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MULTIVARIATE STATISTICAL PROCESS MONITORING

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Original scientific paper

Demands regarding production efficiency, product quality, safety levels and environment protection are continuously increasing in the process industry. The way to accomplish these demands is to introduce ever more complex automatic control systems which require more process variables to be measured and more advanced measurement systems. Quality and reliable measurements of process variables are the basis for the quality process control. Process equipment failures can significantly deteriorate production process and even cause production outage, resulting in high additional costs. This paper analyzes automatic fault detection and identification of process measurement equipment, i.e. sensors. Different statistical methods can be used for this purpose in a way that continuously acquired measurements are analyzed by these methods. In this paper, PCA and ICA methods are used for relationship modelling which exists between process variables while Hotelling's (T^2), I^2 and Q (SPE) statistics are used for fault detection because they provide an indication of unusual variability within and outside normal process workspace. Contribution plots are used for fault identification. The algorithms for the statistical process monitoring based on PCA and ICA methods are derived and applied to the two processes of different complexity. Apart from that, their fault detection ability is mutually compared.

Keywords: *process monitoring, fault detection, fault identification, PCA, ICA, contribution plot*

Multivarijantni statistički nadzor procesa

Izvorni znanstveni članak

U industrijskoj proizvodnji prisutan je stalni rast zahtjeva, u prvom redu, u pogledu ekonomičnosti proizvodnje, kvalitete proizvoda, stupnja sigurnosti i zaštite okoliša. Put ka ispunjenju ovih zahtjeva vodi kroz uvođenje sve složenijih sustava automatskog upravljanja, što ima za posljedicu mjerenje sve većeg broja procesnih veličina i sve složenije mjerne sustave. Osnova za kvalitetno vođenje procesa je kvalitetno i pouzdano mjerenje procesnih veličina. Kvar na procesnoj opremi može značajno narušiti proizvodni proces, pa čak prouzrokovati ispad proizvodnje što rezultira visokim dodatnim troškovima. U ovom radu se analizira način automatskog otkrivanja kvara i identifikacije mjesta kvara u procesnoj mjernoj opremi, tj. senzorima. U ovom smislu mogu poslužiti različite statističke metode kojima se analiziraju podaci koji pristižu iz mjernog sustava. U radu se PCA i ICA metode koriste za modeliranje odnosa među procesnim veličinama, dok se za otkrivanje nastanka kvara koriste Hotellingova (T^2), I^2 i Q (SPE) statistike jer omogućuju otkrivanje neobičnih varijabilnosti unutar i izvan normalnog radnog područja procesa. Za identifikaciju mjesta (uzroka) kvara koriste se dijagrami doprinosa. Izvedeni algoritmi statističkog nadzora procesa temeljeni na PCA metodi i ICA metodi primijenjeni su na dva procesa različite složenosti te je uspoređena njihova sposobnost otkrivanja kvara.

Ključne riječi: *nadzor procesa, detekcija nastanka kvara, identifikacija mjesta kvara, PCA, ICA, dijagram doprinosa*

1 Introduction

Process safety and environment pollution demands are continuously increasing in the process industry. Apart from that, requirements regarding final product quality and production efficiency are higher and higher [1]. This can be achieved by applying advanced process monitoring and control techniques. Process control is heavily dependent on the quality of the data, so it is crucial to measure as many process variables as it is possible and to develop advanced process measurement system [2, 3].

Production outage can be caused by different abnormal situations:

- Equipment failure
  - plant failure (e.g. actuator failure),
  - measurement equipment failure (sensor failure),
  - communication system failure (measurement and control data are not transmitted).
- Large disturbances (when disturbance values exceed compensation limits).

Different plant failures can be very dangerous, especially in chemical plants, so it is important that methods for process monitoring should be able to detect such different abnormal situations. In many cases, equipment failure negatively affects the plant production and product quality. The most dangerous failures are those in measurement equipment because the overall system for production system control relies on measurements. Process control action based on data that come from faulty sensor is at best inefficient and at worst dangerous. Therefore, it is important to check the meaningfulness of the collected measurement data, before they are forwarded to the automatic control system for further processing. In this paper faults of measurement system are considered in more details.

In modern plants there are many process variables which are measured by sensors and logged to process database so the amount of available data is large. Under normal operating conditions these variables are highly correlated due to physical and chemical principles. These relationships can be modelled and the obtained model can then be used to check on new process data in order to detect abnormal process situations [2].

Since the model is built from the plant data, it is important to choose proper modelling technique. Multivariate analysis techniques can be used for analyzing highly correlated process data and process monitoring. Such approach is usually called multivariate statistical process monitoring (MSPM) and has found wide applications in different industrial processes, including chemicals, polymers, microelectronics manufacturing and pharmaceutical processes. Basically, statistical process monitoring is composed of the two main parts: fault detection and fault identification.

MSPM performance depends on how well the model describes relationships between the variables. The most common method for modelling these relationships is Principal Component Analysis (PCA) [2, 4]. However, PCA assumes linear relationships between variables and Gaussian latent variables. Hence, it can be inefficient when dealing with industrial processes which are usually highly nonlinear and have non-Gaussian underlying variables.

Recently, new techniques such as Independent Component Analysis (ICA) [5] and different kernel methods [6] appeared. These methods can sometimes exploit plant data in a more efficient way than PCA method.

The paper is organized as follows. Section 2 describes the basics of PCA and ICA method. Tasks that are part of statistical process monitoring and fault analyzing are described in Section 3 in more details. Section 4 shows the application of the statistical process monitoring algorithms on selected processes. Section 5 provides summary and conclusion of this paper.

