Surrogate-assisted fault detection framework for dynamic process

Baru Chandra Kiran*, Arnab Dutta**

* Chemical Engineering Department, BITS Pilani, Hyderabad Campus, Hyderabad 500 078, Telangana, India (e-mail: h20201010020@hyderabad.bits-pilani.ac.in)

** Chemical Engineering Department, BITS Pilani, Hyderabad Campus, Hyderabad 500 078, Telangana, India (Tel: +9140 66303758; e-mail: arnabdutta@hyderabad.bits-pilani.ac.in)

Abstract: Digitalization is undoubtedly going to play a very important role in revolutionizing the future outlook of process industries. Data-driven models using process data can have diverse applications. The objective of this article is to develop a surrogate assisted framework that can aid in fault detection. In this context, we first develop a surrogate model that captures the dynamics of a process and then use the dynamic surrogate model in conjunction with a binary classification model to perform fault detection for a process. We have implemented a multivariate kriging-based approach to develop the surrogate for a dynamic process and the binary classifier is developed using the support vector machine (SVM) algorithm. We have applied this methodology to a three tank benchmark system. The process data required to train the models are obtained by simulating the three tank system in MATLAB. We have considered both process faults like leakage and plugging of tanks as well as sensor faults. To evaluate the performance and robustness of the methodology, we have tested the framework on different sets of process inputs, types of faults, sequences of faults, and varying magnitudes of faults as compared to those used during the training of these models. Results obtained indicate a minimum fault detection rate of 97.3% and a maximum false alarm rate of 4%. Thus, it is evident that the surrogate-assisted fault detection framework resulted in satisfactory performance.

Keywords: Dynamic surrogate, Kriging, Fault detection, Process faults, Sensor faults, Binary classification, Support vector machine

1. INTRODUCTION

With an increasing need towards industrial digitalization, the concept of surrogate modelling has become extremely relevant in today's world. Surrogate models that can mimic a process effectively can have several applications. One of the most important applications of a surrogate model can be to aid in fault detection. A process can be subjected to different types of faults that may arise from malfunctioning of equipment, sensor failure, etc. A faulty process can not only result in significant economic loss but also hamper process safety leading to catastrophic consequences (Abid et al., 2021; Shokry et al., 2017, 2020; Venkatasubramanian, Rengaswamy, Yin, et al., 2003b). Thus, if an efficient fault detection framework is implemented then it can help the plant personnel to take necessary actions in case of any faulty process scenarios.

Fault detection frameworks can broadly be classified into three categories: model-based, knowledge-based, and data-driven models (Abid et al., 2021; Venkatasubramanian, Rengaswamy, Kavuri, et al., 2003; Venkatasubramanian, Rengaswamy, Yin, et al., 2003a). Model-based frameworks typically rely on the first principle equations. Although first principle equations can accurately capture the dynamics of the process however, it is often not possible to accurately formulate the first principle-based models for complex chemical engineering systems. The knowledge-based method is based on rule of thumbs, which requires extensive knowledge of the entire process. On the other hand, data-based models are developed based on the available historical data. Data-driven models leverage on the historical process data corresponding to different scenarios that the process has encountered. Thus, data driven modeling techniques do not require accurate first principle equations describing the entire process or extensive prior knowledge of the process. Owing to their ease of construction and implementation, data-driven models have been used in different domains like car crash analysis, mineral ores identification, process monitoring, optimization studies, stability analysis, soft sensing (Duddeck and Wehrle, 2015; Klebanov and Georgakis, 2016; Du *et al.*, 2018), etc.

The objective of this study is to develop a data-driven framework that can aid in fault detection. In this context, we rely on process data to develop a surrogate model for a dynamic process under investigation. Surrogates for a process can be developed using various techniques like polynomial response surface methodology (Klebanov & Georgakis, 2016), artificial neural network, kriging (Shokry et al., 2017, 2020), etc. Kriging has become immensely popular in the context of developing surrogate models. The multivariate dynamic kriging approach can be used to develop a surrogate for dynamic systems (Shokry et al., 2017). Besides surrogates that mimic the dynamic system it is also necessary to develop classifier models that can help in classifying whether the process is under normal or faulty state. Machine learning

algorithms like decision tree, logistic neural network, support vector machine (SVM), (Mahadevan & Shah, 2009; Ajagekar & You, 2020) etc. are some of the most popular techniques that can be embedded to develop the classification model.

