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An adaptive DISSIM algorithm for statistical process monitoring

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Abstract: Recently, a novel multivariate statistical process monitoring method, known as dissimilarity algorithm(DISSIM), has been developed based on the idea that a change of operating condition can be detected by monitoring a distribution of process data set, where a dissimilarity index is introduced to quantitatively evaluate the difference between distributions of process data. However, as a fixed-model monitoring technique, it inevitably gives false alarms when applied to real processes involving slow changes. In this paper, an adaptive DISSIM(ADISSIM) algorithm is proposed for on-line updating to consecutively adapt to process slow-varying behaviors. The key to the proposed method is that whenever the old model is judged to be inefficient to capture the current normal operation status, a new monitoring model is developed by integrating the old model and the new updating data. The effectiveness of ADISSIM algorithm is successfully illustrated when applied to simulated data collected from a simple 2×2 numerical process. The results clearly show that the proposed adaptive method is effective to accommodate the normal gradual changes and distinguish them from real process faults, thus providing a new feasible statistical monitoring method for the prevalent slow-varying processes.

1. INTRODUCTION

Proper process monitoring and diagnosis is important not only to quality improvement but also to process safety. Most statistical process monitoring methods are based on principal component analysis (PCA) and partial least squares (PLS) (Kourti and MacGregor, 1995; Kosanovich, Dahl and Piovoso, 1996; Louwerse and Smilde, 2000; Nomikos and MacGregor, 1994, 1995a, 1995b). In recent years, a novel statistical process monitoring method known as DISSIM has been developed and successfully applied in process monitoring(Kano and Hasebe et al. 1999, 2000, 2001, 2002; Zhao and Wang et al. 2007), which detects the change of operating condition by quantitatively evaluating the changes of correlations of process variables using dissimilarity index. A series of successful theory researches and applications have demonstrated that the method can fast and effectively detect the occurrence of process disturbances. However, the monitoring model is constructed based on data from a certain number of observed data. Its major limitation is that the invariant model can't reveal the slow time-varying changes that real industrial processes often experience, such as equipment aging, catalysis deactivation, sensor and process drifting, and degradation of efficiency(Qin, 1998; Li, Yue, Valle-Cervantes and Qin, 2000). Despite the gradual changes of operating conditions, such kind of slow varying behaviours is deemed to be normal features underlying the process operation because they reflect practical process status and won't drastically affect the process correlations. If the gradual process drift is overlooked over evolvement without being differentiated from real process faults, it is not difficult to imagine that the invariant statistical model can often result in false alarms. Therefore it is desirable to develop an adaptive algorithm to update the model based on new normal process data and track the normal slow-varying features effectively. However, it has limitation in updating a DISSIM model online using newly available data. While one could rebuild a new model based on merging the new data and old data, it is computationally inefficient because more and more new process measurements are available consecutively. In the present work, we modify and extend the general DISSIM algorithm so that an adaptive DISSIM(ADISSIM) algorithm can be successfully applied in slow-varying processes. The main advantage of the proposed approach lies in the use of weighted eigenvector so that one can update the monitoring model based on new data in a more parsimonious and smart way without increasing greatly the size of modelling data set. The application to a simple 2×2 numerical process demonstrates the effectiveness of the method.

2. ADISSIM-BASED MONITORING AND UPDATING STRATEGY FOR SLOW-VARYING PROCESSES

2.1 Dissimilarity index

Kano and Hasebe et al.(1999, 2000, 2001, 2002) proposed a statistical process monitoring method based on the dissimilarity analysis of process data. Their method, termed DISSIM, is based on the idea that a change of operating condition can be detected by monitoring the distribution of process data because the distribution reflects the corresponding operating condition. Thus a dissimilarity index is defined to quantitatively evaluate the difference between distributions of process data.

