



Original Article

Quantification of predicted uncertainty for a data-based model

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ARTICLE INFO

Article history:

Received 12 December 2019

Received in revised form

30 July 2020

Accepted 4 August 2020

Available online 8 August 2020

Keywords:

Model uncertainty

Predicted uncertainty

Data-based model

Drift monitoring

Sensor

ABSTRACT

A data-based model, such as an AAKR model is widely used for monitoring the drifts of sensors in nuclear power plants. However, since a training dataset and a test dataset for a data-based model cannot be constructed with the data from all the possible states, the model uncertainty cannot be good enough to represent the uncertainty of estimations. In fact, the errors of estimation grow much bigger if the incoming data come from inexperienced states. To overcome this limitation of the model uncertainty, a new measure of uncertainty for a data-based model is developed and the predicted uncertainty is introduced. The predicted uncertainty is defined in every estimation according to the incoming data. In this paper, the AAKR model is used as a data-based model. The predicted uncertainty is similar in magnitude to the model uncertainty when the estimation is made for the incoming data from the experienced states but it goes bigger otherwise. The characteristics of the predicted model uncertainty are studied and the usefulness is demonstrated with the pressure signals measured in the flow-loop system. It is expected that the predicted uncertainty can quite reduce the false alarm by using the variable threshold instead of the fixed threshold.

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1. Introduction

A data-based model is widely used due to its ease to use and its applicability to a complex system, of which the operating mechanism is not known in detail. Unlike first-principle models which are based on physical equations, it can incorporate all of the functionality of the system by collecting process parameters measured over the operating range of plants. Therefore, it has been implemented to monitor the condition of equipment during operation in nuclear power plants [1]. Especially, it has been played an important role to monitor the drifts of sensors for extending calibration interval since unnecessary calibration might result in not only damage and degradation of sensors but also increase of maintenance cost [2,3].

The data-based model, however, is only accurate when applied to the same or similar operating conditions under which the data were collected. When plant operating conditions are changing, the model extrapolates outside the trained space and the results cannot be trusted. Therefore, it is required to inform the accuracy or the uncertainty of the estimates. Some of data-based models categorized as probabilistic model such as a Gaussian Process Regression

(GPR) model provide uncertainties of the prediction assuming the Gaussian process [4]. Such data-based probabilistic models are actively utilized in many fields including nuclear industries as well as other industries [5,6]. On the other hand, some of data-based models such as an Auto-Associate Kernel Regression(AAKR) model, estimate states without the uncertainty of their prediction since they are not probabilistic models. For the purpose of using those kinds of data-based models for nuclear plants, Electric Power Research Institute (EPRI) of US proposed a concept for quantifying the uncertainty by historical data: the model uncertainty [7].

However, the uncertainties of the prediction are expected to vary with the incoming data to be estimated. Furthermore, it is expected that the uncertainties for inexperienced states increase substantially when the characteristics of the inexperienced states are different from those of the experienced state. According to the above the reasons, the model uncertainty is hardly validated. To overcome the limitations, the new method to quantify the predicted uncertainty depending on the data is proposed. The predicted uncertainty is defined and validated for the case of an AAKR model with the data acquired from the flow loop system and its usefulness is demonstrated. It shows better performance for the inexperienced region of states and reduce the false alarms resulting from the model uncertainty.

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2. Estimation of predicted uncertainties for a data-based model

2.1. Data-based model

A data-based model such as an AAKR model can be utilized to estimate the state of the sensors when the historical data are meaningfully correlated [8,9]. Provided that the number of associated sensors is P and each sensor has N historical data, the memory matrix of an AAKR model is an $N \times P$ matrix M of which each element is denoted by M_{ij} . Then the mathematical expression of the AAKR model in a matrix form is Eq. (1):

$$\hat{X} = \frac{w^T M}{\sum_{i=1}^N w_i} \quad (1)$$

Where,

\hat{X} is a $1 \times P$ vector denoting the estimated states of a $1 \times P$ vector

