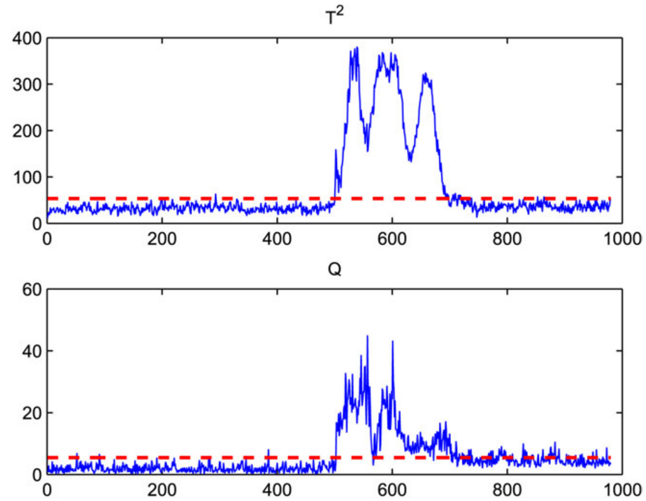

Figure 12. PCA-based monitoring result for a step change in condenser cooling water inlet temperature.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

step is to develop related fault diagnosis and identification methods for the CPLS monitoring framework.

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Appendix A: Calculations of g_x, h_x, g_y, and h_y

The Box's theorem[25] is used to calculate g_y and h_y similar to Eqs. 34 and 35 for Eq. 30. As

$$\begin{aligned}\mathrm{tr}\left[\mathbf{S}_y\left(\mathbf{I}-\mathbf{P}_y\mathbf{P}_y^{\mathrm{T}}\right)\right] &= \mathrm{tr}\left(\mathbf{S}_y\right)-\mathrm{tr}\left(\mathbf{S}_y\mathbf{P}_y\mathbf{P}_y^{T}\right)\\ &= \mathrm{tr}\left(\mathbf{S}_y\right)-\mathrm{tr}\left(\mathbf{P}_y^{\mathrm{T}}\mathbf{S}_y\mathbf{P}_y\right)\\ &= \frac{1}{n-1}\mathrm{tr}\left(\tilde{\mathbf{Y}}_C^{\mathrm{T}}\tilde{\mathbf{Y}}_C\right)-\frac{1}{n-1}\mathrm{tr}\left(\mathbf{T}_y^{\mathrm{T}}\mathbf{T}_y\right)\\ &= \sum_{i=l}^{p}\lambda_{y,i}-\sum_{i=l}^{ly}\lambda_{y,i}\\ &= \sum_{i=l_y+1}^{p}\lambda_{y,i}\end{aligned}$$

and similarly, $\mathrm{tr}\left[\mathbf{S}_y(\mathbf{I}-\mathbf{P}_y\mathbf{P}_y^{\mathrm{T}})\right]^2=\sum_{i=1_y+1}^{p}\lambda_{y,i}^2$, we have

$$g_y\frac{\mathrm{tr}\left[\mathrm{S}_y\left(\mathbf{I}-\mathbf{P}_y\mathbf{P}_y^{\mathrm{T}}\right)\right]^2}{\mathrm{tr}\left[\mathrm{S}_y\left(\mathbf{I}-\mathbf{P}_y\mathbf{P}_y^{\mathrm{T}}\right)\right]}=\frac{\sum_{i=l_y+1}^{p}\lambda_{y,i}^2}{\sum_{i=l_y+1}^{p}\lambda_{y,i}}$$

$$h_y\frac{\left[\mathrm{trS}_y\left(\mathbf{I}-\mathbf{P}_y\mathbf{P}_y^{\mathrm{T}}\right)\right]^2}{\mathrm{tr}\left[\mathrm{S}_y\left(\mathbf{I}-\mathbf{P}_y\mathbf{P}_y^{\mathrm{T}}\right)\right]^2}=\frac{\left[\sum_{i=l_y+1}^{p}\lambda_{y,i}\right]^2}{\sum_{i=l_y+1}^{p}\lambda_{y,i}^2}$$

By analogy,

$$g_x=\frac{\sum_{i=l_x+1}^{m}\lambda_{x,i}^2}{\sum_{i=l_x+1}^{m}\lambda_{x,i}}$$

$$h_x=\frac{\left[\sum_{i=l_x+1}^{m}\lambda_{x,i}\right]^2}{\sum_{i=l_x+1}^{m}\lambda_{x,i}^2}$$

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