Total PLS Based Contribution Plots for Fault Diagnosis

LI Gang[1] QIN Si-Zhao[2] JI Yin-Dong[3] ZHOU Dong-Hua[1]

Abstract Multivariate statistical process monitoring (MSPM) is an efficient data-driven fault detection and diagnosis approach for complex industrial processes. Partial least squares or projection to latent structures (PLS) is one of the latent projection structures used in MSPM, which uses process data X and quality data Y together. In this paper, we discuss a new fault diagnosis approach based on total projection to latent structures (T-PLS). Four kinds of monitoring statistics are used in T-PLS, and a new definition of variable contributions to T^2 of PLS is proposed. Then, definitions of variable contributions to all statistics are derived to identify the faults. Control limits for contribution plots are calculated to identify whether a variable is in abnormal situation or not. Further, the proposed method separates the identified variables into faulty variables related to Y and unrelated to Y more clearly than conventional method. A case study on Tennessee Eastman process (TEP) indicates the efficiency of the proposed approach.

Key words Data-driven, total projection to latent structures (T-PLS), contribution plots, fault diagnosis

On-line monitoring and diagnosis of process operating performance and conditions are extremely important for the safety and reliability of industrial systems or processes. As a data-driven process monitoring methodology, multivariate statistical process monitoring (MSPM) is known to be effective for detecting and diagnosing faults or abnormal operating situations in many industrial processes, such as chemical plants and microelectronics manufacturing plants. Multivariate projection methods such as principal component analysis (PCA) and partial least squares or projection to latent structures (PLS) are used to provide a model for process monitoring, built from a large data set obtained in normal operating condition[1−4]. Using these models, large numbers of highly correlated measured variables are projected onto a low-dimensional latent space and a residual subspace, respectively. Two kinds of statistics are used to monitor the variations in two kinds of subspaces. By observing the statistics on-line, the faults or abnormal situations from the processes can be detected.

PCA structure is widely used to monitor all the abnormal situations that happen in the process variables X. If one is interested in monitoring the abnormal situations that are influential on quality data Y, one should build a PLS from the data X and Y[5]. The purpose of a PLS model is to approximate both process and quality variables and to model the relationship between them. PLS model has been used to estimate quality variables in industrial processes and to monitor process operating performance for a long time[6−8]. Although PLS model is used similar to PCA model, the properties of PLS model are different from PCA model. Li first revealed the geometric properties of PLS for process monitoring and compared the monitoring policies using different PLS models[9].

In regular PLS, there are usually many components extracted from X for predicting Y. As a result, the PLS model is complex to interpret. Furthermore, PLS components also contain the variations orthogonal to Y. In order to improve and modify PLS model, Wold proposed the orthogonal signal correction method[10]. The idea was to remove systematic information in X orthogonal to Y before using PLS algorithm. Fearn then reported another way of estimating the orthogonal components[11]. Trygg and Wold presented orthogonal PLS method based on the regular PLS algorithm[12]. The above methods are all preprocessing methods. On the other hand, the residual part of regular PLS model, which still contains large variations, is not proper for Q statistic to monitor. Zhou proposed the total PLS (T-PLS) algorithm to improve the performance of monitoring based on the regular PLS[13]. T-PLS is a postprocessing algorithm based on the regular PLS algorithm. It divides the whole X-space into four subspaces, and uses four statistics to monitor the variations respectively, which can increase the fault detection rate and reduce the false alarm rate for the faults related to Y.

Once a fault has been detected, it is important to diagnose an assignable cause for it. One of the solutions for this problem is the use of contribution plots, which shows the contribution of each process variable to the calculation of fault detection index[5, 14−17]. A high contribution of a process variable usually indicates a problem with that variable. Although there are other methods in multivariate statistical process monitoring (MSPM) to identify a cause, contribution plots approach seems to work well in practice, as it does not need the historical information of the faults.

In this paper, we propose a fault diagnosis approach based on the T-PLS algorithm. Four kinds of statistics are revisited and analyzed. In particular, we define and derive the variable contributions to all statistics in T-PLS based monitoring. Then, the proposed approach is applied to the Tennessee Eastman process (TEP), which has large amounts of process and quality variables. The fault related to Y attracts more attention usually; hence the T-PLS is efficient to monitor the TEP .

The remainder of this paper is organized as follows. Section 1 presents a brief introduction of T-PLS algorithm. Then, fault detection based on traditional PLS and T-PLS are reviewed in Section 2. In Section 3, the variable contributions to the four monitoring statistics are defined and derived. We describe the TEP and illustrate the fault diagnosis of TEP using the T-PLS based diagnostic method in Section 4. Finally, we present conclusions in the last section.

