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Improvement of the Sensitivity of T² Quality Control Charts by Variable Grouping and Dimension Reducing

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Abstract—**With increasing number of variables the Hotelling's T^2 statistic can detect only larger failures in the variables. A new method is introduced for reducing the dimension of the Hotelling's statistic in order to detect smaller failures. The basic idea is to group some variables into a combined variable and to calculate the T^2 value from this variable and from the remaining variables. As the new calculated variable has not a Gaussian distribution a proper static transformation is applied. Both uncorrelated and correlated data are dealt with. In the latter case principal component analysis is used before calculating T^2. Several simulations show that the sensitivity of the new T^2 control charts is improved. The theory is confirmed by an application of sensor fault monitoring of a gas analyzer.**

I. INTRODUCTION

In the quality control for multivariate data there exist several methods for fault detection and identification (FID). Many methods are based on the T^2 or Q statistic. Several (e.g. five) variables can be simultaneously monitored by using more (e.g. five) control charts. The advantage of this univariate analysis is the fast calculation of control charts and the simple parameterization. However, there are disadvantages like:

- The user has to check several control charts at the same time.
- Only the variances of the variables are taken into account, but not the relations (covariance's) between the variables.

Alternatively Hotelling's T^2 value or Mahalanobis distance D can be monitored as a single variable. If this value exceeds a prescribed limit then at least one of the variables exceeds its limit. The T^2 value is calculated from vector $\mathbf{u}_k \in \Re^{1xm}$ of the measured values, the mean vector $\overline{\mathbf{u}} \in \Re^{1xm}$ and the covariance matrix $\mathbf{S} \in \Re^{mxm}$ by (1), where m indicates the number of variables and k the time.

$$T_k^2 = D_k^2 = (\mathbf{u}_k - \overline{\mathbf{u}})\mathbf{S}^{-1}(\mathbf{u}_k - \overline{\mathbf{u}})^{\mathrm{T}} \quad (1)$$

The mean value and the covariance matrix are estimated usually from a training data set. The quality of this estimation is relevant for the fault detection ability of the control chart. In practice it is often very difficult to separate a training data set which contains no disturbances or outliers. With the standard estimation method the estimation of variance and covariance is adversely affected by disturbances such as outliers, thus the sensitivity of the control chart decreases. In [2] median and MAD (Median Absolute Deviation) are recommended for robust estimation of these parameters. For the ongoing analysis it is assumed that the data have Gaussian distribution and the mean vector and the covariance matrix are known, or they are estimated from a large amount of data. In this case the T^2 value of (1) has χ^2 distribution. [8] The control limit UCL for the number of variables m can be calculated for a given confidence level α by

$$UCL = \chi^2_{\alpha;m} \quad (2)$$

In Fig. 1 the control limits for different number of variables m and a probability $P = 1 - \alpha = 0.9973$, better known as 3 sigma confidence limits in univariate quality control, are shown. As it can be seen the control limits are increased as the error of type I is increased with increasing number of variables m according to (3). This is a well-known problem in the literature e.g. see [8].

$$\alpha_{res} = 1 - (1 - \alpha)^m \quad (3)$$

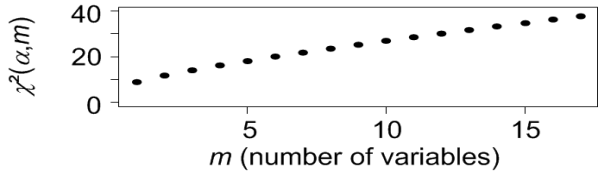

Fig. 1 Control limits for different number of variables m with a probability $P = 1 - \alpha = 99.73\%$

The Mahalanobis distance D is used as a measure of the deviation of the actual measurements from the normal state usually characterized by the mean value. With increasing number of the variables the detectable disturbance is always farther from the mean value. This means, the more variables are monitored the more difficult is to detect small deviations from the normal state. In the literature several methods like PCA, PLS and multi-block methods exist to handle this problem. In this paper a new alternative method based on PCA is presented. By using PCA it is common to separate the principal components in a principal component subspace (PCS) and a residual subspace (RS). This means some (probably) not important principal components (PC's) are excluded from the analysis. For the choice which PC's are not used several evaluation criteria such as 90% of the

