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Data-Driven Fault Diagnostics for Industrial Processes: An Application to Penicillin Fermentation Process

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ABSTRACT We consider the problem of fault detection and isolation for the penicillin fermentation process. A penicillin fermentation process is a highly complex and nonlinear dynamic process with batch processing. A data-driven approach is utilized for fault diagnostics due to the availability of huge batch processing data and the unavailability of an analytical model. To address the non-linearity, a subspace-aided parity-based residual generation technique is proposed by using a just-in-time learning approach. For the just-in-time learning approach, the most similar data samples are selected from the database for incoming test samples and a subspace aided parity-based residual is generated using these samples. The designed fault detection technique is implemented for the penicillin fermentation process to demonstrate real-time health monitoring of the process under sensor noise and process disturbances. Two sensor faults and an actuator fault are considered and successfully detected using the proposed technique. Further, a fault isolation approach is developed to isolate these faults and their location has been identified. A case study is given to show the improvement offered by the proposed technique for the fault detection rate and minimization of the false alarm rate as compared to the existing techniques for the penicillin fermentation process.

INDEX TERMS Data-driven, fault diagnostics, process monitoring, subspace identification, just-in-time learning, penicillin fermentation process.

I. INTRODUCTION

Penicillin is an effective antibiotic that is widely used to treat various contagious ailments. Recently, several natural and synthetic varieties of penicillin are used to cure a wide range of infectious diseases. The penicillin fermentation process (PFP) is a dynamic nonlinear batch process. There are three stages in the process, growth of cell stage, synthesis of penicillin, and the cell autolysis level. In the first stage, the nutrient substance of the starting material is demolished and new cells are continuously synthesized. In the second stage, penicillin synthesis starts and maximizes production until it weakens the capability to synthesize penicillin. The third stage of the process is cell autolysis, where the pH of the fermentation broth enhances and also diminishes the capability of penicillin synthesis. Throughout the complete fermentation process, various elements influence the efficacy of penicillin fermentation, like pH, temperature, dissolved oxygen concentration, substrate concentration [1]. Any abnormality or un-permitted deviation in these process variables may not only affect the product quality but low-quality products may also lead to coordinated effects in human life. The improvement in the safety and reliability of PFP is thus highly desirable. It is of vital importance to decrease and prevent the hazards of faults. To this end, faults must be timely indicated and preventive measures must be taken to look for the issues in the process variables. Therefore, it is important to implement an efficient health monitoring/ fault diagnostic system to ensure the safety and reliability of PFP.

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The fault detection (FD) techniques can be classified as model-based and data-driven techniques. Model-based fault detection techniques are well-established and have a tremendous history of applications [2]–[5]. During the model-based FD design, a mathematical model for the process is first obtained using either the first principle approach or the identification techniques. The mathematical model is then used for the estimation of process outputs. The estimated and actual process measurements are then compared to generate residual signals to detect any anomaly in the process. Model-based fault-detection methods rely heavily on the precision of the mathematical model of the system. Accurate modeling of batch processes is very difficult, due to which data-driven fault diagnosis approaches are more favorable for fermentation processes as huge input-output measurements are available.

The data-driven techniques, on the other hand, rely on the process input and output data. They do not need a mathematical model of the process. The data-driven fault diagnosis techniques are significantly developed in the previous decade [6]–[10]. Among the data-driven techniques, the multivariate statistical approach is commonly applied for batch processes. It is based on principal component analysis (PCA) [11]–[13]. Notice that the PCA-based design primarily estimates the future measurements for online monitoring, then the deviation of inevitable anticipation makes the monitoring outcome unreliable. PCA-based techniques, in general, assume the processes to be linear while the batch processing in PFP is nonlinear and complex. In addition, PCA-based approaches are shown to perform very poorly for the classification of faults. To address the problem of fault diagnosis in complex and nonlinear processes such as PFP, temperature distribution systems, process industry, etc. there exist various data-driven approaches to investigate faults in nonlinear processes. For example, Kernel-based fault detection frameworks have been reported for nonlinear processes [14]–[16]. Fisher discriminant analysis (FDA) and kernel Fisher discriminant analysis (KFDA) has been proposed for fault isolation of industrial processes considering nonlinearity therein [6], [17]–[19]. Besides the successful record of detection and isolation of faults, the limitations of these approaches include huge computations, complexity, and the requirement of the knowledge of both healthy and faulty data for FDA. In addition, certain Kernel functions cannot guarantee the capability of representing the characteristics of the original data. Recently, a detection method based on tnGAN (a generative adversarial network based on the tri-networks form) is proposed in [20] to address the pipeline leak detection problem. The noteworthy feature in this approach is the recovery of missing sensor data which ensures the integrity of data in a pipeline network. Similarly, some new advancement has been made in [21]–[23]. These approaches involve training and validation which required huge data and computation which is the main limitation of these approaches based on neural networks. In addition, nonlinear dynamics and issues of disturbances need further improvement.

Parallel with these developments, subspace identification approaches are proposed [24], [25] which offers an efficient way for data-driven design. In this research work, we have focused on subspace identification approaches due to their feature of simplicity and computationally efficiency in practical implementation. In [7] parity-based data-driven fault detection approach is proposed to detect anomalies in the penicillin fermentation process. In this approach, a subspace identification mechanism is used and a residual generator is constructed based on the computed parity space. The approach proposed in [7] has a limitation in addressing the robustness issue which is of practical concern. In [26], the robust fault detection in PFP is considered. In this work, the low pass filtering and wavelet transformation are used to eliminate high-frequency contents to improve robustness. A worth-mentioning point in the aforementioned literature is the consideration of linear dynamics of the processes. Techniques designed by considering the linear behavior may reduce the efficacy in detecting faults and may sometimes lead to missed detection of a fault.

In [27] a fault-detection scheme is proposed for nonlinear dynamic systems. The primary idea of this detection scheme is to develop a local model using the so-called just-in-time learning (JITL) approach then compare the actual and predicted output. The bottleneck of this method is computational complexity increases from the computation scheme of the optimal local model. Also, this detection method may be less effective in case of inaccurate prediction of the local model. Isolation of simultaneous faults is of vital importance which is also a hard problem using this scheme. To address these issues we have proposed a computationally efficient fault detection scheme based on subspace identification-based fault detection method in [28] using the JITL approach. This method is limited to the detection of faults which should be extended towards the isolation of fault. Motivated by the effectiveness and simple implementation of the subspace identification together with the JITL approach method, this work is extended to address the fault isolation problem.