1 T-PLS algorithm

Given input matrix $X \in \mathbf{R}^{n\times m}$ consisting of n samples with m process variables per sample, and output matrix $Y \in \mathbf{R}^{n\times p}$ with p quality variables per sample, we can use nonlinear iterative partial least squares algorithm (NIPALS) to project (X, Y) to a low-dimensional space defined by a small number of latent variables $(\boldsymbol{t}_1, \cdots, \boldsymbol{t}_A)$, where A

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1. Department of Automation, Tsinghua National Laboratory for Information Science and Technology, Tsinghua University, Beijing 100084, P. R. China 2. Departments of Chemical and Electrical Engineering, Viterbi School of Engineering, University of Southern California, California 90089, USA 3. Research Institute of Information Technology, Tsinghua University, Beijing 100084, P. R. China
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is the PLS component number[5]. In PLS, the scaled and mean-centered X and Y are decomposed as

$$\begin{cases} X = TP^{\mathrm{T}} + E \\ Y = TQ^{\mathrm{T}} + F \end{cases} \tag{1}$$

where $T = [\boldsymbol{t}_1, \cdots, \boldsymbol{t}_A]$ is the score matrix, $P = [\boldsymbol{p}_1, \cdots, \boldsymbol{p}_A]$ is the loading matrix for X, and $Q = [\boldsymbol{q}_1, \cdots, \boldsymbol{q}_A]$ is the loading matrix for Y. In PLS procedure[5], weight matrix W is used to calculate score matrix T. However, W cannot relate T to the original process data X. Therefore, De Jong proposed the original weight matrix R , which can be used to calculate the score matrix T directly from X[18]:

$$T = XR \tag{2}$$

where R is obtained by P and W:

$$R = W(P^{\mathrm{T}}W)^{-1} \tag{3}$$

We obtain the T-PLS based on (1). The T-PLS algorithm for multiple quality variables Y is given in Algorithm 1[13]. Using the T-PLS algorithm, we can model X and Y as

$$\begin{cases} X = T_yP_y^{\mathrm{T}} + T_oP_o^{\mathrm{T}} + T_rP_r^{\mathrm{T}} + E_r \\ Y = T_yQ_y^{\mathrm{T}} + F \end{cases} \tag{4}$$

where $T_y \in \mathbf{R}^{n\times A_y}$, $T_o \in \mathbf{R}^{n\times (A-A_y)}$, and $T_y \in \mathbf{R}^{n\times A_r}$ are three score matrices, and $P_y \in \mathbf{R}^{m\times A_y}$, $P_o \in \mathbf{R}^{m\times (A-A_y)}$, and $P_r \in \mathbf{R}^{m\times A_r}$ are the corresponding loading matrices. $Q_y \in \mathbf{R}^{p\times A_y}$ is the new loading matrix for Y responding to T_y, $E_r = E(I - P_rP_r^{\mathrm{T}})$ is the new residual matrix. A_y is the number of Y-related components, and A_r is the number of Y-unrelated components.

Algorithm 1 (T-PLS algorithm for multiple outputs).

Center and scale the raw data to give matrices$X$ and Y.

Step 1. Perform the NIPALS PLS algorithm on X and Y as shown in (1), where PLS component number A is determined by cross-validation;

Step 2. $\hat{Y} = TQ^{\mathrm{T}} = T_yQ_y^{\mathrm{T}}$, and run PCA on $\hat{Y}$ with A_y components, where $A_y = \mathrm{rank}(Q)$;

Step 3. $\hat{X} = TP^{\mathrm{T}}$, $P_y^{\mathrm{T}} = (T_y^{\mathrm{T}}T_y)^{-1}T_y^{\mathrm{T}}\hat{X}$;

Step 4. $\hat{X}_o = \hat{X} - T_yP_y^{\mathrm{T}} = T_oP_o^{\mathrm{T}}$, and run PCA on $\hat{X}_o$ with $A - A_y$ components;

Step 5. $E = T_rP_r^{\mathrm{T}} + E_r$, and run PCA on E with A_r components, where $A_r < m - A$ is determined using PCA methods.

Compared with PLS model in (1), the T-PLS model in (4) is clear for describing the variations in X according to Y. In the T-PLS model, T_y represents the variations related to Y in score matrix T of regular PLS model, T_o represents the variations orthogonal to Y in T, T_r is the major part of original E, and E_r is the residual part of E which reflects the noise. Theoretical analysis indicates that T-PLS has the same prediction power of Y as PLS. The basic properties of T-PLS are as follows[13].

$$\boldsymbol{t}_i^{\mathrm{T}}\boldsymbol{t}_j = 0, \forall\ \boldsymbol{t}_i, \boldsymbol{t}_j \in \mathrm{Col}\{T_y, T_o, T_r\} \tag{5}$$

$$T_o^{\mathrm{T}}Y = 0 \tag{6}$$

where (5) indicates the orthogonality among score vectors, and (6) shows T_o is orthogonal to Y. Further study shows the equivalence between T-PLS and O-PLS in the decomposition of T.