2 Multivariate statistical methods

Modern industrial plants are often equipped with a large number of sensors which measure different process variables. These measured data, acquired through a couple of years and accumulated in the process database, can be a useful source of information for abnormal situations detection and explanation of their roots. In order to detect abnormal process events a number of multivariate statistical process monitoring (MSPM) approaches were developed. MSPM methods are basically algorithms that can be used for extracting important information from large multivariable data sets such as plant data. Therefore, the key feature of such methods is the possibility to handle highly correlated, highly dimensional and noisy data. MSPM methods describe original data by the reduced set of variables which in turn makes analysis of the data much easier. Usually MSPM consists of the following steps [7]:

1. building data-based model from normal process data (i.e. historical data of normal process operation),
2. new data projection (according to the built model),
3. judging whether the new data are statistically normal or abnormal against the normal process behavior captured by historical normal data,
4. identifying the variables responsible for the process to go out of control,
5. determining the root cause of the abnormality.

Principal Component Analysis (PCA) and Partial Least Squares (PLS) are the two most commonly used methods for process monitoring [2, 8]. Since PCA is a conceptually simpler technique and since it does not require target variable measurements, PCA based monitoring is found more often in practice than PLS based. In recent time another method has gained on popularity, namely independent component analysis (ICA) [5]. However, these methods assume linear variable interrelationship which is rarely found in practice. Nonlinear methods such as kernel PCA (KPCA) and kernel ICA (KICA) [6] have appeared recently and can overcome classical PCA and ICA disadvantages in process monitoring. Time-varying process behaviour is an aspect of great importance in MSPM. Therefore, different adaptive mechanisms for the mentioned methods are continuously being proposed. However, this aspect is beyond the scope of this paper, so adaptive MSPM methods are only briefly mentioned in section 2.3.

2.1 PCA based methods

The starting point in any multivariate analysis is the data matrix, $\boldsymbol{X}$, whose elements are the measured data obtained by measurements carried out in the process. m columns of matrix $\boldsymbol{X}$ are called objects (often correspond to some chemical or process measurement samples), and n rows of matrix $\boldsymbol{X}$ stands for the dimension of input space (corresponds to the number of measured variables that form object).

PCA is a method for the projection of the high-dimensional, correlated input space into the appropriate lower dimensional subspace, a latent space. In the input data space PCA searches for directions with the biggest data variations, provided that these directions are orthogonal, and uses them as a primary axis of a new coordinate system in which the input space is then projected [4]. Thereby PCA transforms correlated variables into the set of new uncorrelated variables which are called principal components (PCs). Apart from being uncorrelated, the new variables are sorted by the size of data variation that they describe. The largest principal components are used for the process variable estimation while the smallest ones are used for the fault detection and fault identification. Illustration of the PCA method is given in Fig. 2.

In PCA the $n \times m$ data matrix $\boldsymbol{X}$ is decomposed into the sum of the product of n pairs of vectors [2, 4]:

$$\boldsymbol{X} = \boldsymbol{T}\boldsymbol{P}^{\mathrm{T}} + \boldsymbol{E} = \boldsymbol{T}\boldsymbol{P}^{\mathrm{T}} + \widetilde{\boldsymbol{T}}\widetilde{\boldsymbol{P}}^{\mathrm{T}} = \begin{bmatrix}\boldsymbol{T} & \widetilde{\boldsymbol{T}}\end{bmatrix}\begin{bmatrix}\boldsymbol{P} & \widetilde{\boldsymbol{P}}\end{bmatrix}^{\mathrm{T}} = \overline{\boldsymbol{T}}\,\overline{\boldsymbol{P}}^{\mathrm{T}}, \quad (1)$$

where $\boldsymbol{T}^{n\times l}$ and $\boldsymbol{P}^{m\times l}$ are the principal component scores and loadings, $\boldsymbol{E}^{n\times m}$ is residual and l is the number of principal components. Since columns of $\boldsymbol{P}$ are eigenvectors of correlation matrix associated with l largest eigenvalues, and $\widetilde{\boldsymbol{P}}$ are the remaining vectors, calculation of the $\boldsymbol{P}$ (PCA model) is reduced to eigenvector problem.

Eigenvectors can be determined one by one, for example by NIPALS method - sequential determination procedure, or all at once, for example by SVD method – simultaneous determination procedure. Once the eigenvectors are determined, projections of the data onto the eigenvectors can be made. These projections are called "scores" and are often useful for showing the relationships between the samples in the data set.

When PCA is applied to data set it is often found that only the first few eigenvectors are associated with systematic variation in the data, i.e., important phenomena in the data, while the remaining eigenvectors are associated with noise, i.e., false phenomena in the data. PCA model is formed by retaining only the eigenvectors which describe systematic variation in the data. Once the PCA model is formed, new data can be viewed as projections onto eigenvectors.

For a reduced order model $\boldsymbol{P}_l$ (where only the first l of total m eigenvectors were retained) and a new sample $\boldsymbol{x}_i^{l\times m}$, its projection is:

$$\widehat{\boldsymbol{x}}_i = \boldsymbol{t}_i\boldsymbol{P}_l^{\mathrm{T}} = \boldsymbol{x}_i\boldsymbol{P}_l\boldsymbol{P}_l^{\mathrm{T}}, \quad (2)$$

where $\widehat{\boldsymbol{x}}_i^{l\times m}$ is the projection of the sample vector on the principal component subspace (PCS), $\boldsymbol{t}_i^{l\times l}$ is a vector of scores of the model $\boldsymbol{P}_l$ for the sample $\boldsymbol{x}_i$.

Different extensions of PCA method were proposed to enhance its monitoring capability (see Fig. 2). In [9] PCA and PLS method is extended to situations where the processes can be naturally blocked into subsections. This multiblock PCA (MBPCA) method is useful in monitoring complex processes [10]. Another useful extension is dynamic PCA (DPCA) method proposed in [11] where lagged measurements were used to take into account process dynamics. Multiscale PCA (MSPCA), which was proposed in [12], combines wavelet analysis and PCA method. MSPCA simultaneously extracts cross-correlation across the sensors (by PCA method) and auto-correlation within a sensor (by wavelet analysis) [13]. Since PCA is a linear method, it can be inefficient, unreliable and misleading when it is used for highly nonlinear process monitoring. To extract nonlinear relationship between variables, nonlinear PCA based monitoring scheme was proposed. Kernel PCA (KPCA) [14] gained much attention recently since it does not involve nonlinear optimization procedure. In [15] dynamic kernel PCA (DKPCA) was developed for monitoring purposes. In [16, 17] wavelet analysis is combined with KPCA which results in multiscale KPCA (MSKPCA). The exstensions and modifications of the PCA method are summarized in Fig. 1.

