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# Dynamic Process Fault Isolation by Partial DPCA

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Original scientific paper
Received: June 28, 2005
Accepted: December 10, 2005

Principal component analysis (PCA) is a popular tool in fault detecting of the complex plant, but offers little support on fault isolation. Partial PCA (PPCA) is well developed for its capability of fault isolation utilizing a structured residual. In this paper, partial dynamic PCA(PDPCA) is proposed to enhance the isolation ability of dynamic process, which is a method combining PPCA and dynamic PCA. Simulation of PDPCA on a CSTR shows the effectiveness of the proposed method.

*Key words:*
Fault isolation, structured residual, dynamic principal component analysis, partial PCA

## 1. Introduction

On-line monitoring of process industry is extremely important for plant safety and product quality, which includes fault detection, fault isolation, fault diagnosis, and fault recovery. Major issues are fault detection and isolation. Due to the complexity of the process, multivariate statistical methods have drawn more and more attention, where principal component analysis (PCA) is one of the most important methods.[1] In PCA monitoring, a statistical model is built using normal data of the process, and faults are detected by referencing the measured process behavior against the model. Though PCA-based monitoring is very effective in detecting abnormal process situations (fault detection), it has been found to be lacking when it came to pinpointing the root-cause of the problem (fault isolation and diagnosis). Contribution Chart, multi-block approach,[2] and pattern recognition technology have been discussed to solve this problem, but none of them can provide a complete solution. Subspace approach based on fault reconstruction is a good tool to identify the occurred fault by assuming that each fault in a candidate fault set is the true fault and comparing to the reconstructed SPE with the control limits.[3] A new index combining SPE and $T^2$ is introduced to improve the identifiability.[4] But the reconstructions of every candidate fault must be computed, which makes the fault identification complex and hard to be implemented online.

Analytical redundancy methods, based on the fundamental model, have well developed fault isolation utilizing a structured or directional residual set, but such a model is not easily obtained due to nonlinearity, complexity, and high dimensionality of a process. *Gertler*[5] (1999) shows that there is a close duality between PCA and parity relations and proves the duality strictly. It gives one direct algebraic method of getting the structured residuals from the full PCA model and implements the fault isolation in the static linear system.

Since most processes are dynamic and nonlinear, which makes the above approach based on PCA not executable, partial NPCA is developed to implement fault isolation in nonlinear system by structured residual.[6,7] But the problem still exists in dynamic system, especially with control loops.

Variable measurements are serially dependent in dynamic process. *Bakshi*[8] (1998) proposed Multi-scale principal component analysis (MSPCA), which combines the ability of PCA to decorrelate the variables by extracting a linear relationship with that of wavelet analysis to extract deterministic features and approximately decorrelate auto-correlated measurements. Modeling utilizing observed disturbance, other than autocorrelated measurement, can eliminate the effects of process dynamics and implement PCA.[9]

In this paper, a dynamic PCA (DPCA) with moving window is introduced to deal with dynamic processes, and a partial DPCA (PDPCA), which can get structured residuals of dynamic process, is proposed to enhance the isolation ability of PCA in dynamic process. This method can isolate the faults of sensor and actuator, but here only sensor faults are discussed. The organization of the paper is as follows. Firstly, a review of the structured residual of PCA is presented. Secondly, moving window dynamic PCA is introduced. Next, the PDPCA is proposed, attainability conditions and implementing procedure are demonstrated in detail. In every section, some problems met in engineering and simulation on CSTR which is described simply are illustrated. Finally, we end this paper with a conclusion.

## 2. Structured residual of PCA

### 2.1 Structured residual of analytical redundancy

Partial PCA was proposed by virtue of the structured residual of analytical redundancy.[10] So it will be discussed first.

Consider a static linear system in which the outputs at time $\tau$ depend on the known (manipulated or measured) inputs and unknown fault (and noise), according to the relationship,

$$\boldsymbol{y}(\tau) = \boldsymbol{A}\ \boldsymbol{u}(\tau) + \boldsymbol{B}\boldsymbol{f}(\tau) \tag{1}$$

where $\boldsymbol{y}(\tau)$ is a $m$-dimensional output vector, $\boldsymbol{u}(\tau)$ is a $k$-dimensional input vector and $\boldsymbol{f}(\tau)$ is a fault vector. $\boldsymbol{A}$ is a model matrix, and $\boldsymbol{B}$ is a fault matrix. A set of residuals is obtained by

$$\xi(\tau) = \boldsymbol{y}(\tau) - \boldsymbol{A}\ \boldsymbol{u}(\tau) = \boldsymbol{B}\boldsymbol{f}(\tau) \tag{2}$$

Residual structures are characterized by an incidence matrix. The rows of this matrix belong to residuals and its columns to faults. A "0" at an intersection indicates that the residual does not respond to the fault while a "1" indicates that it does. Columns of the incidence matrix are the Boolean fault codes obtained in response to the particular faults. The structure is isolating if columns are different, and strongly isolating if, beyond all the columns being different, no column can arise from another column by turning "1"s into "0"s. An easy way of achieving strong isolation is by a column canonical structure, in which all columns have the same number of 1s, all in a different configuration. Table 1 is a strongly isolating structure.

Table 1 – *A strongly isolating incidence matrix*

| | $f_1$ | $f_2$ | $f_3$ |
|---|---|---|---|
| $r_1$ | 0 | 1 | 1 |
| $r_2$ | 1 | 0 | 1 |
| $r_3$ | 1 | 1 | 0 |

Calculate the residuals, make the residual over the thresholds "1", and the fault variables can be isolated according to the residual code column.