2 T-PLS based fault detection

Regular PLS based method monitors the variations in principal subspace by T^2 statistic and residual subspace by Q statistic, respectively. Given a new sample $\boldsymbol{x}$, score and residual are calculated as[5]

$$\begin{aligned} \boldsymbol{t} &= R^{\mathrm{T}}\boldsymbol{x} \\ \tilde{\boldsymbol{x}} &= (I - PR^{\mathrm{T}})\boldsymbol{x} \end{aligned} \tag{7}$$

then, T^2 and Q are calculated as[17]

$$\begin{aligned} T^2 &= \boldsymbol{t}^{\mathrm{T}}\Lambda^{-1}\boldsymbol{t} \sim \frac{A(n^2-1)}{n(n-A)}F_{A,n-A,\alpha} \\ Q &= \|\tilde{\boldsymbol{x}}\|^2 \sim g\chi^2_{h,\alpha} \end{aligned} \tag{8}$$

where $\Lambda = \dfrac{1}{n-1}T^{\mathrm{T}}T$, A is the number of PLS components, and n is the number of training samples. $F_{A,n-A}$ is F-distribution with A and $n - A$ degrees of freedom. $g\chi^2_h$ is the χ^2-distribution with scaling factor g and h degrees of freedom. α defines the significance level $(1 - \alpha) \times 100\,\%$.

T-PLS can be used for process monitoring in a similar way. In the T-PLS, T_y, T_o, and T_r contain the systematic part of the process variation, thus are suitable for T^2 statistics, while E_r represents the residual part of the whole process variation, thus is suitable for Q statistic. For a new or future measured sample $\boldsymbol{x}$, the scores and residual are projected onto the T-PLS model as follows[13]:

$$\boldsymbol{t}_y = Q_y^{\mathrm{T}}QR^{\mathrm{T}}\boldsymbol{x} \in \mathbf{R}^{A_y} \tag{9a}$$

$$\boldsymbol{t}_o = P_o^{\mathrm{T}}(P - P_yQ_y^{\mathrm{T}}Q)R^{\mathrm{T}}\boldsymbol{x} \in \mathbf{R}^{A-A_y} \tag{9b}$$

$$\boldsymbol{t}_r = P_r^{\mathrm{T}}(I - PR^{\mathrm{T}})\boldsymbol{x} \in \mathbf{R}^{A_r} \tag{9c}$$

$$\tilde{\boldsymbol{x}}_r = (I - P_rP_r^{\mathrm{T}})(I - PR^{\mathrm{T}})\boldsymbol{x} \in \mathbf{R}^{m} \tag{9d}$$

Assuming the measured sample follows a multivariate normal distribution, we obtain confidences for T_y^2, T_o^2, and T_r^2 using the F-distribution[14] . On the other hand, the control limit for Q is calculated using the χ^2-distribution[14] on the assumption that a residual vector is multivariate normal. The control limits of statistics are listed in Table 1[13]. For all statistics, 99 % confidence limits are obtained. If the statistics of the new sample fall into these limits, the process is considered to be in control statistically.

Table 1 Monitoring statistics and control limits

Statistic	Calculation	Control limit
T_y^2	$\boldsymbol{t}_y^{\mathrm{T}}\Lambda_y^{-1}\boldsymbol{t}_y$	$\dfrac{A_y(n^2-1)}{n(n-A_y)}F_{A_y,n-A_y,\alpha}$
T_o^2	$\boldsymbol{t}_o^{\mathrm{T}}\Lambda_o^{-1}\boldsymbol{t}_o$	$\dfrac{(A-A_y)(n^2-1)}{n(n-A+A_y)}F_{A-A_y,n-A+A_y,\alpha}$
T_r^2	$\boldsymbol{t}_r^{\mathrm{T}}\Lambda_r^{-1}\boldsymbol{t}_r$	$\dfrac{A_r(n^2-1)}{n(n-A_r)}F_{A_r,n-A_r,\alpha}$
Q_r	$\|\tilde{\boldsymbol{x}}_r\|^2$	$(S/2\mu)\chi^2_{2\mu^2/S,\alpha}$

Notes: $\Lambda_y = \frac{1}{n-1}T_y^{\mathrm{T}}T_y$, $\Lambda_o = \frac{1}{n-1}T_o^{\mathrm{T}}T_o$, $\Lambda_r = \frac{1}{n-1}T_r^{\mathrm{T}}T_r$, S is the sample variance of Q, and μ is the sample mean of Q.

According to the relation between PLS and T-PLS, T^2 and Q statistics in PLS model monitor the same variations as the union of T_y^2 and T_o^2 statistics and the union of T_r^2 and Q_r statistics in T-PLS model, respectively. However, it has been shown that T_y^2 and Q_r detect the faults related to Y while T_o^2 and T_r^2 detect the faults unrelated to Y.

It has been validated further that for the faults related to Y, T-PLS based methods can increase the detection rate and reduce the false alarm rate, compared with PLS based methods[13].

