International Journal of ChemTech Research
CODEN (USA): IJCRGG, ISSN: 0974-4290, ISSN(Online):2455-9555
Vol.11 No.02, pp 266-274, 2018

Fault Detection and Analysis using Statistical Data for Continuous Stirred Tank Reactor (CSTR)

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Abstract : Continuous Stirred Tank Reactor (CSTR) here is considered as a non linear process. CSTR is widely used in many industrial sectors like chemical industries, pharmaceutical, drugs manufacturing, waste water treatment plants and etc.. Due to changes in process parameters the accuracy of final product can be reduced. In order to get the product in desired concentration and temperature, faults developed in CSTR during the chemical reaction need to be analysed. If not, those faults may lead to degrade the performance of the system. For this purpose, there are various fault detection methods are to be considered. Among the methods, the Principal Component Analysis (PCA) can be proposed to detect faults in CSTR. PCA is one of the data based fault detection methods. PCA statistics like Hotelling T^2 statistic and Square Prediction Error (SPE) or Q statistics are used for detecting faults in the process. By detecting various faults, the performance of the process can be improved.

Keywords : Fault detection, Principal component analysis, T^2 and Q statistics, CSTR model.

Introduction

In most chemical plants, monitoring and fault diagnosis are becoming increasingly important safe operation and quality in the process. The Continuous Stirred Tank Reactor (CSTR) system is highly nonlinear, exothermic and irreversible process. In CSTR, when the reactants are added into the tank, the stirrer will stir the reactants to give desired product. Once the equipment is running, it is usually operated at steady state and designed to achieve well mixing. The CSTR also known as vat or back mix reactor, is a common ideal reactor type in chemical engineering. A CSTR refers to a model used to estimate the key unit operation variables when using a continuous agitated tank reactor to reach a specified output. It is widely used in the organic chemicals industry for medium and large scale production. The reactor is operated by three control loops that will regulate the outlet temperature and the inlet flow rate of the reactor tank level. During the process, the heat will be generated and hence the heat of reaction can be removed by a coolant medium that flows through a jacket around the reactor. During the CSTR process, the faults may occur which further leads to inaccurate result. Figure 1 shows a continuous stirred tank reactor.

International Journal of ChemTech Research, 2018,11(02): 266-274

DOI= http://dx.doi.org/10.20902/IJCTR.2018.110232

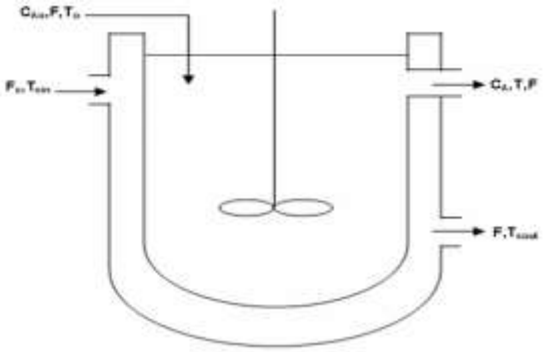

Figure 1 Continuous Stirred Tank Reactor

Mathematical Modelling Of CSTR

Mass and energy balance equation of CSTR [6]

$$V\frac{dC_A}{dt} = F(C_{A0} - C_A) - VK_0 e^{-E/RT} C_A \tag{1}$$

$$V\rho C_p \frac{dT}{dt} = \rho C_p F(T_0 - T) - \frac{aF_c^{b+1}}{F_c + \frac{aF_c^b}{2\rho_c C_{pc}}}(T - T_{cin}) + (-\Delta H_{r\times n}) VK_0 e^{(-E/RT)} C_A \tag{2}$$

where ko 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, FC is the inlet coolant flow rate, V defines the reactor volume, $\Delta Hr\times n$ is the rate of reaction, T_0 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, ρ_c,Cp and Cpc are the densities and specific heats of the CSTR process reacting material and CSTR jacket coolant, respectively.