In this article, a novel fault diagnostic scheme has been proposed and implemented for the Penicillin Fermentation process. A fault isolation scheme is proposed for the classification of sensor and actuator faults for processes with nonlinear dynamics. This technique is generic such that it depends only on the input-output data and the so-called JITL approach is used to address the nonlinear behavior of the process. The parity-based residual generator is used to construct residual in such a way that it ensures robustness against process disturbances and sensor noise, and at the same time sensitivity towards faults. A threshold setting is utilized for fault decisions and to reduce the false alarm rate. The diagnostic technique is implemented for the application of the penicillin fermentation process. The approach proposed in our paper presents diagnostic schemes using input-output data of the nonlinear processes that have the following salient features: 1) The computational complexity is reduced e.g. instead of computing local model just a parity vector is computed; 2) The framework is robust against process disturbances and sensor noise; 3) fault isolation is guaranteed without any additional requirements on data/or designed scheme. The implementation results show that the proposed technique is more effective as compared to existing diagnostic approaches [7], [26] implemented for PFP. The comparative study shows that the proposed technique improves the fault detection rate (FDR) and minimizes the false alarm rate as compare to the existing techniques.

The remaining article is organized as follows. Section II briefly describes the Penicillin fermentation process. The proposed fault diagnostic approach is presented in Section III and residual evaluation and threshold setting are discussed. The implementation results and comparison is presented in Section IV. Finally, a conclusion is drawn in Section V.

II. PENICILLIN FERMENTATION PROCESS

Penicillin is one of the most commonly used antibiotics used for medication. It is discovered in 1928 by Alexander Fleming. The penicillin fermentation process is a typical nonlinear dynamic batch process used for penicillin commercial production. It is a fed-batch process that is performed in aseptic tank reactors of 30 to 100 thousand gallons capacity. The fermentation comprises initial seed growth levels, followed by a fermentation production stage with a cycle of 120 to 200 hours. Numerous substrates including sucrose, glucose, and other crude sugars have been adopted for this process. Nearly 65% of the substrate is consumed for maintenance, 25% is used for growth and the only 10% is utilized for the production of penicillin [29]. For pH value regulation, sugar is too used during the active penicillin production phase. The industrial manufacturing of penicillin is generally classified into two stages, the pre-culture, and the fed-batch stage. Within the first stage, the early quantity of substrate is consumed by penicillin and therefore the substrate is diminished by forcing the penicillin production. Within the next part, the substrate is incessantly maintained as an associated open-loop operation [1].

Mini-production protocols are commonly used in penicillin fermentation. They include the 20-40 percent withdrawal of the fermenter substances and its substitute with the new germ-free medium. This process can be frequently repeated many times during this process deprived of harvest reduction, it can increase the total penicillin harvest. Penicillin is evacuated into the medium and improved in the final stage of fermentation. Entire abstraction is optimum performed at acidic pH, with 2 to 5 percent improvement in overall abstraction efficiency. Substrate abstraction of cool acidified soup is carried out with butyl, amyl, or isobutyl acetate. Nowadays penicillin fermentation processes are highly automated. All the essential antecedents, sugar, ammonia, oxygen, carbon dioxide, etc. are controlled, with comprehensive observing of pH and temperature for optimal penicillin production. The pH is set between 5.5 and 6 throughout the active production phase which can be increased up to 7 due to consumption of lactic acid or discharging of NH3 gas. In case pH exceeds 8 MgCO3 or CaCO3 or phosphate buffer will be added. Agitator power is 30W and aeration rate will be from 30 to 60 L/h which is initially high and later less O_2 [1]. Any abnormality or un-permitted deviation in these process variables may not only affect the product quality but low-quality products may also lead to coordinated effects in human life. The improvement in the safety and reliability of PFP is thus highly desirable. It is of vital importance to decrease and prevent the hazards of faults in order to maintain the continuous quality production of penicillin. The detailed descriptions of biosynthesis and chemical reactions are not focused on in this research work. The structure model of biosynthesis and chemical reactions of PFP as shown in Fig. 1 is summarized in [1] as:

$$\begin{aligned}
X &= f(X; S; C_L; H; T) \\
S &= f(X; S; C_L; H; T) \\
C_L &= f(X; S; C_L; H; T) \\
P &= f(X; S; C_L; H; T; P) \\
CO_2 &= f(X; H; T) \\
H &= f(X; H; T)
\end{aligned}$$

where X is the biomass concentration, C_L is the dissolved oxygen concentration, S is the substrate concentration, CO_2 is the concentration of carbon dioxide, P is the penicillin concentration, H refers to the pH and T represents the temperature. A simulation package of the penicillin fermentation process is introduced by Bajpai et. al in 1980 [30]. The environmental effects such as temperature, pH are not included in this model. Furthermore, the effect of input variables like agitator power, aeration rate, feed flow rate of the substrate on biomass is not considered. This modular simulation package was extended by Birol *et al.* in 2002, in which effects of input and environmental variables are also addressed [1] as shown in Fig. 2. In order to control environmental variables, two PID controllers are introduced by using input variables as control variables. This modular package is flexible and user-friendly. The controls, input variables can be changed and outputs can be measured offline. In this research work, the PenSim v2.0 package is used provided by Ali Cinar for the implementation of the diagnostic system. Using this simulator normal and faulty batches are produced for diagnostic purposes. In this model, the effects of environmental variables like pH, Temperature, and input variables such as agitator power, aeration rate, and feed flow rate of glucose on biomass and penicillin concentrations are considered. Two PID controllers are installed to control the temperature and pH, using cooling water and base/acid flow rate as control variables. The simulation package gives the user flexibility of varying sampling and total simulation time. In bio-processes, variables like penicillin concentrations and biomass are measured offline by a quality analysis laboratory, therefore introducing lag in measurements. Thus sampling time is adjusted accordingly. The description of the process model is given in Table 1.