3 Contribution analysis for fault diagnosis

When an abnormal variation, which does not meet normal operating condition, is detected by the monitoring statistic, a further analysis may be needed to diagnose which variables may cause the abnormal event. One of the popular approaches for fault diagnosis in data-driven methods is to use a contribution plot. A contribution plot represents the contribution of each process variable to the statistic which exceeds the control limit. In regular PLS based monitoring, three kinds of contribution plots are commonly considered: the contributions of each variable to T^2, Q, and each score. Here, we propose a new calculation of contribution to T^2 statistic, and meanwhile derive the contributions to four statistics that are used in T-PLS based monitoring.

3.1 Variable contributions to $\boldsymbol{Q_r}$

The Q_r monitors the abnormal situation in the residual subspace, which is not present in the normal operation condition data. As Q_r can be seen as the sum of the squared residuals of each variables:

$$Q_r = \|\tilde{\boldsymbol{x}}_r\|^2 = \sum_{i=1}^{m} \tilde{x}_{r,i}^2 \tag{10}$$

the contributions to Q_r are defined as

$$C(Q_r, i) = \tilde{x}_{r,i}^2 \tag{11}$$

where $\tilde{x}_{r,i}$ represents the i-th element of $\tilde{\boldsymbol{x}}_r$.

3.2 Variable contributions to $\boldsymbol{T}^2$ statistics

In regular PLS based monitoring, there have been several approaches to calculate the contribution of each variables to T^2 statistics. Nomikos suggested the variable contribution to the T^2 statistics as follows[14]:

$$C(T^2, i) = \sum_{k=1}^{A} t_k \lambda_{kk}^{-1} p_{ik} x_i \tag{12}$$

where t_k is the k-th score, λ_{kk} is the variance of t_k, and p_{ik} is the element of P in i-th row and k-th column k. This calculation assumes that the loading matrix P is orthogonal, which is satisfied in PCA model but not in PLS model. In order to extend the above approaches into PLS and other models, Westerhuis defined a generalized contribution to T^2 statistic as follows[15]:

$$C(T^2, i) = \boldsymbol{t}^{\mathrm{T}} \Lambda^{-1} [(P^{\mathrm{T}} P)^{-1} \boldsymbol{p}_i^{\mathrm{T}} x_i] \tag{13}$$

where $\boldsymbol{p}_i \in \mathbf{R}^{A\times 1}$ is the i-th row of P, and

$$\boldsymbol{t} = (P^{\mathrm{T}} P)^{-1} P^{\mathrm{T}} \boldsymbol{x} \tag{14}$$

is the new calculation of scores. This new definition of variable contributions to T^2 works if score vectors and loading vectors are not orthogonal. However, this approach is still an approximation in the case of PLS based monitoring[17]. As the two previous methods mentioned above result in negative contributions[15], Qin defined the variable contribution as[16]

$$C(T^2, i) = \|\Lambda^{-1/2} \boldsymbol{p}_i^{\mathrm{T}} x_i\|^2 \tag{15}$$

which is suitable for PCA-based monitoring. As an extension of the above approach, Choi proposed the calculation suitable for the PLS model as[17]

$$C(T^2, i) = \|\Lambda^{-1/2} \boldsymbol{r}_i^{\mathrm{T}} x_i\|^2 \tag{16}$$

where $\boldsymbol{r}_i \in \mathbf{R}^{A\times 1}$ is the i-th row of weighing matrix R for original data matrix X.

However, this definition does not meet the decomposition condition, that is,

$$T^2 = \boldsymbol{x}^{\mathrm{T}} R \Lambda^{-1} R^{\mathrm{T}} \boldsymbol{x} = \|\sum_{i=1}^{m} \Lambda^{-1/2} \boldsymbol{r}_i^{\mathrm{T}} x_i\|^2 \neq \sum_{i=1}^{m} C(T^2, i)$$

In this paper, we provide a new definition of variables to T^2 types of statistics. Let $\Gamma = (R\Lambda^{-1}R^{\mathrm{T}})^{1/2}$; the T^2 statistic can be rewritten as

$$T^2 = \|\Gamma \boldsymbol{x}\|^2 = \sum_{i=1}^{m} \|\boldsymbol{\gamma}_i \boldsymbol{x}\|^2 \tag{17}$$

where $\boldsymbol{\gamma}_i$ is the i-th row of Γ. So, the exact variable contributions to T^2 statistic can be defined as

$$C(T^2, i) = \|\boldsymbol{\gamma}_i \boldsymbol{x}\|^2 \tag{18}$$

Unlike the above approaches, (18) shows the contribution of one variable to T^2 is related to not only itself but also other variables, which is consistent with the variable contributions to Q or Q_r statistic. In T-PLS, T_y^2, T_o^2, and T_r^2 are all T^2 type of statistics, so the variable contributions to these statistics can be defined as (18) according to Table 2.