In this article we propose a data-driven framework to develop a kriging-based surrogate model for a dynamic process. A SVM-based classification model is then developed for detecting whether the process is at a normal or faulty state. The proposed SVM-based classification model is solely based on the residuals i.e., the deviation of the output from the kriging model and the actual plant. The framework takes into consideration not only the presence of a single fault but also multiple faults simultaneously. The framework also considers various sequences of faults with different magnitudes as well as sensor faults. The article is organized as follows: in section 2 we present the methodology to develop the proposed framework; in section 3 we present a case study to demonstrate the application of the proposed framework and evaluate the performance of the framework; this is followed by concluding remarks in section 4.

2. METHODLOGY

The proposed methodology broadly consists of two steps: 1. development of a surrogate model; 2. development of a classification model to perform fault detection. In subsequent sections, we enumerate the above two steps to develop a surrogate-assisted fault detection framework.

2.1 Dynamic surrogate model development

For a dynamic system, we have developed the surrogate model using a multivariate dynamic kriging approach. The available data (obtained either directly from the process or generated using a simulator) is used to train the model such that it can capture the future state of the system over one-time interval. The kriging model predicts the future value of the output variable as a function of the past values of outputs and inputs. Mathematically this is represented by equation 1 as follows:

$$
\left.
\begin{aligned}
\widehat{X}_1^{prd}(t+1) \\
= f_{prd,1}\left(\widehat{X}(t),..,\widehat{X}(t-L),U(t),..,U(t-L)\right) \\
\widehat{X}_2^{prd}(t+1) \\
= f_{prd,2}\left(\widehat{X}(t),..,\widehat{X}(t-L),U(t),..,U(t-L)\right) \\
\widehat{X}_3^{prd}(t+1) \\
= f_{prd,3}\left(\widehat{X}(t),..,\widehat{X}(t-L),U(t),..,U(t-L)\right)
\end{aligned}
\right\}
\quad (1)
$$

Here, $U(t)$ represents the set of input variables and $X(t)$ represent a set of output variables at a given time instant, t. L represents a specific time lag or delay that can be determined using a trial and error approach by setting prediction accuracy as the metric. The f_{prd} here denotes the kriging model that maps the output at a future instant with inputs and outputs at the previous time instants. The set of surrogate models developed is then used recursively to predict the outputs at several time steps ahead in the future. At each time step, the output is predicted using the input and the predicted output variables from the previous time instants. The performance of the developed dynamic surrogates is accessed by their prediction accuracies in terms of NRMSE (normalized root mean square) values over significantly larger time horizons.

2.2 Binary classifier development

We have developed a binary classifier that can detect if the process is under normal or faulty state. The binary classifier is developed based on the SVM algorithm. At any given time instant, the kriging-based dynamic surrogate is used to predict the output variables. The output predicted from the kriging model is compared with the actual values of the output (obtained either directly from the process or generated using a simulator). The residuals i.e., the difference between the actual output and that predicted by the dynamic surrogate is used as the input to the classifier. This input along with the actual labels (1: Normal and 0: Faulty) is used to train the classifier using the nonlinear SVM algorithm. The hyperparameters associated with the SVM algorithm ($i.e., c$ and γ) are tuned using a five-fold cross validation technique to obtain the optimal values of hyperparameters ($c_{optimal} = 0.1$ and $\gamma_{optimal} = 0.01$). The performance of the classifier is assessed based on the fault detection rate (FDR), false alarm rate (FAR), and overall accuracy (Ajagekar & You, 2020), as given by equations 2, 3, and 4, respectively. FDR ranges from 0 (worst value) to 1 (best value). FAR represents the percentage of normal samples that are misclassified as faulty. FAR ranges from 0 (best value) to 1 (worst value).

$$
\text{FDR (\%)} = 100 \frac{\text{number of fault samples detected as faulty}}{\text{total number of fault samples}} \quad (2)
$$

$$
\text{FAR (\%)} = 100 \frac{\text{number of normal samples detected as faulty}}{\text{total number of normal samples}} \quad (3)
$$

$$
\text{Accuracy (\%)} = 100 \frac{\text{number of samples detected correctly}}{\text{total number of samples}} \quad (4)
$$