To achieve that each residual is sensitive to a particular subset of faults and each fault triggers a different subset of residual, as described by incidence matrix in table 1, they need to be transformed to

$$\boldsymbol{s}(\tau) = \boldsymbol{W}\,\xi(\tau) = \boldsymbol{W}\,\boldsymbol{B}\,\boldsymbol{f}(\tau) \tag{3}$$

where $\boldsymbol{W}$ is a transforming matrix. $\boldsymbol{s}(\tau)$ is a structured residual. Structured residuals are so designed that each residual is sensitive to a particular subset of fault.

### 2.2 Structured Residual of PCA

When PCA is used, we put all variables together, combine input and output used above, and get

$$\boldsymbol{x}(\tau) = \begin{bmatrix} \boldsymbol{u}(\tau) \\ \boldsymbol{y}(\tau) \end{bmatrix} \tag{4}$$

$\boldsymbol{x}(\tau)$ is a vector composed of process variables. Choosing process training data, free from fault at $n$ observation points ($n > k+m$), we can get

$$\boldsymbol{X}_{(k+m)\times n} = [\boldsymbol{x}(1),\ \boldsymbol{x}(2),\ldots \boldsymbol{x}(n)] \tag{5}$$

This matrix will be used to model. After being normalized, it can be decomposed as

$$\boldsymbol{X}_{(k+m)\times n} = \boldsymbol{P}\boldsymbol{T}' + \boldsymbol{E} = \sum_{i=1}^{k} \boldsymbol{p}_i\,\boldsymbol{t}_i' + \boldsymbol{E} \tag{6}$$

where $\boldsymbol{T}$ is a $n \times k$ orthogonal matrix, being called scores matrix. $\boldsymbol{t}_i$. is a $n$-dimensional vector, being called principal component (PC) scores. $\boldsymbol{P}$ is an $(k+m)\times k$ orthonormal matrix, $\boldsymbol{p}_i$ is eigenvectors of the covariance matrix, being called loadings vectors. Every column of $\boldsymbol{X}$ is corresponding to one sample time. The methods of determining $k$ are in section 3.3. $\boldsymbol{E}$ is called model residual matrix, expressed by

$$\boldsymbol{E} = \boldsymbol{X} - \boldsymbol{P}\boldsymbol{T}' = \boldsymbol{X} - \boldsymbol{P}\boldsymbol{P}'\boldsymbol{X} = \overline{\boldsymbol{P}\boldsymbol{P}'}\boldsymbol{X} \tag{7}$$

where $\overline{\boldsymbol{P}} = [\mathbf{p}_{k+1}\ldots\ldots\mathbf{p}_{k+m}]$, $\boldsymbol{T} = \boldsymbol{P}'\boldsymbol{X}$

So any column of $E$ can be expressed in vector form.

$$\boldsymbol{e}(\tau) = \overline{\boldsymbol{P}\boldsymbol{P}'}\boldsymbol{x}(\tau) \quad \tau = 1\ldots n \tag{8}$$

Eq. (8) indicates that the residuals are the linear combinations of $\boldsymbol{p}_{k+1}\ldots\ldots\boldsymbol{p}_{k+m}$.

To solve the problem better, the residual can be described in the residual subspace (RS), in term of $\boldsymbol{p}_{k+1}\ldots\ldots\boldsymbol{p}_{k+m}$ coordinates.

$$\varepsilon(t) = \overline{\boldsymbol{P}'}\boldsymbol{x}(\tau) \tag{9}$$

Eq. (9) shows that new residuals are linear combinations of the observation $\boldsymbol{x}(\tau)$, and $\boldsymbol{p}_{k+1}\ \ldots\ \boldsymbol{p}_{k+m}$ are coefficients.

Since $\boldsymbol{x}(\tau)$ is the observed value, it can be expressed as

$$\boldsymbol{x}(\tau) = \boldsymbol{x}^0(\tau) + \Delta\boldsymbol{x}(\tau) \tag{10}$$

where $\boldsymbol{x}^0(\tau)$ is the true value, which approximately exists in the PC subspace and is orthogonal to the RS. So $\boldsymbol{x}^0(\tau)$ is orthogonal to the RS and (9) can be rewritten as

$$\varepsilon(\tau) = \overline{\boldsymbol{P}'}\boldsymbol{x}(\tau) = \overline{\boldsymbol{P}'}\boldsymbol{x}_0(\tau) + \overline{\boldsymbol{P}'}\Delta\boldsymbol{x}(\tau) \cong \overline{\boldsymbol{P}'}\Delta\boldsymbol{x}(\tau) \tag{11}$$

$\varepsilon(\tau)$ is computed by $\boldsymbol{x}(\tau)$, but depends on $\Delta\boldsymbol{x}(\tau)$ only.

The structured residual of a new observation at time $t$ can be obtained by the transformation:

$$\eta(t) = \boldsymbol{V}\varepsilon(t) = \boldsymbol{V}\overline{\boldsymbol{P}}'\Delta\boldsymbol{x}(t) \tag{12}$$

where $\eta(t)$ is structured residual and can be of any dimension by choosing $V$. By comparing (3) and (12), the same residual form between analytical redundancy and PCA can be found. The duality has been proved.[5] The $i$th elements $\eta_i(t)$ of $\eta(t)$ is corresponding with $i$th row of the incidence matrix.

