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A Revised State Space Modelling Approach and Improved Fault Detection Using Combined Index Monitoring for Dynamic Processes

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Abstract: Larimore's state space model derivation and stochastic estimation algorithm, first published in 1983, have been the adopted standard for deriving the state variables and parameters of the five (5) matrices state space model representation which continues to be applied extensively in the literature for applications ranging from controls, system identification and process monitoring. This paper presents an alternate derivation and stochastic estimation algorithm. The paper also discusses how strategic classification of the process inputs may, for some applications, facilitate the use of a simplified stochastic estimation algorithm. The alternative state space modeling approaches demonstrated better fault monitoring statistic performance for specific types of faults simulated. The canonical variate based state space modeling approaches were evaluated on a simulate CSTR process – with recycle through a heat exchanger. The results demonstrates the potential benefits to be derived from using a combined monitoring index based upon monitoring statistics derived from independent state space models for improved overall fault detecting capabilities and reliability of the fault monitoring scheme.

Keywords: Dynamic modeling, Stochastic modeling, State space modeling, Fault detection, Canonical Variate Analysis, Combined Index.

1. INTRODUCTION

The application of canonical correlation analysis, stochastic estimation and system identification was pioneered by Akaike (1976). However, his work primarily involved the fitting of autoregressive moving average ARMA time series model. The first application of a state space modelling approach was proposed by Larimore (1983). There are in general about three different form of state space representation appearing in the literature parameterized by three (3) to five (5) matrices. The 3-matrices representation is only applicable to systems with no exogenous inputs, one example of its application is by Negiz and Cinar (1997) for modelling Vector Autoregressive Moving Average (VARMA) type of time series model. Larimore (1983, and 1990) employed a 5-matrices state space model which explicitly defined exogenous inputs in the representation. Stubbs et al (2009) proposed a return to a 3-matrices state space representation citing it to be more appropriate for fault monitoring applications as opposed to controls based applications. His proposal, however, also included a slight redefining of the process of extracting the state variables to ensure that the state variables captured the information contribution of the exogenous inputs and that the model, therefore, remain broadly applicable.

Despite the simpler stochastic estimation procedure associated with the 3-matrices state space representation, the 5-matrices state space model has been the more popular choice of representation employed for fault monitoring applications. Invariably, researchers applying the 5-matrices state space model employ Larimore's stochastic estimation technique for model parameterization. In this paper an alternative stochastic estimation derivation and equations based upon minimization of the state and output residuals is proposed. The paper also proposes and consider yet another alternative method of deriving the state variables which will be demonstrated to achieve simplification of the stochastic estimation algorithm and a unification of the both Larimore's stochastic estimation algorithm and that proposed by the author.

The Hotelling's T^2 and square prediction error SPE (Q) statistics on the output and state residuals for the three variants of the state space models developed highlights the fact that the most effective monitoring statistics in terms of speed of detection is subject to the fault simulated and the state space model employed. This observation led to the investigation of applying a combined monitoring index that would effectively merge the benefits of the three independent monitoring schemes. The method of merger was inspired by that proposed by Yue and Qin (2001) and Cherry and Qin (2006), for merging the monitoring of SPE (Q) and Hotelling's T^2 principal component analysis PCA based statistics. For this application, however, statistics of the same type obtained from two independently derived state space models were merged. The fault monitoring performance of the combine index proved to have indeed inherited the strengths of the two independent monitoring schemes.

2. Canonical Variate CV Based State Variable Extraction

2.1 Canonical Variate Analysis

The main idea behind canonical correlation analysis is to extract the relationship between two sets of variables. It achieves this by finding corresponding sets of linear combinations (the canonical variates) of the original data sets. The transform seeking to maximize the correlation between derived canonical variates:

$$V = YL \tag{1}$$

$$U = XJ \tag{2}$$

$$\text{Maximise } U^T V = \frac{J^T R_{xy} L}{\sqrt{J^T R_{xx} J}\sqrt{L^T R_{yy} L}} \tag{3}$$

where $R_{xx} = E(X^T X)$, $R_{yy} = E(Y^T Y)$, and $R_{xy} = E(X^T Y)$.

