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Multivariate Statistical Based Process Monitoring using Principal Component Analysis: An Application to Chemical reactor

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Abstract : The monitoring of industrial chemical plants and diagnosing the abnormalities in those set ups are crucial in process system domain as they are the deciding factors for the betterment of overall production quality in the process. Various statistical based malfunction detection methods have been included in the literature, namely, univariate and multivariate techniques. The univariate techniques are limited for monitoring only a single variable at a time whereas multivariate techniques can handle multiple correlated variables. Principal component analysis (PCA), a multi-variate technique, has been successfully used in the domain of process monitoring. PCA is used along with its two fault detection indices, T2 and Q statistics for detecting faults in any process. In the present study, a benchmark Continuous stirred tank reactor (CSTR) model is used to test the performance of the proposed PCA method. The simulated results show the effectiveness of the proposed method in handling different sensor faults in a CSTR process.

Keywords: Fault detection; Principal component analysis; T2 and Q statistics; CSTR model.

1. INTRODUCTION

In most chemical plants, monitoring and fault diagnosis are becoming increasingly important to maintain safe operation and quality in the process. Fault detection (FD), an important component of Abnormal Event Management System (AEM), is required to successfully detect, isolate and eliminate faults before the performance of the process is affected [1]. An abnormal event, also referred to as fault, is a continuous step where a variable undergoes change from its acceptable range of behavior leading to a malfunction and thus, huge losses in chemical plants. Several FD techniques have been proposed in the last two decade for the successful detection of faults in process industry, which could be broadly classified into model-based and process history based techniques. While a background knowledge of the system is required for a model based method, huge data set is required for a data based method [2].

The modelling based FD method involves comparing the measured variables of the system with the useful information that have been obtained from a mathematical model of the process [9]. Few commonly applied model based methods for process diagnosis include statistical based hypothesis testing strategies, observer based strategies, and interval based strategies and parity-space strategies [3]. For complex industrial processes involving large variables, deriving and developing models could be a challenging task, thus making model based methods highly non-applicable for many applications.

In contrast to the model based approaches, statistics based FD strategy is performed by collecting historical data and applying various techniques for monitoring the process [12]. In general, data based

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fault detection methods are divided as univariate methods and multivariate methods. Univariate methods are used in applications that monitor only one process variable at a given time and include methods like shewart charts, exponentially weighted moving average (EWMA) and cumulative sum (CUSUM) technique [4]. In contrast, multivariate techniques are used for monitoring multiple variables and are capable of successful monitoring in complex plants that involve large number of variables [13]. Some of the important multivariate FD strategies are partial least square (PLS), principal component analysis (PCA), Principal component regression (PCR), canonical variate analysis (CVA) and independent component analysis (ICA).

PCA is an important multiple variable regression technique used for compressing and extracting useful information from a given data [7]. It has been applied in various disciplines of science and engineering ranging from face recognition, compressing data to visualization and fault detection [10]. In the field of fault detection it has been successfully applied for process monitoring in various applications as given in [8][10[11]. PCA technique will project a given data from a multi-dimensional space with a dimension m (m defines the number of input variables) to a much lower principal component subspace with a dimension l (l < m) (l defines the number of principal components) by the maximization of variance of the projections. The resulting model would have the number of principal components (PC's) either equal to or lesser than the number of original variables in an observed data. The lower dimensional PCA model along with the two fault detection indices, T2 and Q statistics, are used to detect faults in a given process. This paper proposes a FD strategy based on Principal Component Analysis (PCA) model for a continuous stirred tank rector (CSTR) model.

2. PRINCIPAL COMPONENT ANALYSIS (PCA)

Principal Component Analysis (PCA) is a method that would transform the variables of a correlated data on to a new set of variables (principal components or PC's), which are not correlated and contain most of the information from the original data [13]. The transformation is developed such that the first PC has the largest possible capture (first PC would account for as much of the variability in the data as possible), and each following principal component in turn has the highest variance possible with an underlying constraint that each PC is orthogonal to the preceding PC. The PCA model is developed by decomposing a data set $X \in R_{nxm}$ using the singular value decomposition (SVD) as follows:

$$X = TP^T \tag{1}$$

where T is a matrix containing principal components or score vectors and P is a matrix, of orthogonal loading vectors that are eigen vectors derived from the application of SVD on the covariance matrix of data set X, n is the number of samples and m is the number of variables of the data set. Score vectors contain useful information about the relation between the samples and loading vectors contain useful information regarding the relationship between the variables. The covariance matrix of X, $\hat{G}$ is defined as:

$$\hat{G} = \frac{1}{n-1} X^T X = P£P^T \tag{2}$$

£ is a diagonal matrix having decreasing arrangement of eigien values.