When residual structure is designed, the residual can be obtained by (12) and

$$\boldsymbol{v}_i'(\overline{\boldsymbol{P}}')^i = 0 \tag{13}$$

where $\boldsymbol{v}_i'$ is the $i$th row of $\boldsymbol{V}$, $(\overline{\boldsymbol{P}}')^i$ is the column corresponding with the "0"of the $i$th residual. Get,

$$\begin{aligned}\eta_i(t) &= \boldsymbol{v}_i\varepsilon(t) = \boldsymbol{v}_i\overline{\boldsymbol{P}}'\boldsymbol{x}(t)\\ &= \boldsymbol{v}_i[(\overline{\boldsymbol{P}}')^{(i)}(\overline{\boldsymbol{P}}')^i]\begin{bmatrix}\boldsymbol{x}^{(i)}(t)\\ \boldsymbol{x}^i(t)\end{bmatrix}\\ &= \boldsymbol{v}_i(\overline{\boldsymbol{P}}')^{(i)}\boldsymbol{x}^{(i)}(t)\\ &\cong \boldsymbol{v}_i(\overline{\boldsymbol{P}}')^{(i)}\Delta\boldsymbol{x}^{(i)}(t)\end{aligned} \tag{14}$$

where $\eta_i(t)$ is the $i$th residual, $(\overline{\boldsymbol{P}}')^{(i)}$ and $\boldsymbol{x}^{(i)}(t)$ are parts of $\overline{\boldsymbol{P}}'$ and $\boldsymbol{x}(t)$ corresponding with the "1" of the $i$th residual.

So the residual is decoupled with some variables designated in the residual structure and only sensitive to partial process variables. Eq. (13) is often used to design transformation matrix $V$, and can also be satisfied by

$$\operatorname{rank}(\overline{\boldsymbol{P}}')^i \le m-1 \tag{15}$$

To guarantee that $\eta_i(t)$ respond to all corresponding fault, the following rank condition has to be satisfied:

$$\operatorname{Rank}[(\overline{\boldsymbol{P}}')^i\,\boldsymbol{p}_{*\,\mathrm{g}}] = \operatorname{Rank}(\overline{\boldsymbol{P}}')^i + 1 \tag{16}$$

where $\boldsymbol{p}_{*\,\mathrm{g}}$ is any column of $(\overline{\boldsymbol{P}}')^i$.

If Eqs. (15), (16) are not satisfied, the selected row-structure is not attainable. If any two columns of $\overline{\boldsymbol{P}}'$ are linear dependent, the respective faults are not isolable.

## Dynamic PCA (DPCA)

### Moving Window DPCA

Dynamic systems are naturally described by differential equations or difference equations. In the difference equation model, the variables appear with a number of past samples, in addition to the present one. If past samples are there only for the output variables, the model is autoregressive (AR). If only the input variables have their past samples, the model is moving average (MA). If both, the model is autoregressive–moving average (ARMA). In this paper, only AR model is discussed to simplify the problem, the similar to MA model and ARMA model.

AR model can be expressed as

$$\boldsymbol{y}^0(t) = \boldsymbol{A}\boldsymbol{u}^0(t) - \sum_{g=1}^{h}\boldsymbol{D}_{\mathrm{g}}\,\boldsymbol{y}^0(t-g) \tag{17}$$

where superscript '0' still indicates true values, $\boldsymbol{A}$ and diagonal matrices $\boldsymbol{D}_{\mathrm{g}}$ are the coefficient matrices of $\boldsymbol{u}^0$(t) and $\boldsymbol{y}^0(t-g)$, $h$ is the process order, i.e. past outputs number.

Here the process output $\boldsymbol{y}$ at time $t$ is linearly related to the $h$ past outputs. When PCA, which is based on samples from a stationary process, is applied to this dynamic process, the information of the auto-correlations is not taken into account. Dynamic PCA (DPCA) was proposed to solve this problem, which augmented each dynamic vector with the previous $h$ observations and stacked the data matrix in the following manner:

$$\boldsymbol{X}_1' = \begin{bmatrix}\boldsymbol{y}'(t) & \boldsymbol{y}'(t-1) & \dots & \boldsymbol{y}'(t-h) & \boldsymbol{u}'(t)\\ \boldsymbol{y}'(t+1) & \boldsymbol{y}'(t) & \dots & \boldsymbol{y}'(t+1-h) & \boldsymbol{u}'(t+1)\\ & & \dots & & \\ \boldsymbol{y}'(t+n) & \boldsymbol{y}'(t+n-1) & \dots & \boldsymbol{y}'(t+n-h) & \boldsymbol{u}'(t+n)\end{bmatrix} \tag{18}$$

$$\boldsymbol{x}'(t) = [\boldsymbol{y}'(t)\ \ \boldsymbol{y}'(t-1)\ \dots\ \boldsymbol{y}'(t-h)\ \ \boldsymbol{u}'(t)] \tag{19}$$

The matrix contained $n+1$ observations. It is clear that the columns in the above matrix are linearly related to each other. Moreover, for each sample (row), only the first vector's observation is new, while all others are merely replications of the row above, so less information is introduced into the matrix. So the matrix is not constructed well. Instead, we construct a matrix in the form of a moving window of constant width that does not contain overlapping rows:

$$\boldsymbol{X}_2' = \begin{bmatrix}\boldsymbol{y}'(t)\,\boldsymbol{y}'(t-1) & \dots & \boldsymbol{y}'(t-h) & \boldsymbol{u}'(t)\\ \boldsymbol{y}'(t+h+1) & \dots & \boldsymbol{y}'(t+1) & \boldsymbol{u}'(t+h+1)\\ & \dots & & \\ \boldsymbol{y}'(t+n(h+1))) & \dots & \boldsymbol{y}'(t+n(h+1)-h) & \boldsymbol{u}'(t+n(h+1))\end{bmatrix} \tag{20}$$

where $h+1$, is the moving window's width, and $n+1$ is the number of windows used in the matrix. Matrix $\boldsymbol{X}_2$ has full information and eliminates the auto-correlation. The procedure is illustrated in Fig. 1.