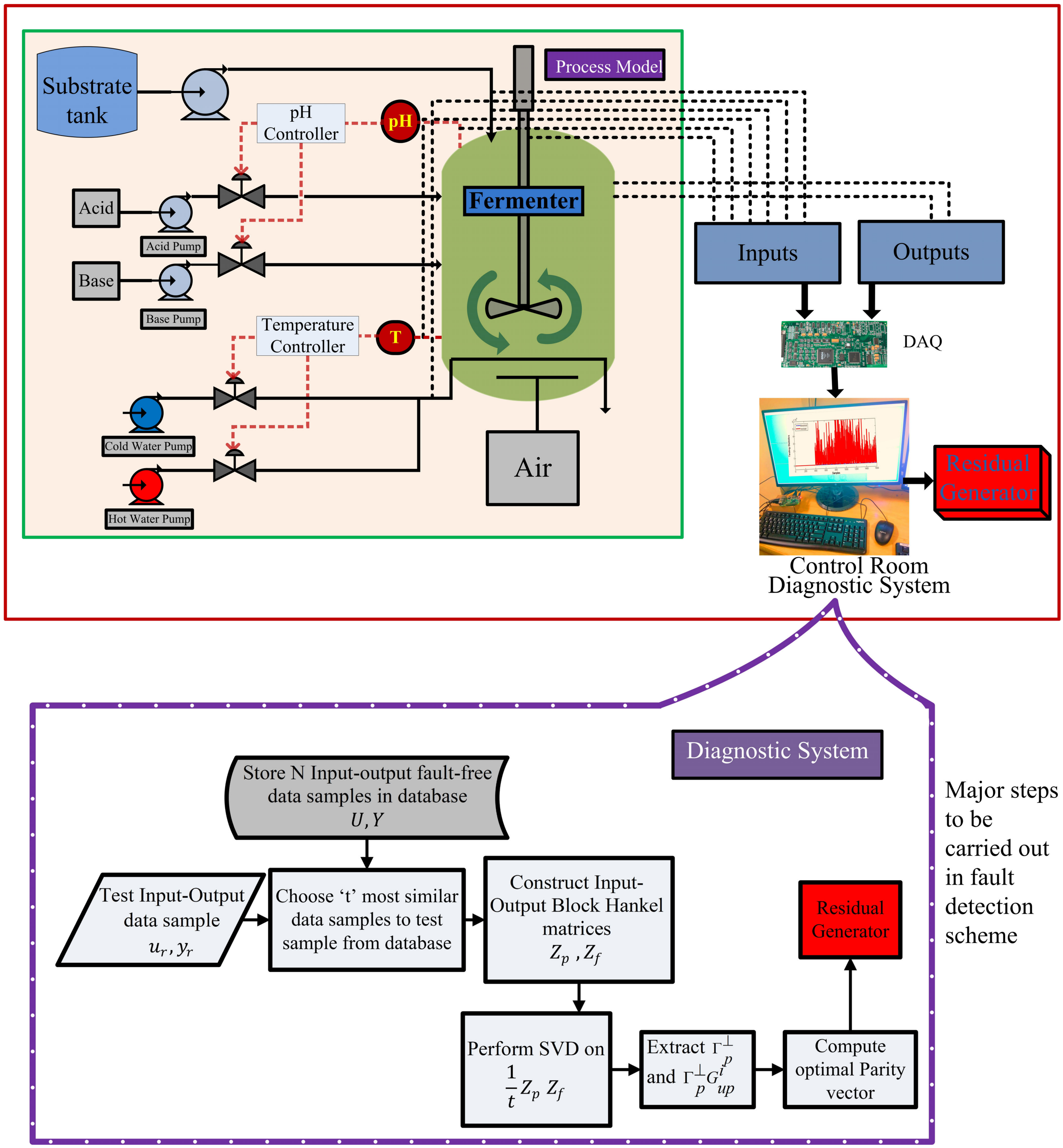


FIGURE 1. Schematics of fault detection of Penicillin fermentation process.

III. DESIGN OF PROPOSED FAULT DIAGNOSTIC SCHEME

In this article, we consider the problem of fault diagnostics (detection and isolation) for the PFP with nonlinear dynamics. Fault detection is the binary decision about the presence of a fault. Fault isolation is the identification of fault location. It is of prime importance to detect the fault in time and identify the position of fault that occurs in order to take appropriate preventive actions to avoid consequential damages well before the incipient fault evolves to a failure. A data-driven diagnostic approach is utilized for the detection and isolation of faults due to the availability of huge processing data and the unavailability of an analytical model. The so-called JITL

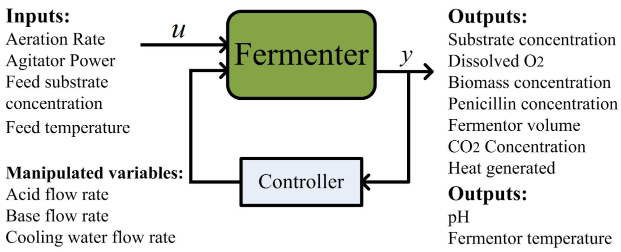


FIGURE 2. Fed batch penicillin fermentation process.

TABLE 1. Description of process variables [1].

Number	Variable	Value
1	Agitator power	30 W
2	Aeration rate	8 L/h
3	Substrate concentration	15 g/L
4	Substrate feed flow rate	0.045 L/h
5	Substrate feed temperature	296 K
6	Biomass concentration	0.1 g/LK
7	Dissolved O_2 concentration	1.16 mmol/L
8	Culture volume	100 L
9	Penicillin concentration	0 g/L
10	Carbondioxide concentration	0.5 mmol/L
11	pH	5.5
12	Heat generated	0 kcal
13	Temperature	298 K
14	Cooling water flow rate	0L/h
15	Acid flow rate	0mL/h
16	Base flow rate	0mL/h

based fault detection technique is presented in our previous work in [28] that addresses the nonlinear effect of the process. This work is extended for fault isolation which is an important part of fault diagnostics. To address the non-linearity, the so-called JITL techniques are utilized wherein, the t input-output data samples based on similarity index are selected to generate residual signals.

The fault detection technique is briefly presented in Algorithm 1 and schematics of fault detection of the PFP is demonstrated in Fig. 1. For each incoming test sample, the most relevant samples are selected from the stored samples, and then optimal robust parity vector (P_p) is constructed to generate the residual signal. The interested reader are referred to [28].

The robust fault isolation algorithm is proposed for fault isolation of industrial processes is based on decoupling the effect of faults other than the desired fault from specific residual. The weighted parity vector is designed in such a way that it shows the effect of i^{th} fault on i^{th} residual and nullifies the effect of remaining faults on i^{th} residual. For example, the i^{th} residual $\gamma_i(k)$ indicates the i^{th} position of fault is sensitive towards i^{th} fault and decoupled from all remaining faults. A bank of residuals is generated for the isolation of a single fault.

To this end, consider a nonlinear dynamic process as:

$$\begin{aligned} x(k+1) &= f(x(k), u(k)) + d(k) \\ y(k) &= g(x(k), u(k)) + n(k) \end{aligned} \tag{1}$$

where, $x(k) \in R^n$ is the state of the system, $u(k) \in R^l$ is the input and $y(k) \in R^m$, is the output of the system. The variables $d(k)$ represents process disturbance and $n(k)$ represents sensor noise.

Algorithm 1 Fault Detection Approach

1: Store N input-output samples in healthy condition.
2: Compute similarity index p_i between test input sample u_r and healthy samples u_i, $i = 1, \cdots, N$ in database by using (2).
3: Select t most relevant data samples based on similarity index.
4: Construct t input-output data samples in form of past and future input-output block Hankel matrices Z_p and Z_f respectively.
5: Perform SVD on $\frac{1}{t} Z_f Z_p^T$.
6: Compute the terms $\Gamma_p^{\perp}$, $\Gamma_p^{\perp} G_{up}^i$ by using (10).
7: Construct the optimal parity vector by using (11) and (12).
8: The residual is generated using (13).
9: Repeat steps 2-6 to generate residuals for other test samples.