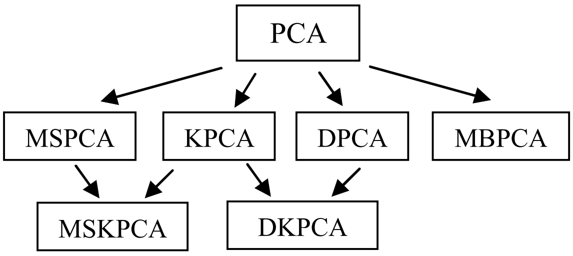

Figure 1 PCA based methods

2.2 ICA based methods

Statistical process monitoring method that uses Independent Component Analysis (ICA) was proposed in [18, 19]. While PCA projects correlated variables onto the set of new variables which are uncorrelated, the goal of ICA is to decompose data into linear combinations of statistically independent components (ICs). Since the measured process variables are usually a combination of independent variables that are not directly measurable, process monitoring based on ICA method can be quite superior to the PCA based monitoring.

The measured variables are assumed to be linear mixtures of some unknown latent variables (ICs), where the mixing matrix of coefficients is also unknown. m measured variables that are collected in matrix $\boldsymbol{X}^{m\times n}$ can be presented as a linear combination of l $(l\leq m)$ unknown independent components (note that ICA uses transposed data matrix in respect to PCA):

$$\boldsymbol{X} = \boldsymbol{AS} + \boldsymbol{E}, \tag{3}$$

where $\boldsymbol{A}^{m\times l}$ is the unknown mixing matrix, $\boldsymbol{S}^{l\times n}$ is the independent component matrix and $\boldsymbol{E}^{m\times n}$ is the residual matrix. Therefore, ICA seeks to extract these independent components as well as the mixing matrix of coefficients only from the available measured data. This objective of ICA can be defined alternatively, i.e. to find demixing matrix $\boldsymbol{W}^{l\times m}$ such that rows of reconstructed component matrix $\hat{\boldsymbol{S}}$ [19]:

$$\hat{\boldsymbol{S}} = \boldsymbol{WX}, \tag{4}$$

become independent of each other as much as possible. Demixing matrix $\boldsymbol{W}$ is found by the following equation:

$$\boldsymbol{W} = \boldsymbol{B}^{\mathrm{T}}\boldsymbol{Q}, \tag{5}$$

where $\boldsymbol{B}$ is orthogonal matrix obtained by the whitening transformation and $\boldsymbol{Q}$ is matrix which is obtained by the eigendecomposition of covariance data matrix [19]. In [20] fast and robust fixed point algorithm for calculating matrix $\boldsymbol{B}$ (and demixing matrix $\boldsymbol{W}$ respectively), known as FastICA, can be found.

Dimension reduction in ICA is based upon belief that measured variables are the mixtures of a smaller number of independent variables. In contrast to PCA method, selection of independent components is not trivial task. In this paper L_2 norm of rows in demixing matrix $\boldsymbol{W}$ is used for choosing the most important independent components [5].

Since original ICA algorithm has several drawbacks, extensions of ICA method were made to enhance ICA based process monitoring. In original ICA number of ICs is equal to the number of measured variables which means that some unimportant ICs are also extracted from the measured data. Apart from that, ICs are not sorted according to their importance like in PCA method. In [7] modified ICA is proposed which extracts only few dominant ICs, determine the order of ICs and gives a consistent solution. To take process dynamics into consideration, dynamic ICA (DICA) was proposed in [21] and its further modification in [22]. Also different nonlinear versions of the ICA method were reported (e.g. [23]) or hybridizations with SVM or PCA (e.g. [24, 25]).

2.3 Adaptive multivariate statistical methods

Static models which are usually used in MSPM have some major drawbacks. Sometimes available normal operating data are not sufficient for developing reliable process model. Therefore, it is desirable to update the model with every new sample which is found to be normal. Apart from that, industrial processes usually exhibit some kind of time-varying behavior which static models can interpret as a fault. To decrease the number of false alarms the model should be updated in order to better represent current state of the process.

Adaptive models are models which possess the ability to automatically change their properties during online operation [26]. Generally there are two ways to adapt the model. First one updates offline built model in moving window manner in a way that the model is recalculated on the data contained in a window which slides across the data as the new data are collected. More efficient approach is recursive which combines the old model with the newly acquired data. Adaptive process monitoring can be found in [27-29].

3 Dealing with faults

When a model is built from normal process data by using PCA or ICA method, the model can be used for detecting and identifying unusual process conditions such as process and sensors faults. Monitoring statistics are used for fault detection and contribution plots are usually used for fault identification. In the following sections sensors faults will be examined in more details.

3.1 Fault detection

Fault detection is determining whether a fault has occurred. Multivariate statistical techniques can be used to detect the following abnormal sensor conditions:

- the measurements reach unusual values, often caused by a major sensor failure,
- multiple sensors can deviate from normal correlations,
- the monitored process undergoes transient variations [30].

For fault detection, the PCA model of the process is developed, based on normal operating process data, and then used to check new measurement data. The differences between the new measurement data and their projections to the built model, the residuals, are then subjected to some sort of statistical test to determine if they are significant. Usually the Q statistic, also called squared prediction error (SPE), and the Hotelling's (T^2) statistic are used to represent the variability in the residual subspace and principal component subspace [2].