These two nonlinear differential equations 2 and 3 cannot be solved analytically. The linearized equations in deviation variables are

$$\frac{dC_A'}{dt} = a_{11}C_A' + a_{12}T' + a_{13}C_{Ao}' + a_{14}F_c' + a_{15}T_o' + a_{16}F' \tag{3}$$

$$\frac{dT'}{dt} = a_{21}C_A' + a_{22}T' + a_{23}C_{Ao}' + a_{24}F_c' + a_{25}T_o' + a_{26}F' \tag{4}$$

The coefficients are

$$a_{11} = -\frac{F}{V} - K_o e^{-E/RT_s},\ a_{12} = -\frac{E}{RT_s^2} K_o e^{-E/RT_s} C_{As},\ a_{13} = \frac{F}{V},\ a_{14} = 0,\ a_{15} = 0,\ a_{16} = \frac{(C_{Ao} - C_A)_s}{V},$$

$$a_{21} = -\frac{\Delta H_{r\times n} k_o e^{-E/RTs}}{\rho C_p},\ a_{22} = -\frac{F}{V} - \frac{UA_s^*}{V\rho C_p} + (-\Delta H_{r\times n})\frac{\frac{E}{RT_s^2}}{\rho C_P} k_0 e^{-E/RTs} C_{As},\ a_{23} = 0,\ a_{25} = \frac{F}{V},$$

$$a_{26} = \frac{(T_o - T)_s}{V},$$

$$a_{24} = \frac{-abF_{cs}^{b}\left(F_{cs} + \frac{a}{b}\frac{aF_{cs}^{b}}{2\rho_c C_{pc}}\right)[T_s - (T_{cin})_s]}{(V\rho C_p)\left(F_{cs} + \frac{aF_{cs}^{b}}{2\rho_c C_{pc}}\right)^2}$$

The resulting transfer function

$$\frac{T(s)}{F_c(s)} = \frac{a_{24}s + (a_{21}a_{14} - a_{24}a_{11})}{s^2 - (a_{11} + a_{22})s + (a_{11}a_{22} - a_{12}a_{21})} \qquad (5)$$

Based on the specific parameters of continuous stirred tank reactor model, the appropriate coefficients are to be calculated and the corresponding transfer function can be obtained.

Fault Detection Methods

The term fault is generally defined as a departure from an acceptance range of an observed variable. A failure is a permanent interruption of a system ability to perform a required function under specified operating conditions [1]. The fault can be identified using various methods. Fault detection and analysis is an important problem in process engineering [15]. Early detection of process fault while the plant is still operating in a controllable region can help to avoid abnormal event progression and to reduce productivity loss. The basic classifications of fault detection method is represented in the Figure 2.