Notice that in the design of a data-driven based fault diagnosis scheme, a sufficiently large amount of data samples are collected. For our purpose, the N number of healthy input-output data samples are collected. The collected data sample are stored as $U = [u_1 \cdots u_N]^T \in R^{N \times l}$ input samples and $Y = [y_1 \cdots y_N]^T \in R^{N \times m}$ as output samples. Among these samples t most similar data samples are selected using the so-called JITL approach where $t \gg n$ [27]. The idea of JITL is that for each incoming test sample, the most relevant samples from the stored samples will be selected based on the similarity index. Then parity space is computed using these selective data samples. In the conventional subspace-aided parity base approach, a constant parity space is computed. Meanwhile, in the proposed technique the parity space is adaptive and computed for each test sample in order to address the non-linear dynamics. The similarity index (s) depends on the distance and angle between test input and stored data samples. The similarity index of test input (u_q) and stored input (u_i) is:

$$s_i = \alpha \sqrt{e^{d^2}} + (1 - \alpha) \cos\theta_i \tag{2}$$

where, α is freedom variable i.e. $0 < \alpha < 1$, d is Euclidean distance between test input u_q and stored input u_i and θ_i is angle between u_q and u_i.

The selected t most relevant data samples are organized within the descending order based on similarity index (s_i). The input-output data samples are organized within the type of block Hankel matrices for these t data samples.

$$U_f = \begin{bmatrix} u_o & u_1 & \cdots & u_{t-p} \\ u_1 & u_2 & \cdots & u_{t-p+1} \\ \vdots & \ddots & \ddots & \vdots \\ u_p & u_{p+1} & \cdots & u_t \end{bmatrix}$$

$$Y_f = \begin{bmatrix} y_o & y_1 & \cdots & y_{t-p} \\ y_1 & y_2 & \cdots & y_{t-p+1} \\ \vdots & \ddots & \ddots & \vdots \\ y_p & y_{p+2} & \cdots & y_t \end{bmatrix}$$

After the selection of similar data samples based on similarity index from the database, now for such data samples, we can assume the linear dynamics of the system to generate the parity vector. Considering an LTI system as:

$$\begin{aligned} x(k+1) &= A_{d_i}x(k) + B_{d_i}(u(k) + f_a(k)) + w(k) \\ y(k) &= C_{d_i}x(k) + D_{d_i}(u(k) + f_a(k)) + v(k) + f_s(k) \end{aligned} \quad (3)$$

Here, $A_{d_i} \in R^{n\times n}$, $B_{d_i} \in R^{n\times l}$, $C_{d_i} \in R^{m\times n}$, $D_{d_i} \in R^{m\times l}$ are constant matrices and $x(k) \in R^{n\times 1}$ is state vector, $u(k) \in R^{l\times 1}$ is input vector, $f_s(k), f_a(k)$ are sensor and actuator fault vectors respectively. $w(k)$, $v(k)$ are disturbances, and sensor noise respectively and are speculated having normal distribution with zero means.
The output of system in (3), for $p \geq 0$ is considered as

$$\begin{aligned} y_p(k) = \Gamma_p x_p(k) + G_{up}(u_p(k) + f_{ap}(k)) \\ + G_{dp}w_p(k) + v_p(k) + f_{sp}(k) \end{aligned} \quad (4)$$

where,

$$w_p(k) = \begin{bmatrix} w(k-p) \\ w(k-p+1) \\ \vdots \\ w(k) \end{bmatrix}, \quad v_p(k) = \begin{bmatrix} v(k-p) \\ v(k-p+1) \\ \vdots \\ v(k) \end{bmatrix}$$
$$f_{sp}(k) = \begin{bmatrix} f_s(k-p) \\ f_s(k-p+1) \\ \vdots \\ f_s(k) \end{bmatrix}, \quad y_p(k) = \begin{bmatrix} y(k-p) \\ y(k-p+1) \\ \vdots \\ y(k) \end{bmatrix} \quad (5)$$

and

$$G_{up} = \begin{bmatrix} D_d & 0 & \cdots & 0 \\ C_d B_d & D_d & \ddots & 0 \\ \vdots & \ddots & \ddots & 0 \\ C_d {A_d}^{p-1} B_d & \cdots & C_d B_d & D_d \end{bmatrix},$$
$$G_{dp} = \begin{bmatrix} 0 & 0 & \cdots & 0 \\ C_d & 0 & \ddots & 0 \\ \vdots & \ddots & \ddots & 0 \\ C_d {A_d}^{p-1} & \cdots & C_d & 0 \end{bmatrix} \quad (6)$$

For subspace aided data-driven approach (4) can be written as:

$$Y_f = \Gamma_p X_i + G_{up}^i U_f + G_{dp}^i W_f + N_f \quad (7)$$

where, Γ_p is known as the external observability matrix, U_f is the block Hankel matrix of future inputs and Y_f includes future outputs and X_i is the state matrix. G_{up}^i is lower block Toeplitz deterministic fault coupling matrix and G_{dp}^i is stochastic disturbances coupling matrix. W_f is the block Hankel matrix represent disturbances while N_f represents noise.
Equation (7) can also be represented as:

$$Z_f = \begin{bmatrix} Y_f \\ U_f \end{bmatrix} = \begin{bmatrix} \Gamma_p & G_{up}^i \\ 0 & I \end{bmatrix} \begin{bmatrix} X_i \\ U_f \end{bmatrix} + \begin{bmatrix} G_{dp}^i W_f + N_f \\ 0 \end{bmatrix}$$

where Z_f^T is input-output block Hankel matrices comprising the inputs-outputs respectively. Subdividing the total number of samples (t) and post multiplying Z_f^T on both sides, the above equation turns out to be as:

$$\frac{1}{t} Z_f Z_f^T = \frac{1}{t} \begin{bmatrix} \Gamma_p & G_{up}^i \\ 0 & I \end{bmatrix} \begin{bmatrix} X_i \\ U_f \end{bmatrix} Z_f^T + \frac{1}{t} \Xi Z_f^T,$$
$$\Xi = \begin{bmatrix} G_{dp}^i W_f + N_f \\ 0 \end{bmatrix}$$

Perform singular value decomposition of $\frac{1}{t} Z_f Z_f^T$.

$$\frac{1}{t} Z_f Z_f^T = U_z \Sigma_z \tilde{V}_z \quad (8)$$

where,

$$\begin{aligned} U_z &= \begin{bmatrix} U_{z11} & U_{z12} \\ U_{z21} & U_{z22} \end{bmatrix} \in R^{(m+l)p\times(m+l)p} \\ U_{z11} &\in R^{(m+p)\times(pl+n)}, \quad U_{z12}^T \in R^{(mp-n)\times(mp)} \\ U_{z22} &\in R^{(lp)\times(pm-n)} \end{aligned} \quad (9)$$