After the application of SVD, choosing the right number of principal components is a very crucial since it describes the goodness of a PCA model. Choosing more number would introduce noise that would mask few important parameters in data whereas choosing less number could lead to losing of few important features in the data, thus leading to degradation in the quality of the PCA model [4]. The cumulative percentage variance (CPV) technique has been used in the present task to determine the exact number of score components. Once a reference PCA model is been developed from a normal fault-free data, it is employed along with the Hotelling's T2 and Q statistics for diagnosis in a faulty data [8]. The Hotelling's T2 is a statistical based method for capturing the nature of the exact PCs retained through CPV technique. It is defined as:

$$T^2 = X^T P\Lambda_a -1 P^T X \tag{3}$$

Λ a is a diagonal matrix having the eigien values that is associated with the retained PC's. The application process is said to be in control if T^2 value is less than the limit, which is described as [5] :

$$T_\alpha^2 = \frac{(n^2-1)}{n(n-a)} F_\alpha(a, n-a) \tag{4}$$

In contrast, the Q statistic data is used to measure variations of data which are not measured by the T^2 statistics, and this would provide an idea of how good the data fits the developed PCA model and it is defined as:

$$Q = r^T r \tag{5}$$

where $r = (I - PP^T)x$. The confidence limits for Q statistics are considered as given in [6].

The whole PC based fault detection process can be explained as shown in Figure 1:

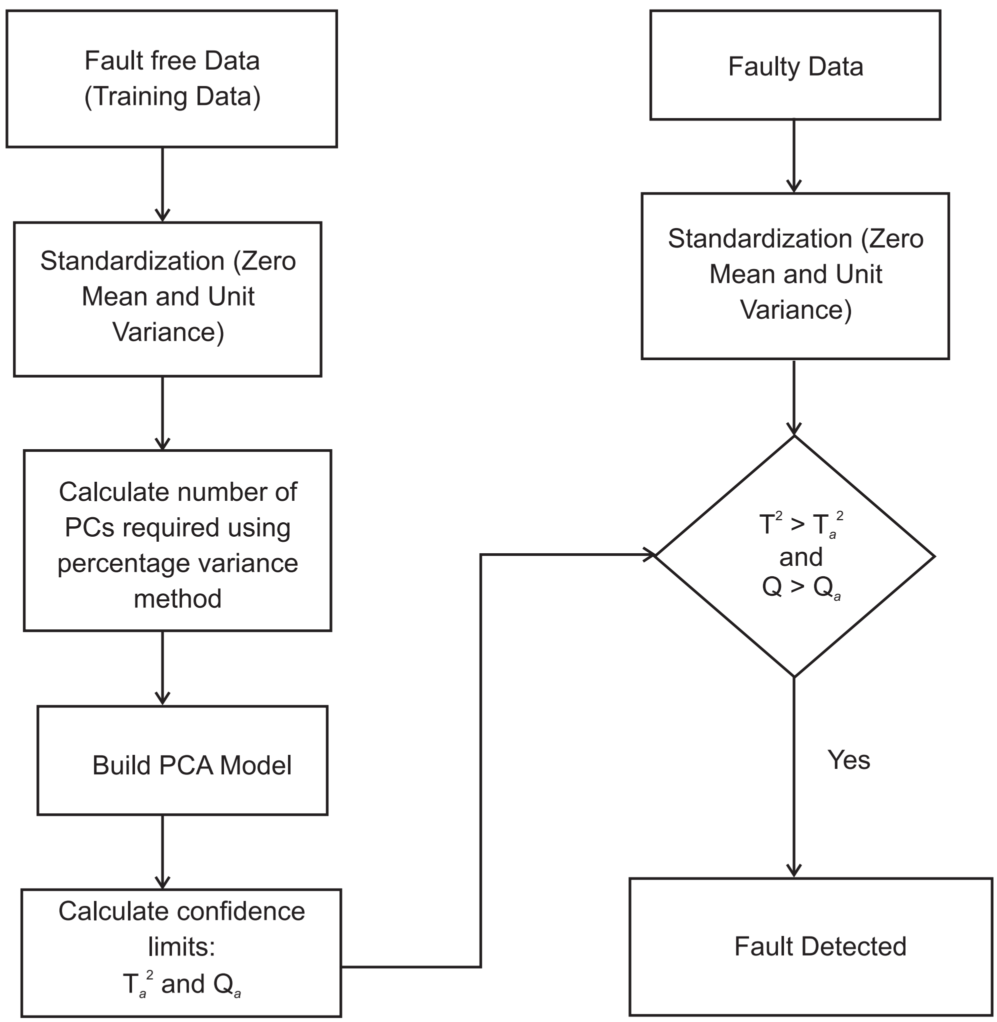

Figure 1: Fault detection process using PCA

3. CONTINUOUS STIRRED TANK REACTOR (CSTR)

The efficient performance of the developed monitoring strategy would be tested on the data derived from a simulated CSTR bench mark problem. A Continuous Stirred Tank Reactor (CSTR) is an important unit operation in many chemical plants that has very large operating range. Chemical reactions in the stirred tank process are either exothermic or endothermic in nature. They need that energy can either be added or removed to the process for maintaining a constant temperature. In the CSTR process where a non-isothermal, non-reversible first order reaction A → B occurs. The dynamics of CSTR can be explained with the following equations:

$$\frac{dCa}{dT} = \frac{F}{V}(C_{AO} - C_A) - k_0 \exp\left(-\frac{E}{RT}\right)C_A \tag{6}$$

$$\frac{dT}{dT} = \frac{F}{V}(T_O - T) - \left(-\frac{H_r}{\rho C_\rho}\right)k_0 \exp\left(-\frac{E}{RT}\right)C_A - Q/V\rho_1 C_p \tag{7}$$

$$Q = \frac{aF_c^{b+1}}{\left(F_C + \left(\frac{aF_c^b}{2\rho C_{pc}}\right)\right)}(T - T_{cin}) \tag{8}$$

where k_o is the rate constant of the reaction, E defines the activation energy of the reaction, R is the gas constant, F defines the feed flow rate, F_C is the inlet coolant flow rate, V defines the reactor volume, H_r is the rate of reaction, T_O is the temperature at the inlet, T is the reactor temperature, T_{cin} defines the coolant inlet temperature, C_{AO} and C_A are the concentration of inlet and reactor concentration of liquid A, respectively and ρ_1, ρ,C_p and C_{pc} are the densities and specific heats of the CSTR process reacting material and CSTR jacket coolant, respectively.

4. DATA GENERATION

In the present work, the reactor is used for generating the data set through simulations. The data is divided into two categories: training data set and testing data set. The training data would be used to build a PCA model and developed model would be used for finding faults in the testing data set. Simulations are carried to get 400 observations of the CSTR model that would be used as training data for the PCA model. The data for execution would include four variables that are combination of two input and two output variables. They are flow rate of the coolant (Fc), flow rate of the input feed (F) the concentration at the outlet (Ca), and the temperature at the output of reactor (T). The two input variables Fc and F, are pseudo-random binary sequence (PRBS) with frequencies of 0.05 and 0.01 respectively. Hence, the data set to be used for developing the PCA model after the normalization of all the variables, would constitute 400 rows and 4 columns. As discussed in section 2, the Cumulative Percentage Variance technique is used for determining the right number of PCs with a 90% limit and in this case, it results in retaining three PC's. Similarly, 400 rows and 4 columns of the CSTR model would be generated to be used for testing the developed PCA model. Different kind of faults would be added to the steady state reactor temperature (Ts) variable and effect of developed PCA model would be checked. The nominal simulated parameter values for the CSTR plant are as given in [14].

5. RESULTS AND DISCUSSION

In the following section, the developed PCA FD model performance is being checked for detecting faults in a CSTR data having several fault scenarios. In the first scenario, one variable from testing data set is with additive bias faults *i.e*. bias sensor fault (case A). Secondly, fault with degraded precision for a sensor is being taken, where the variable is contaminated by an additional random noise (case B). This is followed by a scenario where it is assumed that the variable is having an aging fault (case C). Finally, a case of outlier type of sensor fault is also considered (case D).

Case A: Sensor bias fault

A scenario where sensor bias additive fault is being added to the Steady state reactor temperature (Ts) variable. The fault is inserted in the variable Ts from samples 300 to 350. This type fault can be shown by a constant amplitude of 500 in variable Ts and this could be easily detected b. On simulation, it can be seen that both T2 and Q indices exceed their threshold value between the samples 300 and 350, as shown in figure 2.