Figure 1 below illustrates the proposed surrogate assisted framework for fault detection.
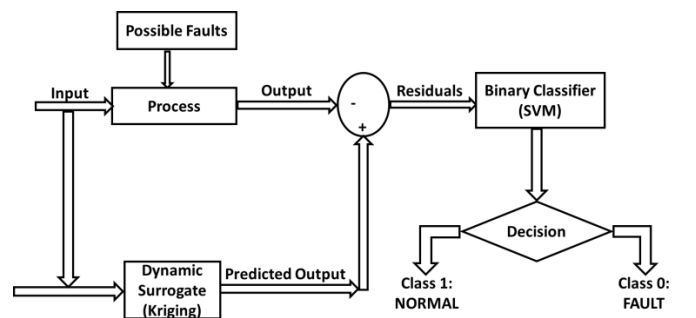

Figure 1: Surrogate-assisted fault detection framework.

3. APPLICATION

3.1 Three-tank system

The proposed methodology is applied to a benchmark problem involving three interconnected tanks as shown below in Figure 2. The system consists of three cylindrical tanks of each area $A = 0.0154\ m^2$, $s_{13} = s_{23} = s_0 = 0.005\ m^2$ area

of cylindrical pipe, and flow coefficients of $a_1 = 0.6836$, $a_2 = 0.4819$, $a_3 = 0.4819$. Two pumps fill the tanks at flow rates of $Q_1(t)$ and $Q_2(t)$, which range from 0 to $0.003\frac{m^3}{s}$. The levels of each tank (i.e., h_1, h_2, and h_3) are the process outputs and Q_1 & Q_2 are considered as inputs to this process. The three tank system is modelled as a set of ordinary differential equations as shown in equation 5. The process is subjected to faults such as leakage and plugging in tanks and drift in level measurement of tanks. Leakage and plugging for a tank is modelled using an additional flowrate term represented by Q_{f1}, Q_{f2}, and Q_{f3}. Values of these flowrates usually vary between $\pm 10 - 25\%$ of the maximum flowrate, $[Q_{Max} = 0.003\frac{m^3}{s}]$ (Shokry et al., 2020). Positive values of these flowrates denote plugging whereas negative values represent leakage in a tank.

$$
\left.
\begin{aligned}
A\frac{dh_1}{dt} &= -a_1 s_{13} \mathrm{sgn}(h_1 - h_3)\sqrt{2g|h_1 - h_3|} \\
&\quad + Q_1 + Q_{f1} \\
A\frac{dh_2}{dt} &= -a_3 s_{23} \mathrm{sgn}(h_3 - h_2)\sqrt{2g|h_3 - h_2|} \\
&\quad - a_2 s_0\sqrt{2gh_2} + Q_2 + Q_{f2} \\
A\frac{dh_3}{dt} &= -a_1 s_{13} \mathrm{sgn}(h_1 - h_3)\sqrt{2g|h_1 - h_3|} \\
&\quad - a_3 s_{23} \mathrm{sgn}(h_3 - h_2)\sqrt{2g|h_3 - h_2|} + Q_{f3}
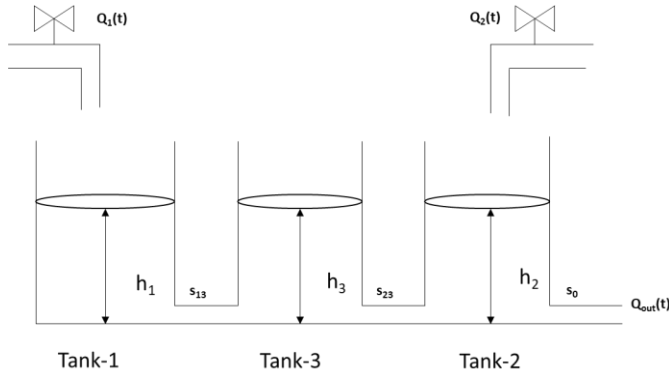\end{aligned}
\right\}
\quad (5)
$$

Figure 2: Three tanks system.