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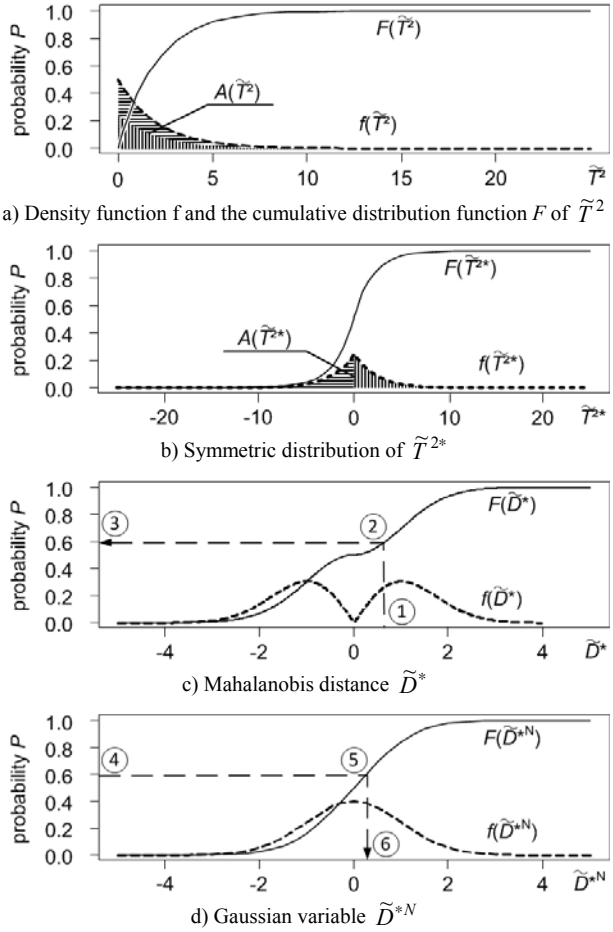
explained variance, Kaiser or elbow criterion are known. But these criteria are not good enough as deviations in the non-monitored / not used PC's can never be detected. An alternative but more complicated way is to observe the important PCS with a T^2 value and the non-important RS with the *SPE* value (Squared Prediction Error). As all the variables are considered, there is no information lost. But it is necessary to observe two quality values T^2 and *SPE*. For more details see [10]. By using the separation in PCS and RS it is useful to work with combined indices. A linear combination of T^2 and *SPE* is defined in [12] and [11] define a weighted version. In [1] a modified covariance matrix for the RS is used. However the evaluation of *SPE* is more difficult for a practitioner than using the T^2 control chart.

II. NEW METHOD FOR IMPROVING THE SENSIBILITY OF T^2

In this article an alternative, new method is presented for improving the sensibility of T^2. By this method which is easier than the combined calculation of T^2 and *SPE* charts there is no information loss.



a) Density function f and the cumulative distribution function F of $\tilde{T}^2$

b) Symmetric distribution of $\tilde{T}^{2*}$

c) Mahalanobis distance $\tilde{D}^*$

d) Gaussian variable $\tilde{D}^{*N}$

Fig. 2. Density and sum functions during the transformation

In this procedure some variables are grouped to a new, calculated variable. As the new variable has not a Gaussian distribution it is transformed to a Gaussian distribution. From this Gaussian variable and the other remaining, non-grouped variables the T^2 value is calculated and monitored in a single control chart. As the dimension of the variables in the T^2 control chart is less than the total number of variables, the failures in the non-grouped variables can be detected easier. Also the deviations in the grouped variables can be detected, even they become smaller. Please don't confuse grouping methods with sub-grouped data and with individual observations. Using grouped variables with sub-grouped data means to calculate one quality parameter e.g. T^2 from N measurements of each m variables. Some detailed explanations can be found in [5] and [8]. The new method deals only with individual observations, which mean a T^2 value is calculated from one measurement of each m variables [8]. This is rather similar to the grouping with multi-block PCA, see [9], [10] and [13]. Because here the data are grouped in e.g. parts of a plant and in a second step these groups are combined in a quality parameter. There exist several methods how to interpret a T^2 signal. [8] and [6] try to decompose the variable T^2 into independent components. An overview about several methods can be found in [7]. But all these methods start their work if the T^2 control chart has detected an abnormal state. Therefore, it is important to improve the sensibility of the T^2 calculation and exactly this is proposed in the present paper.