According to [24], we can obtain the $\Gamma_p^{\perp}$ and $\Gamma_p^{\perp} G_{up}^i$ by using the relations

$$\Gamma_p^{\perp} = U_{z12}^T, \; \Gamma_p^{\perp} G_{up}^i = -U_{z22}^T \quad (10)$$

It is noticed that U_{z12}^T spans parity space and also rows of U_{z12}^T are the parity vectors [31]. So, parity space is equal to $\Gamma_p^{\perp}$ such that $\Gamma_p^{\perp}\Gamma_p = 0$. In order to construct an optimal parity vector which can ensure sensitivity towards faults as well as robustness against disturbances, the following performance index [32]is used:

$$J = \max_{\Gamma_p^{\perp}} \frac{\Gamma_p^{\perp} G_{up}^i {G_{up}^i}^T \Gamma_p^{\perp,T}}{\Gamma_p^{\perp} G_{dp}^i {G_{dp}^i}^T \Gamma_p^{\perp,T}} \quad (11)$$

This performance index includes two terms that are G_{up}^i and G_{dp}^i. The term G_{up}^i represents the influence of faults on residual signals while the term G_{dp}^i represents the effect of disturbances as mention in (7). In order to compute optimal robust parity vector we have to maximize the performance index that means to maximize the term $\Gamma_p^{\perp} G_{up}^i$ that enhance the impact of the fault and at the same time minimize the term $\Gamma_p^{\perp} G_{dp}^i$ which minimize the influence of disturbances. The performance index (11) is solved by expressing it as an associate eigenvalue problem.

$$\ell_{p,max}(\Gamma_p^{\perp} G_{up}^i {G_{up}^i}^T \Gamma_p^{\perp,T} - \lambda_{p,max} \Gamma_p^{\perp} G_{dp}^i {G_{dp}^i}^T \Gamma_p^{\perp,T}) = 0 \quad (12)$$

where, $\ell_{p,max}$ is the maximum eigenvector and $\lambda_{p,max}$ is the maximum eigenvalue.

$P_p = \ell_{p,max}\Gamma_p^{\perp}$ is the optimal robust parity vector that diminishes the influence of the disturbances and enhances the impact of the fault on residual. The residual is computed by using the subsequent relation.

$$\gamma(k) = P_p(y_p(k) - G_{up}u_p) \tag{13}$$

where P_p is the optimal robust parity vector.

A. CLASSIFICATION OF SENSOR FAULTS

Consider the parity based residual generator given as

$$\begin{aligned}\gamma(k) &= \Gamma_p^{\perp}(y_p(k) - G_{up}u_p(k)) \\ &= \Gamma_p^{\perp}(G_{up}f_{ap}(k) + f_{sp}(k) + G_{dp}w_s(k) + v_s(k))\end{aligned} \tag{14}$$

By ignoring the effect of disturbances and noise, it can be written as:

$$\gamma(k) = \Gamma_p^{\perp}G_{up}f_{ap}(k) + \Gamma_p^{\perp}f_{sp}(k) \tag{15}$$

where, $\Gamma_p^{\perp}$ is the parity vector and G_{up} and $\Gamma_p^{\perp}$ is computed using JITL parity space approach as discussed (10). $f_{ap}(k)$ and $f_{sp}(k)$ are the actuators and sensors faults respectively.

$$f_{sp}(k) = \begin{bmatrix} f_s(k-s) \\ f_s(k-s+1) \\ \vdots \\ f_s(k) \end{bmatrix}, \; f_{ap}(k) = \begin{bmatrix} f_a(k-s) \\ f_a(k-s+1) \\ \vdots \\ f_a(k) \end{bmatrix} \tag{16}$$

and

$$f_a(k) = \begin{bmatrix} f_{a_1}(k) \\ \vdots \\ f_{a_j}(k) \\ \vdots \\ f_{a_\ell}(k) \end{bmatrix}, \quad f_s(k) = \begin{bmatrix} f_{s_1}(k) \\ \vdots \\ f_{s_j}(k) \\ \vdots \\ f_{s_m}(k) \end{bmatrix} \tag{17}$$

$$\begin{aligned} f_{sp_{\bar{j}}}(k) = [&f_{s_1}(k-s) \cdots f_{s_{j-1}}(k-s) f_{s_{j+1}}(k-s) \cdots \\ &f_{s_m}(k-s) \cdots\cdots f_{s_{j-1}}(k) f_{s_{j+1}}(k) \cdots f_{s_m}(k)]^T \end{aligned} \tag{18}$$

$$\begin{aligned} f_{ap_{\bar{j}}}(k) = [&f_{a1}(k-s) \cdots f_{a_{j-1}}(k-s) f_{a_{j+1}}(k-s) \cdots \\ &f_{a_p}(k-s) \cdots\cdots f_{a_1}(k) \cdots f_{a_{j-1}}(k) f_{a_{j+1}}(k) \\ &\cdots f_{a_p}(k)\,]^T \end{aligned} \tag{19}$$

$$f_{sp_j}(k) = [f_{s_j}(k-s) f_{s_j}(k-s+1) \cdots\cdots f_{s_j}(k)]^T \tag{20}$$

$$f_{ap_j}(k) = [f_{a_j}(k-s) f_{a_j}(k-s+1) \cdots\cdots f_{a_j}(k)]^T \tag{21}$$

where $'\ell'$ is the total number of actuators, $'m'$ is the total number of sensors and $'j'$ is the jth actuator or sensor fault. In order to isolate the jth sensor fault, parity space $(\Gamma_{s,sen,j}^{\perp})$ is selected in such a way that it decouples the remaining sensors faults. For $'m'$ sensor faults $'m'$ residual signal will be computed, each residual signal indicates a specific sensor fault. For jth sensor fault, the residual equation (14) can be written as:

$$\begin{aligned}\gamma_j(k) &= \Gamma_p^{\perp}G_{up}f_{ap}(k) + \Gamma_p^{\perp}f_{sp}(k) \\ &= \Gamma_{s,sen,j}^{\perp}\Gamma_p^{\perp}G_{up}f_{ap}(k) + \Gamma_{s,sen,j}^{\perp}[\Gamma_{s,j}^{\perp} \quad \Gamma_{s,\bar{j}}^{\perp}] \begin{bmatrix} f_{sp_{\bar{j}}}(k) \\ f_{sp_j}(k) \end{bmatrix}\end{aligned} \tag{22}$$

such that $\Gamma_{s,sen,j}^{\perp}\Gamma_{s,j}^{\perp} = 0$.