This is equivalent to solving the constraint optimization:

$$\emptyset = \mathrm{J}^T R_{xy} \mathrm{L} + \lambda_x (I_x - \mathrm{J}^T R_{xx} \mathrm{J}) + \lambda_y (I_y - L^T R_{yy} L) \tag{4}$$

where $\boldsymbol{I}_x$ and $\boldsymbol{I}_y$ are unity matrix.

The solution is given by:

$$SVD\left(R_{xx}^{-1/2} R_{xy} R_{yy}^{-1/2}\right) = \hat{J} S \hat{L}^T \tag{5}$$

$$J = R_{xx}^{-1/2} \hat{J};\ L = R_{yy}^{-1/2} \hat{L} \tag{6}$$

The main diagonal of the $\boldsymbol{S}$ matrix contains the correlation coefficients. The application of CCA to state space modeling involves the use of only one of set of the canonical variates to be used as state variables. The matrix X and Y is replaced with what is traditionally referred to as the past $\boldsymbol{P}$ and future $\boldsymbol{F}$ matrix respectively, defined as:

$$\boldsymbol{P}(t) = \left[y_{t-1}^T ; y_{t-2}^T, \ldots . y_{t-l_y}^T, u_{t-1}^T, u_{t-2}^T, \ldots . u_{t-l_u}^T\right] \tag{7}$$

$$\mathbf{F}(t) = \left[y_t^T ; y_{t+1}^T, \ldots . y_{t+f}^T\right] \tag{8}$$

where l_y, l_u, f are the window lengths of the lag and lead windows of the input and output vectors. The state vector $\boldsymbol{X(t)}$ is computed from the canonical variate transform $\boldsymbol{J}$ of the past vector P :

$$\mathbf{X}(t) = \mathbf{P}(t)\mathbf{J} \tag{9}$$

2.2 Selecting the number of state variables.

Several methods have been proposed for selection of the number of state variables to be used for the state space model development. The number of states to be used is equivalent to selecting the number of columns of the **J** matrix. Negiz and Cinar (1997) proposed using the eigenvalues of the Hankel matrix. However, the far more popular technique is to apply Akaike Information Criterion AIC, Larimore (1990) and Simoglou et al (1999 & 2002). Thus, the method used in this paper explored both the option of inspection of the decomposed scaled Hankel matrix diagonal elements as well as application of the AIC criterion. The p x f correlation matrix $\boldsymbol{S}$ of the decomposed scaled Hankel matrix comprises of an f x f diagonal sub-matrix and a (p - f) x f zero matrix, where p is the number of vectors of the past matrix $\boldsymbol{P}$ and f is the number of vectors of the future matrix $\boldsymbol{F}$. Fig. 1 shows a trend consistent with all models evaluated, for correlation values significantly less that 1, inclusion of the columns associated with the diagonal element provided comparatively minimal improvement in the model residual sum squared RSS error. Therefore the number of state variables used was dependent upon the number of unity (or approximately unity) correlation diagonal elements of the $\boldsymbol{S}$ matrix. As can be observed the reduction in the residual sum squared RSS error of the model diminishes with each successive orthogonal vector included and more so as its associated correlation value deviates from unity. The AIC value corroborates the selection based upon the diagonal inspection as shown in Fig. 1 both selection method aligns with the state order selection of 5.