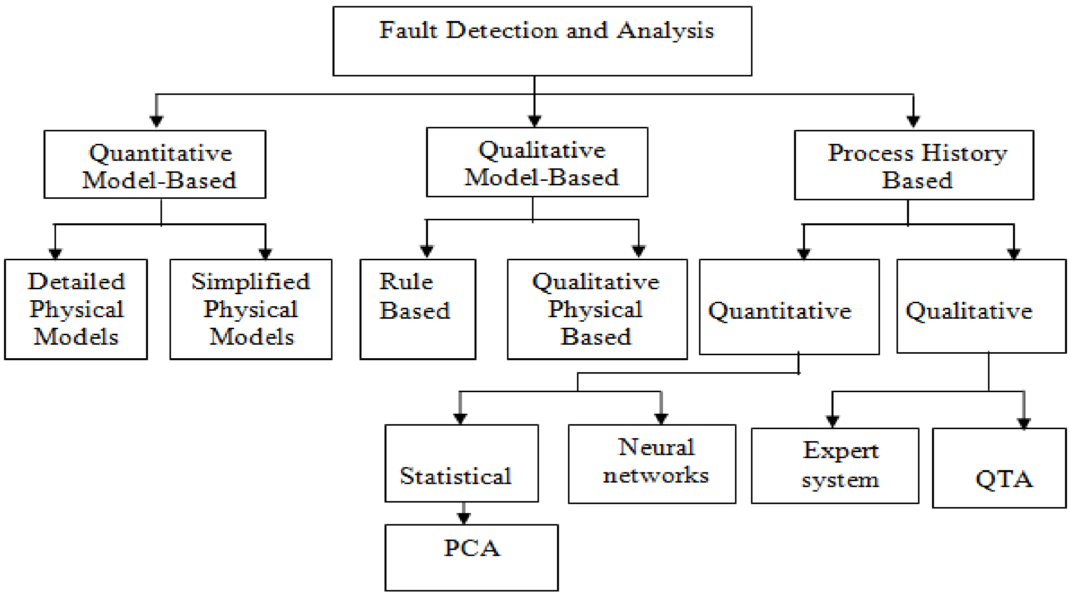

Figure 2 Classification of Fault Detection methods

Quantitative model based methods include those based on detailed physical models as well as those based on simplified models of the physical processes. These models can be steady-state, linear dynamic or nonlinear dynamic.

Qualitative model- based approaches include rule-based system and models based on qualitative physics. For rule-based systems, it is necessary to distinguish between those based on expert rules for which there may be no underlying first principles from physics, rules derived from first principles, and simple limit checks which serve as the basis for alarms.

In contrast to the first two groups where a priori knowledge of the process is assumed, the third group is based fully on process history, i.e., a large amount of historical data is assumed to be available [3]. These models include quantitative and qualitative methods. Here the fault diagnosis is done mainly based on the process history based methods. The process history based methods are classified into quantitative and qualitative methods. The quantitative methods include neural network and statistical. The qualitative methods include expert system and Qualitative Trend Analysis (QTA). Principal Component Analysis (PCA)/Partial Least Squares (PLS) and statistical pattern classifiers form a major component of statistical feature extraction methods.

Principal Component Analysis

Principal Component Analysis (PCA) is a statistical procedure that uses an orthogonal transformation to convert a set of observations by decomposing a data set $X \in R^{n \times m}$ using the singular value decomposition (SVD) as follows

$$X = PT^T$$

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, , nis 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 Σ is defined as

$$\Sigma = \frac{1}{n-1} X^T X = P \wedge P^T$$

$$\wedge = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_m)$$

$$(\lambda_1 > \lambda_2 > \ldots\ldots > \lambda_m)$$

is a diagonal matrix containing the eigen values in a decreasing order

Hotelling's T^2 statistic

The Hotelling's T^2 statistic which measures the variations in the principal components at different time samples, is defined as

$$T^2 = X^T P \wedge^{-1} P^T X$$

For each new test data, the T^2 statistic is calculated and a threshold, T_α is calculated as

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

Where,

F(a,n-a,α) is the F-distribution with (a,n-a) degrees of freedom with significance level α, n is the number of observations of the training data, a is the number of selected principal components. If the T^2 statistic exceeds T_α, then the fault is considered as detected.

Q statistic

The Q statistic measures the projection of a data sample on the residual subspace, which provides an overall measure of how a data sample fits the PCA model. The Q-statistic measures the square of error not captured by principal components in approximation.

$$Q = \left\| \left(I - PP^T \right) X \right\|^2$$

The Q-statistic value is estimated and it is compared to a threshold Q_α. The Q_α defined as

$$Q_\alpha = \theta_1 \left[\frac{h_o c_\alpha \sqrt{2\theta_2}}{\theta_1} + 1 + \frac{\theta_2 h_o (h_o - 1)}{\theta_1^{\,2}} \right]^{\frac{1}{h_o}}$$

where c_α is the standard normal distribution with a significance level, θ_i and h_o are defined as follows:

$$\theta_i = \Sigma_{j=a+1}^{m} \lambda_j^i \,, \quad h_o = 1 - \frac{2\theta_1\theta_3}{3\theta_2^2}$$

where m is the number of variables. PCA based fault detection process is explained in Figure 3.