The Q statistic shows how well a new sample fits into the PCA model built on previous measurement data. It is a measure of the difference (residual) between the sample and its projection onto the l principal components retained in the model. The residual $\boldsymbol{r}_i$ for sample $\boldsymbol{x}_i$ is given by:

$$\boldsymbol{r}_i = \boldsymbol{x}_i - \hat{\boldsymbol{x}}_i = \boldsymbol{x}_i(\boldsymbol{I} - \boldsymbol{P}_l\boldsymbol{P}_l^{\mathrm{T}}). \tag{6}$$

The magnitude of the residual for any sample $\boldsymbol{x}_i$ is:

$$Q = \|\boldsymbol{r}_i\| = \boldsymbol{r}_i\boldsymbol{r}_i^{\mathrm{T}} = \boldsymbol{x}_i(\boldsymbol{I} - \boldsymbol{P}_l\boldsymbol{P}_l^{\mathrm{T}})\boldsymbol{x}_i^{\mathrm{T}}, \tag{7}$$

and represents the "goodness of fit" of the new sample to the model $\boldsymbol{P}_l$ as a scalar. It can be calculated by taking the sum of squares of the components of $\boldsymbol{r}_i$.

Approximate confidence limits can be calculated for the model residual, Q, provided that all the eigenvalues of the covariance matrix are known:

$$Q_\alpha = \Theta_1\left[\frac{c_\alpha\sqrt{2\Theta_2 h_0^2}}{\Theta_1} + 1 + \frac{\Theta_2 h_0(h_0-1)}{\Theta_1^2}\right]^{\frac{1}{h_0}}, \tag{8}$$

where:

$$\Theta_i = \sum_{j=k+1}^{n}\lambda_j^i \quad \text{za } i = 1,2,3, \tag{9}$$

$$h_0 = 1 - \frac{2\Theta_1\Theta_3}{3\Theta_2^2}, \tag{10}$$

where:
Q_α – upper confidence limit for the model residual Q with significant level α,
c_α – normal deviate corresponding to the upper (1 – α) percentile.

The measurements of three process variables together with the result of PCA method are shown in Fig. 2. Two "suspicous" samples can be also observed. The sample with large Q value is out of the plane of the model, although its projection into the model is not unusual. The calculated Q limit is based on the data used to form the PCA model. It defines a distance off the plane, formed by eigenvectors, that is considered unusual. Therefore, Q statistic represents variations not explained by the retained PCs.

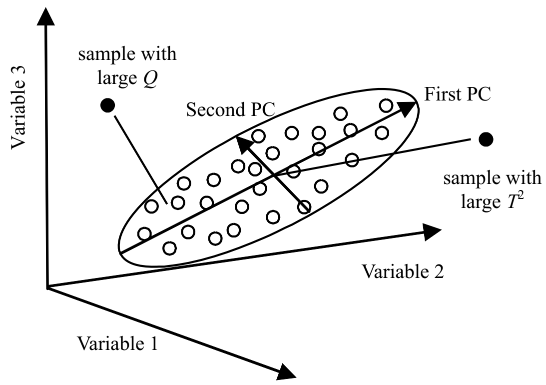

Figure 2 Data projection on two PCs

Hotelling's (T^2) statistic provides an indication of unusual variability within the normal subspace. The value of T^2 for one sample is equal to the sum of squares of the adjusted (unit variance) scores on each of the principal components in the model:

$$T^2 = \sum_{i=1}^{l}\left(\frac{\boldsymbol{t}_i}{\lambda_i}\right)^2. \tag{11}$$

T^2 represents the squared length of the projection of the current sample into the space spanned by the PCA model of the data. It is an indication of how far the PCA estimate of the sample (2) is from multivariate mean of the data, i.e., the intersection of the principal components (Fig. 2). Therefore, if sample has an abnormal value of T^2 but Q value below the limit, it is not necessarily a fault – it can also be a change of the operating region. The statistical confidence limits for the values of T^2 can be calculated according to statistical F-distribution as follows:

$$T_{l,n,\alpha}^2 = \frac{l(n-1)}{n-l}F_{l,n-l,\alpha}, \tag{12}$$

where:
n – number of samples in the data set used in the calculation of the PCA model,
l – number of retained principal components,
α – parameter of the standard normal deviate.

The T^2 limit defines an ellipse on the plane within the data are assumed to be normal (Fig. 2).

Process monitoring based on ICA is similar to the monitoring based on PCA. When ICA model is derived from normal process data with FastICA algorithm, matrices $\boldsymbol{W}$, $\hat{\boldsymbol{S}}$, $\boldsymbol{B}$, $\boldsymbol{Q}$ and $\boldsymbol{A}$ are obtained. By selecting the most dominant ICs reduced matrix $\boldsymbol{W}_l$ and remaining matrix $\boldsymbol{W}_e$ are formed. Matrices $\boldsymbol{B}_l$ and $\boldsymbol{B}_e$ are obtained according to the equation (5). Now, $\hat{\mathbf{s}}_l$ and $\hat{\mathbf{s}}_e$ for the new sample $\boldsymbol{x}_i^{m\times l}$ can be calculated:

$$\hat{\mathbf{s}}_l = \boldsymbol{W}_l\boldsymbol{x}_i, \tag{13}$$

$$\hat{\mathbf{s}}_e = \boldsymbol{W}_e\boldsymbol{x}_i. \tag{14}$$

In ICA based monitoring three statistics are used for process monitoring. I^2 statistics is defined as sum of the independent scores:

$$I^2 = \hat{\boldsymbol{s}}_l^{\mathrm{T}} \hat{\boldsymbol{s}}_l. \tag{15}$$

I^2 statistics is used to monitor the systematic part of process variations. I_e^2 statistic is similarly defined but it monitors the non-systematic part of measurements and therefore provides detection of some special events that enter the process. Q or SPE statistic is defined like in PCA based monitoring:

$$Q = (\boldsymbol{x}_i - \hat{\boldsymbol{x}}_i)^{\mathrm{T}} (\boldsymbol{x}_i - \hat{\boldsymbol{x}}_i), \tag{16}$$

where $\hat{\boldsymbol{x}}_i$ is defined as:

$$\hat{\boldsymbol{x}}_i = \boldsymbol{Q}^{-1} \boldsymbol{B}_d \boldsymbol{W}_d \boldsymbol{x}_i. \tag{17}$$

Since the variables in ICA do not follow Gaussian distribution, kernel density estimators are used for calculating confidence limit of I^2, I_e^2 and Q statistics [19]:

$$f(x) = \frac{1}{nh} \sum_{i=1}^{n} K\left(\frac{x - x_i}{h}\right), \tag{18}$$

where f is density function, n is number of samples, h is smoothing parameter, x_i are observed values and K is kernel function. Control limit of normal operating data is point occupying 99 % of area under density function. In this paper kernel density estimator with Gaussian kernel function is used.