Xw is the $N \times 1$ wt vector

w_i is the i -th weight

For each sensor,

$$\hat{X}_j = \frac{\sum_{i=1}^N w_i M_{ij}}{\sum_{i=1}^N w_i} \text{ for } j = 1, 2, \dots, P \quad (2)$$

$$w_i = K(D_i, h) = \frac{1}{\sqrt{2\pi}h^2} e^{-\frac{D_i^2}{2h^2}} \quad (3)$$

$$D_i = \sqrt{\sum_{j=1}^P (M_{ij} - X_j)^2} \text{ for } i = 1, 2, \dots, N \quad (4)$$

Where,

\hat{X}_j is the j -th element of \hat{X} and is the estimate of a vector Xw_i is the i -th weight when the Gaussian Kernel is used.

h is a hyperparameter

D_i is the Euclidean distance between X_j and M_{ij}

2.2. Model uncertainty of a data-based model

Provided that X_j is the j -th row vector of the matrix X of Section 2.1 and \hat{X}_j is that of their state estimates. In general, the model uncertainty of a data-based model is estimated with Eq. (5) through Eq. (7) where $\hat{\sigma}_e^2$ is the variance of the noise from independent factors of X_{tst} . X_{tst} is the test data for calculating the model uncertainty, and A is $N_{tst} \times 1$ matrix for calculating bias, respectively [7].

$$MSE(\hat{X}_{tst}) = \frac{1}{N_{tst}} \sum_{i=1}^{N_{tst}} (\hat{X}_{tst,i} - X_{tst,i})^2 \quad (5)$$

$$Bias(\hat{X}_{tst}) = A \cdot MSE(\hat{X}_{tst}) - Var(\hat{X}_{tst}) - A \cdot \hat{\sigma}_e^2 \quad (6)$$

$$U = \sqrt{Var(\hat{X}_{tst}) + [Bias(\hat{X}_{tst})]^2} \quad (7)$$

Where,

$\hat{\sigma}_e^2$ is the variance of the noise

The above model uncertainty is defined to be used as the criteria of the classification [7]. However, since the model uncertainty

depends only on the test data, that cannot represent the uncertainty of the prediction for the unseen data which may happen in the future. In fact, the test data cannot include all the possible states and the model uncertainty cannot cover all the range of the uncertainties.

2.3. Predicted uncertainties for a data-based model

In general, the test data used for evaluating the model uncertainty cannot be obtained from all the possible states of the processes. Therefore, the model uncertainty is not good enough to denote the performance of the model. To overcome this limitation of the model uncertainty, the predicted uncertainty is proposed to represent the uncertainty of prediction.

The predicted uncertainty is defined as Eq. (8) which is very similar to the uncertainty definition as in eq. (9) which is root-square-average of the difference between the data and the estimate. In fact, the predicted uncertainty can be considered as the weighted uncertainty depending on the importance of data which is similar concept of the AAKR model. Therefore, the same equations for AAKR model are used to calculate weights and distance as in Eq. (3) and Eq. (4), respectively. Weights can be modeled with the various Kernel functions with hyperparameter h and distance is the Euclidean distance. They determine the effective range of the memory data to be used for estimation.

$$U_{predict} = \sqrt{\frac{\sum_{i=1}^N w_i \sum_{j=1}^P (M_{ij} - \hat{X}_j)^2}{\sum_{i=1}^N w_i}} = \sqrt{\sum_{i=1}^N \frac{w_i}{N_{eq}} |M_i - \hat{X}|^2} \quad (8)$$

$$U = \sqrt{\frac{\sum_{i=1}^N (x_i - \bar{x})^2}{N}} = \sqrt{\sum_{i=1}^N \frac{1}{N} (x_i - \bar{x})^2} \quad (9)$$

Where,

M_i is the row vector of matrix $M\hat{X}$ is the estimated vector

N_{eq} is the equivalent number of data

x_i is the data to be used for estimation

\bar{x} is the mean of x_i 's

N is the number of data

The predicted uncertainty interval is defined as Eq. (10) using t -distribution considering the size of the data to be evaluated.

$$U_{predict} = t_c(\beta N_{eq}, 95\%) U_{predict} \quad (10)$$

Where,

t_c is the critical value of the student t -distribution with the 95% confidence level and degree of freedom βN_{eq} .