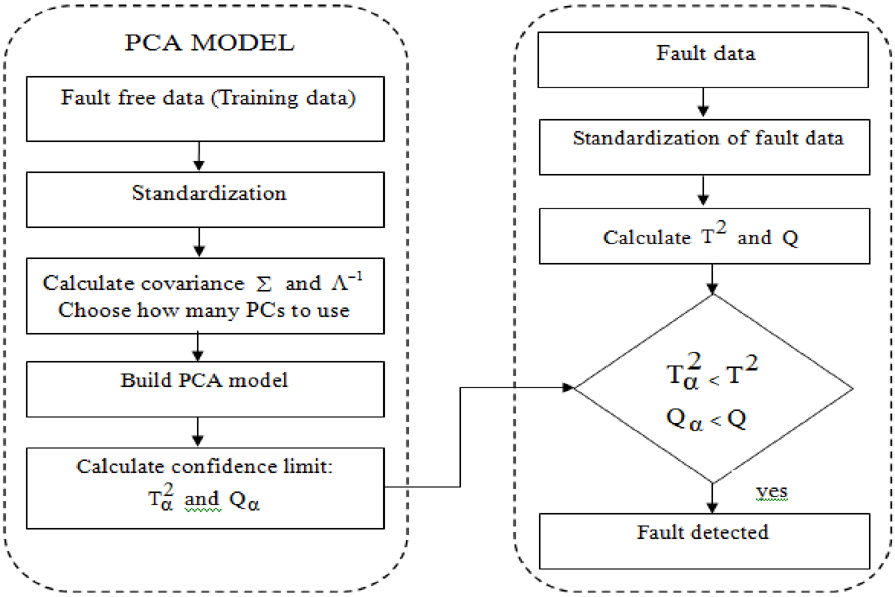

Figure 3 Fault detection process using PCA

Data Generation

There are various faults occur in CSTR. Some of the common faults considered here are actuator fault, sensor faults and process faults. For CSTR it is also considered Principle Component Analysis under faultless condition. Table 1 shows some of the data under faultless condition.

able 1 Data under Faultless Condition

S. No	Coolant flow rate F_c (lpm)	Concentration(mol/l)	Reactor temperature R_T(^{o}K)
1.	181	0.1897	356
2.	178	0.1878	359
3.	176	0.1863	361
4.	174	0.1841	363
.	.	.	.
.	.	.	.
74.	56	0.0406	488

Sensor faults

A sensor is an object whose purpose is to detect events or changes in its environment, and then provide a corresponding output. It is otherwise known as a transducer if it is provided with suitable signal conditioning circuit. The sensor considered here is Thermometer-Temperature sensor. Table 2 shows some of the data considered with sensor fault condition.

Actuator faults

The operation of a control valve involves positioning its movable part relative to the stationary seat of the valve. The purpose of the valve actuator is to accurately locate the valve plug in a position dictated by the control signal. The actuator accepts a signal from the control system and in response moves the valve to a fully open or fully closed position. Table 3 shows some of the data considered with actuator fault condition.

Table 2 Data under Sensor Fault Condition

S.No	Coolant flow rate F_c (lpm)	Concentration(mol/l)	Reactor temperature R_T (^oK)
1.	88	0.0692	790
2.	86	0.0672	771
3.	84	0.0653	773
4.	82	0.0642	874
.	.	.	.
.	.	.	.
25.	60	0.0438	903

Table 3 Data under Actuator Fault Condition

S.No	Coolant flow rate F_c (lpm)	Concentration(mol/l)	Reactor temperature R_T (^oK)
1.	0	0.0734	1200
2.	5	0.0701	1100
3.	7	0.0692	1050
4.	8	0.0672	1000
	.	.	.
	.	.	.
24.	1200	0.064	160

Process faults

The process faults occur due to hard failures in equipment. This results in changes in the information flow between various variables. Both quality and reliability may be affected from process faults. Table 4 shows some of the data considered with process fault condition.