3.2 Surrogate model performance evaluation

The dynamic surrogate for the above three tank system is developed using the multivariate dynamic kriging approach with zero-lag as explained in section 2.1. The process data is generated by solving equation (5) using MATLAB as the simulator under normal scenario i.e., by setting the flowrates of Q_{f1}, Q_{f2}, and Q_{f3} to 0 and Q_1 & Q_2 are assigned random flowrate values within the range of $[0 - Q_{Max}]$. The data obtained from our simulations is used to train the dynamic surrogate. We have developed three surrogates corresponding to each of the process output (i.e., h_1, h_2, and h_3). To evaluate the robustness of the developed kriging models, we have performed validation w.r.t. a different dataset as compared to the training dataset. The input profile depicting the flowrates of Q_1 & Q_2 considered for validation is shown in Figure 3. The actual and predicted heights (using kriging models) over 1800 time steps ahead in the future are illustrated in Figure 4. The NRMSE values for the three

models are obtained as 0.37%, 0.04%, and 0.26%. Thus, it is evident that the developed surrogate models can approximate the system behavior with reasonably high accuracy and can be reliably used within the fault detection framework.
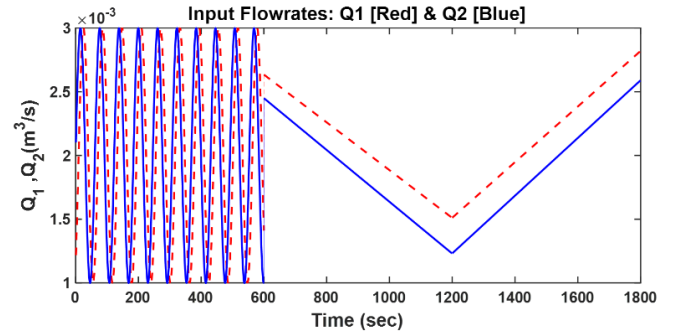

Figure 3: Input profile for Q_1 & Q_2 to test the performance of surrogate model.
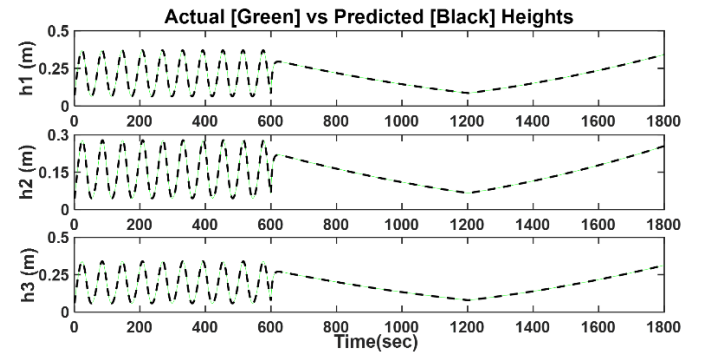

Figure 4: Actual and predicted heights using kriging models.

3.3. Binary classifier model evaluation

The binary classifier is developed using the nonlinear SVM (rbf kernel) algorithm in MATLAB based on the procedure given in section 2.2. To train the SVM model we have used the same input profile for Q_1 & Q_2 as shown in Figure 3. However, we have introduced a sequence of fault as shown in Figure 5. The same fault sequence has been repeated thrice to encompass 1800 time steps. To evaluate the robustness of the trained SVM model, we have tested the classifier under various scenarios. It is to be noted that the input profiles of Q_1 & Q_2, sequence of faults, type of faults, and magnitude of faults in all of these scenarios are different from what is used during training of the classification model. The input profile depicting the flowrates of Q_1 & Q_2 considered for testing the performance of the developed binary classifier is shown in Figure 6. Keeping the input profile same we have generated the following test scenarios:

Test scenario 1: During the training of the classifier we have always used any one fault at a given time instant. In reality there can be more than one fault present at a given time instant. Thus, in this scenario, we have introduced multiple faults at the same time instant. Also, in reality faults may be present with different intensity. It is particularly important to see if the proposed framework can detect faults even when

the magnitude is significantly lower compared to the training case. To take this factor into account, we have also reduced the magnitude of each fault as compared to that used during training the classifier. The classifiers are trained using fault magnitudes of $\pm25\%$ of Q_{Max} (i.e., $0.00075\frac{m3}{s}$), whereas for test scenarios fault magnitudes as low as $\pm10\%$ of Q_{Max} (i.e., $0.0003\frac{m3}{s}$), are implemented. Besides these, we have also changed the sequence in which faults are introduced into the process. Figure 7 demonstrates the fault sequence for test scenario 1. The actual heights and the predicted heights obtained from the kriging model are shown in Figure 8. Based on the residuals as inputs to our classification model, it classifies whether at any given time instant the process is at normal or faulty state. The FDR, FAR, and accuracy for this test scenario are found to be 99.3%, 4%, and 98.2% respectively.
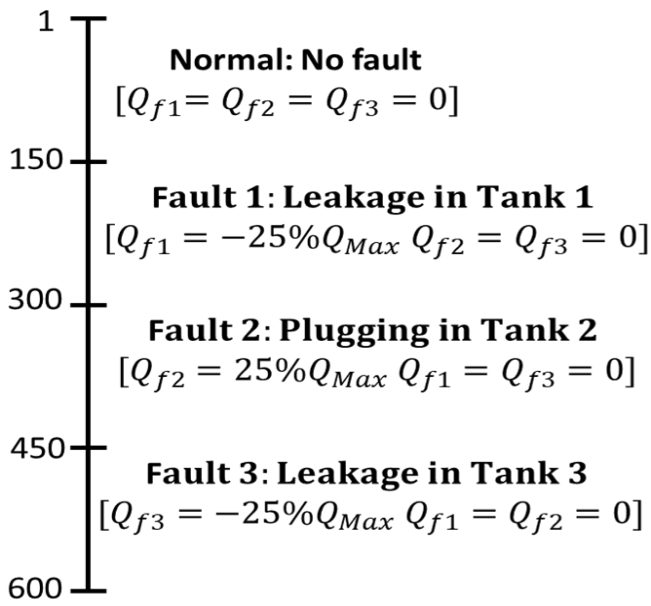

Figure 5: Fault sequence to train the classifier.
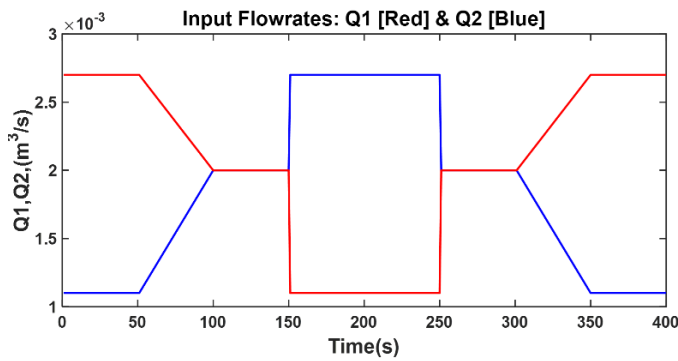

Figure 6: Input profile for Q_1 & Q_2 to test the performance of the classifier model.
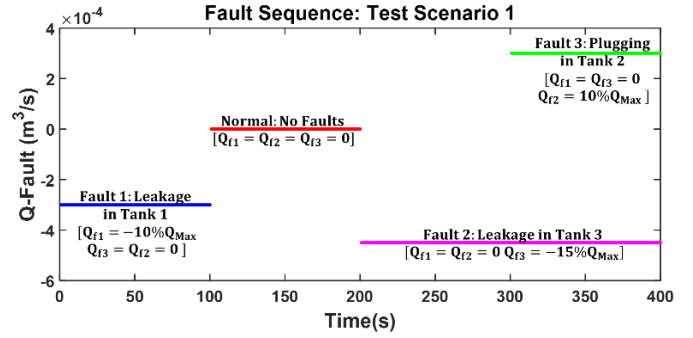
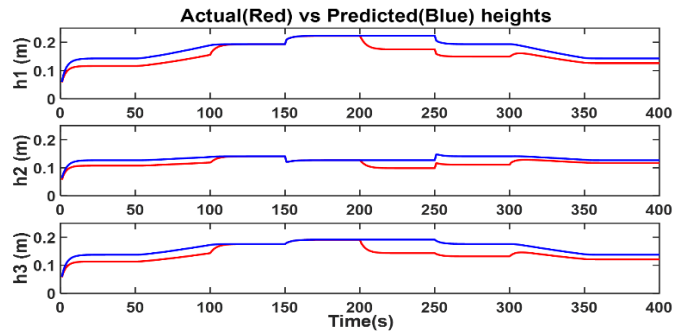

Figure 7: Fault sequence for test scenario 1.