3.2 Fault identification (fault diagnosis)

After a fault is detected, it is important to diagnose the cause of failure. So far, the most popular approach to diagnosis is the use of contribution plots. A faulty sensor usually breaks down the normal correlation with the remaining sensors. This feature can be used to identify the faulty sensor after an abnormal condition is detected. The contribution plot uses the residual of each sensor at every sample to identify the sensors related to a detected fault. The sensor with the largest error is considered faulty, since it has a major contribution to the squared prediction error used for fault detection. To show the contribution of each variable to the total amount of the residual, equation (7) is written in the form:

$$Q = \sum_{i=1}^{m} \boldsymbol{r}_i^2 = \sum_{i=1}^{m} Q_i, \tag{19}$$

where $\boldsymbol{r}_i$ is contribution of the i-th variable. Variable contribution for PCA T^2 statistics and ICA I^2 statistics can be found in [5].

Usually it is possible to reconstruct sensor faults based on multivariate statistical models to maintain process control and optimization [1].

4 Implementation of the derived algorithms for fault detection and identification

Based on the theoretical expressions, PCA and ICA based algorithms for fault detection and identification are derived and implemented. To analyze fault detection and identification ability of those methods, proposed algorithms are applied to the two different processes whose simulation models were made in Matlab/Simulink.

The first one is the process of liquid storage in two coupled tanks (Fig. 3). In this process, common sensor errors like drift and bias are simulated. The algorithm based on PCA is used for detection and identification of these conditions. The second process is the more complex process of liquid storage (Fig. 4). Data obtained by the simulation were used for PCA and ICA model building which are then used for detection of faulty samples.

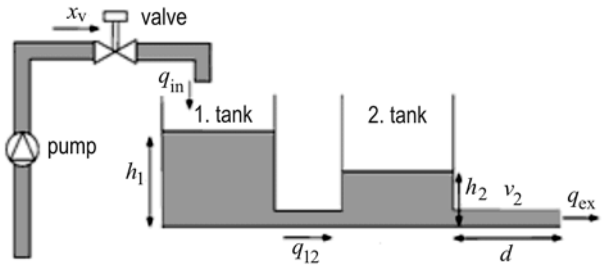

Figure 3 Process of liquid storage in the two coupled tanks

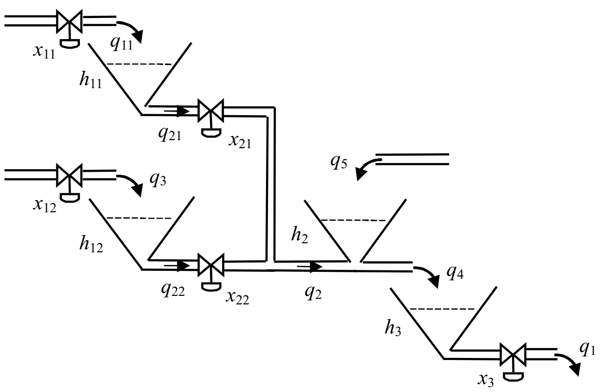

Figure 4 Principal schema of complex fluid storage process

4.1 Statistical process monitoring based on PCA

The basic procedure for the SPM based on the PCA method can be derived according to the section 2.1 that covers PCA model building and sections 3.1 and 3.2 that deal with fault detection and fault identification. The proposed algorithm for a fault detection and identification consists of the following steps:

1. Data standardization:
- Scaling and centering of the input data matrix that is used for process model building.
2. PCA model building:
- Covariance matrix calculation based on standardized input data matrix,
- Eigenvalues and eigenvectors calculation,
- Number of principal components selection that will be retained in the model,
- Q (SPE) and Hotellings (T^2) confidence limits calculation.

3. Test of the new data:
- Scaling and centering of the new data,
- Projection of new data to the existing PCA model,
- Q and T^2 values calculation for each sample,
- If Q or T^2 sample values exceed the confidence limits, fault has occurred.

If any abnormality is detected, draw contribution plot and find the responsible variables (sensors).

A. MSPM of the fluid storage process in the two coupled tanks

Simple process of the liquid flow and level control in the two coupled tanks is shown in Fig. 3. These tasks are very common in the process industry. Regulation is implemented through a controllable valve at the entrance. Measured data are generated by simulation and algorithms for fault detection and identification are applied on the obtained data. Three variables are measured: input flow q_{in}, output flow q_{ex} and flow q_{12}. In order to obtain more realistic process data, a noise was added to the simulated measurement data. Obtained data matrix consists of 3 variables and 1000 samples. Once the data have been normalized, PCA method can be applied. Implementation of PCA method in Matlab is based on singular value decomposition. Tabs. 1 and 2 show the obtained eigenvectors and variances described by the PCA model.