Table 2 Variable contributions to T^2 type of statistics

Contribution	Calculation	Γ^2
$C(T_y^2, i)$	$\|\boldsymbol{\gamma}_{y,i}\boldsymbol{x}\|^2$	$RQ^{\mathrm{T}}Q_y\Lambda_y^{-1}Q_y^{\mathrm{T}}QR^{\mathrm{T}}$
$C(T_o^2, i)$	$\|\boldsymbol{\gamma}_{o,i}\boldsymbol{x}\|^2$	$R(P^{\mathrm{T}} - Q^{\mathrm{T}}Q_yP_y^{\mathrm{T}})P_o\Lambda_o^{-1}\times$ $P_o^{\mathrm{T}}(P - P_yQ_y^{\mathrm{T}}Q)R^{\mathrm{T}}$
$C(T_r^2, i)$	$\|\boldsymbol{\gamma}_{r,i}\boldsymbol{x}\|^2$	$(I - RP^{\mathrm{T}})P_r\Lambda_r^{-1}P_r^{\mathrm{T}}(I - PR^{\mathrm{T}})$

3.3 Control limits for contribution plots

In the early application of contributions, one used to compare contributions of different variables to the same statistic and choose the variables corresponding to the relatively large contributions as the possible causes for abnormal situation. However, it is not reasonable to compare the absolute magnitudes of variable contributions because they are usually different even in the normal process condition. It is necessary to derive a control limit for fault diagnosis just as fault detection policy. Westerhuis proposed the idea of deriving the control limits for variable contributions to statistics[15]. Choi provided the upper control limits for each variable contribution to four monitoring statistics based on the multi-block PLS model[17]. In our study, we use the calculations for each variable contribution C to statistics in T-PLS as follows[17]:

$$C_\alpha = \mu(C) + 2.3263 \cdot s(C) \tag{19}$$

where $\mu(C)$ and $s(C)$ are the sample mean and standard deviation of the contribution C, respectively, assuming that the variable contribution is approximately normally distributed. The confidence level α is selected as 99 %.

Instead of comparing the absolute contribution and the corresponding control limit, the use of the relative contribution of C/C_α is a more convenient way to identify faulty variables[17]. In this case, the relative contributions of all variables are equivalent statistically under normal conditions.

4 Application study: Tennessee Eastman process

In order to demonstrate the efficiency of T-PLS based contribution plots, the Tennessee Eastman benchmark data are used for fault detection and diagnosis. The TEP was created by the Eastman Chemical Company to provide a realistic industrial process for evaluating process control and monitoring methods[19]. The process consists of five major units: a reactor, condenser, compressor, separator, and stripper; it contains eight components: A, B, C, D, E, F, G, and H. The gaseous reactants A, C, D, and E and the inert B are fed to the reactor where the liquid products G and H are formed. The species F is a by-product of the reactions. The reactions in the reactor are

$$\begin{array}{rcl} \mathrm{A(g)+C(g)+D(g)} & \rightarrow & \mathrm{G(liq)} \\ \mathrm{A(g)+C(g)+E(g)} & \rightarrow & \mathrm{H(liq)} \\ \mathrm{A(g)+E(g)} & \rightarrow & \mathrm{F(liq)} \\ \mathrm{3D(g)} & \rightarrow & \mathrm{2F(liq)} \end{array} \tag{20}$$

4.1 Process and fault description

The reactions are irreversible, exothermic, and approximately first-order with respect to the reactant concentrations. The reaction rates are Arrhenius functions of temperature where the reaction for G has a higher activation energy than the reaction for H, resulting in a higher sensitivity to temperature. The reactor product stream is cooled through a partial condenser and then fed to a vapor-liquid separator. The vapor exiting from the separator is recycled to the reactor feed through a compressor. A portion of the recycle stream is purged to keep the inert and by-product from accumulating in the process. The condensed components form the separator (stream 10) are pumped to a stripper[20].

The TEP contains two blocks of variables: the manipulated variable (MV) block of 12 manipulated variables and measurement variable (MEAS) block of 41 measured variables[20]. Process measurements are sampled with interval of 3 minutes. 19 composition measurements are sampled with time delays that vary from 6 minutes to 15 minutes, which are taken from streams 6, 9, and 11. This time delay has a potentially critical impact on product quality control within the plant. This implies that the fault effect on product quality cannot be detected until the next sample of Y is available. During this time, the products are produced with uncontrolled quality. PLS based monitoring methods can detect the fault more related to Y compared with PCA based methods, and thus it has received wide applications in industrial cases.

There are sixteen known faults and five unknown faults in TEP[20], denoted by IDV 1∼21. IDV 1∼7 are associated with a step change in a process variable, e.g. in the cooling water inlet temperature. IDV 8∼12 are associated with an increase in the variability of some process variables. IDV 13 is a slow drift in the reaction kinetics. IDV 14, IDV 15, and IDV 21 are associated with sticking valves.

The process used here is operated under closed-loop control. The simulation code for the TEP in closed loop can be found on the Web site http://brahms.scs.uiuc.edu. TEP has been widely used as a benchmark process for evaluating the process diagnosis methods such as PCA, multiway PCA, support vector machine, and Fisher discriminant analysis (FDA)[20]. PLS based method has also been applied to the TEP[21].