β is the hyperparameter which is related to the size of memory matrix.

The hyperparameter h and β should be determined to make the predicted uncertainty be approximated to the model uncertainty for the experienced region. However, if the incoming data were located far from the memory data, the equivalent number of data N_{eq} would reduce according to the distance from the memory data. As the equivalent number of data is smaller, the uncertainty interval $U_{predict}$ is larger based on the t -distribution. Since the equivalent number of data is dependent on the size of the memory data, β is designed to controls the predicted uncertainty interval for the inexperience region. The predicted uncertainty interval of the data-based model can be estimated for every incoming data.

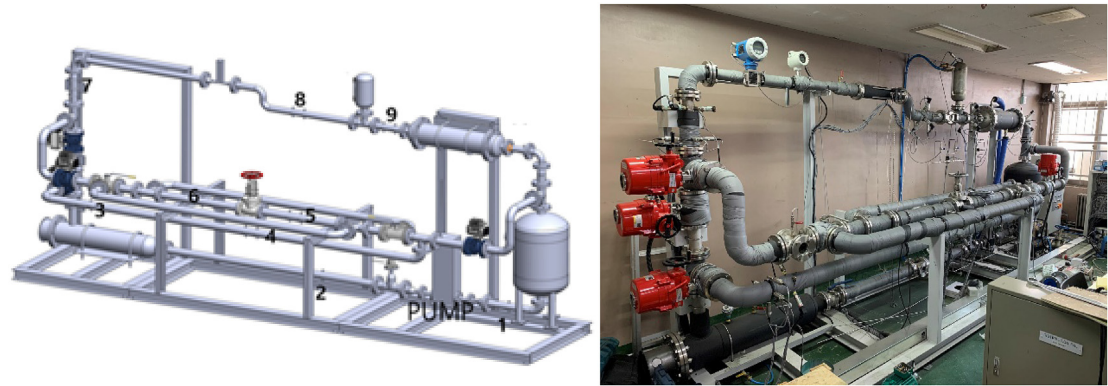


Fig. 1. The flow loop system.