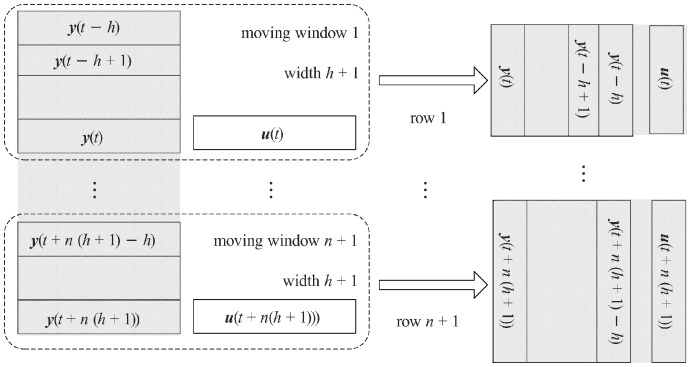



Fig. 1 – *Procedure of construct matrix by moving window*

To distinguish from general PCA we call this method moving window DPCA. Its advantage can be seen in the following application.

It is clear that the model form and the lag order $h$ are important to construct matrix of DPCA. In PCA modeling, past samples pose as "pseudo variables." Pseudo variables in plant models increase the number of variables without changing the number of equations. Experience indicates that $h$=1 or 2 is usually appropriate when DPCA is used.[11] The optimal order, used by process statistical model, can be determined by the criterion that the number of new relationships will increase with the order until it is optimal.[12]

In addition, it is important to determine the variables with auto-correlations, which can be implemented by virtue of the analysis model in our application, while the Durbin-Watson test is used in engineering.[13] The $D$ statistic can be compared to two (lower and upper) critical values, $D_L$ and $D_U$. When $D < D_L$, the null hypothesis that there is no correlation between the successive variables is rejected; when $D > D_U$, it is not rejected. If $D_L < D < D_U$, the test is inconclusive.

## Process of CSTR

A nonisothermal continuous stirred tank chemical reactor (Fig. 2), a dynamic nonlinear system

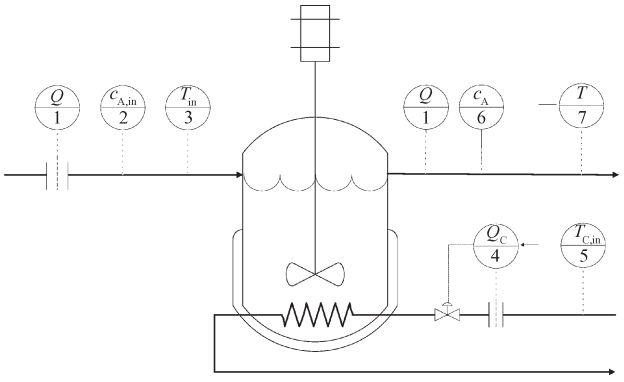



Fig. 2 – *CSTR process*

is used in the application of the paper. The reaction is of 1st order (A → B). It is assumed that the tank is well mixed and the physical properties are constant. The process has one feed stream, one product stream, and one cooling water stream. The cooling water flow controls the outlet temperature (T) by feed back control. The flow rate of inlet and outlet can be adjusted to be equal.

The CSTR model can be expressed as

$$\frac{dc_A}{dt} = \frac{Q}{V}c_{A,in} - \frac{Q}{V}c_A - k_0 e^{\frac{E}{RT}}c_A \qquad (21)$$

$$V\rho c_p \frac{dT}{dt} = Q\rho c_p(T_{in} - T) - kVc_A\Delta H - \frac{\alpha Q_c^{\beta+1}(T - T_{c,in})}{Q_c + \frac{\alpha Q_c^{\beta}}{2\rho c_{p,c}}} \qquad (22)$$

Here Eq. (21) is the mass balance equation and (22) is the energy balance equation for CSTR. Seven variables are involved in the process: flow rate ($Q$), inlet concentration of A ($c_{A,in}$) inlet temperature ($T_{in}$) flow rate of cooling water ($Q_c$) cooling temperature ($T_{c,in}$) outlet concentration of $A$ ($c_A$) and outlet temperature ($T$).

The proportional feedback control relation is

$$Q_c(t) = 15 + K_C \cdot (T_{set} - T(t)) \qquad (23)$$

In this paper, the parameters are

$V$ = 1m$^3$, $\rho = \rho_c = 10^6$ g m$^{-3}$, $E/R$ = 8330.1K,

$c_p = c_{p,c} = 1$ (cal g$^{-1}$ K$^{-1}$), $k_0 = 10^{10}$ (m$^3$ kmol$^{-1}$ min$^{-1}$)

$a = 1.678 \cdot 10^6$ cal min$^{-1}$ K$^{-1}$, $b$ = 0.5,

$\Delta H = -1.3 \cdot 10^7$ cal kmol$^{-1}$,

initial values:

$T_{in}$ = 370.0 K, $T_{C,in}$ = 365.0 K, $Q$ = 1 m$^3$ min$^{-1}$,

$Q_C$ = 15 m$^3$ min$^{-1}$, $c_{A,in}$ = 2 kmol m$^{-3}$,

$T$ = 368.25 K, $c_A$ = 0.8 kmol m$^{-3}$.

Coefficient of proportional feedback control: $K_C = -1.5$.