Consider the following two data sets, X_1 and X_2. X_i consists of N_i samples of J variables. Here, without special statement, they are both scaled to zero-mean and unit-variance. The covariance matrices are given by

$$R_i = \frac{1}{N_i} X_i^T X_i \tag{1}$$

And the covariance matrix of the mixture of both data sets is given by R.

$$R = \frac{N_1}{N_1 + N_2} R_1 + \frac{N_2}{N_1 + N_2} R_2 \tag{2}$$

On the basis of the fact that the covariance matrix R can be diagonalized by an orthogonal matrix P_0

$$P_0^T R P_0 = \Lambda \tag{3}$$

Where, Λ is a diagonal matrix whose diagonal elements are eigenvalues of R. Then the original data matrices X_i are transformed into Y_i.

$$Y_i = \sqrt{\frac{N_i}{N_1 + N_2}} X_i P_0 \Lambda^{-\frac{1}{2}} = \sqrt{\frac{N_i}{N_1 + N_2}} X_i P \tag{4}$$

Where, P is a transformation matrix defined as $P = P_0 \Lambda^{-1/2}$.

The covariance matrices of the transformed data matrix

$$\begin{aligned} S_i &= \frac{1}{N_i} Y_i^T Y_i = \frac{N_i}{N_1 + N_2} P^T \frac{X_i^T X_i}{N_i} P \\ &= \frac{N_i}{N_1 + N_2} P^T R_i P \end{aligned} \tag{5}$$

satisfy the following equations:

$$S_1 + S_2 = I \tag{6}$$

By application of eigenvalue decomposition to the covariance matrices

$$S_i \omega_i^j = \lambda_i^j \omega_i^j \tag{7}$$

Here, λ_i^j and ω_i^j are the eigenvalues and the corresponding eigenvectors, respectively. The superscript j denotes the $j-th$ eigenvalue or eigenvector. From Eqs. (6) and (7), the following relationships

$$S_2 \omega_1^j = (1 - \lambda_1^j) \omega_1^j \tag{8}$$

$$1 - \lambda_1^j = \lambda_2^j \tag{9}$$

can be derived. The above two relationships mean the transformed data matrices, Y_1 and Y_2, have the same set of principal components and the principal components are reversely ordered. In other words, the most important correlation for the transformed data set Y_1 is equivalent to the least important correlation for the other transformed data set Y_2, and vice versa.

Finally, the following index D was defined for evaluating the dissimilarity of data sets.

$$D = diss(X_1, X_2) = \frac{4}{J} \sum_{j=1}^{J} (\lambda_j - 0.5)^2 \tag{10}$$

where, λ_j denotes the eigenvalues of the covariance matrix of the transformed data matrix and J is the number of process variables. When data sets are quite similar to each other, the eigenvalues λ_j must be near 0.5, and then D should be near zero. On the other hand, when data sets are quite different form each other, the largest and the smallest eigenvalues should be near one and zero respectively and D should be near one. Therefore, the index D changes between zero and one.

2.2 ADISSIM monitoring and updating algorithm

For continuous process modelling using DISSIM method, one reference data set under normal operating conditions is defined. Then the dissimilarity indices between time series data sets spanning other time regions and the reference one are compared to determine the control limit simply by sorting the vector data of a variable from the lowest to largest values and then taking 99.9% and 0.1% percentile of the data to be the upper and lower control limits respectively. So it assumes that future process features exactly behave in the same way as those used for model identification. However, industrial processes commonly exhibit slow time-varying behaviours, such as catalyst deactivation, equipment aging, sensor and process drifting, and preventive maintenance and cleaning. Therefore they induces slow and normal process changes in most real chemical process, including their mean, variance, and correlation structure among their measurement variables. Different from real process abnormalities, they are deemed as normal process dynamics. The monitoring performance will lose sensitiveness thus inducing false fault indications when an invariant model is used to monitor such slow-varying processes, which significantly compromise the reliability of the monitoring system. In order to accommodate the normal slow varying in operating conditions, an adaptive algorithm should be developed by updating the model structures recursively with accumulation of new normal data. Several methods(Qin, 1998; Li, Yue, Valle-Cervantes and Qin, 2000; Lee, Yoo, and Lee, 2003; Zhao, Chai and Wang, 2005) based on recursive PCA/PLS have been proposed to resolve the kind of monitoring problem, which have greatly promoted and extended the development of multivariate statistical process control(MSPC). Similarly, considering the inherent characteristics of slow-varying processes, only one invariant reference data set as monitoring model to calculate the dissimilarity values is not enough, in which dissimilarity values between different time-serial data sets and the reference model may change along time without tracking the similar trajectory as before. Here, an adaptive DISSIM algorithm(ADISSIM) is explored based on simple updating strategy for the slow-varying processes.