Case B: Precision degradation fault

In this scenario, the problem of detecting precision degradation fault to the Steady state reactor temperature (Ts) variable is considered. Towards the end, the fault free output variable Ts is corrupted using random Gaussian noise from sample 300 till sample 400. On simulation, it can be seen that the T^2 and Q indices exceed their threshold value after the sample 300 as shown in figure 3.

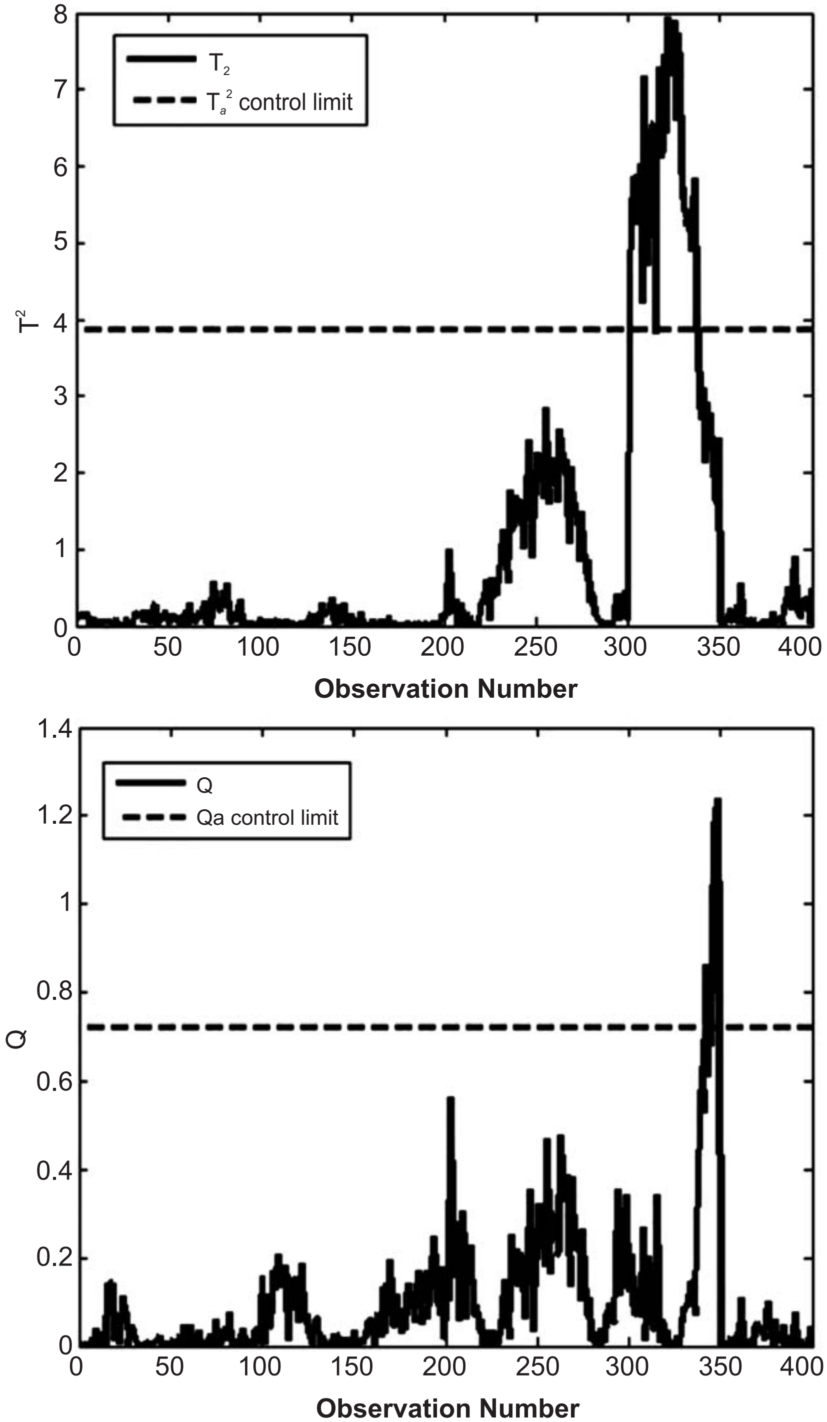

Figure 2: T^2 and Q statistics in presence of sensor bias fault

Case C: Aging fault

For checking aging or a drift sensor fault, a ramp signal with a 0.6 slope, is being inserted into the variable Ts from sample 300 of the simulation data set. As seen in the figure, the Q statistic value gradually increases with aging fault increasing, and it begins to exceed the threshold limit as the fault magnitude becomes larger and larger. However, the drift fault was not detected by the Hoteling's T^2 statistic as shown in figure 4.