A. Principle of the new method

The measurement matrix $\mathbf{U} \in R^{Nxm}$ is given with N measurement of m variables. By using the PCA the corresponding score vector $\mathbf{T}$ and loading matrix $\mathbf{P}$ can be determined. Equation (4) show the relation between the measurement matrix $\mathbf{U}$ and the score matrix $\mathbf{T}$ with the mean vector $\overline{\mathbf{U}}$.

$$\mathbf{T} = \mathbf{P}^T\left(\mathbf{U} - \overline{\mathbf{U}}\right) \tag{4}$$

In the observation phase only one measurement of each variable is available, $\mathbf{u}_k \in R^{1xm}$. The score vector can be separated in two parts, see (5). The first one $\hat{\mathbf{T}}_k$ span the principal component subspace (PCS) which includes $t_{k,i} \quad i \in 1,...,l$ and the second $\tilde{\mathbf{T}}_k$ span the residual subspace (RS) which includes $t_{k,i} \quad i \in l+1,...,m$. In the formulation $t_{k,i}$ stands for the i^{th} column of the score vector $\mathbf{T}_k$.

$$\mathbf{T}_k = \left[\hat{\mathbf{T}}_k \quad \tilde{\mathbf{T}}_k\right] \tag{5}$$

If $\mathbf{S}$ is the covariance matrix of $\mathbf{U}$ then $\mathbf{\Lambda} = diag\left(\lambda_1,...,\lambda_m\right)$ is the covariance matrix of the scores, where λ_i are the eigenvalues of $\mathbf{S}$ [10]. Also $\mathbf{\Lambda}$ can be separated into two parts, see (6).

$$\mathbf{\Lambda} = \begin{bmatrix} \hat{\mathbf{\Lambda}} & 0 \\ 0 & \tilde{\mathbf{\Lambda}} \end{bmatrix} = \begin{bmatrix} diag\left(\lambda_1,...,\lambda_l\right) & 0 \\ 0 & diag\left(\lambda_{l+1},...,\lambda_m\right) \end{bmatrix} \tag{6}$$

The $\tilde{\mathbf{T}}_k$ vector contain $\tilde{m} = m - l + 1$ variables. The $\tilde{T}_k^2$

value of the $\tilde{m}$ variables follow a χ^2 distribution, see Fig 2a. In the ideal normal condition there is no deviation between the mean value $\bar{\mathbf{u}}$ and the measured value $\mathbf{u}$. This point $\mathbf{u}-\bar{\mathbf{u}}=0$, is in the middle of a symmetric Gaussian distribution. The normal state of the $\tilde{T}_k^2$ value is also zero. But the point $\tilde{T}_k^2=0$ is at the left edge of a non-symmetric χ^2 distribution. Before using the grouped variables ($\tilde{T}_k^2$ value) as a new input variable in a T^2 control chart there are some aspects to be considered:

- The ideal normal condition of T^2 value must lie in the middle of a symmetric distribution.
- The transformed symmetric distribution of the grouped variables has to be a Gaussian distribution. Otherwise the new grouped variable might not be used in a new T^2 control chart.
- The transformation to a Gaussian distribution should be static and exactly defined, because a reverse calculation should be possible if a disturbance is detected.

To solve the first problem the normal calculation of a T^2 value which was defined in (1) is extended by a factor C_k.

$$\tilde{T}_k^2=\tilde{\mathbf{T}}_k\tilde{\mathbf{\Lambda}}^{-1}\tilde{\mathbf{T}}_k^{\mathrm{T}} \qquad \tilde{T}_k^{2*}=\tilde{\mathbf{T}}_k\tilde{\mathbf{\Lambda}}^{-1}\tilde{\mathbf{T}}_k^{\mathrm{T}}\cdot C_k \quad with \quad C_k=\prod_{i=1}^{\tilde{m}}\frac{\tilde{t}_{k,i}}{|\tilde{t}_{k,i}|} \tag{7}$$