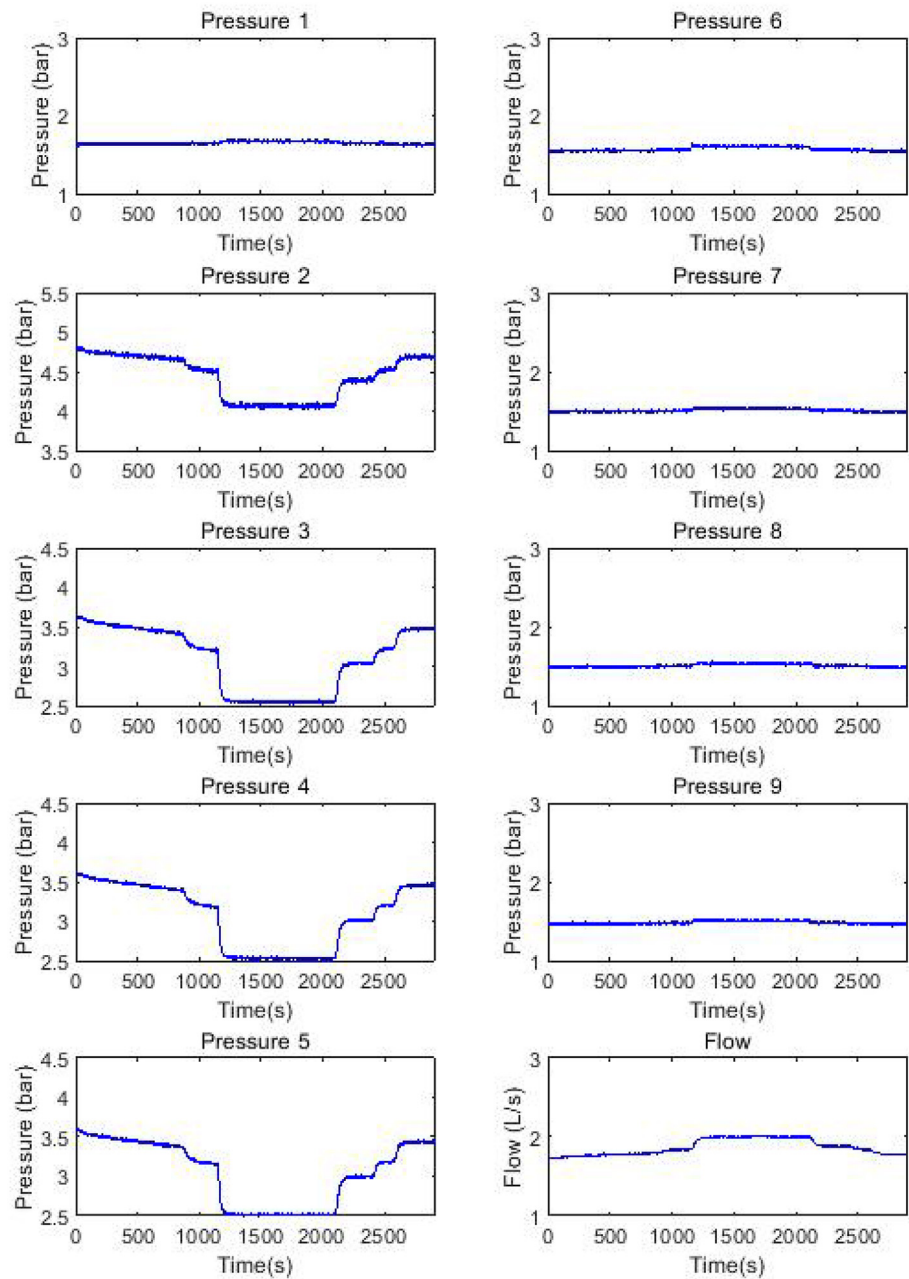


Fig. 2. Pressure signals at 9 locations depicted in Fig. 1 and flow rate signal.

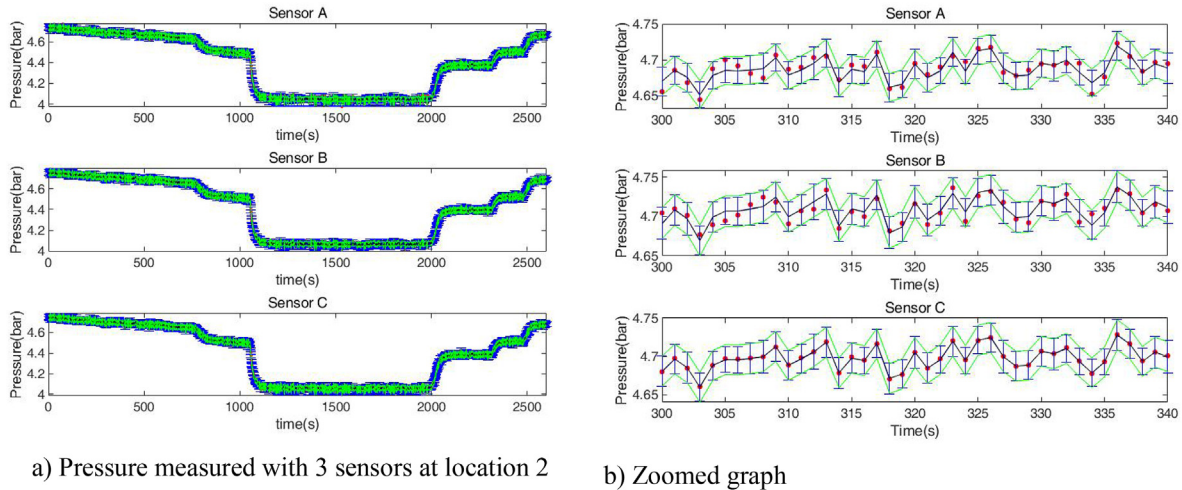


Fig. 3. The model uncertainty interval and the predicted uncertainty interval when the test data are estimated. (Red dot: measured signal, black line: estimated signal, green lines: model uncertainty interval, vertical bars: predicted uncertainty interval). (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