Figure 8: Actual and predicted heights for test scenario 1.

Test scenario 2: During the training of our classification model we have specifically considered leakage in tank 1 and 3 and plugging in tank 2 (as shown in Figure 5). In reality, leakage or plugging can be associated with any of the three tanks. Thus, in this scenario we wanted to see the performance of the proposed framework when we introduce a different nature of fault into a tank as compared to our training scenario. In this test scenario, we considered leakage in tank 1 and 2 and plugging in tank 3. The fault magnitudes used in this scenario is also comparatively lower with respect to that used during the training phase. Figure 9 demonstrates the fault sequence for test scenario 2. The actual heights and the predicted heights obtained from the kriging models are shown in Figure 10. Based on the residuals as inputs, the SVM model classifies whether at a given time instant the process is at normal or faulty state. The values of FDR, FAR, and accuracy for this scenario are found to be 99%, 4%, and 98.5% respectively.
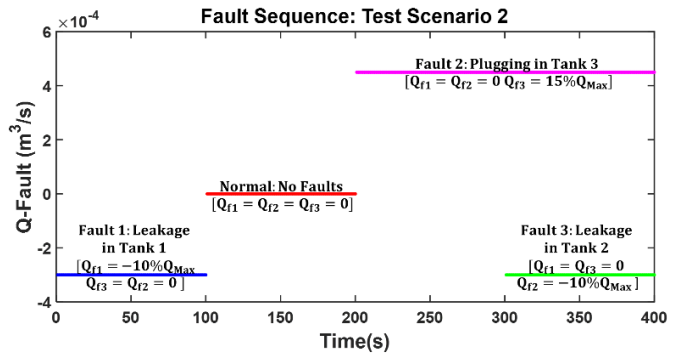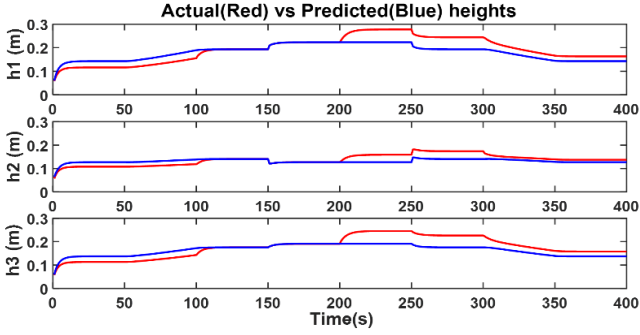

Figure 9: Fault sequence for test scenario 2.

Figure 10: Actual and predicted heights for test scenario 2.

Test scenario 3: The classifier is trained using constant values of fault magnitudes. However, a fault may not always have a constant magnitude rather the magnitude of a fault can vary with time. In this test scenario, we consider that leakage in tank 1 and 3 and plugging in tank 2 are changing exponentially. Figure 11 demonstrates the fault sequence for test scenario 3. The actual heights and the predicted heights obtained from the kriging model are shown in Figure 12. Based on the residuals as inputs, the SVM classifier results in an FDR, FAR, and accuracy values of 97.3%, 0%, and 98% respectively. We see that although there is a slight reduction in FDR and accuracy as compared to the previous two test scenarios, there is no case of false alarm.
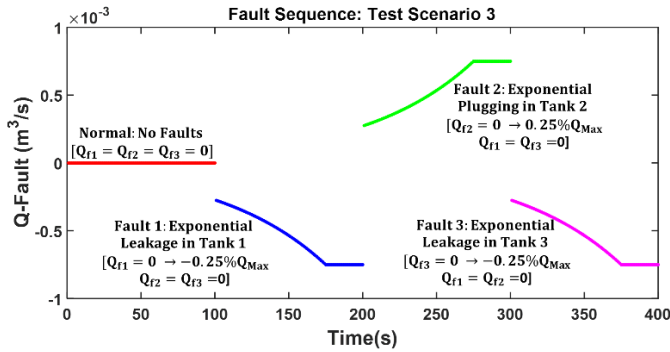