To compute $\Gamma_{s,sen,j}^{\perp}$ organize $\Gamma_p^{\perp}$ as: $\Gamma_p^{\perp} = [\Gamma_{s,1}^{\perp}\Gamma_{s,2}^{\perp}\cdots\Gamma_{s,s}^{\perp}]$, where $\Gamma_{s,k}^{\perp} \in R^{\mu\times n}$ and $k = 1, 2\cdots s$

Subdivide the term $\Gamma_{s,k}^{\perp} = [\Gamma_{s,k,1}^{\perp}\Gamma_{s,k,2}^{\perp}\cdots\Gamma_{s,k,m}^{\perp}]$ such that $\Gamma_{s,k,i}^{\perp} \in R^{\mu}$, $i = 1,\cdots m$, where m is the number of outputs or sensors.

Now compute the parity space for jth fault such that $\Gamma_{s,sen,j}^{\perp} = null(\Gamma_{s,j}^{\perp})$, where $\Gamma_{s,j}^{\perp}$ can be written as:

$$\begin{aligned}\Gamma_{s,j}^{\perp} = [&\Gamma_{s,1,1}^{\perp} \cdots \Gamma_{s,1,j-1}^{\perp}\Gamma_{s,1,j+1}^{\perp} \cdots \Gamma_{s,2,m}^{\perp}\Gamma_{s,2,1}^{\perp} \cdots \\ &\Gamma_{s,2,j-1}^{\perp}\Gamma_{s,2,j+1}^{\perp}\cdots \Gamma_{s,2,m}^{\perp} \cdots \Gamma_{s,s,1}^{\perp} \cdots \Gamma_{s,s,j-1}^{\perp} \\ &\Gamma_{s,s,j+1}^{\perp} \cdots \Gamma_{s,s,m}^{\perp}]\end{aligned} \tag{23}$$

Considering the effect of noise and disturbances as shown in (14), the parity vector should compute that ensure robustness against noise and disturbances and sensitivity towards faults. In order to construct such an optimal parity vector $P_{sen,j}$ for jth sensor following performance index will be solved as mentioned in (12)

$$J_{sen} = \max_{\Gamma_{s,sen,j}^{\perp}} \frac{\Gamma_{s,sen,j}^{\perp}G_{up}^{i}G_{up}^{i\;T}\Gamma_{s,sen,j}^{\perp,T}}{\Gamma_{s,sen,j}^{\perp}G_{dp}^{i}G_{dp}^{i\;T}\Gamma_{s,sen,j}^{\perp,T}} \tag{24}$$

The optimal robust parity vector for jth residual will be $P_{sen,j} = \ell_{s,max}\Gamma_{s,sen,j}^{\perp}\Gamma_p^{\perp}$. The residual is generated for jth sensor by using following relation.

$$\gamma_{sen,j}(k) = P_{sen,j}(y_p(k) - G_{up}u_p(k)) \tag{25}$$

The proposed fault classification approach for sensor fault is briefly mentioned in Algorithm 2.

Algorithm 2 Proposed Sensor Fault Isolation Approach

1: Compute similarity index p_i between test input sample u_r and healthy samples u_i, $i = 1,\cdots, N$ in database by using (2).
2: Select t most relevant data samples based on similarity index.
3: Compute the terms $\Gamma_p^{\perp}$ and $\Gamma_p^{\perp}G_{up}^{i}$ by using (10).
4: Organize $\Gamma_p^{\perp}$ as: $\Gamma_p^{\perp} = [\Gamma_{p,1}^{\perp}\Gamma_{p,2}^{\perp}\cdots\Gamma_{p,s}^{\perp}]$, where $\Gamma_{p,k}^{\perp} \in R^{\mu\times n}$ and $k = 1, 2\cdots s$
5: Subdivide the term $\Gamma_{p,k}^{\perp} = [\Gamma_{p,k,1}^{\perp}\Gamma_{p,k,2}^{\perp}\cdots\Gamma_{p,k,m}^{\perp}]$ such that $\Gamma_{p,k,i}^{\perp} \in R^{\mu}$, $i = 1,\cdots m$, where m is the number of outputs. Construct $\Gamma_{p,j}^{\perp}$ as mentioned in (23).
6: Now compute the parity space for jth fault such that $\Gamma_{p,sen,j}^{\perp} = null(\Gamma_{p,j}^{\perp})$.
7: Construct the optimal parity vector $P_{sen,j}$ for jth sensor by solving the performance index (24).
8: The bank of residual signal is generated by using (25).

$$\gamma(sen, j) = P_{sen,j}(y_p(k) - G_{up}u_p)$$

B. CLASSIFICATION OF ACTUATOR FAULTS

In order to isolate the jth actuator fault, parity space $(\mathcal{H}_{p,act,j})$ is computed in such a way that it decouple the remaining actuator faults. For *jth* actuator fault (14) can be written as:

$$\gamma_j(k) = \mathcal{H}_{p,act,j}(\Gamma_p^{\perp} G_{up} \begin{bmatrix} f_{ap_{\bar{j}}}(k) \\ f_{ap_j}(k) \end{bmatrix} + \Gamma_p^{\perp} f_{sp}(k)) \quad (26)$$

Consider $\mathcal{H} = \Gamma_p^{\perp} G_{up}^i$, (26) can be written as:

$$\begin{aligned} \gamma_j(k) &= \mathcal{H}_{p,act,j}\mathcal{H} \begin{bmatrix} f_{ap_{\bar{j}}}(k) \\ f_{ap_j}(k) \end{bmatrix} + \mathcal{H}_{p,act,j}\Gamma_p^{\perp} f_{sp}(k) \\ &= \mathcal{H}_{p,act,j}[\mathcal{H}_{p,j} \quad \mathcal{H}_{p,\bar{j}}] \begin{bmatrix} f_{ap_{\bar{j}}}(k) \\ f_{ap_j}(k) \end{bmatrix} + \mathcal{H}_{p,act,j}\Gamma_p^{\perp} f_{sp}(k) \end{aligned} \quad (27)$$

such that $\mathcal{H}_{p,act,j}\mathcal{H}_{p,j} = 0$.

To compute $\mathcal{H}_{p,act,j}$, organize $\mathcal{H}$ as: $\mathcal{H} = [\mathcal{H}_{p,1}\mathcal{H}_{p,2}\cdots \mathcal{H}_{p,s}]$, where $\mathcal{H}_{p,k} \in R^{\mu\times l}$ and $k = 1, 2\cdots s$, where $\Gamma_{p,k}^{\perp} \in R^{\mu\times n}$ and $k = 1, 2\cdots s$.

Subdivide the term $\mathcal{H}_{p,k} = [\mathcal{H}_{p,k,1}\mathcal{H}_{p,k,2}\cdots\mathcal{H}_{p,k,\ell}]$ such that $\mathcal{H}_{p,k,i} \in R^{\mu}, i = 1, \cdots \ell$, where ℓ is the number of actuators.