4.2 T-PLS model for TEP

In this study, the compositions of G and H in stream 9, i.e., MEAS 35 and MEAS 36, are chosen as quality variable Y with a time delay of 6 minutes. 22 process measurements and 11 manipulated variables, i.e., MEAS 1∼22 and MV 1∼11, are chosen as X. MV 12 is not included because it does not change during the whole simulation. The 960 normal samples are used to build a T-PLS. First, the samples are centered to zero mean and scaled to unit variance. 6 components are kept for PLS components according to cross validation. A_y is 2 in this model, and A_r=17 according to PCA based methods. Fig. 1 shows the prediction of composition of G in stream 9 using T-PLS model. Note that the T-PLS model has the same prediction power as PLS model. Based on the normal data, we calculate the control limits both for monitoring statistics and for variable contributions to these statistics.

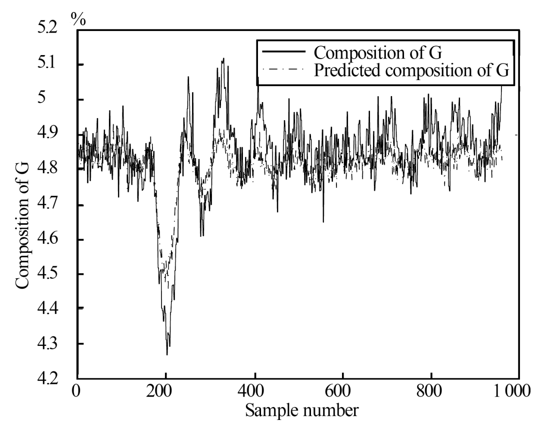

Fig. 1 T-PLS model of composition of G

4.3 Example and discussion

Here, we take the IDV 1 for an example to illustrate the proposed approach. When the fault IDV 1 occurs, a step change is induced in the A/C feed ratio in stream 4, which decreases the composition of A in stream 6 (MEAS 23) and a control loop reacts to increase the A feed in stream 1 (MEAS 1). The variations in the flow rate and compositions of stream 6 to the reactor cause the variations in the reactor level (MEAS 8), which affects the flow rate in stream 4 (MEAS 4) through a cascade control loop[21]. Furthermore, the variables associated with reaction such as pressure and composition of reactants, are also affected correspondingly. Fig. 2 shows the variations in the significant variables.

The faulty data set consists of 960 samples with sampling interval of 3 minutes. The simulation starts with no fault, and the fault is introduced to the process from the 8 simulation hours (#160 sample). The fault is detected both by the T^2 and Q in PLS based monitoring as shown in Fig. 3. In T-PLS based monitoring, T_y^2 and Q_r detect the variations related to Y, while T_o^2 and T_r^2 detect the variations unrelated to Y, which provides detailed monitoring. Fig. 4 indicates that the effect by a fault to each part is different. This detailed monitoring describes how seriously the fault affects the output Y. As shown in Fig. 4. T_y^2 does not exceed the control limit for such a long time as other statistics. This is because TEP is operated under a closed-loop control, which keeps pulling the quality Y back to the set value after the fault occurs. If the process is operated under an open-loop control, the fault effect will last for the whole fault period. The fault can be seen as related to Y, as Y is indeed affected by the fault. For faults unrelated to Y, Y is never affected during the whole fault period.