This factor in (7) is used to get a $\tilde{T}_k^{2*}$ value which follows a symmetric distribution. The new symmetric density function of $\tilde{T}_k^{2*}$ is defined in (8), see. Fig. 2b. The factor C_k assigns 50% of the $\tilde{T}_k^{2*}$ values a positive sign ||||||| and to the other 50% a negative sign ≡, see Fig. 2b. Therefore the $\tilde{T}_k^{2*}$ value is also defined in the negative region. Because the area $A(\tilde{T}^2)$ and $A(\tilde{T}^{2*})$ under the density function in Fig. 2a and 2b have to be equal the maximum of $f(\tilde{T}^{2*})$ is only 50% of $f(\tilde{T}^2)$.

$$f(\tilde{T}^{2*})=\begin{cases}\chi^2_{0.5+2\alpha;\tilde{m}}\cdot\frac{1}{2} & for\ C_k>0\\ \chi^2_{0;\tilde{m}}\cdot\frac{1}{2} & for\ C_k=0\\ \chi^2_{2\alpha;\tilde{m}}\cdot\frac{1}{2} & for\ C_k<0\end{cases} \tag{8}$$

In the next step the Mahalanobis distance $\tilde{D}_k^*$ is calculated by a simple Box-Cox transformation, see (9).

$$\tilde{D}_k^*=\left(\tilde{T}_k^{2*}\right)^{0.5} \tag{9}$$

The resulting functions are shown in Fig. 2c. As $\tilde{D}_k^*$ is not normally distributed, it is transformed by (10) to the Gaussian variable $\tilde{D}_k^{*N}$.

$$\tilde{D}_k^{*N}=\tilde{D}_k^*\cdot f(\tilde{D}_k^*,\tilde{m}) \tag{10}$$

The nonlinear function $f(\tilde{D}_k^*,\tilde{m})$ is shown in Fig. 3. The mathematical definition of this function is given in (11). For a given deviation $\tilde{D}_k^*$ the corresponding probability $P(\tilde{D}_k^*)=1-\alpha$ of the $\tilde{D}^*$-distribution is determined. In a following step the same probability is used to determine the new quantile $quant(P(\tilde{D}_k^*))$ of the $\tilde{D}^{*N}$-distribution.

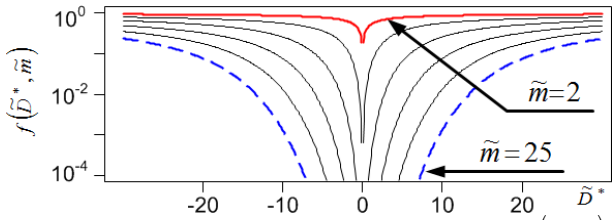


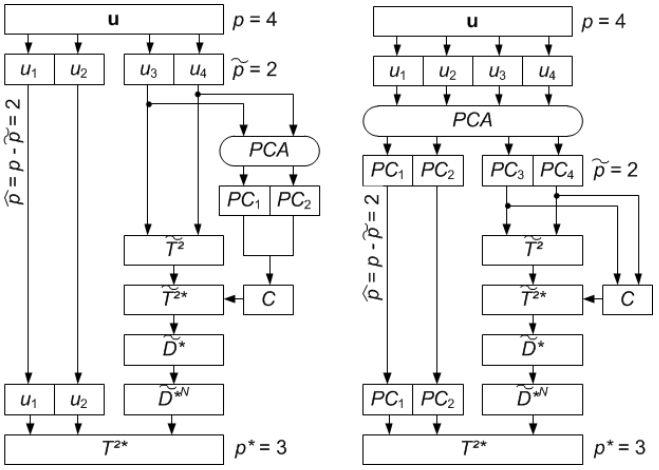
Fig. 3 example for the nonlinear transformation function $f(\tilde{D}^*,\tilde{m})$