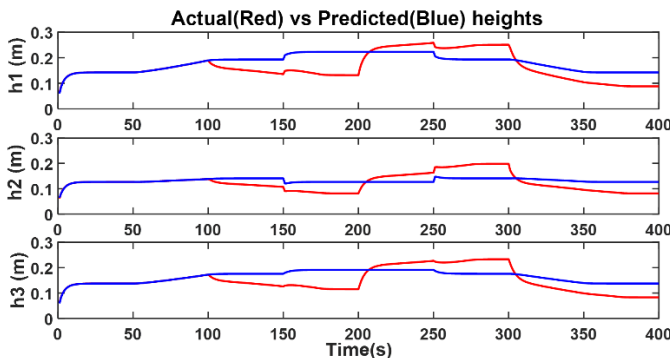Figure 11: Fault sequence for test scenario 3.

Figure 12: Actual and predicted heights for test scenario 3.

Test scenario 4: In this test scenario, we consider that the tanks in this process are not subjected to any faults. However, there is a drift in sensor readings corresponding to the level measurement for tank 1 and 2. We have incorporated a positive drift in level measurement of tank 1 whereas a negative drift in level measurement of tank 2. Figure 13 shows the fault sequence for test scenario 4. The actual heights and the predicted heights obtained from the kriging model are shown in Figure 14. The drifts in the sensor readings are introduced at time instant 101 and continued till 400 as shown in Figure 13. Our framework is able to detect it from time instant 107 onwards i.e., there is a lag of 6 time steps before the drift can be detected. However, there was no case of false alarm in this scenario. From our results obtained, we observed that the values of FDR, FAR, and accuracy are 98%, 0%, and 98.5% respectively.
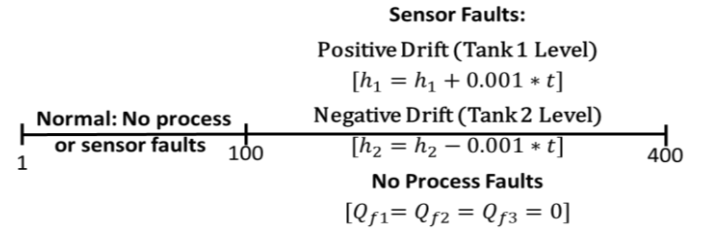

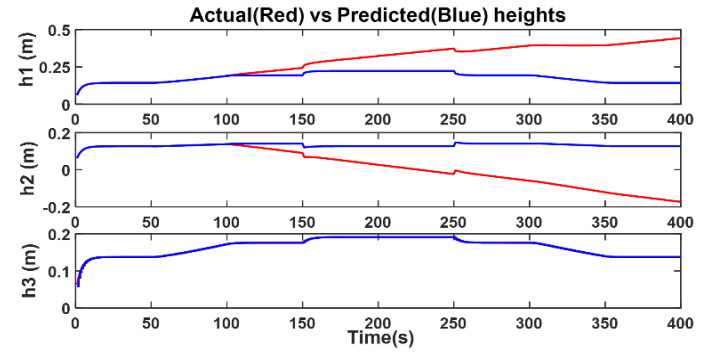Figure 13: Fault sequence for test scenario 4.

Figure 14: Actual and predicted heights for test scenario 4.

4. CONCLUSION

In this study, we have proposed a surrogate-assisted fault detection framework and applied it to a three tank benchmark system. The proposed kriging-based dynamic surrogate model resulted in a significantly lower NRMSE values, thus enhancing the reliability of the surrogate mimicking the actual process output under normal (i.e., no faults) scenarios. Based on the residuals i.e., difference in the predicted output from the kriging model and the actual plant output, a SVM-based binary classification model is proposed to detect fault(s), if any. To evaluate the robustness and performance of the developed methodology, we have tested it on a variety of scenarios different from that considered during the training phase. We have not only considered process faults like leakage and plugging of tanks but also accounted for sensor faults. The framework has been tested for different magnitudes of faults as well as a variety of fault sequences that are completely different from the ones used during the training phase. Besides this, we have incorporated not only single fault but also the presence of multiple faults simultaneously. The proposed framework not only performed

well under different types of faults and sequences of faults but also successfully detected faults with significantly lower magnitudes as compared to the training phase.