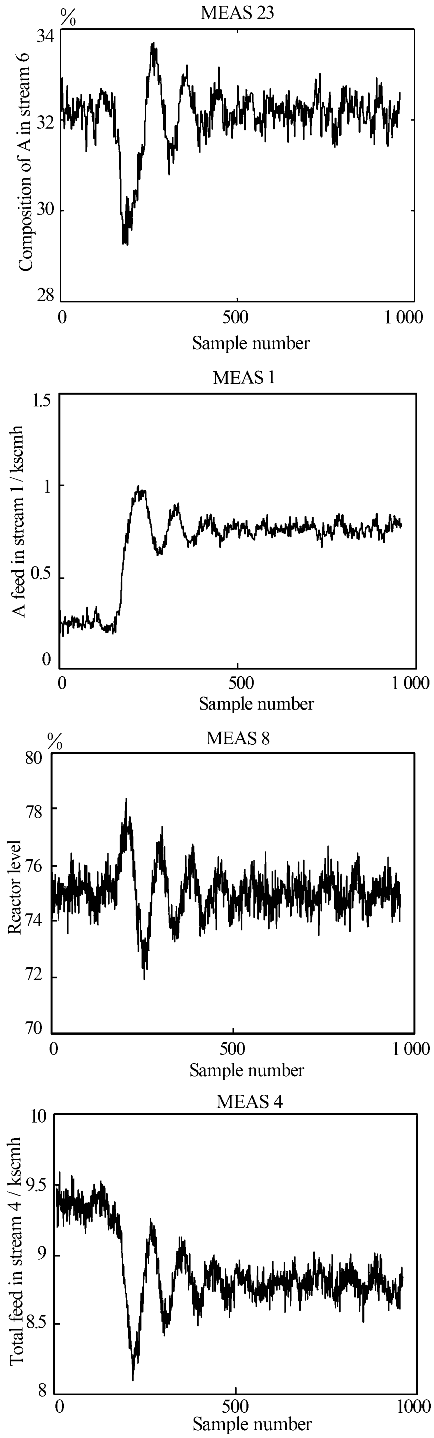

Fig. 2 Dynamics of measured variables for IDV 1 (kscmh means kilo standard cubil meters per hour.)

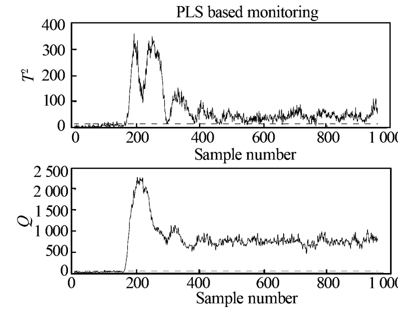

Fig. 3 On-line Q and T^2 charts for fault detection using PLS (Dotted line represents the 99 % control limit for statistics.)

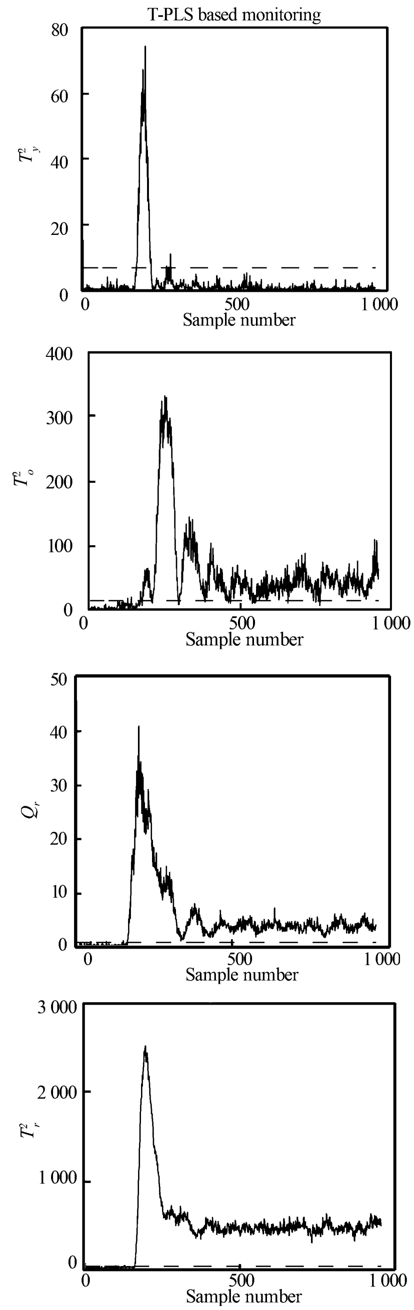

Fig. 4 On-line Q_r and T_y^2, T_o^2, T_r^2 charts for fault detection using T-PLS (Dotted line represents the 99 % control limit for statistics.)

After the fault is detected, the relative variable contributions to each statistic are observed to identify the variables responsible for this situation. Figs. 5∼7 show the relative contributions to statistics in PLS and T-PLS. As mentioned above, the fault affects quality data significantly in the early period. Thus, we choose the initial samples (e.g. #170) after the fault occurs to identify the faulty variables. In the relative contribution plots, the variables with contribution greater than one can be seen as abnormal and the variables with top contributions can be seen as the source to the fault.

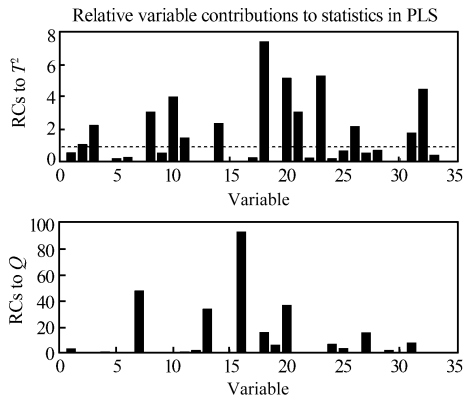

Fig. 5 Relative variable contribution plots for Q and T^2 at the sample #170 (Dotted line represents 1 and RCs means relative contributions.)

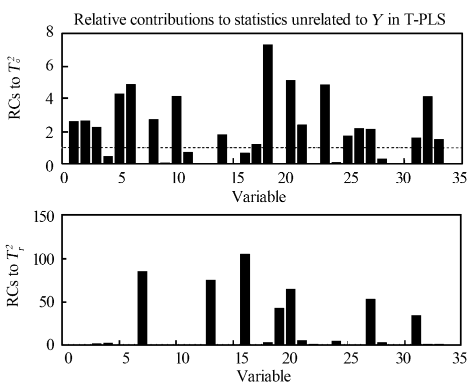

Fig. 6 Relative variable contribution plots for T_r^2 and T_o^2 at the sample #170 (Dotted line represents 1 and RCs means relative contributions.)