$\tilde{m}\in(2, 5, 10, 15, 20, 25)$

$$f(\tilde{D}_k^*,\tilde{m})=\tilde{D}_k^*/quant(P(\tilde{D}_k^*)) \tag{11}$$

The new variable $\tilde{D}_k^{*N}$ have a Gaussian distribution, with zero mean. The new score vector $\mathbf{T}_k^*$ and the covariance matrix $\mathbf{\Lambda}^*$ can be formulated as shown in (12). Note that the covariance vector $\mathbf{cov}_{Dt}$ between the new variable $\tilde{D}^{*N}$ and the scores $\hat{\mathbf{T}}$ are different from zero and have to be determined in a training phase from a probably fault free dataset.

$$\mathbf{T}_k^{*T}=\begin{bmatrix}\hat{\mathbf{T}}_k\\ \tilde{D}_k^{*N}\end{bmatrix} \qquad \mathbf{\Lambda}^*=\begin{bmatrix}diag(\lambda_1,\ldots,\lambda_l) & \mathbf{cov}_{Dt}^T\\ \mathbf{cov}_{Dt} & \sum_{i=(l+1)}^{m}\lambda_i\end{bmatrix} \tag{12}$$



a) If some information about the process is available

b) If the covariance`s are not zero

Fig. 4. Overview of the different calculation methods (PC_i means the scores corresponding to the i^{th} principal component)

The new combined variable is used now instead of the grouped variables. Now the T^2 value is calculated by (13) from this new grouped variable and from the so far non-grouped, remaining $\hat{m}=m-\tilde{m}$ variables that means altogether from $m^*=m-\tilde{m}+1=\hat{m}+1$ variables.

$$T_k^{2*}=\mathbf{T}_k^*\mathbf{\Lambda}^{*-1}\mathbf{T}_k^* \tag{13}$$

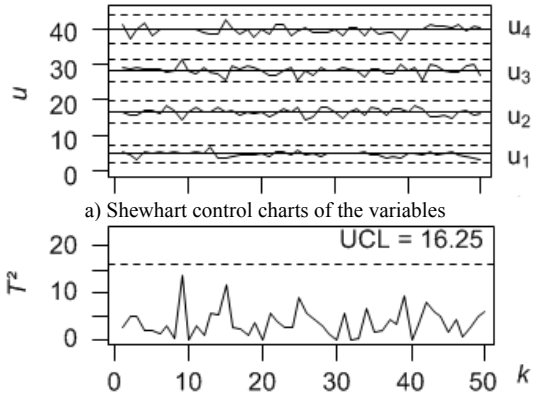
An overview of the whole transformation is shown in Fig. 4. Since $m^*<m$ the control limit UCL^* becomes smaller as if T^2 would have been calculated from all the variables

according to (1) or (7a). Therefore smaller deviations can be detected.

$$UCL^* = \chi^2_{\alpha;m^*} \quad < \quad \chi^2_{\alpha;m} = UCL \tag{14}$$

B. Example

In Fig. 5a the measured data of four independent normally distributed variables are plotted. It can be seen that there is no value outside the control limits (dashed lines). All control limits are calculated for a significance level $\alpha = 1 - P = 0.0027$. The calculated T^2 values are drawn in Fig. 5b. Neither of the plots shows any abnormal condition.



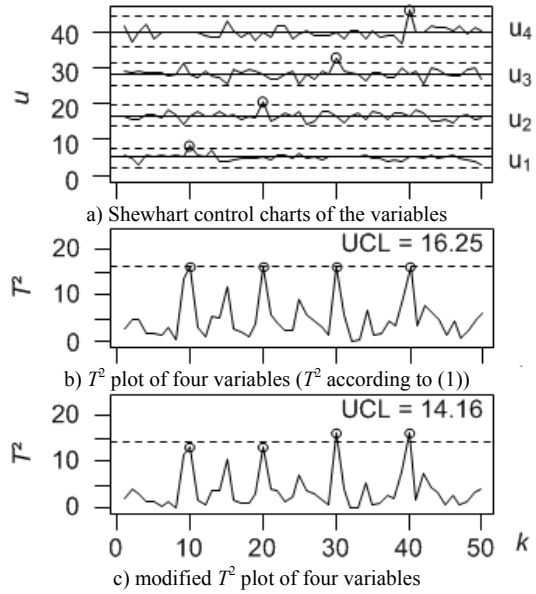
a) Shewhart control charts of the variables