Table 1 Eigenvectors

Loadings coefficients	Eigenvector 1	Eigenvector 2	Eigenvector 3
1.	0,5629	0,6915	0,4528
2.	0,6092	0,0231	–0,7927
3.	0,5585	–0,7221	0,4083

Table 2 Variance described by the PCA model

Eigenvector	Eigenvalue	%Variance	%Total variance
1.	2,6755	89,1831	89,1831
2.	0,3137	10,4561	99,6392
3.	0,0108	0,36080	100,0000

It can be seen that the first eigenvector describes 89 % of the variance in the data and that the first two eigenvectors together describe even more than 99 % of the total variance in the data. From this it can be concluded that the observed process variables are strongly correlated. Also, by looking at the eigenvalues, it can be seen that the eigenvector with the biggest eigenvalue describes the biggest variance in the data. It represents the first principal component, and since it captures most data variation (89 %), it is enough to remain only this first component in the PCA model. So, the data will be projected onto the one principal component.

Obtained PCA model could be used to check for new measurement data and sensor fault detection. In order to detect sensor fault, confidence limits must be determined according to equations (8) and (12):

Q confidence limit = 2,61,

T^2 confidence limit = 7,99.

Now, when confidence limits are calculated, the built model can be used to check on new data. The first example of sensor fault is sensor drift which was simulated by the slope of 0,00005 that was added to the sensor value and which takes effect after 50 seconds. The new data matrix has 11 samples. To detect sensor failure, new data have to be standardized firstly, but with the standardization parameters that were used in model building procedure. Then, based on the obtained model and new standardized data, Q and T^2 values for the new measurement samples are calculated. The obtained values are shown in Figs. 5 and 6. Confidence limits are marked with lines. It can be seen that the T^2 values of all the samples are below the limit. However, Q values of some samples have exceeded the confidence limit, from which it can be concluded that sensor fault has occurred. Contribution plots are used for faulty sensor identification. Since Q values actually represent the amount of residual for each sample, it is necessary to find the variable (sensor) that most contributes to the large amount of residual. Fig. 7 shows the contributions of individual variables to the residuals of each sample. It can be concluded that the first sensor is faulty.

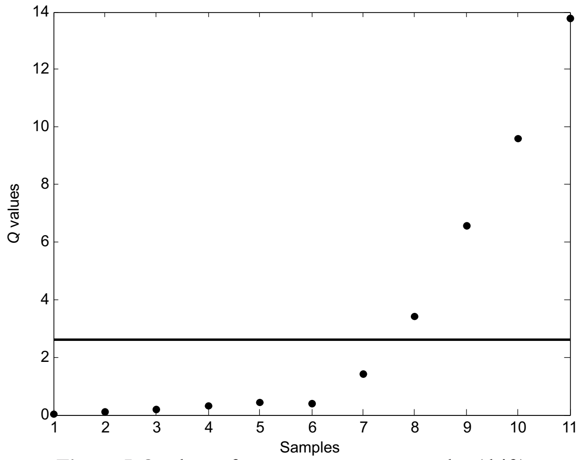

Figure 5 Q values of new measurement samples (drift)

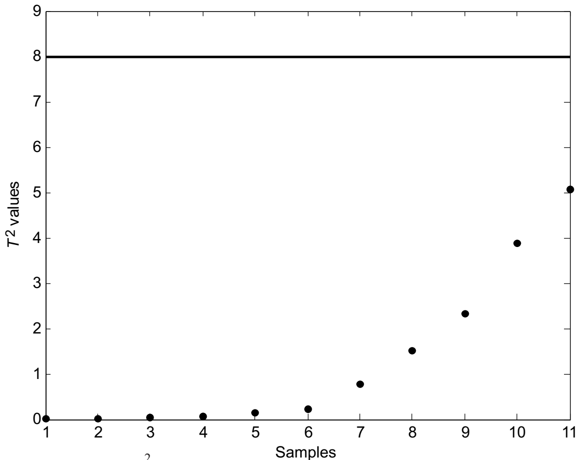

Figure 6 T^2 values of new measurement samples (drift)

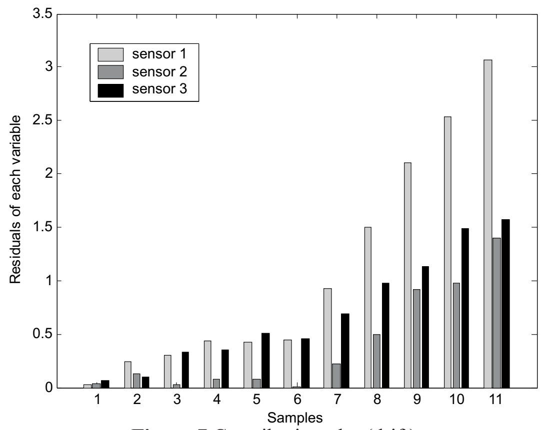

Figure 7 Contribution plot (drift)

Another type of possible sensor failure is bias. In order to simulate bias in Matlab/Simulink, a constant amount of 0,005 is added to the second sensor. The resulting Q and T^2 values of the samples are shown in Figs. 8 and 9. In this case, T^2 and Q values of all the samples are above the confidence limits. The contribution plot in Fig. 10 shows that the second sensor is faulty.

B. SPM of the complex process of liquid storage

Second process is the complex process of liquid storage (Fig. 4). Simulation model of the process was made and sets of measurement data with different properties were formed. The process consists of four liquid tanks with sloping walls, of which the first three are mutually coupled. Controllable valves are located at the entrances and exits of the first two tanks and at the exit of the fourth tank. The third tank,

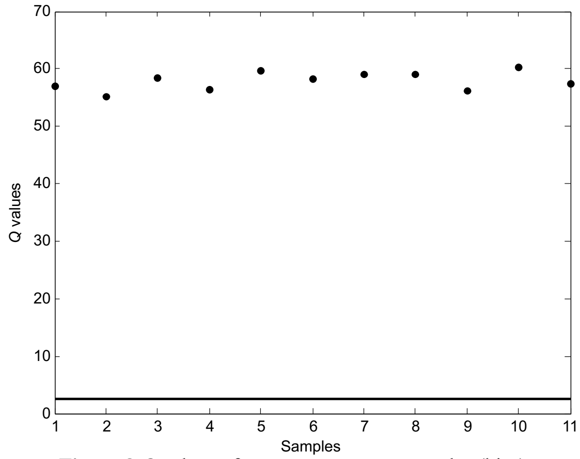

Figure 8 Q values of new measurement samples (bias)