Now compute the parity space for *jth* actuator fault such that $\mathcal{H}_{p,act,j} = null(\mathcal{H}_{p,j})$, where $\mathcal{H}_{p,j}$ can be written as:

$$\begin{aligned} \mathcal{H}_{p,j} = [&\mathcal{H}_{p,1,1}\cdots\mathcal{H}_{p,1,j-1}\ \mathcal{H}_{p,1,j+1}\cdots\mathcal{H}_{p,2,m}\ \mathcal{H}_{p,2,1}\ \cdots \\ &\mathcal{H}_{p,2,j-1}\ \mathcal{H}_{p,2,j+1}\cdots\mathcal{H}_{p,2,m}\cdots\mathcal{H}_{p,s,1}\cdots\mathcal{H}_{p,s,j-1} \\ &\mathcal{H}_{p,s,j+1}\ \cdots\ \mathcal{H}_{p,s,m}] \end{aligned} \quad (28)$$

Considering the effect of noise and disturbances as shown in (14), the parity vector should be computed that ensure robustness against sensor noise and process disturbances as well as sensitivity towards faults. In order to construct such an optimal parity vector ($P_{act,j}$) for *jth* actuator fault following performance index will be solved as mentioned in (12)

$$J_{act} = \max_{\mathcal{H}_{p,act,j}} \frac{\mathcal{H}_{p,act,j} G_{up}^i {G_{up}^i}^T \mathcal{H}_{p,act,j}^T}{\mathcal{H}_{p,act,j} G_{dp}^i {G_{ds}^i}^T \mathcal{H}_{p,sen,j}^T} \quad (29)$$

The optimal robust parity vector for *jth* actuator residual will be $P_{act,j} = \ell_{s,max}\mathcal{H}_{p,act,j}\Gamma_p^{\perp}$. The residual is generated for *jth* actuator by using following relation.

$$\gamma_{act,j}(k) = P_{act,j}(y_s(k) - G_{up}u_s) \quad (30)$$

The proposed actuators fault classification approach is briefly mentioned in Algorithm 3

C. RESIDUAL EVALUATION AND THRESHOLD SETTING

The unavoidable disturbances and noise may affect the residual and generate false alarms. It is important to differentiate faults from such unavoidable influences. The threshold setting is used in order to make decisions for fault alarms and minimize false alarms. The fault alarm should be generated only when the residual surpasses the particular threshold level. There are various types of threshold settings discussed in [2], [3] and the references therein. In this work, we have used the Generalized likelihood ratio (GLR) based threshold design for the decision of fault. GLR has been proved as a valuable fault decision rule that guarantees the maximal fault

Algorithm 3 Proposed Actuator Fault Isolation Approach

1: Consider $\mathcal{H} = \Gamma_p^{\perp} G_{up}^i$
2: Organize $\mathcal{H}$ as: $\mathcal{H} = [\mathcal{H}_{p,1}\mathcal{H}_{p,2}\cdots\mathcal{H}_{p,s}]$, where $\mathcal{H}_{p,k} \in R^{\mu\times l}$ and $k = 1, 2\cdots s$
3: Subdivide the term $\mathcal{H}_{p,k} = [\mathcal{H}_{p,k,1}\mathcal{H}_{p,k,2}\cdots\mathcal{H}_{p,k,\ell}]$ such that $\mathcal{H}_{p,k,i} \in R^{\mu}, i = 1, \cdots p$, where $p\ell$ is the number of actuators. Construct $\mathcal{H}_{p,j}$ as mentioned in (28)
4: Now compute the parity space for *jth* actuator fault such that $\mathcal{H}_{p,act,j} = null(\mathcal{H}_{p,j})$.
5: Compute the optimal parity vector $P_{act,j}$ for *jth* actuator by solving the performance index (29).
6: The bank of residual signals are generated by using (30).

$$\gamma(act, j) = P_{act,j}(y_s(k) - G_{up}u_s)$$

detection rate (FDR) and minimum false alarm rate (FAR) [2]. By considering the residual generator (13),

$$\gamma(k) = f(k) + d(k) \quad (31)$$

where $\gamma(k)$ represents the residual signal, $f(k)$ indicates the fault and $d(k)$ is white noise $\in \mathcal{N}(0, \sigma_r^2)$. Considering the false alarm rate (FAR) is not more than β, Algorithm-4 briefly defines the execution steps of threshold setting by using GLR.

Algorithm 4 GLR Based Threshold Computation

1: By using chi-square distribution table, compute χ_a such that $P[\chi^2 > \chi_a] = \beta$.
2: The threshold level will be: $J_{TH} = \frac{\chi_a}{2}$.
3: The testing statistic is processed as $J = \frac{1}{2\sigma_r^2 N_w}(\sum_{k=1}^{N_w}\gamma(k)^2)$. where, $\gamma(k)$ is the residual signal.
4: The fault alarm is set if $J > J_{TH}$.

IV. IMPLEMENTATION RESULTS

The PenSim v2.0 package is used for simulation purposes provided by Ali Cinar. Using this simulator healthy and faulty batches are produced for FDI purposes. For the implementation of the FDI scheme, 20 batches are obtained under normal conditions with a sampling time (Ts) of 0.5hrs. The simulation time is set to 400hrs for each batch process. A total of 16,000 samples are collected for the purpose of FDI. p is chosen to be 10. The variables penicillin concentrations and biomass served as outputs whereas inputs variables are temperature, pH, dissolved O_2 concentration, CO_2 concentration, culture volume, and cooling water flow rate as shown in Fig. 1 Three faults that are aeration rate fault, biomass concentration fault, and penicillin concentration fault are considered for testing.

Figs. 3-5 show the implementation results of the FD technique. For each incoming test sample, the most similar data samples are collected from the stored samples then the optimal robust parity vector is constructed using these selective samples for the generation of the residual signals. The fault

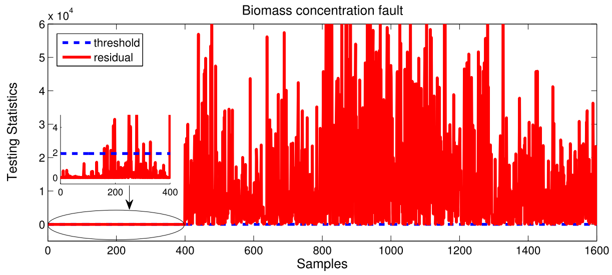


FIGURE 3. Biomass concentration fault.

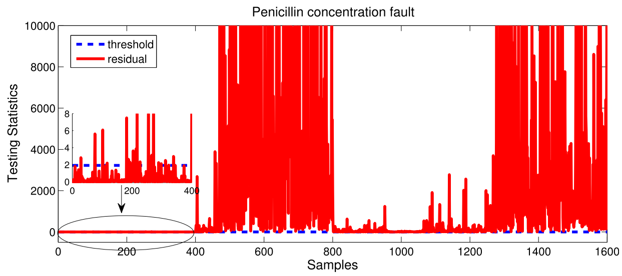


FIGURE 4. Penicillin concentration fault.