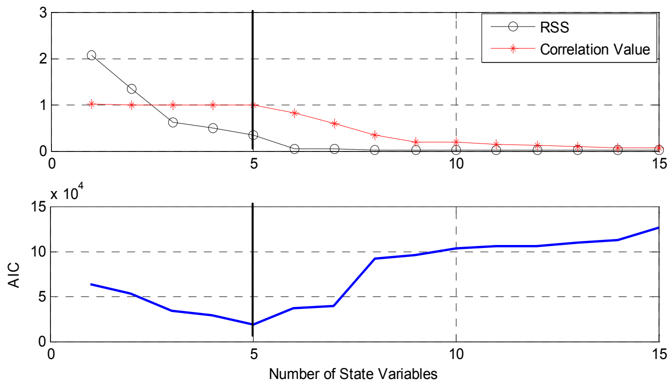

Fig. 1 Plot of RSS, correlation values diagonal of S matrix, and AIC. State variable selection is 5.

3. PARAMETRIC STATE SPACE MODEL ESTIMATION

3.1 Proposed Stochastic Estimation Derivation

The advent of Larimore's state space representation given in (10) offer several improvements to the previous work by Akaike in the area of stochastic realization and system identification.

$$X_{t+1} = X_t A + U_t B + e_x$$

$$Y_t = X_t C + U_t D + e_y \tag{10}$$

The improvements include the inclusion of inputs in the representation to facilitate controls and make the model more broadly applicable to different process applications and accounting for the correlation between the state and output residuals. The correlation is accounted for by the representation of the total measurement (output) noise using $e_x(t)\boldsymbol{E} + e_y(t)$. Accounting for the correlation between the residuals ensures a minimal order state space model for a given process, Sharper et al. (1994).

The proposed stochastic estimation of matrices **A**, **B**, **C**, **D** and **E** of (10) to be presented in the following is based upon minimizing the RSS of the state and output equation.

Consider the expansion of the squared state residuals:

$$e_x^T e_x = X_{t+1}^T X_t - 2X_{t+1}^T X_t \boldsymbol{A} - 2X_{t+1}^T U_t \boldsymbol{B} + \boldsymbol{A}^T X_t^T X_t \boldsymbol{A} + \boldsymbol{B}^T U_t^T U_t \boldsymbol{B} - 2\boldsymbol{A}^T X_t^T U_t \boldsymbol{B} \tag{11}$$

Owing to the method used to derive the states, $X_t^T X_t = X_{t+1}^T X_{t+1} = I_k$, therefore minimization with respect to **A** matrix is given by:

$$\frac{d(e_x e_x^T)}{d\boldsymbol{A}} = -X_{t+1}^T X_t + \boldsymbol{A}^T - \boldsymbol{B}^T U_t^T X_t = 0;$$

$$\boldsymbol{A}^T = X_{t+1}^T X_t + \boldsymbol{B}^T U_t^T X_t \tag{12}$$

Now differentiating (11) with respect to B gives:

$$\frac{d(e_x e_x^T)}{d\mathbf{B}} = -X_{t+1}^T U_t + \boldsymbol{B}^T U_t^T U_t - \boldsymbol{A}^T X_t^T U_t \tag{13}$$

Substituting (12) into (13) and solving for B yields:

$$\boldsymbol{B}^T U_t^T U_t - \boldsymbol{B}^T U_t^T X_t X_t^T U_t = X_{t+1}^T X_t X_t^T U_t + X_{t+1}^T U_t \tag{14}$$

Let $\boldsymbol{Q} = \boldsymbol{X}_t^T \boldsymbol{U}_t$, then the solution for **A** and **B** maybe expressed as:

$$\boldsymbol{B}^T = \left(X_{t+1}^T U_t + X_{t+1}^T X_t Q\right)\left[U_t^T U_t - Q^T Q\right]^{-1} \tag{15}$$

$$\boldsymbol{A}^T = X_{t+1}^T X_t + \boldsymbol{B}^T Q^T \tag{16}$$

Derivation of the matrices of the output equation follows essentially the same path. In this case however, the equation for the square residual is simplified by now noting the fact that both the state and current input vector is orthogonal to the state equation residuals:

$$X_t^T e_x = 0;\; U_t^T e_x = 0; \tag{17}$$

the output square residuals reduces to:

$$e_y^T e_y = Y_t^T Y_t - 2Y_t^T X_t \boldsymbol{C} + \boldsymbol{C}^T X_t^T X_t \boldsymbol{C} - 2Y_t^T U_t \boldsymbol{D} + \boldsymbol{C}^T X_t^T U_t \boldsymbol{D} - 2Y_t^T e_x \boldsymbol{E} + \boldsymbol{E}^T e_x^T e_x \boldsymbol{E} \tag{18}$$