3. Evaluation of the proposed predicted uncertainty

3.1. Experimental set-up and the predicted uncertainty interval

To examine the characteristics of the proposed predicted uncertainty, the data were measured from a flow loop system as in Fig. 1. The system consists of a pump, an electrical heater, control valves, a pressurizer, a heat exchanger, and pipes. The flow rates and the pressure are controlled by the variable speed pump and the flow control valve. Fig. 2 shows examples of the pressure signals measured at 9 locations in Fig. 1 and the flow rate signal. Pressures vary according to the flow rates and the locations. In nuclear power plants, multiple sensors are placed to increase sensing reliability at important locations. At location 2, three pressure sensors (Sensor A, Sensor B and Sensor C) are installed and the pressures were measured at the same time. All sensors are calibrated and normal. The train dataset, the validation dataset and the test dataset are randomly sampled from the whole range of the data at location 2 in various flow conditions as in Fig. 2. The AAKR model for estimating the pressure at location 2 was developed with those datasets.

Fig. 3 shows the model uncertainty interval (between two green lines), the predicted uncertainty interval (blue bar) centered at the estimates of the model (black line) and the measured points (red dots) of each 3 pressure sensors when the data from the test dataset are estimated as incoming data. Since the test dataset was sampled from the same region as the training dataset, model estimations are very accurate and the uncertainty intervals are very small. The predicted uncertainty intervals look similar to the model uncertainty interval. The measured data are located within not only the model uncertainty intervals but also the predicted uncertainty interval of the estimations as expected since the sensors are normal. This means that the predicted uncertainty is statistically a good performance indicator as the model uncertainty for the trained and tested region. However, the uncertainty of prediction for inexperienced data could be different from the model uncertainty.

3.2. Uncertainty interval for inexperienced data

To classify the drift of the sensor, the residuals, which is the difference between the measured data and the estimates by the model are compared with the uncertainty intervals. If the residuals are located within the uncertainty interval, the sensor is classified

as normal. Therefore, the data-based model should provide the estimates and the uncertainty at the same time. Furthermore, the model should be developed by the data of normal states since the estimates of the model are assumed to be normal. However, the training dataset cannot include all the normal state of the system. Thus, the effect of the inexperienced data should be examined.

There are two kinds of inexperienced data. One is the abnormal-state inexperienced data and the other is out-of-range normal-state inexperienced data since the train dataset cannot include all the operating range of the process in general. It is also obvious that the uncertainty of the data-based model for the inexperienced region cannot be the same as that for the experienced.

To examine the former case, one of three pressure signals at location 2 (Pressure 2 of Sensor B) was intentionally made drifted slightly starting from the time of 2100 s as in Fig. 4. The blue line is the normal signal and the red line is the drifted signal. Fig. 5 shows the measured signal (red dot), the estimated signal (black line), the model uncertainty interval (green lines) and the predicted

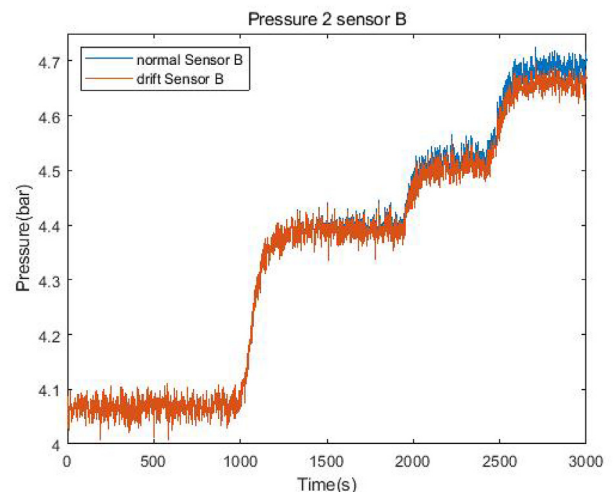


Fig. 4. Pressure 2 signal measured with Sensor B (blue line) and the drift signal made intentionally of the measured pressure 2 (red line). (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