Generally, based on common adaptive idea, new process information can be infused into the monitoring models by merging the new process measurement consecutively since it is a time-wise modelling approach. However, the typical updating algorithm involves time-consuming and repetitive calculation since more and more new process data are added into the modelling database, which will augment the size of modelling data set infinitely with time evolving. Thus it is desirable to improve the computation efficiency if the previous calculation result can be made better use of. In the present work, the ADISSIM algorithm can adapt the model based on new data and the old model, thus avoiding re-modelling the old data and the over-increase of modelling data.

From Eq. (3), by application of eigenvalues decomposition, we can readily deduce the following relationship:

$$
\begin{aligned}
&\frac{1}{N}X^T X = P\Lambda P^T \\
&= \frac{1}{J}\left[J(P\Lambda^{0.5})(P\Lambda^{0.5})^T\right] = \frac{1}{J}\widetilde{P}\widetilde{P}^T
\end{aligned}
\tag{11}
$$

where $\widetilde{P} = \sqrt{J}P\Lambda^{0.5}$, here it is termed as weighted eigenvector. Λ is a diagonal matrix whose diagonal elements are eigenvalues of $\frac{1}{N}X^T X$.

Moreover, combined with the DISSIM algorithm in section 2.1, it is clear that performing dissimilarity analysis on $\widetilde{P}_i$ and $\widetilde{P}_j$ results in the same dissimilarity index value as performing on data pair X_i and X_j . Based on such idea, the weighted eigenvector can naturally take the place of process measurements as monitoring model. Especially, instead of storing old reference data set in memory, we can simply replace them with the weighted eigenvector. Thus instead of integrating old data set and new data set to updating the reference model, the ADISSIM can update the model using the old model $\widetilde{P}_{ref}$ and new process measurements, X_{new} . Whenever model updating is required, the new modelling data set $X_{ref}^{new} = \begin{bmatrix} \widetilde{P}_{ref}^T \\ X_{new} \end{bmatrix}$ are formulated and new monitoring model $\widetilde{P}_{ref}^{new}$ are thus developed. Moreover, in the present work, we use nonparametric kernel density estimation method(Levinson, 1997; Chen, Wynne, Hiden, Sandoz, 2000; Martin, Morris, 1996) to develop the control limits for D -statistic. Based on normal operating data, the univariate kernel density estimator is used to estimate the density function of these normal dissimilarity index values. The point, occupying certain quantile area of density function, can be obtained and employed as the control limit of normal operation conditions. One major advantage of kernel density estimation is that it needs no specific statistical distribution prior and the determined control limits follows the data more closely. With enough train samples, no matter which kernel function is adopted, a reliable density estimation result can be finally obtained in theory. However, using kernel estimation method might be sometimes dangerous for designing thresholds. The kernel itself increases variance from the histogram of data, and in particular in the tails this is critical.

It should be noted that n the adaptive updating algorithm, a potential adaptation problem is that the model may adapt not only to normal process evolution, but also to process disturbances and failures. To prevent this, it is necessary and vital to exactly distinguish the normal gradual variations from the real abnormal variability so that the adaptation of monitoring model to slow-varying features won't impact disadvantageously on the accuracy and sensitivity of process fault detection.

According to what is analyzed above, an adaptive DISSIM algorithm with respect to modelling, monitoring and updating may be implemented in the following manner:

(1) Acquire time series data as the training database when a process is operated under a normal condition. The current time is denoted as k_{ref} . Determine the size of time window, l . Generate data set with l samples from the data by moving the time window. Select a reference data set X_{ref} by trial and error and normalize it to zero mean and unit variance. Moreover, the 'rest training data windows' are also scaled using the mean and variance obtained from reference data.

(2) Then the weighted eigenvector $\widetilde{P}_{ref}$ is obtained as the initial monitoring model by eigenvalues decomposition on the selected reference data set in step (1). Dissimilarity analysis can thus be performed between those 'rest training data windows' and $\widetilde{P}_{ref}$. Consequently, the control limits are derived from those obtained D -statistic values, $DISS_{ref}$, using kernel-based density estimation method.