From Figs. 5 and 6, it can be seen that the identified faulty resources by T^2 and Q of PLS are nearly the same as those by Y-unrelated statistics of T-PLS, which are quite different from the results by Y-related statistics of T-PLS. This phenomena is general with samples in the early stage of the fault, which is because the variations monitored by Y-unrelated statistics are greater than those monitored by Y-related statistics. With the mixture property of T^2 and Q, PLS based contributions are affected mostly by the Y-unrelated faulty source, which fail to identify the Y-related faulty resources in this situation. Therefore, the T-PLS based contribution plots can separate the identified fault source variables into Y-related and Y-unrelated variables.

However, as contributions can smear from one variable to another, the variable which is not affected may have a high contribution. Hence, we should deal with the results of contribution plots approach carefully based on the process knowledge.

5 Conclusions

Decomposing the two subspaces of PLS model into four subspaces further, and performing the fault diagnosis based on the T-PLS model are very meaningful in monitoring the processes when the quality variables Y attract much attention. In this paper, we have dealt with the diagnosis of the problem using the T-PLS model. First, we reviewed the four kinds of monitoring statistics based on T-PLS model. Then, we derived and defined the contributions to these statistics: T_y^2 and Q_r are related to Y, T_o^2 and T_r^2 are unrelated to Y. The upper control limit of each contribution was obtained. The relative contribution was used to identify the variables responsible for the abnormal situations efficiently.

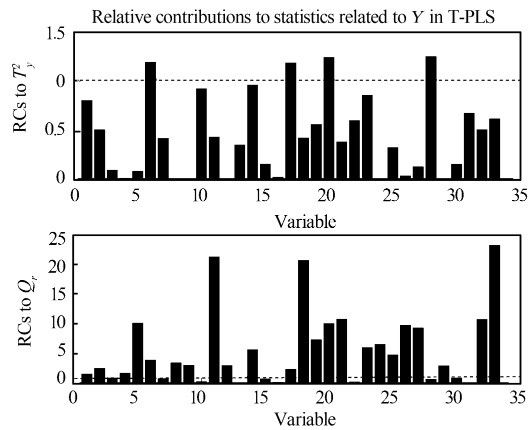

Fig. 7 Relative variable contribution plots for T_y^2 and Q_r at the sample #170 (Dotted line represents 1 and RCS means relative contributions.)

The TEP was taken as an application case study in this paper. The compositions of products G and H, which we may concern as the quality variable Y, were modeled and predicted on-line using a T-PLS model. The fault diagnosis approach based on the T-PLS model clearly seperated the identified fault resources into the faulty variables related and unrelated to Y.

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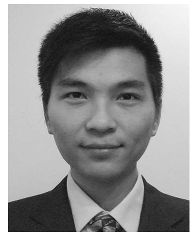

LI Gang Ph. D. candidate in the Department of Automation, Tsinghua University. He received his bachelor degree from the Department of Precision Instruments and Mechanology, Tsinghua University in 2004. His research interest covers statistical process monitoring, data-driven fault diagnosis and prognosis.
E-mail: dlg00@mails.thu.edu.cn

QIN Si-Zhao Fluor professor at the Viterbi School of Engineering at University of Southern California, USA. He received his bachelor and master degrees in automatic control from Tsinghua University in 1984 and 1987, respectively, and his Ph. D. degree in chemical engineering from University of Maryland at College Park, USA in 1992. He worked as a principal engineer at Fisher-Rosemount from 1992 to 1995. His research interest covers statistical process monitoring and fault diagnosis, model predictive control, system identification, run-to-run control, semiconductor process control, and control performance monitoring.
E-mail: sqin@usc.edu.cn

JI Yin-Dong Associate professor at the Research Institute of Information Technology (RIIT), Tsinghua University. He received his bachelor and master degrees from the Department of Automation, Tsinghua University, in 1985 and 1989, respectively. His research interest covers digit signal processing, fault diagnosis, and control engineering.
E-mail: jyd@mail.tsinghua.edu.cn

ZHOU Dong-Hua Professor in the Department of Automation, Tsinghua University. He received his bachelor, master, and Ph. D. degrees from Shanghai Jiao Tong University, in 1985, 1988, and 1990, respectively. He was an Alexander von Humboldt research fellow (1995 ∼ 1996) in the University of Duisburg, Germany, and a visiting professor at Yale University, USA (July 2001 ∼ January 2002). His research interest covers fault diagnosis, fault prediction, reliability prediction, and predictive maintenance. Corresponding author of this paper. E-mail: zdh@tsinghua.edu.cn