Measurement noise of every variable and disturbance (process noise) on every input are normal process with zero means, and the variances are listed in table 2.

Table 2 – *Variances of measurement and process noise*

| | Measurement noise | Process noise |
|---|---|---|
| $Q$ | 4e-6 | 1.9e-3 |
| $c_{A,in}$ | 1e-2 | 6.44e-3 |
| $T_{c,in}$ | 2.5e-3 | 4.75e-2 |
| $T_C$ | 2.5e-3 | 4.75e-2 |
| $Q_C$ | 1e-2 | |
| $c_A$ | 2.5e-5 | |
| $T$ | 4e-4 | |

## Principal component subspace of CSTR process

To describe the modeling ability of DPCA in focus, 400 normal observations without measurement noise, generated by above process under control, are used to identify the principal component subspace (PCS) of CSTR. PCS should explain 100 % variance of process variables without measurement noise

It is obvious that the process of CSTR in section 3.2 is first order dynamic system, which can be expressed by the following model.

$$\boldsymbol{y}(t+1) = \boldsymbol{y}(t) + f(\boldsymbol{u}(t), \boldsymbol{y}(t)) \qquad (24)$$

So, according to Eq. (24) and section 3.1, the matrix $\boldsymbol{X}_1(399\times9)$ for general DPCA in Eq. (18) and $\boldsymbol{X}_2$ (200×9) for moving window DPCA in Eq. (20) can be constructed as $\boldsymbol{x}(t)=[\boldsymbol{u}(t)\,\boldsymbol{y}(t)\,\boldsymbol{y}(t+1)]$, which includes 9 (pseudo) variables. $\boldsymbol{X}(400\times7)$, for PCA is still constructed as $\boldsymbol{x}(t)=[\boldsymbol{u}(t)\,\boldsymbol{y}(t)]$, which includes 7 variables.

After mean-centering and scaling $\boldsymbol{X}$, $\boldsymbol{X}_1$ and $\boldsymbol{X}_2$, the principal components (PCs) model was identified and the explanation to data variances of PCs can be got as Fig. 3.

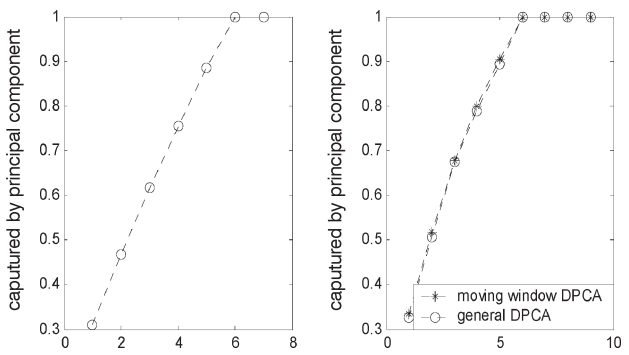



Fig. 3 – *Variance explained by PC*

It is well known that the dimension of RS of PCA model is equal to the number of the linear relationships among the monitored variables. Fig. 3a, based on PCA, shows that the first 6 PCs explain near 100 % variance. The dimension of PCS is 6, and that of RS is 1. Therefore, PCA model only deal with the linear relationship of feedback control, and the information of two differential equations is neglected. Fig. 3b, based on DPCA, shows that the first 6 PCs still explain near 100 % variance and PCS has dimension 6, but RS has dimension 3, due to introducing pseudo variables. So, three linear relationships extracted from one feedback control and two differential equations are described by the DPCA model.

It is noticeable in fig. 3b, that the moving window DPCA has the same ability to identify the PC model as general DPCA, only dealing with half size matrix of $\boldsymbol{X}_1$. The detailed explanation of each PC is listed in table 3, where the first 6 PCs of two methods both capture 99.998 % variance, and the first 5 PCs of moving window DPCA capture more variance than the latter.

Table 3a – *Percent variance captured by general DPCA model*

| PC no. | Eigenvalues | By this PC | Total |
|---|---|---|---|
| 1 | 2.9473 | 32.75 | 32.75 |
| 2 | 1.6098 | 17.87 | 50.63 |
| 3 | 1.5064 | 16.74 | 67.37 |
| 4 | 1.0242 | 11.38 | 78.75 |
| 5 | 0.95657 | 10.63 | 89.38 |
| 6 | 0.95551 | 10.61 | 99.998 |
| 7 | 1.5731e-004 | 0.002 | 100 |
| 8 | 2.8018e-005 | 0 | 100 |
| 9 | 2.1718e-032 | 0 | 100 |

Table 3b – *Percent variance captured by moving windows DPCA model*

| PC no. | Eigenvalues | By this PC | Total |
|---|---|---|---|
| 1 | 3.0023 | 33.36 | 33.36 |
| 2 | 1.6595 | 18.44 | 51.80 |
| 3 | 1.4441 | 16.05 | 67.84 |
| 4 | 1.0913 | 12.13 | 79.97 |
| 5 | 0.95262 | 10.58 | 90.55 |
| 6 | 0.85001 | 9.445 | 99.998 |
| 7 | 1.6035e-004 | 0.002 | 100 |
| 8 | 2.3121e-005 | 0 | 100 |
| 9 | 1.0884e-031 | 0 | 100 |

Although, strong nonlinearity exists in CSTR process, it can be considered as a linear system in this paper for the little variation of inputs. The fig. 3b and table 3 validate this point, where PCS represents 99.998% of the total variance. So, the three linear relationships can approximately represent the CSTR model, and the DPCA, based on linear system, can be performed on this process