(3) For online monitoring, the data window X_k , representing the current operating condition at time interval k , is obtained consecutively by moving the time-window step by step, and is scaled by the same mean and variance derived from reference data set in step (1). Then the dissimilarity values between them and the monitoring model $\widetilde{P}_{ref}$ are calculated, and process monitoring is conducted by continuously comparing the obtained D -statistic with the predetermined control limits. Whenever a new normal process measurement is available, it will be archived into the candidate updating database.

(4) If the current D_k is outside the control limits, there are two potential causes. One may result from the real operation abnormality, and the other may be due to the failure of old monitoring model in pursuing the current new operating status. To identify the two cases, the reliability of the old models can be checked online. That is, those available normal time serial measurements newly archived in updating database from k_{ref} to the current time enter into the reference dataset forming the new modelling data set as $X_{ref}^{new} = \begin{bmatrix} \widetilde{P}_{ref}^T \\ X_{new} \end{bmatrix}$. New monitoring model, $\widetilde{P}_{ref}^{new}$ is readily recalculated in the same way as $\widetilde{P}_{ref}$. By doing so, the new monitoring model will accommodate the evolving slow changes of process features and more process operation information. Thus using the newly obtained monitoring model, new D -statistic values, termed as $DISS_{new}$, are recalculated for those time windows acted on by X_{new} . Then the reference $DISS_{ref}$ used for estimating the control limits will be augmented to include $DISS_{new}$, $DISS_{ref}^{new} = \begin{bmatrix} DISS_{ref} \\ DISS_{new} \end{bmatrix}$, where $DISS_{ref}^{new}$ is gradually filled by the new statistic values along time evolving. Correspondingly, the control limits will be adjusted in the same way as step (2).

(5) The current sampling time window is re-monitored using the newly designed models. If the dissimilarity statistic returns below the control limits, it indicates that the previous alarm indication is caused by the failure of old model and thus the new model should replace the old ones as the current monitoring tool to adapt to the new process operating feature. Otherwise, if fault alarm is still exposed, it reveals that a real process abnormality has occurred, resulting from the unknown disturbances rather than the normal slow-varying dynamics. Correspondingly, the process should be analyzed in detail to give the possible cause for the fault.

3. APPLICATION TO 2×2 PROCESS

In this section, the proposed monitoring method, ADISSIM, is applied to on-line monitoring problems of a simple 2×2 process, which initially is a typical continuous process. The monitoring results demonstrate the effectiveness of the proposed method to adapt easily to slow-varying processes.

For simplicity, the 2×2 multivariate process(Ku et al., 1995) is described as follows:

$$x(t)=\begin{bmatrix}0.118 & -0.191\\ 0.847 & 0.264\end{bmatrix}x(t-1)+\begin{bmatrix}1.0 & 2.0\\ 3.0 & -4.0\end{bmatrix}u(t-1) \quad (15)$$

$$y(t)=x(t)+v(t) \quad (16)$$

Where u is the correlated input:

$$u(t)=\begin{bmatrix}0.811 & -0.266\\ 0.477 & 0.415\end{bmatrix}u(t-1) + \begin{bmatrix}0.193 & 0.689\\ -0.320 & -0.749\end{bmatrix}w(t-1) \quad (17)$$

The input w_i in w are uncorrelated Gaussian signals with zero mean and unit variance. The output y_i in y is corrupted by uncorrelated Gaussian errors with zero mean and variance 0.1. The input u and the output y are measured, and their measurements are used for monitoring.