The overall accuracy of the model is found to be at least 98%, irrespective of the scenarios considered. Across scenarios, the maximum value of false alarm is found to be only 4% and the minimum value of fault detection is observed to be 97.3%. Thus, the proposed surrogate-assisted fault detection framework showed satisfactory performance for the three-tank benchmark system. The future work will be directed towards evaluating the performance of the proposed surrogate-assisted residual-based classification framework for fault detection in other dynamic processes.

5. REFERENCES

Abid, A., Khan, M. T., & Iqbal, J. (2021). A review on fault detection and diagnosis techniques: basics and beyond. *Artificial Intelligence Review*, *54*(5), 3639–3664. https://doi.org/10.1007/s10462-020-09934-2

Ajagekar, A., & You, F. (2020). Quantum computing assisted deep learning for fault detection and diagnosis in industrial process systems. *Computers and Chemical Engineering*, *143*, 107119. https://doi.org/10.1016/j.compchemeng.2020.107119

Du, D., Yan, S., Yang, F., Zhu, Z., Song, Q., & Yang, G. (2018). Kriging interpolation for evaluating the mineral resources of cobalt-rich crusts on magellan seamounts. *Minerals*, *8*(9), 9–16. https://doi.org/10.3390/min8090374

Duddeck, F., & Wehrle, E. (2015). Recent Advances on Surrogate Modeling for Robustness Assessment of Structures with respect to Crashworthiness Requirements. *10th European LS-DYNA Conference*, *June*.

Klebanov, N., & Georgakis, C. (2016). Dynamic Response Surface Models: A Data-Driven Approach for the Analysis of Time-Varying Process Outputs. *Industrial and Engineering Chemistry Research*, *55*(14), 4022–4034. https://doi.org/10.1021/acs.iecr.5b03572

Mahadevan, S., & Shah, S. L. (2009). Fault detection and diagnosis in process data using one-class support vector machines. *Journal of Process Control*, *19*(10), 1627–1639. https://doi.org/10.1016/j.jprocont.2009.07.011

Shokry, A., Ardakani, M. H., Escudero, G., Graells, M., & Espuña, A. (2017). Dynamic kriging based fault detection and diagnosis approach for nonlinear noisy dynamic processes. *Computers and Chemical Engineering*, *106*, 758–776. https://doi.org/10.1016/j.compchemeng.2017.03.016

Shokry, A., Baraldi, P., Zio, E., & Espuña, A. (2020). Dynamic Surrogate Modeling for Multistep-ahead Prediction of Multivariate Nonlinear Chemical Processes. *Industrial and Engineering Chemistry Research*, *59*(35), 15634–15655. https://doi.org/10.1021/acs.iecr.0c00729

Shokry, A., Vicente, P., Escudero, G., Pérez-Moya, M., Graells, M., & Espuña, A. (2018). Data-driven soft-sensors for online monitoring of batch processes with different initial conditions. *Computers and Chemical Engineering*, *118*, 159–179. https://doi.org/10.1016/j.compchemeng.2018.07.014

Venkatasubramanian, V., Rengaswamy, R., Kavuri, S. N., & Yin, K. (2003). A review of process fault detection and diagnosis. *Computers & Chemical Engineering*, *27*(3), 327–346. https://doi.org/10.1016/s0098-1354(02)00162-x

Venkatasubramanian, V., Rengaswamy, R., Yin, K., & Kavuri, S. N. (2003a). A review of fault detection and diagnosis. Part III: Process history based methods. *Computers and Chemical Engineering*, *27*, 327–346.

Venkatasubramanian, V., Rengaswamy, R., Yin, K., & Kavuri, S. N. (2003b). A review of process fault detection and diagnosis part I: Quantitative model-based methods. *Computers and Chemical Engineering*, *27*(3), 293–311. https://doi.org/10.1016/S0098-1354(02)00160-6