In engineering, 85 % of captured variance is used to determine the number of PCs roughly. The method in this paper can be obtained after the measurement noises are filtered. Cross validation method can determine the dimension of PCS by data including measurement noise.[13,14] Variance of reconstruction error, based on fault reconstruction, is also proposed to select the number of retain PCs,[15] which is compared with several other method in Valle(1999).[16]

## Partial DPCA (PDPCA)

Now, a better method, moving window DPCA, can be used to process auto-correlation data. Let

$$\boldsymbol{B} = [-\boldsymbol{I},\ -\boldsymbol{D}_1\ \ldots\ -\boldsymbol{D}_h,\ \boldsymbol{A}] \tag{25}$$

AR model (17) can be described as:

$$\boldsymbol{B}\ \boldsymbol{x}^0(t) = 0 \tag{26}$$

So we can get structured residual in the dynamic process as section 2.2. Since the structured residual $\eta(t)$ used above is distinguished from the standard PCA, the method of computing residual threshold is also different from standard PCA. What is more, there are strong dynamics in some complex process, where the computing of transformation matrix $\boldsymbol{V}$ becomes difficult due to the pseudo variables, especially when control loops exist.

To implement fault isolation by structured residual in dynamic system, the partial PCA is proposed on the basis of structured residual of PCA in section 2.2, and is combined with DPCA.

### Partial PCA (PPCA)

Partial PCA is a PCA performed on a reduced vector $\boldsymbol{x}^{(i)}(\tau)$ (as described by section 2.2), where some variables in $\boldsymbol{x}(\tau)$ are missing. Therefore, the residual (Q statistic in general) will only be sensitive to faults associated with the variables which are present in the reduced vector $\boldsymbol{x}^{(i)}(\tau)$.[10] Faults associated with variables eliminated from the partial PCA, corresponding to '0' in the incidence matrix, will leave the residuals within the nominal thresholds. These residuals, corresponding to an incidence matrix, are referred to as structured residuals of partial PCA.

Designing incidence matrix, each subset should include at least one linear relationship on which PPCA is performed. It can also be guaranteed by Eq. (15) in linear static system.

### Partial dynamic PCA (PDPCA)

During Partial PCA the structured residuals, corresponding to incidence matrix, can be got by standard PCA on every data subset, without transformation matrix. So structured residual can be easily introduced into the dynamic process with control loop, and there moving window DPCA, substituted for standard PCA, is performed on every subset. This approach to obtain the structured residual of dynamic system, combining DPCA and PPCA, is referred to as partial DPCA (PDPCA). It should be noticed, that the method of using DPCA and PDPCA on AR model can also be applied to other model.

Although, trouble in transformation matrix do not exist in PDPCA, the attainability conditions of incidence matrix can not be given by Eqs. (15)(16).

It has been discussed in section 4.1 that every subset where PPCA performed on should include one linear relationship at least. In dynamic linear process, the linear relationships of $\boldsymbol{X}_2$ in Eq. (20) result from the auto-correlation variables.

So **attainability condition** 1 of the incidence matrix is that not less than one auto-correlation variable is included in every subset. In this paper's application, two output variables are easily determined to be auto-correlative according to the analytical model. In practice Durbin – Watson test is used to do it.

When the incidence matrix satisfying above condition is designed, the partial DPCA can be run to implement the fault isolation of dynamic process.

### Implementation of Partial DPCA

The specific procedure of the PDPCA is given.

1. Choose the width $h$+1 of the moving windows, process model form and variables with auto-correlation, construct normal data matrix $\boldsymbol{X}_2$ by moving windows. Mean-center and scale it.

2. Perform a DPCA on $\boldsymbol{X}_2$ to determine the number of relations m.

3. Construct an incidence matrix according to attainability condition, preferably with strong isolation properties.

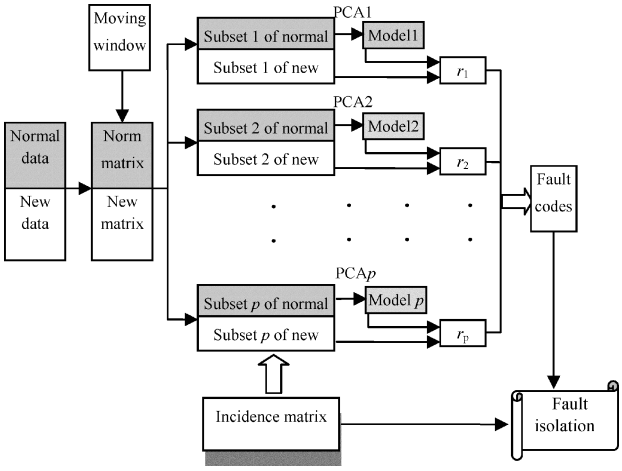
4. Select subset data matrix from $\boldsymbol{X}_2$ and perform a set of partial DPCAs with each one implementing a row of the incidence matrix. Determine the thresholds beyond which abnormality is indicated and according fault code is set "1". Now, get

loading vector and thresholds of every subset, which is PDPCA model of every subset.

5. When new data come, select data belonging to *i*th subset and calculate the residual $r_i$ (SPE) in PDPCA model which correspond to fault code '1', if beyond the threshold of *i*th subset.

6. Compare the fault code of structured residuals to every column of incidence matrix to attain fault isolation.

The procedure is also illustrated in Fig. 4.