Therefore, the equations defining the matrices **C** and **D** are given by:

$$\boldsymbol{D}^T = \left(Y_t^T U_t + Y_t^T X_t Q\right)\left[U_t^T U_t - Q^T Q\right]^{-1} \tag{19}$$

$$\boldsymbol{C}^T = Y_t^T X_t + \boldsymbol{D}^T Q^T \tag{20}$$

The central difference in the derivation approach outlined by Larimore (1990) and that being presented in this paper, is that the resulting equations explicit identifies the relationship and dependency of the derived parameters of one matrix relative to the other. Note that the parameters of matrix **A** as given by (12) will be directly dependent upon the derived parameters of matrix **B.** Likewise, equation (20) outlines the dependency of **C** on **D**. In both cases the dependency is linked by the previously defined ***Q*** matrix. The set of equations could be simplified, therefore, if the ***Q*** matrix was a zero matrix but that would require the state vector $\boldsymbol{X}_t$ being orthogonal to the current input vector $\boldsymbol{U}_t$ which would only be possible if there existed no serial or cross correlation in the set of define input variables**.** Such condition was approximated by classifying the controller actuating signals as outputs in the simulation case study used for this paper. The set of simplified stochastic equations is given by:

$$\boldsymbol{A}^T = X_{t+1}^T X_t \tag{21}$$

$$\hat{\mathbf{B}} = X_{t+1}^T U_t \left(U_t^T U_t\right)^{-1} \tag{22}$$

$$\hat{\mathbf{C}} = Y_t^T X_t \tag{23}$$

$$\hat{\mathbf{D}} = Y_t^T U_t \left(U_t^T U_t\right)^{-1} \tag{24}$$

Finally, minimization of the output residuals with respect to ***E*** gives the solution:

$$E^T = Y_t^T e_x \left[e_x^T e_x\right]^{-1} \tag{25}$$

3.2 Larimore's Stochastic Estimation Algorithm

Larimore's stochastic estimation procedure is summarised by equations (26&27). The stochastic algorithms simultaneous derives covariance matrix of the state and output residuals ($\boldsymbol{\Phi}_\mathbf{x}$, $\boldsymbol{\Phi}_\mathbf{y}$) along with the parameters of the **E** matrix:

$$\begin{bmatrix} \hat{A} & \hat{B} \\ \hat{C} & \hat{D} \end{bmatrix} = \begin{bmatrix} \mathbf{X}_{t+1} \\ \boldsymbol{Y}_t \end{bmatrix} \begin{bmatrix} \mathbf{X}_t & \mathbf{U}_t \end{bmatrix}^T \left\{ \begin{bmatrix} \mathbf{X}_t \\ \mathbf{U}_t \end{bmatrix} \begin{bmatrix} \mathbf{X}_t & \mathbf{U}_t \end{bmatrix}^T \right\}^{-1} \tag{26}$$

$$\begin{bmatrix} \Phi_x & \Phi_x E \\ E^T \Phi_x & E^T \Phi_x E + \Phi_y \end{bmatrix} = \begin{bmatrix} \tilde{\mathbf{X}}_{t+1} \\ \tilde{\boldsymbol{Y}}_t \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{X}}_t & \tilde{\boldsymbol{Y}}_t \end{bmatrix}^T \tag{27}$$

where

$$\tilde{\boldsymbol{X}}_{t+1} = \boldsymbol{X}_{t+1} - \left(\boldsymbol{X}_t \hat{\mathbf{A}} + \boldsymbol{U}_t \hat{\mathbf{B}}\right)$$

$$\tilde{\mathbf{Y}}_\mathrm{t} = \mathbf{Y}_\mathrm{t} - \left(\mathbf{X}_\mathrm{t} \hat{\mathbf{C}} + \mathbf{U}_\mathrm{t} \hat{\mathbf{D}}\right)$$