Table 4 Data under Process Fault Condition

S.No	Coolant flow rate F_c (lpm)	Concentration(mol/l)	Reactor temperature R_T (^oK)
1.	10	0.019	850
2.	11	0.02	800
3.	13	0.025	750
.	.	.	.
.	.	.	.
24.	1200	8	160

Results and Discussion

Principle Component Analysis under Faultless Condition

During the normal process, Principle Component Aanalysis is performed for 73 samples. By the simulation, it can be identified that the Hotelling's T^2 and Q statistics have not exceeded their threshold value. Figure 4 shows the Principle Component Analysis during normal operation of CSTR

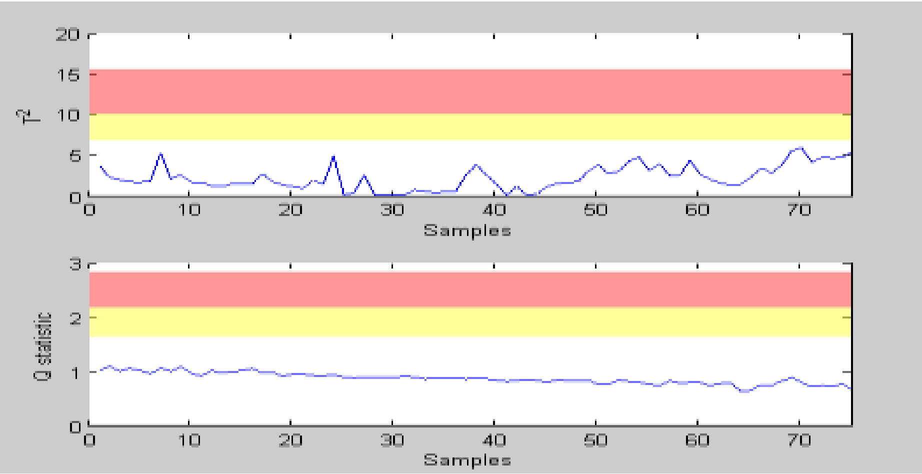

Figure 4 Principle Component Analysis during Normal Operation of CSTR

Fault Detection during Actuator Fault Condition

During the normal process, it is considered that there is an actuator fault happened from the samples 50 to 73. By the simulation, it can be identified that the Hotelling's T^2 and Q statistics exceeded their threshold value after the sample 51. Figure 5 shows the fault detection of the CSTR during actuator fault condition.

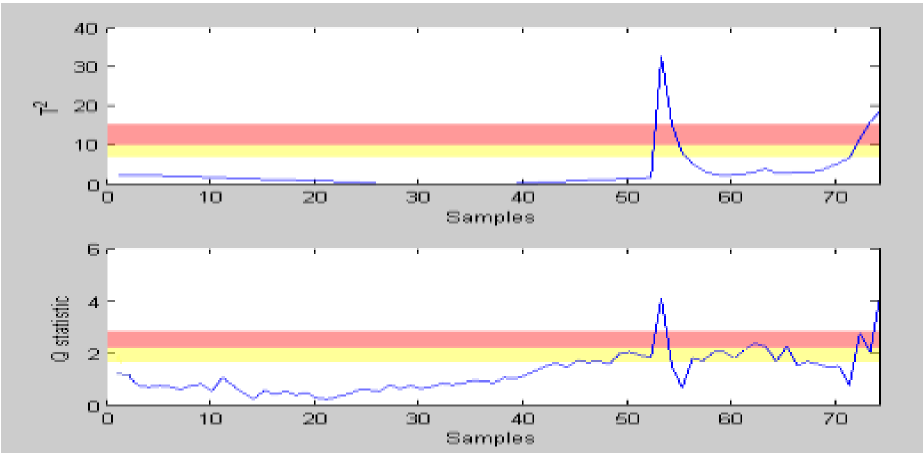

Figure 5 Fault Detection during Actuator Fault Condition

Fault Detection during Process Fault Condition

During the normal process, it is considered that there is an process fault happened from the samples 50 to 73. By the simulation, it can be identified that the Hotelling's T^2 and Q statistics exceeded their threshold value after the sample 51. Figure 6 shows the fault detection of the CSTR during process fault condition.