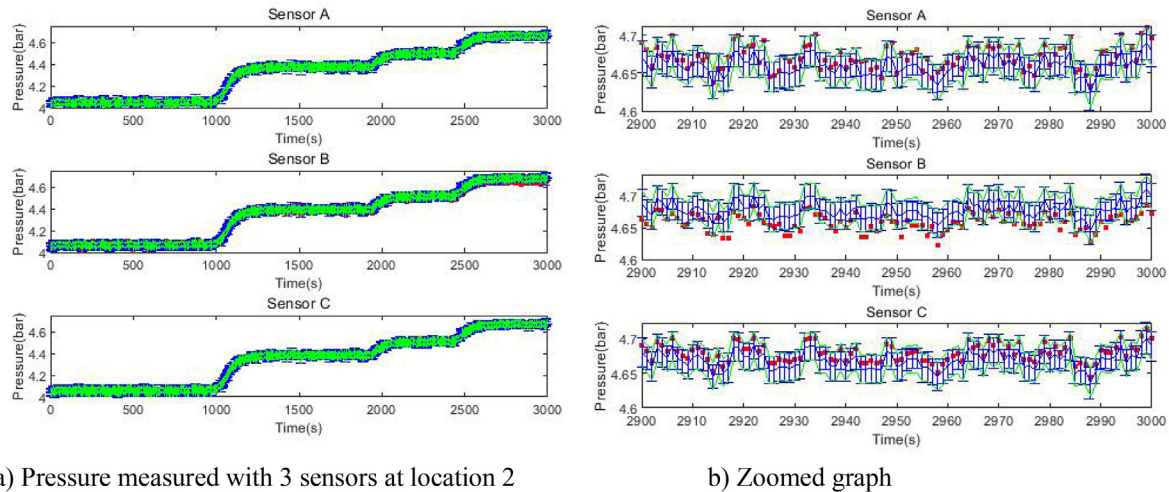


Fig. 5. Uncertainty intervals of Sensor A, B and C (Red dot: measured signal, black line: estimated signal, green lines: model uncertainty interval, vertical bars: predicted uncertainty interval). (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

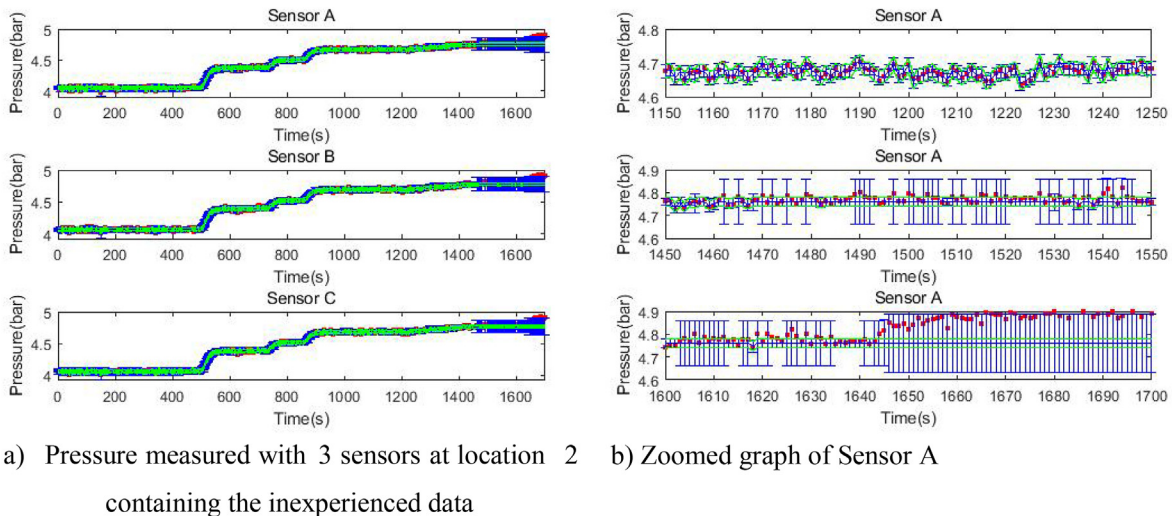


Fig. 6. Model estimates and uncertainty intervals for inexperienced data (Red dot: measured signal, black line: estimated signal, green lines: model uncertainty interval, vertical bars: predicted uncertainty interval). (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

uncertainty intervals (vertical bar). Both the model uncertainty interval and the predicted uncertainty intervals are almost same in the whole region as in Fig. 5 a) since the measured data are in the range of training dataset. For Sensor A and Sensor C, the data are located within the uncertainty intervals but it can be noticed that the drifted data are out of uncertainty intervals for Sensor B as in Fig. 5 b). It means that both the model uncertainty and the predicted uncertainty are good indicator to identify the drift sensors even when the sensors are abnormal if the measured data are in the range of training dataset.