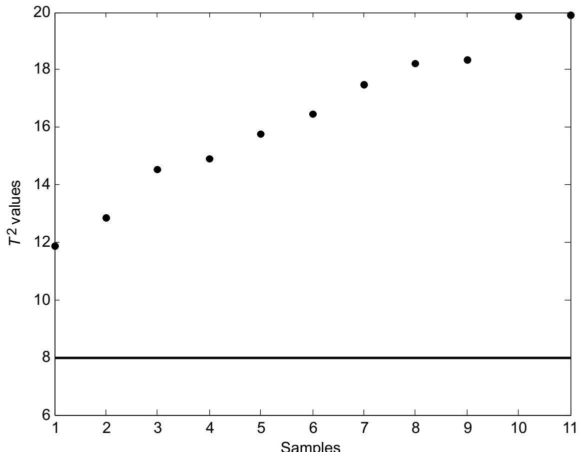

Figure 9 T^2 values of new measurement samples (bias)

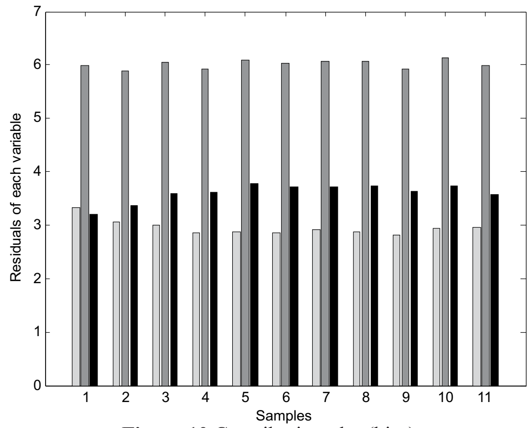

Figure 10 Contribution plot (bias)

except the resulting flow from the first two tanks has an additional liquid flow, which by nature is a random variable. 13 variables are measured: positions of all the controllable valves (in total there are 5) and all the flow rates (input and output flows of the first two tanks, the resultant flow in the third tank, the additional flow of the third tank, the output flow of the third tank and the output flow of the fourth tank). 1000 samples with a noise were generated which represent normal process behavior and which are used for PCA model building. By applying the PCA method, 13 eigenvectors were obtained from which 5 remained in the model, i.e., measurement data were projected to the 5 principal components. Confidence limits are obtained according to (8) and (12):

Q confidence limit = 11,69,

T^2 confidence limit = 15,25.

The built model is used to check the test data. 50 test samples with the noise were generated. To simulate sensor errors of random magnitude were added to 21 test sample. Q and T^2 values of the test measurement samples are shown in Figs. 11 and 12.

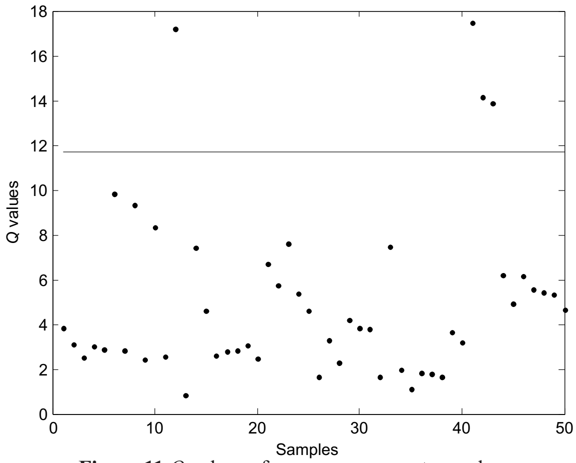

Figure 11 Q values of new measurement samples

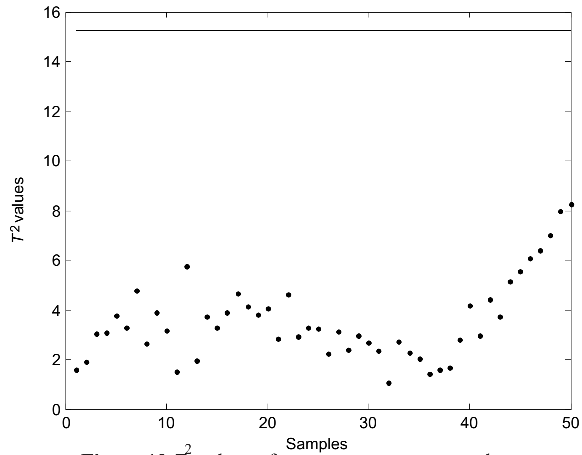

Figure 12 T^2 values of new measurement samples

In this case, statistics did not register all incorrect measurements probably because the added errors were small in magnitude. Identification of the faulty sensor can be done in similar way like in first example using contribution plots. However, there are more variables used for modelling and there can be several faulty sensors at the same time, so contribution plots are not so clear as in Figs. 7 and 10. Hence, it is more difficult to detect which sensor is faulty.

4.2 Statistical process monitoring based on ICA

The basic procedure for the SPM based on the ICA method can be derived according to the section 2.2 that covers ICA model building and sections 3.1 and 3.2 that deal with fault detection and fault identification. The proposed algorithm for a fault detection and identification consists of the following steps:

1. Data standardization:
   - Scaling and centering of the input data matrix that is used for process model building.
2. ICA model building:
   - Calculation of matrices ***B***, ***W*** and ***Q*** with FastICA algorithm**,**
   - Selection of independent components according to the L_2 norm of rows in the matrix ***W***,
   - Q (SPE) and I^2 statistics confidence limits calculation.
3. Test of the new data:
   - Scaling and centering of the new data,
   - Projection of the new data to the existing ICA model,
   - Q and I^2 values calculation for each sample,
   - If Q or I^2 sample values exceed the confidence limits, fault has occurred.