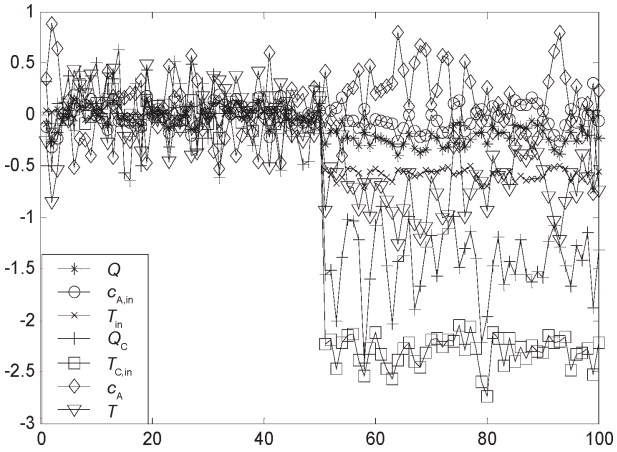

F i g . 4 – *Procedure of PDPCA*

## Application on CSTR

Sensor faults include reading deviating, floating, sensor invalidating completely and accuracy decrease. Here only reading deviating and sensor invalidating are considered, and the others are similar as viewed from fault isolation.

From time 401, 400 × 7 observations are sampled from CSTR process respectively working under 7 faults: flow sensor bias +0.1 $m^3\ min^{-1}$, input stream concentration –0.2 $kmol/m^3$, input stream temperature +1 °C, cool water flow +0.2 $m^3\ min^{-1}$, cool water temperature –1 °C, output stream temperature –1 °C and 'A' concentration sensor invalidation of output stream, pointing to 0.8 kmol $m^{-3}$.

Contribution plot, which is the commonest tool of fault isolation, is first used to deal with +1°C fault of cooling water temperature sensor. After the $T_{c,in}$ fault is detected in $X_2$ (200 × 7 matrix, composed of 400 observations), for clear drawing contribution plot in Fig. 5, first 50 rows of $X_2$ under normal and fault station are used. It can be seen that an evident fault occurs from point 51 and the contribution of $T_{c,in}$ to SPE is the largest. Then fault of $T_{c,in}$ occurs in all probability. Meanwhile, contribution of $Q_c$ is also large. It can not be decided whether or not the fault of $Q_c$ occurs. Thus, contribution plots can not give a totally unambiguous isolation.




F i g . 5 – *Fault detect and isolation by contribution plot*

Next, PDPCA is applied to fault isolation of CSTR process. The incidence matrix with strong isolability is designed as table 4.

T a b l e 4 – *Incidence matrix with strong isolability of CSTR*

| | $Q$ | $c_{Ain}$ | $T_{in}$ | $Q$c | $T_{c,in}$ | $c_A$ | $T$ |
|---|---|---|---|---|---|---|---|
| $r_1$ | 0 | 0 | 1 | 1 | 1 | 1 | 1 |
| $r_2$ | 1 | 0 | 0 | 1 | 1 | 1 | 1 |
| $r_3$ | 1 | 1 | 0 | 0 | 1 | 1 | 1 |
| $r_4$ | 1 | 1 | 1 | 0 | 1 | 0 | 1 |
| $r_5$ | 1 | 1 | 1 | 1 | 0 | 0 | 1 |
| $r_6$ | 1 | 1 | 1 | 1 | 0 | 1 | 0 |
| $r_7$ | 0 | 1 | 1 | 1 | 1 | 1 | 0 |

In each row of seven, corresponding to a variable subset, two variables are missing, each time differently. Note, that when the data matrix $X_2$ for PDPCA is constructed, the dynamic variable should exist in or be eliminated from a subset together with its $h$ time lag pseudo variables. It can be tested that the linear relationships numbers of respective subsets are (3, 3, 2, 1, 2, 1, 1), and the matrix meets the attainability condition 1. After loading vector and thresholds are determined, based on the 200 normal data, the structured residuals (i.e. SPE of every subset here) for single fault of 7 faults can be obtained by PDPCA. The responses to fault are plotted in Fig. 6, where each column corresponds to a fault code given in table 4. In each subplot, the first 200 samples are normal data, and the next 200 are faulty data.

By comparing Fig. 6 with table 4, it can be seen that the responses of every subset to most faults ($Q$, $Q_c$, $c_A$, $T$) are in agreement with the incidence matrix and these faults can be isolated. But (4,2), (5,2), (6,3), (7,3), (7,5), which denote (row number, column number) of corresponding subplots in Fig. 6, show that some subsets can not response to faults of ($c_{Ain}$, $T_{in}$, $T_{cin}$). The reason is that these variables, called independent variable, which are independent of the linear relationships in a subset, appear in this subset, such as $c_{Ain}$ in subset 5 and 6, $T_{in}$ in subset 6 and 7, and $T_{cin}$ in subset 7. The information of these variables exists in the PCS, not the RS, which represents the linear relationships. So, the SPE statistic from RS does not response when these variables' faults occur. Only attainability condition 1 can not guarantee the attainability of the incidence matrix.

**Attainability condition 2:** If SPE is used as the residual, every subset can not include variables independent of the linear relationships in this subset. To meet this condition, an auto-correlation variable is eliminated from a subset together with the variables only correlative with this dynamic variable. According to analytical model of CSTR, $c_{A,in}$ is only correlative with $c_A$, while $T_{in}$ and $T_{cin}$ are only correlative with $T$. Thus, the incidence matrix can be improved as table 5.