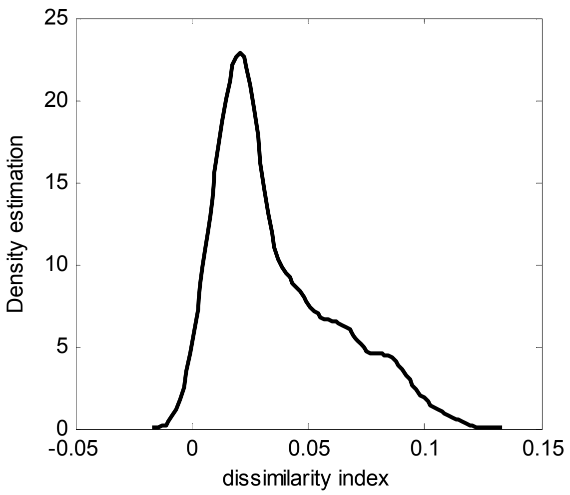

Fig. 1 Density estimate for dissimilarity values

Under the normal operating conditions, a time-series data set $X(500\times 4)$ can be obtained from the continuous process with the development of time. The window length is set to be 50 by trial and error and then 451 moving windows are generated. Using the modelling procedure mentioned in section 2.2, one data window is selected properly to build a reference model. Then focusing on the process variation along time direction, the other moving windows are used as training data sets to determine the control limits of D -statistic. Without prior statistical distribution knowledge, the density distribution rule can be readily obtained using nonparametric kernel estimation method as visually shown in Fig. 1. However, considering that the dissimilarity index values are positive, the estimated density corresponding to negative values, here termed "losing density", is improper. Thus the subsequently calculated control limits might be not accurate enough under its influence. Naturally, some modification should be made to better adapt to the specific circumstance. Here, the control limits are properly raised to make for those "lost density". This is carried out by modifying the imposed quantile used to compute the control limits until a certain OTI(overall type I error) value, for instance 0.05, is met(Camacho and Picó, 2006).

Once the model is developed, it can be used for online application. To quantitatively evaluate the performance of the proposed method in comparison with DISSIM method, two performance indices can be used in the simulation: the overall type I error(OTI) and the relative action signal time(AST). The OTI is the proportion of faults in the process representing normal operation conditions. The AST is defined as the time elapsed between the introduction of an error and the out-of-control signal in the control chart. In the present work, we mimic the slow-varying behaviours by introducing the gradual increase on the mean of w_1 from 0 to 0.5 within 500 time intervals. Despite the gradual increase, the process is regarded as normal because this change will not drastically affect the other process variables. Fig. 2 shows the monitoring result with the fixed model without updating, where the D -statistic demonstrate an obvious trend to violate the confidence limits after about 200^{th} time interval. Hence the reliability of initial model has been compromised.

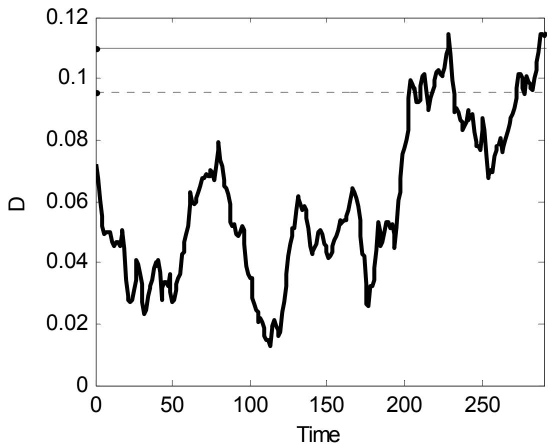

Fig. 2 Monitoring result for normal case before updating (solid line, 99% control limit; dashed line, 95% control limit; bold line, D-statistic)

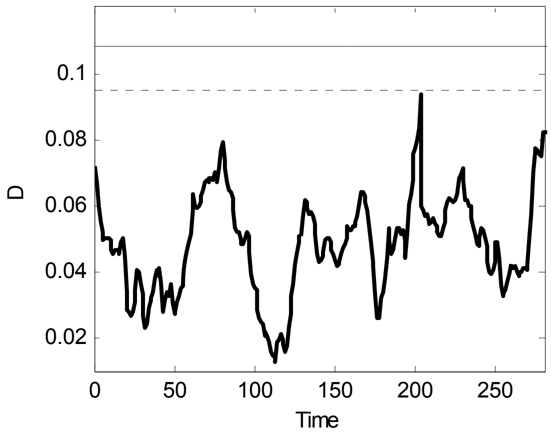

Fig. 3 Monitoring result for normal case after updating (solid line, 99% control limit; dashed line, 95% control limit; bold line, D-statistic)

However, for practical application in industrial processes, there is no prior knowledge about the inherent alarm cause. Thus we need to check whether the alarm is induced by real process fault or the failure of monitoring model. Using the proposed method, the reference model is put into updating and then the monitoring result using the updated model is shown in Fig. 3. It can be seen that after updating, the alarms disappear, revealing that the false alarms are caused by the failure of old model in tracking slow-varying behaviours. Thus updating procedure is necessary to accommodate the norm gradual changes and adapt to the new operation conditions.