To examine the case of the out-of-range normal-state inexperienced data, the signals including the higher-pressure operating condition than that of the training dataset were used as incoming data. As shown in Fig. 6 a). The front part of the graph belongs to the range of the training dataset and the latter part of the graph starting from around 1460 s comes from the data of the inexperienced region. All the sensors are calibrated and normal. In the inexperience region, however, the measured data are outside the model uncertainty interval, which leads to identify that all the sensors are drifted. This shows that the model uncertainty interval is not good

enough to be used as the threshold to classify the drift and that the errors of the model in the inexperience region are greater than the model uncertainty.

However, the predicted uncertainty can be estimated in every estimation considering the characteristics of the incoming data. Since the predicted uncertainty is defined using the same weights as the AAKR model, it has statistically similar characteristics as the AAKR model in dealing with the importance of data. It also become larger as the incoming data go farther from the training dataset since the equivalent number of data to be used to calculate the uncertainty reduces. Those characteristics of the predicted uncertainty are shown in Fig. 6 b). The top graph of Fig. 6 b) shows that the measured data are within the range of the predicted uncertainty intervals and that the classification can be made with small uncertainty since it is in the experienced region. In the middle graph of Fig. 6 b) which comes from both the experienced and the inexperienced region, the measured data are noticed to be out of the model uncertainty interval due to the estimation error of the data-based model even though the sensors are normal. However, the predicted uncertainty intervals cover the errors of the

estimation by increasing the intervals and prevent the wrong decision which the model uncertainty might cause in the inexperienced region. Finally, in the last graph of Fig. 6 b), it is shown that the predicted uncertainties go bigger as the incoming data points are farther from the experienced region. Even though the predicted uncertainty intervals do not cover for all the incoming data, they show much better performance than the model uncertainty interval in reducing the false alarm due to the estimation errors.

4. Conclusions

A data-based model estimates the normal state of the incoming data but errors of the estimation depend on the characteristics of the incoming data. Errors of the estimation increase substantially when the characteristics of the incoming data are different from those of training and test dataset. Therefore, it has been required that the uncertainty of estimation should be quantified in every estimation considering the characteristics of the incoming data.

In this paper, the predicted uncertainty is introduced and its characteristics are studied comparing with those of the model uncertainty which has been used for deciding the threshold of classification. To demonstrate the benefits of the predicted uncertainty, the pressure data were measured with 3 pressure sensors at the same location in the flow-loop system. One of the pressure signal was made drifted on purpose. The predicted uncertainties have similar values in magnitude as the model uncertainty when the incoming data belong to the same operating range of training dataset. Therefore, the detection of the drifted signal can be made by either the predicted uncertainty or the model uncertainty. However, when the incoming data are out of range of the training dataset, it is noticed that the residuals increase beyond the model uncertainty interval and the sensors are classified as drifted sensors even though they are all well calibrated since the data-based model provides rather large error which cannot be covered by the model uncertainty. This means that the model uncertainty may lead to the wrong conclusion due to the bigger error. On the other hand, the predicted uncertainties depend on the incoming data and provide reasonable results. When the incoming data are out of the training dataset, the predicted uncertainty grows big and it covers the errors made by the data-based model. Therefore, it is possible to make false alarms be substantially reduced with the predicted uncertainty. In conclusion, the proposed method to calculate the predicted uncertainty is useful for monitoring the drift sensors by quantifying the uncertainty in every estimation considering the

characteristics of the incoming data.

Funding

This work was supported by the Nuclear Safety Research Program through the Korea Foundation Of Nuclear Safety(KoFONS) using the financial resource granted by the Nuclear Safety and Security Commission(NSSC) of the Republic of Korea (No. 1805007).

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.net.2020.08.002>.

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