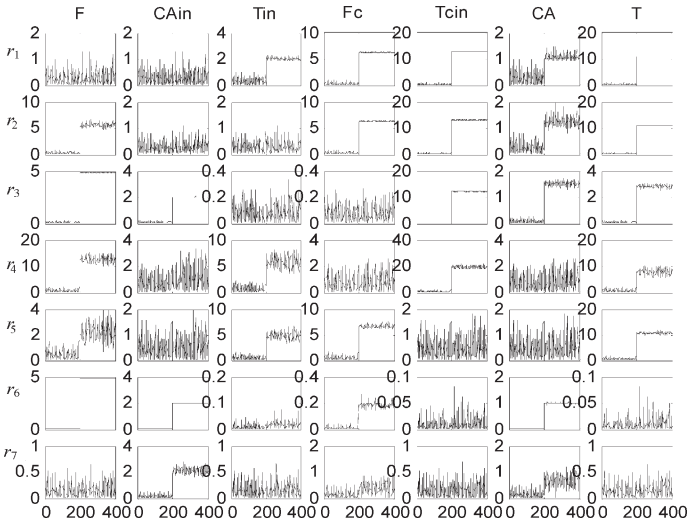



Fig. 6 – *Response to 7 faults of CSTR*

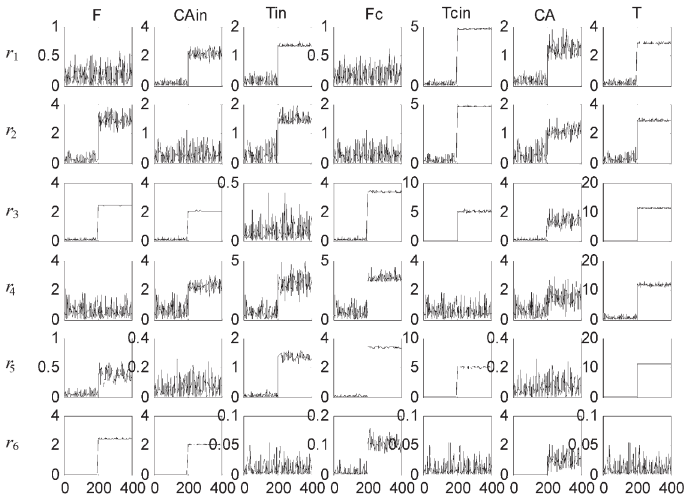



Fig. 7 – *Response to 7 faults of CSTR after improvement*

Table 5 – *Improved incidence matrix*

| | $Q$ | $c_{A,in}$ | $T_{in}$ | $Q_c$ | $T_{c,in}$ | $c_A$ | $T$ |
|---|---|---|---|---|---|---|---|
| $r_1$ | 0 | 1 | 1 | 0 | 1 | 1 | 1 |
| $r_2$ | 1 | 0 | 1 | 0 | 1 | 1 | 1 |
| $r_3$ | 1 | 1 | 0 | 1 | 1 | 1 | 1 |
| $r_4$ | 0 | 1 | 1 | 1 | 0 | 1 | 1 |
| $r_5$ | 1 | 0 | 1 | 1 | 1 | 0 | 1 |
| $r_6$ | 1 | 1 | 0 | 1 | 0 | 1 | 0 |

The numbers of linear relationships in respective subset are (2,2,3,3,2,1) and condition 1 is met. After PDPCA is performed again, response is got as Fig. 7, where the residual is sensitive to all faults associated with the variables in its subset, and is within in-control limit when variable with fault does not exist in its subset. For new observation, the variable with fault can be found by comparing the response of every subset with table 5.

The isolation property may be not strong any longer for meeting attainability condition 2. In addition, some knowledge of process or fault data is needed to determine the independent variables in one subset.

## Conclusion

Multivariate statistical method plays an important role in the process monitoring, where PCA is the main approach. But PCA is found to be lacking in fault isolation. Another, standard PCA can not be used in dynamic system. Structure residual is useful for fault isolation. By performing PCA on subsets of variables, i.e. partial PCA based on the link between PCA and parity relations, a set of structured residuals can be obtained for sensor/actuator fault isolation. In addition, structure residual for process parameter fault can be obtained from PCA models established from a full training data set containing a fault one at a time, not partial. So process fault is not discussed in this article. In this paper, moving window DPCA is introduced and PDPCA combin-

ing moving DPCA and PPCA is proposed to resolve the sensor/actuator fault isolation of the dynamic process. To implement PDPCA, two attainability conditions of incident matrix are given. Problem that moving DPCA and PDPCA will meet in engineering is discussed in detail. Simulation on the CSTR shows the better effect of this method. Though there is some difficulty in determining the variable independent with the subset linear relation in complexity dynamic system, further research on PDPCA is a challenging subject.

*ACKNOWLEDGEMENT*

*This work is supported by National Natural Science Foundation of China (60421002).*

## Nomenclature

AR – autoregressive
CSTR – continuous stirred tank reactor
PCA – principal component analysis.
PDPCA – partial dynamic principal component analysis
PCS – principal component subspace
PCs – principal components
RS – residual subspace

## Notation

$t$ – scalar
$\boldsymbol{t}$ – vectors
$\boldsymbol{T}$ – matrix
$k$ – number of input
$m$ – dimension of RS, number of output
$n$ – number of samples
$r$ – residual

## Superscripts

$^0$ – true value
$'$ – transpose

## List of symbols

$c$ – conentration, kmol m$^{-3}$
$c_p$ – specific heat capacity, cal g$^{-1}$ K$^{-1}$
$H$ – molar enthalpy, cal kmol$^{-1}$
$k$ – rate coefficient, m$^3$ kmol$^{-1}$ min$^{-1}$
$Q$ – volume flow rate, m$^3$ min$^{-1}$
$t$ – time, min
$T$ – temperature, K
$V$ – volume, m$^3$
$\rho$ – density, g m$^{-3}$

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