Equation 26 can be re-expressed to include the **Q** matrix as follows:

$$\begin{bmatrix}\hat{A} & \hat{B}\\ \hat{C} & \hat{D}\end{bmatrix} = \begin{bmatrix}\mathbf{X}_t^T\mathbf{X}_{t+1} & \mathbf{X}_{t+1}^T\mathbf{U}_t\\ \mathbf{X}_t^T\mathbf{X}_t & \boldsymbol{Y}_t^T\mathbf{U}_t\end{bmatrix}\begin{bmatrix}\mathbf{X}_t^T\mathbf{X}_t & \boldsymbol{Q}_t\\ \boldsymbol{Q}_t^T & \boldsymbol{U}_t^T\mathbf{U}_t\end{bmatrix}^{-1} \quad (28)$$

Solving the above would yield a different and even more complex set of equations than (15,16, 19 & 20), however, if the $\boldsymbol{Q}$ matrix is approximately a zero matrix, the solution reduces to the set of equations given by (21-24).

4. APPLICATION TO CSTR FAULT MONITORING

4.1 CSTR Model and Fault Simulation

The CSTR system shown in Fig. 2 is an adaptation of a similar model used by Zhang J. et al (1996) to evaluate the detection and diagnostic capable of principal component analysis PCA based monitoring scheme. The reaction model is one of an irreversible heterogeneous catalytic exothermic conversion of a reactant A to a product B. The control objective is to maintain the product concentration at a desired level by indirect control of the temperature, residence time and mixing conditions in the CSTR. A recycle product stream circulated via a heat exchanger (HTX) is used to facilitate the temperature control and ensure well-mixed condition. The reactor temperature is controlled by manipulating the flow rate of the cold water feed to the heat exchanger via a cascade control loop. The residence time is controlled by maintaining the level in the reactor.

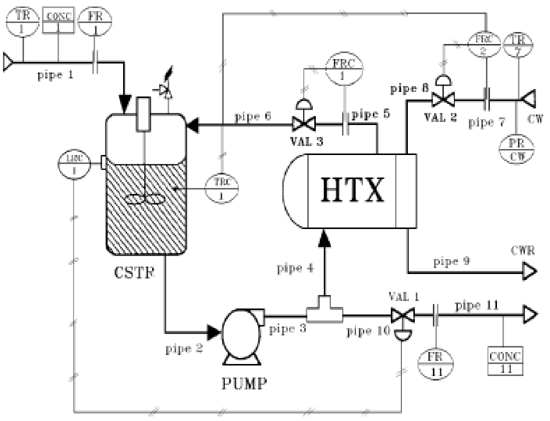

Fig. 2. Continuous Stirred Tank Reactor CSTR with recycle loop via Heat Exchanger HTX.

The impact of the coolant flow-rate on the heat-transfer coefficient UA value was also accounted for by using an analytical expression taken from a publication by Yoon and MacGregor (2001). A notable change to the model also included the use of a dynamic instead of a steady-state model for the heat exchanger unit. There are 19 possible on-line measurements that could be simulated, of which 11 were used in the model with lead and lag order of 3 and state vector dimension of 5.

Both incipient and sudden type faults were simulated to represent temperature and flow sensor drift type faults along gradual heat exchanger fouling faults and sudden valve sticking faults. The heat-exchanger fouling faults were implemented by reducing the UA of the heat-exchanger at a fix time rate.

4.2 Fault Detection

For the fault detection metrics both the Hotelling's T^2 statistics based on the first k state variables and SPE (Q) metrics based on the residuals of the state and output matrix were applied. It was observed that the best detection statistics was dependent upon the fault being simulated and the state space model being employed in terms of the stochastic estimation algorithm employed to parameterize the model. This observation motivated investigations into the use of a combined index monitoring with the goal of merging the benefits of the two independent monitoring schemes. The method of merger was inspired by the publications of Yue and Qin (2001) and more recently Cherry and Qin (2006).