Similarly like in PCA based monitoring, if any abnormality is detected, contribution plots can be used to find the responsible variables (sensors).

ICA based process monitoring is applied only to the complex process of liquid storage to show advances over PCA method. Like in PCA based monitoring, ICA model was developed on 1000 samples which represent normal process behavior. 13 independent components were obtained and, according to the L_2 norm of rows of matrix ***W*** (see Fig. 13), it is sufficient to retain only first four independent components.

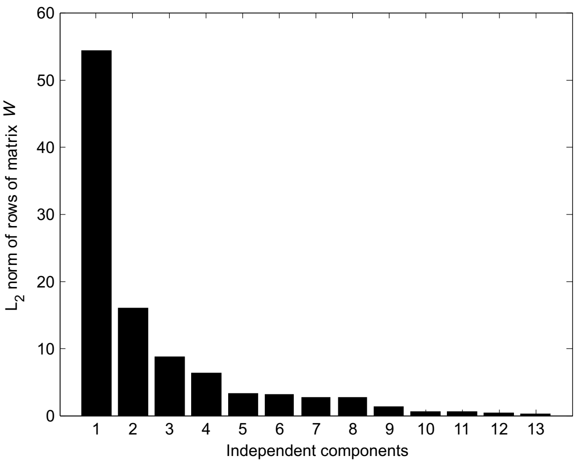

Figure 13 L_2 norm of rows of matrix ***W***

Confidence limits are obtained according to (13), (14) and (16) with kernel density estimators:

I^2 confidence limit = 14,37,

I_e^2 confidence limit = 37,40,

Q confidence limit = 30,45.

From Fig. 14 it can be noticed that ICA based monitoring is more sensitive, i.e. it has better detection capabilities than PCA method (ICA based monitoring revealed 14 while PCA detected only 4 faults of total 21 sensor faults). This means that ICA can extract true factors that drive the process. However, it is interesting to notice that in ICA based monitoring all faults were detected by I^2 statistics while in PCA based monitoring with Q statistics. Since I^2 statistic is similar to T^2 statistic, it measures systematic variations in IC subspace. So, it can be concluded that erroneous samples violate normal correlation between variables in ICA based monitoring. However, this can also indicate change of the operating region. I_e^2 statistic for the test samples is not presented because it did not show any important information about sensor faults.

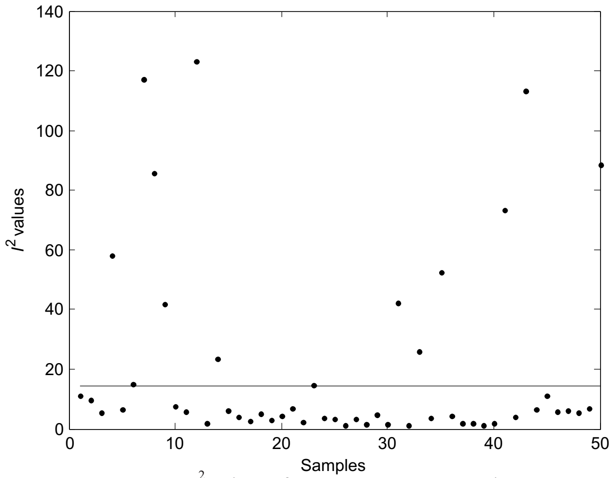

Figure 14 I^2 values of test measurement samples

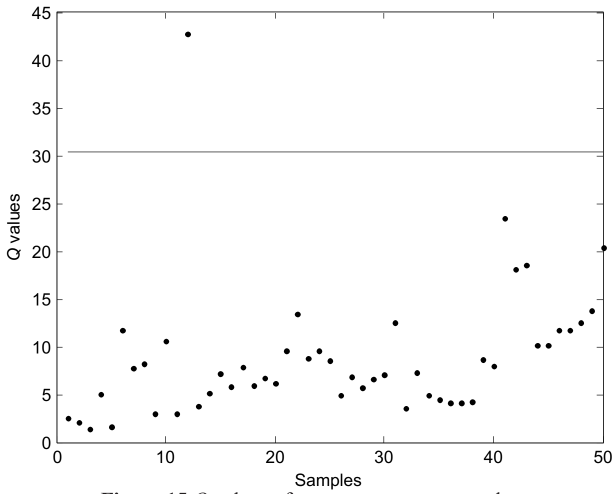

Figure 15 Q values of test measurement samples

5 Conclusion

Automatic fault detection and identification in the process measurement system is very important for quality process control. In modern industrial plants there are many process variables which are measured by sensors and the measurements are recorded to the plant database. Under normal operating conditions these variables are highly correlated. Multivariate statistical methods can be used to model relationships between process variables. Built models can be used to check the new measurements that are acquired and to judge whether abnormal process situation occurred or not. When such abnormal situation is detected and identified on time, additional appropriate actions can be carried out.

This paper shows fault detection and fault identification based on PCA and ICA methods. Apart from that, a short review of available modifications of PCA and ICA methods is also given. Hotelling's (T^2), Q (SPE) and I^2 statistics are used for sensor fault detection. Faulty sensor identification is performed by the use of contribution plots which proved to be simple and useful diagnostic tool. However, it can be difficult to identify faulty sensors from contribution plot when error occurs in a couple of sensors at the same time. Basic PCA and ICA equations are given together with the equations and guidelines for MSPM based on these methods. Structure of the PCA and ICA based algorithms for fault analysis is also derived. The proposed algorithms are applied to the two simulated processes. Presented results show that ICA based monitoring is more sensitive than PCA method, i.e. ICA revealed more sensor faults. On the other hand, PCA method is much simpler than ICA method regarding computational cost and optimization procedure which must be taken into consideration when such methods are implemented in the plant supervision and control system. The value of the faulty sensor process variable can be estimated from the remaining sensors with different soft-sensing techniques.

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