b) T^2 plot of the four variables

Fig. 5. Normal state without any failure

In a second example Fig. 6a shows almost the same data as in Fig. 5a. Each variable is once disturbed with a value of 4.03 times the standard deviation from the mean value. At the same time the non-disturbed variables are equal to their mean value. Therefore the disturbance is similar to the Mahalanobis distance D. All four values are above the upper control limits and are marked by circles. The remaining values are identical to those in Fig. 5 and lie within the control limits. The T^2 values calculated according to (1) are plotted in Fig. 6b. The disturbed values are marked again by circles. As it can be seen, they are located exactly on the control limit (dashed line) in all four cases. The control limit has a value of UCL = 16.25. That means all Mahalanobis distance D_k less than 4.03 are below the control limits. Therefore always a normal state is detected. In Fig. 6c a new T^2 value is shown. For this calculation the first two of the four variables are grouped to a new, normally distributed variable. The T^2 value is calculated by (1) from the new variable and the remaining non-grouped variables (variable 3 and 4). It can be seen, that the disturbances in the grouped variables at k = 10 and k = 20 with a T^2 value of 13.18 are not detected. Only the disturbances in the non-grouped variables at k = 30 and k = 40 with a T^2 value of 16.25 are above the control limit, with a value of UCL = 14.16. Therefore the last two disturbances are detected as abnormal states.

In a third example variable 1 and 2 have a Mahalanobis distance of D = 4.16 and the variables 3 and 4 of D = 3.76. All new T^2 values with grouped variables are equal to the



a) Shewhart control charts of the variables

b) T^2 plot of four variables (T^2 according to (1))

c) modified T^2 plot of four variables

Fig. 6. Four variables with always a single failure

control limit UCL^* = 14.16. If the T^2 value is calculated by (1) without grouped variables, then the last two disturbances at k = 30 and k = 40 are below the control limit with a T^2 value of 14.16. The first two disturbances at k = 10 and k = 20 are above the control limit UCL = 16.25 with a T^2 value of 17.28. By comparing the examples the following points can be found:

- The residual subspace should be grouped.
- The sensitivity for detecting disturbances in the grouped variables is decreased.
- The sensitivity for detecting disturbances in the non-grouped variables is increased.
- A bad sensitivity for the residual subspace is better than calculation of T^2 value without considering it.

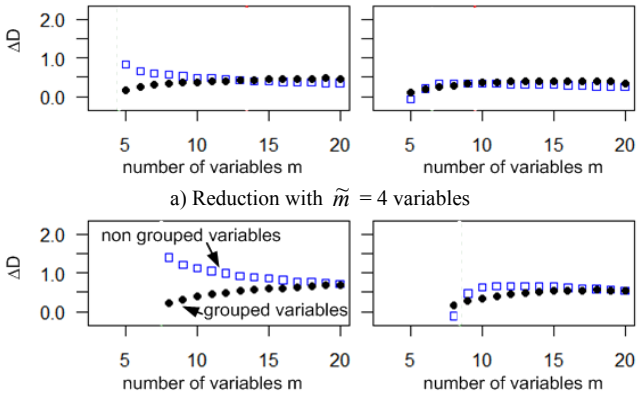
C. Using the new method

In the above section the principle of the new method was explained. The question remains: How too chose the grouped variables. As shown in Fig. 4 there are two possibilities; the first one to use principal components (Fig. 4b) and the second one to use the measured variables (Fig. 4a). In the first case some common known procedures like Kaiser criterion can be used to define the PC's for the residual subspace. By using the presented new method the PC's of the residual subspace have to be grouped. In the second case it is possible to use physical information about the process and the measured data. For example some measurements of machine are observed. Then it is possible to separate variables which indicate faults with a high risk and some with a lower risk. A variable which indicates a fault with high risk could be an acceleration measurement, because the disturbance increases very fast. A variable with lower risk could be the oil temperature, because the disturbance increases slower than the unbalance. The variables with lower risk can be grouped into the residual subspace in the new method. If there is some covariance

