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Feature Based Fault Detection for Pressure Swing Adsorption Processes

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Abstract: Over the past few decades, there has been widespread development of pressure swing adsorption (PSA) systems, with their applications expanding from traditional bulk gas separation and drying, to CO_2 sequestration, trace contaminant removal, and many others. With extensive industrial applications, there is a significant need for effective monitoring methods to detect and diagnose process abnormalities in real-time, as well as to facilitate predictive maintenance for avoiding major production disruptions ahead. Although periodic operations such as PSA have been used widely in chemical and petrochemical industries, the process monitoring of these operations has received limited attention compared to non-periodic continuous or batch processes. A potential reason is that the monitoring of periodic processes is significantly more challenging than that of processes operated at steady-state. In this work, we propose a data-driven feature space monitoring (FSM) approach for PSA processes. We show that the FSM based fault detection naturally addresses the challenges in monitoring periodic processes, such as unequal step and/or cycle time that requires trajectory alignment or synchronization for the traditional statistical process monitoring (SPM) methods. In addition, we demonstrate the superior fault detection performance of the proposed method compared to the conventional SPM methods using both simulated faults and real faults from an industrial PSA process.

Keywords: pressure swing adsorption, fault detection, fault diagnosis, statistical process monitoring, statistics pattern analysis, feature space monitoring.

1. INTRODUCTION

In the past few decades, pressure swing adsorption (PSA) processes have gained increasing commercial acceptance as an energy efficient separation technology (Jiang et al., 2004). PSA applications range from traditional bulk gas separation and drying, to CO_2 sequestration, trace contaminant removal, and other. With its extensive industrial applications, PSA has drawn significant research interests from the process systems engineering community recently. The research has focused mainly on PSA system modelling and simulation (Choi and Wen-Chung, 1994; Chou and Huang, 1994; Nikolic et al., 2008), design and optimization (Boukouvala et al., 2017; Jiang et al., 2004, 2003). Although there is a significant need for effective monitoring methods to detect and diagnose PSA process abnormalities in real-time to avoid major production disruptions, research in this area has been scarce. This is mainly due to the non-stationary and periodic nature of the process, which pose special challenges to the monitoring of such a process. For example, the application of the conventional multivariate statistical process monitoring (MSPM) methods, such as principal component analysis (PCA) and its variants, can lead to frequent false alarms and/or missed faults (Pan et al., 2004). To address this challenge, Pan et al. (2004) proposed a process monitoring approach for continuous processes with periodic characteristics by identifying a stochastic state space model that captures the statistical behavior of changes occurring from period to period. The approach was validated using a waste water treatment process (WWTP). While there are similarities between WWTP and PSA processes, there are also differences. For example, the activated sludge process, which is a main part of a WWTP, is a natural periodic process with somewhat constant cycle time that is driven by the diurnal temperature and light fluctuations. In contrast, PSA is a forced periodic process with cycle time dynamically controlled to address many disturbances that affect the PSA operations (e.g., increased or decreased product throughput to meet customer demand or to minimize cost by scheduling based on electricity pricing, raw material feed composition variations), even weather conditions can affect the plant operations. As a result, the cycle time is heavily and frequently adjusted, which renders the approach proposed in (Pan et al., 2004) less effective for PSA processes. Another difference is that while the biological process in the WWTP is a very slow process, PSA is a very fast process. Recently, Wang et al. (2017) proposed a geometric framework for the monitoring and fault detection of periodic processes. The proposed approach was applied to two simulated periodic processes with superior performance compared to the conventional dynamic PCA (DPCA) and multiway PCA (MPCA). For the simulated 2-bed PSA process, a total of 26 variables relating to the flow rate of the feed, as well as pressures and concentrations in and across both beds were used for observation. However, in industrial PSA processes, not all of these variables were measured, especially the concentrations in and across the beds. In addition, pressure is the major process variable to be monitored, in this case the proposed method is not applicable as there is no centroid for a single variable. Another method specifically proposed for

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monitoring industrial PSA processes is a US patent (Arslan et al., 2014). In this method, a moving window discrete Fourier transform (DFT) was applied to process the data such as pressure profile. A number of "relevant" peaks were identified from the frequency spectra (i.e., their frequencies and amplitudes). Then calculate the logarithm of the amplitude ratio of peak k between beds i and j, which is defined as $\mathcal{R}$ in this work as the following.