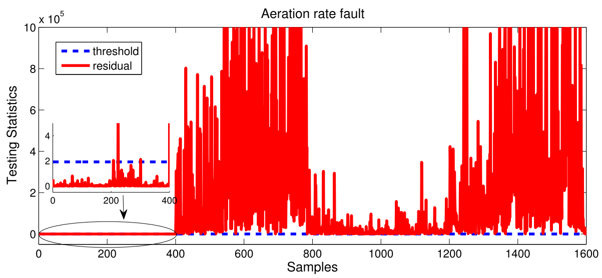


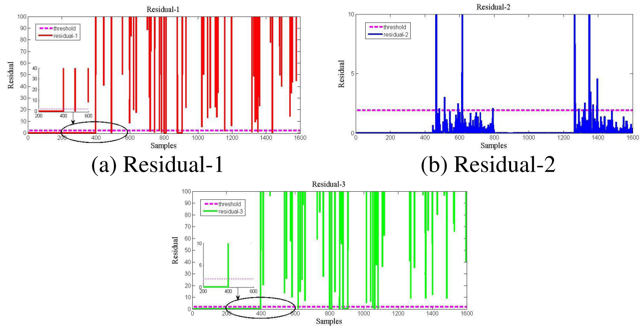
FIGURE 5. Aeration rate fault.

TABLE 2. Comparison of FD approaches.

Technique	False alarm rate	Fault detection rate
Shen et.al [7]	9 %	80 %
Rehman et. al [26]	12.09 %	94.89 %
Proposed	4.5 %	98 %

decoupling approach as discussed earlier is used for the classifications of fault positions. In Fig. 3 biomass concentration fault is introduced up to 15 percent after 400th samples and penicillin concentration fault is inserted up to 20 percent in Fig. 4. Aeration rate fault is introduced after the 400th sample by adding up to 10 percent fault in Fig. 5. All mentioned faults are successfully detected. The effect of disturbances is also included that may affect the residual signal and cause somewhere false alarms. The worth noticing point here is that FAR has been reduced and FDR has been maximized as shown in Table 3. A comparison with recently reported techniques (Table 3) shows that our proposed FD framework performs well and superior.

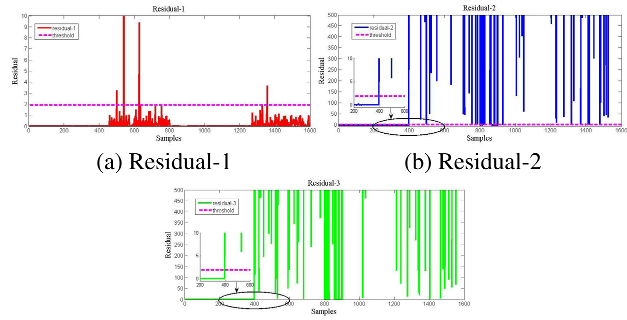
Fault isolation is shown in Figs. 6-8. It is obvious from the figures that all the faults are successfully isolated. Fig. 6 shows the biomass concentration fault for which residual-1 and residual-3 are greater than threshold while residual-2 is less than a threshold level. In the case of sensor faults, the residuals representing the actuator faults will be greater than a threshold as their parity space will be insensitive towards the sensors fault coupling matrix as discussed earlier. Similarly, in the case of actuator faults, the residuals representing sensor faults will be greater than the threshold as their parity space will be insensitive towards actuator fault coupling matrix Fig. 7 reflects the penicillin concentration fault that clearly indicates that the residual-2 which represents



(a) Residual-1 (b) Residual-2

(c) Residual-3

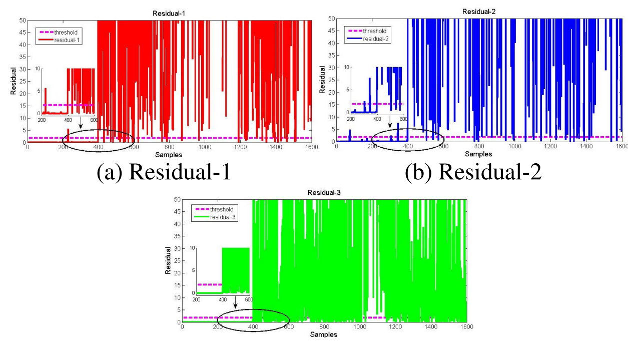
FIGURE 6. Biomass concentration fault.



(a) Residual-1 (b) Residual-2

(c) Residual-3

FIGURE 7. Penicillin concentration fault.



(a) Residual-1 (b) Residual-2

(c) Residual-3

FIGURE 8. Aeration rate fault.

TABLE 3. Decision table for fault isolation.

Fault	Residual-1	Residual-2	Residual-3
Biomass concentration	1	0	1
Penicillin concentration	0	1	1
Aeration rate fault	1	1	1

the penicillin concentration fault is greater as compared to threshold along residual-3 which represent aeration rate fault. The aeration rate fault is shown in Fig-3 in which all residual signals are greater than the threshold level.
The table 3 shows the decision table for the proposed fault isolation scheme that indicates the final result about a fault in a specific component for the penicillin fermentation process. '1' indicates the residual is greater than the threshold and '0' represents the residual is less than the threshold level.

V. CONCLUSION

We have developed and implemented a data-driven fault diagnostic scheme for the Penicillin fermentation process. The so-called just-in-time learning approach is used to address the non-linear behavior of the process. For incoming test samples, the data samples are chosen based on similarity and by using these samples appropriate parity space is generated. The designed diagnostic scheme improves the fault detection rate and decreases the false alarm rate as compared to the previous fault diagnostic approaches implemented for the Penicillin fermentation process. It is noticed that the designed scheme is effective for industrial processes like the Penicillin fermentation process having a high sampling period. The online computational complexity is still one of the problems specifically for processes with low sampling periods which need further attention. In a typical large-scale complex industrial process, there are hundreds and thousands of sensors. The input and output information is coming from various channels. Using this big chunk of data, the design of a process monitoring system is a challenging problem. In practice, the analysis of such big data reveals that the performance of the process can be monitored by a group of sensors. This can reduce the demand for storing the whole data and consequently its analysis. This idea can lead us to the so-called identification of key performance indicators which is highly important for designing and implementation diagnostic systems. It is worth noticing that identification of Key Performance Indicators among the whole input and output space of a large-scale process and based on these indicators constructing an appropriate diagnostic scheme is still a challenging task that needs to be explored. In the future, the research work will be performed to develop an effective diagnostic scheme based on Key Performance Indicators for industrial processes. Also, the just-in-time learning based approach can be extended to develop a fault-tolerant control design for nonlinear dynamic processes to ensure continued operation of the process with reasonable performance in presence of tolerable faults.

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