between the grouped and ungrouped data, and the new method without PCA (Fig. 4a) is used, it is important to know that in this case the information about covariance between oil temperature (grouped data) and unbalance (ungrouped data) gets lost. In the above example u_1 and u_2 respectively PC_3 and PC_4 are grouped. If a second T^2 value is calculated from the grouped and transformed variable $\tilde{D}^{*N}$ and the PC's which are not used until now, no information is lost (4 independent variables with covariance equal to zero). If an abnormal state is detected, a reverse calculation can be done and the reason for the disturbance can be identified. Thereby disturbances in the ungrouped variables or principal components ($T_k^{2*} \Rightarrow \hat{\mathbf{T}}_k \Rightarrow \mathbf{u}_k$) and also in the grouped variables or grouped principal components ($T_k^{2*} \Rightarrow \tilde{D}_k^{*N} \Rightarrow \tilde{D}_k^{*} \Rightarrow \tilde{T}_k^{2*} \Rightarrow \tilde{T}_k^{2*} \Rightarrow \tilde{\mathbf{T}}_k \Rightarrow \mathbf{u}_k$) can be identified.

D. Test of the new method

The new method was tested for both uncorrelated and correlated data. Here only two examples are shown, how the fault detection sensitivity is increasing for the not grouped variables. For the ungrouped variables (□) Fig. 7 shows the difference ΔD between the smallest detectable disturbance calculated by (1) and the new method. For the grouped variables (●) the difference between the new method and the calculation with (1) is shown.



a) Reduction with $\tilde{m} = 4$ variables

b) Reduction with $\tilde{m} = 7$ variables

Fig. 7 Fault detection sensitivity for m variables uncorrelated on the left side and m correlated variables on the right side.

By comparing the simulated results the following points can be marked out:

- By increasing amount of variables m the difference between the sensitivities in the cases covariance's are zero (left side in Fig. 7) and any covariance (right side in Fig. 7) decrease.
- The sensitivity for smaller amounts of variables m is higher than for many variables, see ΔD. It is easy to see that the difference ΔD corresponds to the difference between the UCL for m variables and UCL* for m* variables. The sloop of the $\chi^2(\alpha,m)$ value defined by (3) in Fig. 1 is for smaller m greater than for more variables.
- The sensitivity increases with the number of grouped variables $\tilde{m}$, see ΔD. Here the same arguments like before can be used. By increasing $\tilde{m} = m - \hat{m}$ variables the difference between UCL and UCL* increases as well.
- The theoretical assumptions are confirmed by the simulations.

III. APPLICATION FOR A GAS ANALYZER

A. Description of the test plant

CO_2 concentration is measured by the gas analyzer AO2000 of ABB. Fig. 8 shows the principal workflow of the test system. The gas is pumped to the detector after drying and absorbing CO_2. The treatment was necessary as the zero point has to be measured by zero (neutral) gas.

It is usual that such a gas analyzer is calibrated once in a week in the industry. In this experiment the calibration was made in every hour. The zero point was measured by air in the room which was prior dried and free of CO_2 because of the absorber. The end point was measured with a cuvette filled with gas with known concentration. The calibration sequence is shown in Fig. 8. If the measured concentrations do not coincide with the known concentration of the calibration gas then the analyzer is recalibrated. These calibration values characterize the quality of the analyzer. Changes in the quality parameter of the gas analyzer are stored as absolute calibration offsets, which mean offsets to an initial value. The changes are scaled as a percentage of the measurement range MR%.

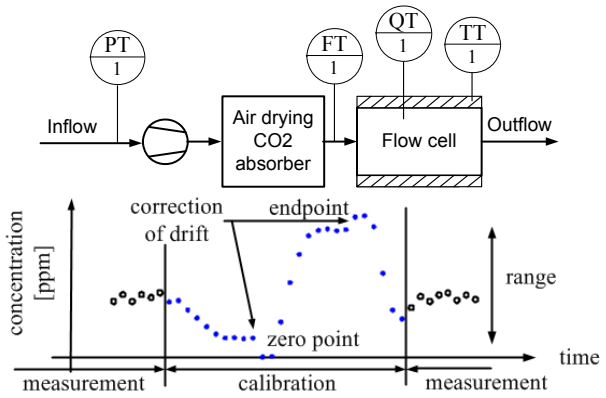


Fig. 8. The test system and the steps of a calibration circuit

The detector unit is tempered in order to keep consistent results. If the cover was opened for maintenance work, a temperature drop could be observed even the case was closed quickly. The flow is measured in order to detect pump failures and absorber blocking. There are two calibration parameters with primary priority:

- zero point offset,
- end point offset

and the three parameters of secondary priority:

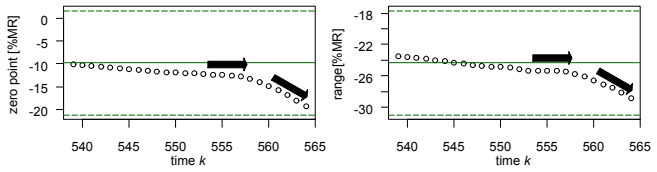
- gas flow,
- detector temperature,

• air pressure in the laboratory

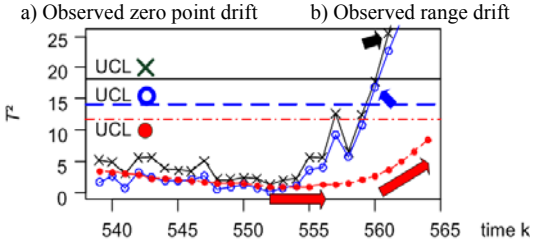
Altogether 5 system parameters are measured and monitored which characterize the analyzer quality.

B. *Off-line analysis of the measured data*

Fig. 9a and b shows typical measurements over 25 samples. At the beginning normal variations caused from changes in temperature, pressure and the CO_2 absorber unit can be seen. The set value (mean value of the training data) is labeled with the solid horizontal line and the Shewhart control chart limits for a probability of P = 99.73% are marked by the dashed lines. From sample k = 550 a drift can be seen. It is caused by students in the same room. Thereby the CO_2 level in the room increased and the room temperature changed.



a) Observed zero point drift b) Observed range drift



c) 3 T^2 values calculated with different methods

Fig. 9. Typical measurements of a gas analyzer in the experimental setup

In Fig. 9c three different T^2 values for the same time period are shown. The first row of T^2 values which is marked by solid circles ● is calculated by (1) from the two primary quality parameters, zero point and range. The corresponding control level is marked by the dot-dashed line. In the observed time period no abnormal condition is detected but an increasing T^2 value can be monitored. If the secondary quality parameters are not used the abnormal condition is not detected even after 12 samples. For the T^2 values which are marked with X also the secondary quality parameters (temperature, pressure and flow) are used for the calculation by (1). The corresponding control level is marked by the solid line. It can be seen, that the abnormal condition is detected at k = 561. So we can conclude, the time difference between the first student enter the laboratory at k = 554 and the detection of the abnormal condition (student in the laboratory) is Δk = 9 samples. For the T^2 values which are marked with ○ all five quality parameters are used. The secondary quality parameters are grouped and transformed to a new Gaussian distributed variable with the new method presented in this paper. The corresponding control level is marked by the dashed line. Now the abnormal condition is detected at k = 560, this means after Δk = 8 samples which is smaller than the second row (X). If the sloop of the drift would be smaller than in the above example then the new method would be more advantageous.

IV. Conclusion

A new method was introduced for reducing the dimension of the Hotelling's statistic in order to detect smaller failures. The basic idea is to group some variables into a combined variable and to calculate the T^2 value from this variable and from the remaining variables. As the new calculated variable has non Gaussian distribution a proper transformation was applied to ensure a Gaussian distribution of the calculated variable. It was shown that those variables or PC's have to be grouped which build the residual subspace or produce faults with lower risk. Comprehensive simulations confirmed the presented method. In an off-line analysis the advantages of the new method where shown exemplary. In the presented application sensor fault of a gas analyzer was detected. Additional practical examples are published in [4]. As explained this new alternative method is different to the observation with sub-grouped data and to multi-block PCA and to the known combined indices based on PCA. A comparative sensitivity analysis of all these methods is planned as a next step. Of course the new method can be applied together with some other methods like T^2 statistic with sub grouped data and can improve their efficiency.

Appendix

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