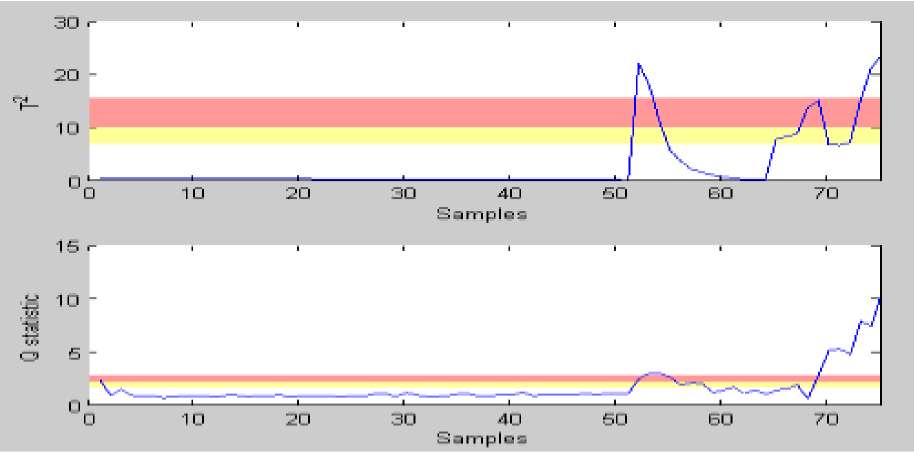

Figure 6 Fault Detection during Process Fault Condition

Fault Detection during Sensor Fault Condition

During the normal process, it is considered that there is an sensor fault happened from the samples 50 to 73. By the simulation, it can be identified that the Hotelling's T^2 and Q statistics exceeded their threshold value after the sample 50. Figure 7 shows the fault detection of the CSTR during sensor fault condition.

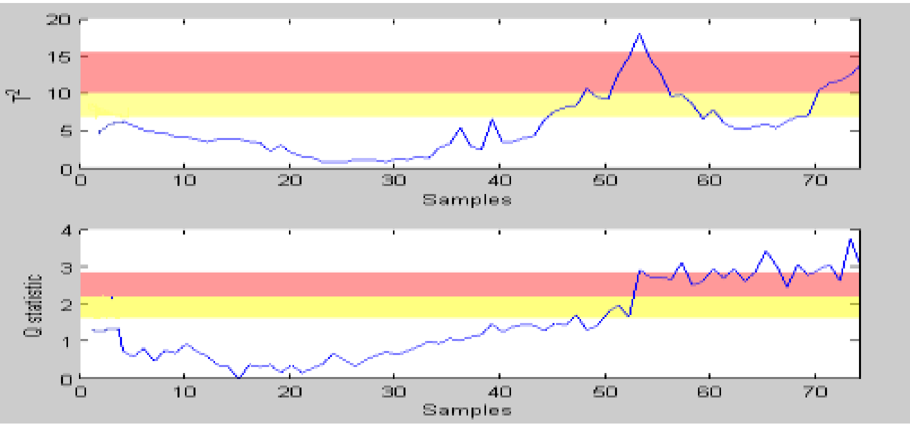

Figure 7 Fault Detection during Sensor Fault Condition

Conclusion

The application of Continuous Stirred Tank Reactor is very essential nowadays. The fault detection in CSTR is very important. The various faults such as sensor faults, actuator faults, process faults present in CSTR are detected using Principle Component Analysis.

References

1. Fouzi Harrou, Mohamed N. Nounou , Hazem N. Nounou and Muddu Madakyaru, Statistical fault detection using PCA-based GLR hypothesis testing, Elsevier Journal of Loss Prevention in the Process Industries, 2013, 26, 129-139.
2. Farid Kadrib, Fouzi Harrou, Sofiane Khadraouic and Yin Sun, Ozone measurements monitoring using data-based approach, Elsevier Journal of Process Safety and Environmental Protection, 2016, 100, 220-231.
3. Garcia-Alvarez.D, Fault detection using Principal Component Analysis (PCA) in a Wastewater Treatment Plant (WWTP), 62th International Student's Scientific Conference, International Society of Automation, 2009, 13-17.