The merger in this application involved combining statistics of the same type obtained from independently derived state space models. The combined index is defined as the summation of the metrics (Hotelling's T^2 or SPE statistics) weighted against their independent control limits:

$$SPE_c = \sum_{i=1}^{n} \frac{SPE_i}{\delta_i^2} \quad (29)$$

$$T_c^2 = \sum_{i=1}^{n} \frac{T_i^2}{\tau_i^2} \quad (30)$$

where the subscript index indicates the state space model from which the statistic is derived and SPE_c and T^2_c are the combined index square prediction residuals and Hotelling's T^2 statistics, respectively. In this application the combine index was derived from three state space model: model **A** refers to the state space model derived using Larimore's stochastic estimation algorithm (26&27), model **B** applied the author's proposed alternative stochastic estimation algorithm (15,16,19&20) and model **C** is based upon the simplified set of stochastic equations given by (21-24) assuming the $\boldsymbol{Q}$ matrix zero condition holds.

The Hotelling's T^2 statistics on the state on output residuals of model **B** was on average better performing than model A whereas Hotellings T^2 on the state vector using model **A** was on average slightly better detecting than model **B**. Likewise, model **C** for some of the faults analyzed came out with the best detection, refer to Fig. 3a. However, they are no clear winner, the combine index monitoring is refer to as model A+**B+C** and has can be seen from the two examples given, it is most influenced equally by the independent statistics and it also provides a great trade off between detection speed and reliability hence resulting in less misdetection and false alarm conditions. Two examples of the combine index statistics performance is provided in Fig. 3, the faults were introduce at sample time instance 4000.

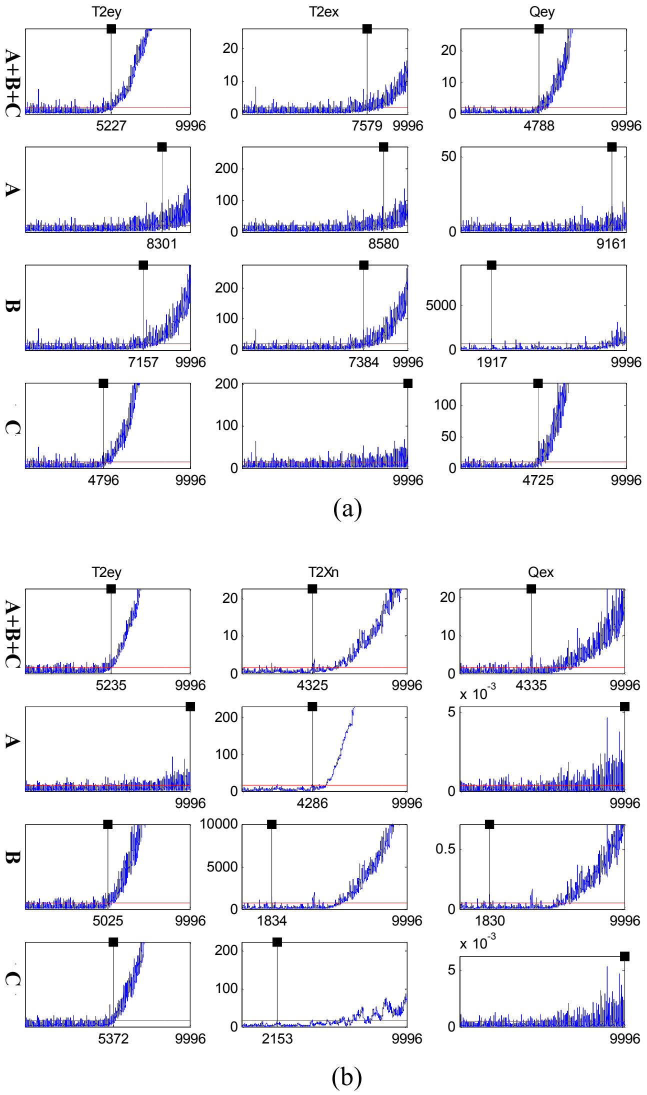

Fig. 3. (a) T^2 on output and state residual, and Q statistics on the output residuals for heat exchanger fouling fault (b) T^2 statistics on output residual and state vectors, and Q statistics on state residuals for temperature sensor drift fault.