Moreover, to verify the fault detection performance of the proposed updating algorithm, two kinds of process disturbances are taken into account. One is step shift from 0 to 0.5 in case of the mean of w and the other is the step change of a coefficient relating u_1 with x_2 from 3.0 to 4.5. Different from normal slow variations, they are believed to be real process faults because the abrupt changes have seriously affected the process correlations. Thus with time evolving, those fault data are entering the time windows and checked by means of dissimilarity index. As shown in Figs. 4 and 5, both of the two significant deviations are correctly detected soon after the occurrence of fault using the updated model visually which shows that updating algorithm doesn't compromise the performance of the process fault detection. Therefore, normal slow-varying behaviours are correctly distinguished from real significant process faults. In case of the normal slowing varying and the above two faults, the serials of monitoring results have demonstrated the swiftness and effectiveness of the proposed method for process monitoring and fault detection. Thus it is viable to monitor such slow-varying processes using consecutively updating algorithm, in which the adjustment considering the successive slow variation in evolution is reasonable and will benefit the efficiency of process monitoring.

However, it should be noted that the algorithm has the potential problem that the newly updated model sometimes might adapt itself to faulty data when the fault is small and slow varying. In the present work, we only put emphasis on the detection of significant faults. To correctly distinguish the normal slow varying behaviours from slow faults, some process expertise may be necessary. On the other hand, the dissimilarity index only concerns the covariance matrix, i.e., the underlying process correlations, without considering the varying in mean of data. Moreover, due to the smoothing function of moving window, the monitoring results suffer a time delay. Therefore, the selection of an appropriate time-window size is crucial for the effective function of ADISSIM method. In the modelling procedure, we have chosen the time-window length by trial and error.

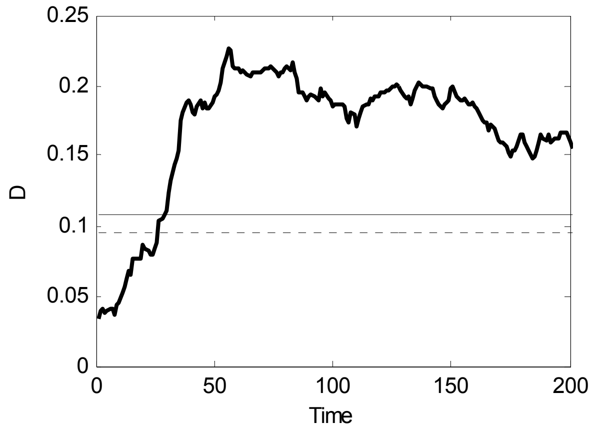

Fig. 4 Monitoring result for fault 1 with updating model (solid line, 99% control limit; dashed line, 95% control limit; bold line, D-statistic)

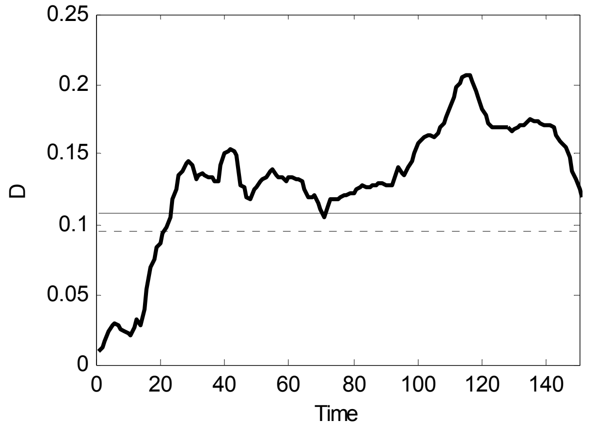

Fig. 5 Monitoring result for fault 2 with updating model (solid line, 99% control limit; dashed line, 95% control limit; bold line, D-statistic)

4. CONCLUSIONS

A new monitoring and adaptively updating method has been proposed as a response to these problems in the case of slow-varying processes. This method, termed ADISSIM, supplies a simple and promising updating way to adapt to the common slow-varying dynamics in real industrial processes, which reduces false alarms and provides greater reliability. Meanwhile, a more accurate control limit is developed properly using kernel-based density estimation method. The results of application to a simple 2×2 process indicate that the method is feasible and competent used as a monitoring tools when applied to the monitoring of processes whose normal operating conditions undergo normal gradual changes. Therefore, a process monitoring system based on dissimilarity analysis of moving windows will be promising.

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