4. Jie Bai, Simon X. Yang and Zhu, A Multi-Fault Diagnosis Method for Sensor Systems Based on Principle Component Analysis, Journal of Sensors, 2010, 10, 241-253.
5. Joe Qin.S, Survey on data-driven industrial process monitoring and diagnosis, Elsevier Journal of Annual Reviews in Control, 2012, 36, 220-234.
6. Marlin.T, Process control: Designing processes and control systems for dynamic performance, Second Edition, McGraw-Hill, New York, 2000.
7. Mohamed-Faouzi Harkat, Gilles Mourot, Jose´ Ragot, An improved PCA scheme for sensor FDI: Application to an air quality monitoring network, Elsevier Journal of Process Control,2006, 16, 625-634.
8. Mahmud Ahmed, M Baqqar, Fengshou Gu and A D Ball, Fault Detection and Diagnosis using Principal Component Analysis of Vibration Data from a Reciprocating Compressor,IEEE, UKACC International Conference on Control, 2012, 461-466.
9. Peter Fogh Odgaard , Bao Lin and Sten Bay Jorgensen, Observer and Data-Driven-Model-Based Fault Detection in Power Plant Coal Mills, IEEE Transactions On Energy Conversion, 2008, 23, 219-227.
10. Mahmud Ahmed, M Baqqar, Fengshou Gu and A D Ball, Fault Detection and Diagnosis using Principal Component Analysis of Vibration Data from a Reciprocating Compressor,IEEE, UKACC International Conference on Control, 2012, 461-466.
11. Peter Fogh Odgaard , Bao Lin and Sten Bay Jorgensen, Observer and Data-Driven-Model-Based Fault Detection in Power Plant Coal Mills, IEEE Transactions On Energy Conversion, 2008, 23, 219-227.
12. Q.Chen, U.Kruger, M.Meronk and A.Y.T. Leung, Synthesis of T2 and Q statistics for process monitoring, Elsevier Journal of Control Engineering Practice, 2004, 12, 745-755.
13. Ramakrishna Kini.K and Muddu Madakyaru, Multivariate Statistical Based Process Monitoring using Principal Component Analysis: An Application to Chemical reactor, International Journal of Computer Technology and Application,2016, 9, pp.303-311.
14. Raoudha Baklouti, Mohamed Nounou, Hazem Nounou,Ahmed Ben, HamidaMajdi Mansouri1, Mohammed and Nazmul Karim, Statistical Fault Detection of Chemical Process - Comparative Studies, Elsevier Journal of Chemical Engineering & Process Technology, 2016, 7, 352-363.
15. Shyamapada mandal, N Sairam, S Sridhar and P Swaminathan, Nuclear power plant sensor fault detection using singular value decomposition-based method, Indian Academy of Sciences, 2017, 42, 1473–1480.
16. Thamara Villegas, Maria Jesus Fuente, Miguel Rodríguez, Principal Component Analysis for Fault Detection and Diagnosis. Experience with a pilot plant, 9th WSEAS international conference on computational intelligence, man-machine systems and cybernetics, 2010, 147-152.
17. Venkat Venkatasubramanian, Raghunathan Rengaswamy, Surya N. Kavuri and Kewen Yin, A review of process fault detection and diagnosis Part I: Quantitative model-based methods, Elsevier Journal of Computers and Chemical Engineering, 2003, 27, 293- 311.
18. Venkat Venkatasubramanian, Raghunathan Rengaswamy, Surya N. Kavuri and Kewen Yin, A review of process fault detection and diagnosis Part III: Process history based methods, Elsevier Journal of Computers and Chemical Engineering, 2003, 27, 327- 346.

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