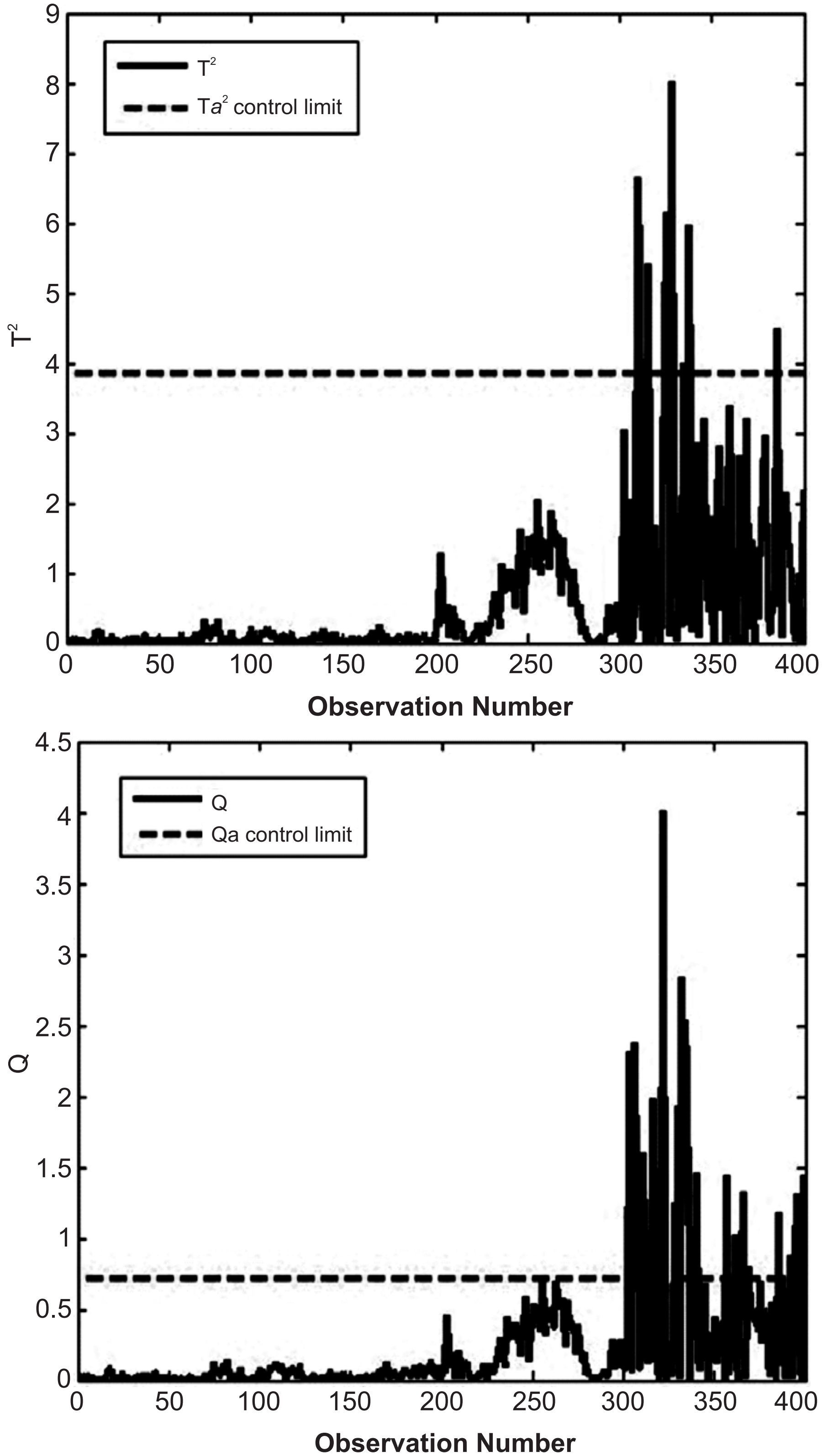

Figure 3: T^2 and Q statistics in presence of precision degradation fault

Case D: Sensor outlier fault

The effect of sensor outlier fault was checked by applying variations to the steady state reactor temperature (T*s*). The variable is corrupted by applying multiple outlier faults between samples n = 200 to 204 and n = 300 to 304, respectively. On simulation, the T^2 and Q graphs, as shown in figure 5 are obtained, which clearly show that the calculated T2 and Q value exceed the control limits:

6. CONCLUSION

Fault diagnosis and detection has been a critical issue in the domain of process monitoring since it directly effects the safety and financial condition of any industrial process. Process data malfunction detection methods have been used for handling complex data in the chemical processes. Principal component analysis (PCA) is a popular multivariate strategy, widely used for data compression as well as fault detection. The developed PCA model along with its two fault detection indices is illustrated to detect different sensor faults through a simulated CSTR data. The simulated results show that the multivariate methods have a clear advantage over the univariate methods for monitoring multiple correlated data. The results show that the developed algorithm is successfully able to detect different variants of sensor faults.

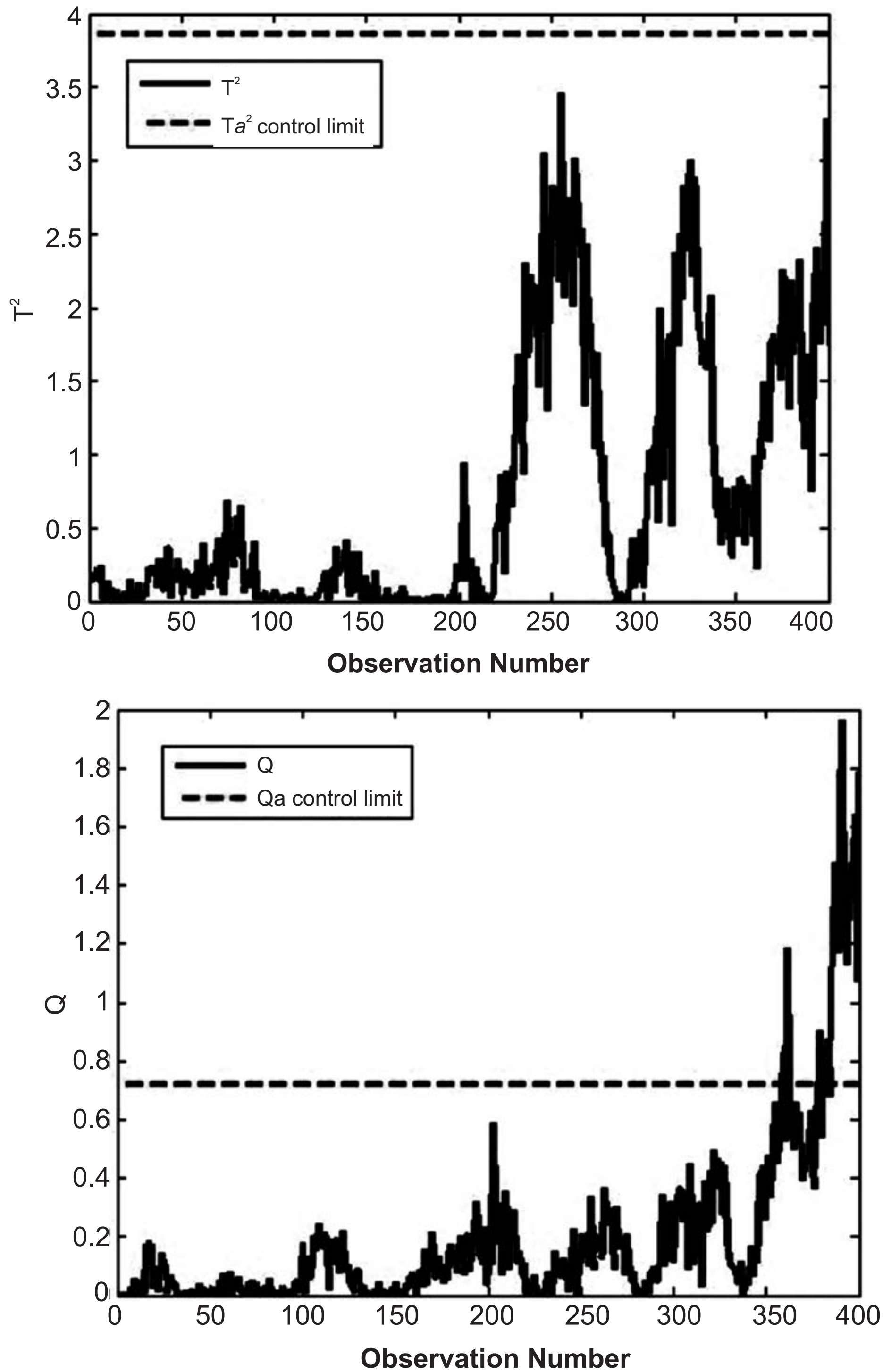

Figure 4 : T^2 and Q statistics in presence of aging fault

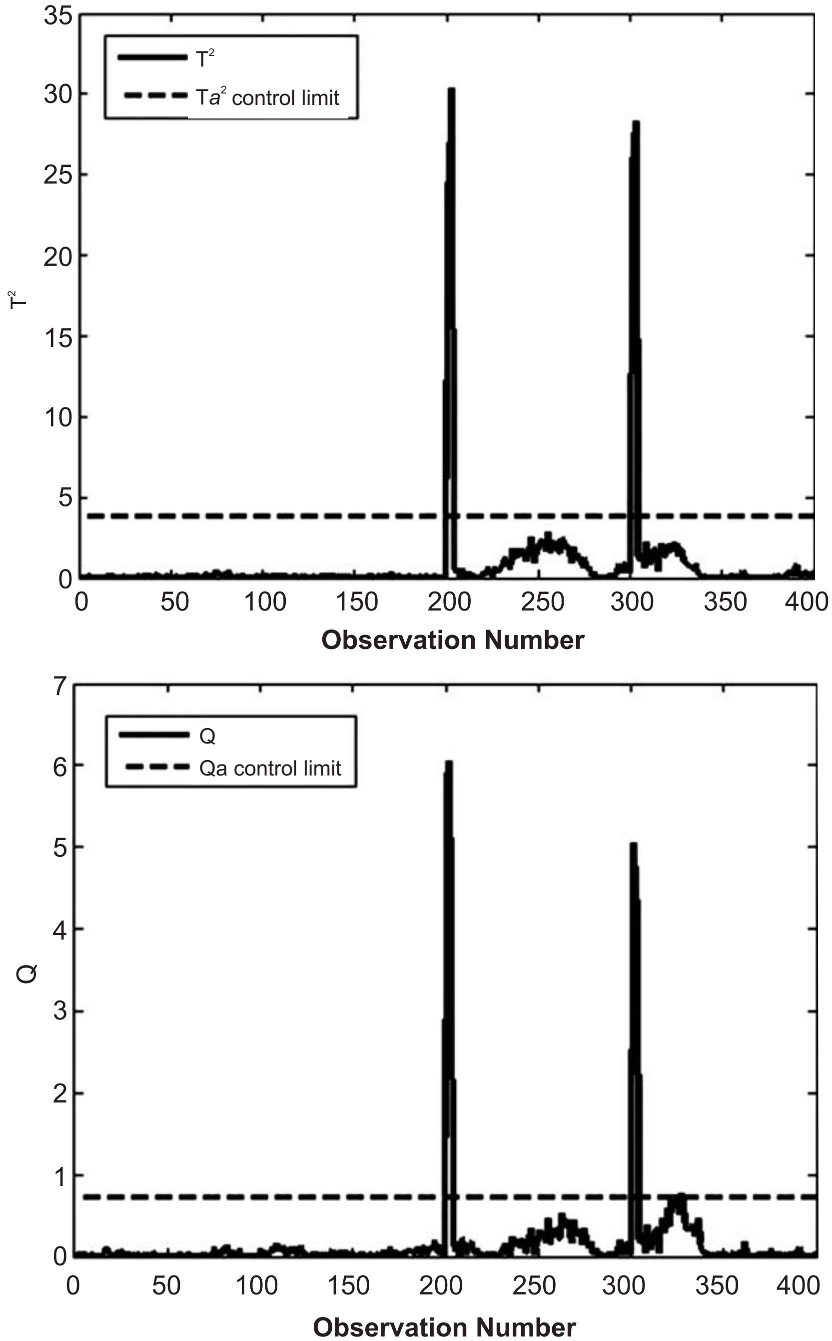

Figure 5 : T^2 and Q statistics in presence of sensor outlier fault

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