Table 1 provides a list of the incipient type faults tested and the best performing combine index statistics. The fault growth rate was set at 1.43 x 10^{-3}% per sample interval. The speed of detection measurement is given as the observed percentage drift of the faulty process variable or parameter at the time of detection relative to its steady state value prior to fault initiation. Expressing the detection delay in sample intervals, therefore requires multiplying by the growth rate of the fault. The sudden valve sticking faults simulated were both instantaneously detectable by the CVA state space model, however, the PCA statistics only had partial success in detection of the such faults as shown in Fig. 4.

Table 1. Fault detection of CVA SS model

Fault No.	Fault Description	Percent Drift	Det. Stats.
1	Reactor temp. sensor	0.92	T^2_{Xc}
2	Input stream temperature sensor	2.64	T^2_{Xc}
3	Recycle stream temperature sensor	1.61	T^2_{Xc} & T^2_{X}
4	Recycle-pump pressure sensor	2.90	T^2_{eyc} & T^2_{Xc}
5	Analysis sensor- input stream	2.02	Q_{ey} & T^2_{ey}
6	Analysis sensor – product stream	1.0	Q_{ey}
7	Reactor level sensor	0.75	T^2_{X}
8	Input-stream flow sensor	0.01	T^2_{Xc}
9	Recycle-Input flow sensor	0.80	T^2_{X}
10	Tank-output flow sensor	2.60	Q_{ey}
11	Product-output flow sensor	1.42	T^2_{X}
12	Cool-water flow sensor	2.06	T^2_{X}

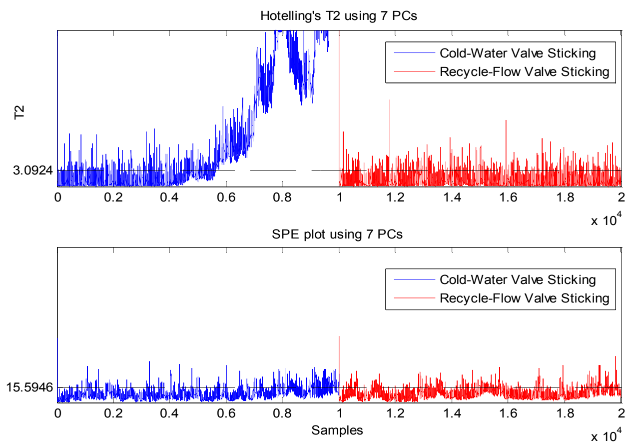

Fig. 4 Detection of Cool-Water and Recycle flow valve sticking using T^2 and Q statistics of a PCA model.

5. CONCLUSIONS

For all the state space SS model evaluated, there was no clearly superior fault detecting model. The best detecting statistical metric was dependent upon the fault being evaluated and the model employed. The only overall clear winner was the monitoring scheme based upon the combine index of the independent models which seem to achieve filtering out of misdetection and false alarms and provided reliable and relatively quick detection in comparison to its PCA counterpart. The superior fault detection was attributed to the CVA SS model's being more capable of detecting changes in the correlation structure between variables along with general shift in steady-state condition.

Using the approximate simplifier set of stochastic equations did not appear to have any adverse effect on the state space model fault detection capabilities. This is attributed to the model development path used in which the controller actuating signals were classified as process outputs and not inputs, leaving only the measurements on the process input streams and other disturbances variables to be consider as the process inputs.

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