$$\mathcal{R} = log\left(\frac{A_{i,k}}{A_{j,k}}\right) \quad (1)$$

where A is peak amplitude, i and j are the bed or vessel indices, k is the peak index. $\mathcal{R}$ is then monitored over time, where the control upper and lower limits were calculated based on normal operation data. In this work, we propose a completely different method based on a feature space monitoring (FSM) framework we proposed recently (Peter He and Wang, 2018). The basic idea of the proposed approach is that instead of monitoring the original pressure profile of a PSA process, we characterize the pressure profile of each PSA step by statistics and shape or morphology features. These features are then grouped by cycles and monitored by a linear or nonlinear MSPM method such as PCA for process monitoring (i.e., fault detection and diagnosis). The rest of the paper is organized as follows. Sec. 2 discusses some of the characteristics of the industrial PSA process and the challenges posed to the conventional MSPM methods by these characteristics. Sec. 3 briefly reviews statistics pattern analysis (SPA), which is the predecessor and a special case of FSM. Sec. 4 introduces the proposed FSM method for PSA processes. Sec. 5 presents several case studies, including simulated and real faults in an industrial PSA process to demonstrate the performance of the proposed method, which is compared to those of the conventional MSPM methods. Because only pressure was used for PSA process fault detection and diagnosis in this study, the method proposed by Wang et al. (2017) does not apply. While for the patent filed by Arslan et al. (2014), because there are no technical details as how the peaks were defined or classified as "relevant", and the criteria used for peak selection and control limits determination are unknown, it is not compared either. Sec. 6 discuss the results and Sec. 7 draws conclusions.

2. PROCESS AND DATA CHARACTERISTICS

In this section, we discuss the unique characteristics of a PSA process and how these characteristics pose challenges to process monitoring. Fig. 1 shows the typical pressure profile of a multi-bed PSA process. Due to the sensitivity of the actual operation and production data of the process, all axis tick labels in this and other figures based on real operation data were omitted. To reduce clutter, only the pressure profiles from three beds are plotted. This type of pressure time series plot is good for visualizing and observing between-bed variations. However, only obvious deviations/faults can be observed from this type of plot and it can become very cluttered and difficult to read if all beds were plotted on the same figure. Fig. 2 plots the overlapping of multiple cycles of a single bed, which can be used to visualize within-bed variations. Fig. 3 plots the durations of the cycles over a period

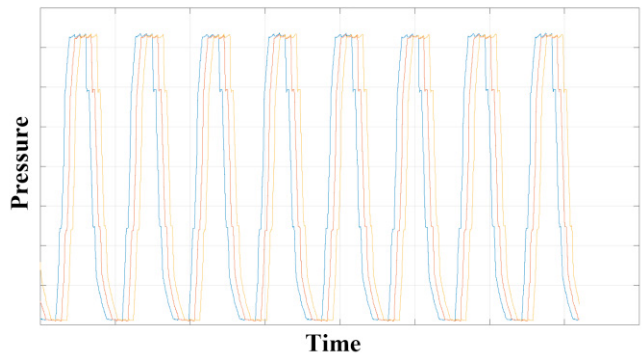


Fig. 1 Typical pressure profiles of three beds in a multi-bed PSA process

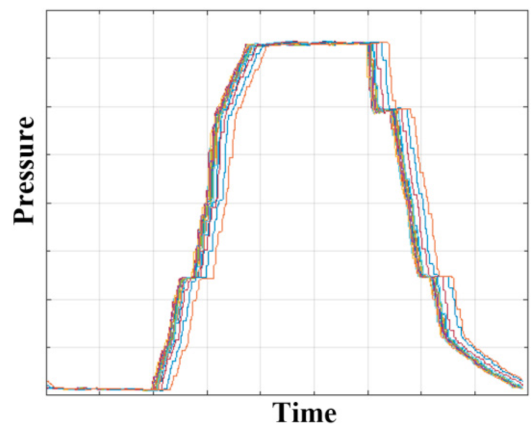


Fig. 2 Overlapping pressure profiles of a single bed over multiple cycles

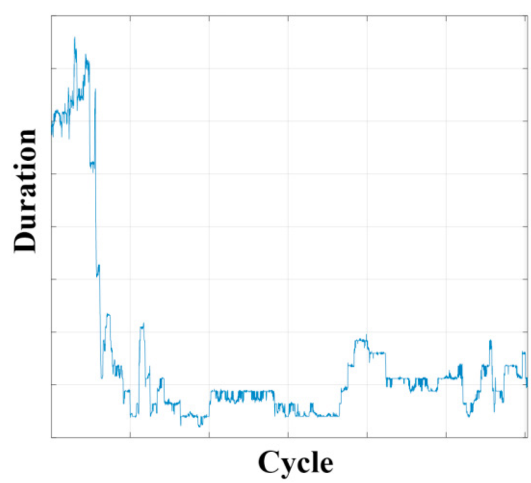


Fig. 3 The cycle duration varies significantly from cycle to cyle

of time. There are several points that can be made based on these three figures. First, the cycles are asynchronous across different beds as shown in Fig. 1. They do not exactly overlap each other after unfolding for the same bed as shown in Fig. 2, even for the onset, i.e., the start of the repressurization step, of the cycle. Second, the cycle duration, as well as the durations of the steps, vary from cycle to cycle as shown in Fig. 3. These durations are dynamically controlled to ensure product quality in response to dynamic scheduling, and/or disturbances such as demand change and weather conditions. Third, the process is highly nonlinear as shown in

Figs. 1 and 2. These characteristics pose significantly challenges to conventional MSPM methods such as multi-way PCA (MPCA), trilinear decomposition (TLD) and parallel factor analysis (PARAFAC) (Wise et al., 1999), or recently proposed methods such as multi-way independent component analysis (MICA) (Yoo et al., 2004) and kernel PCA (KPCA) (Choi et al., 2005). All these methods require the construction of a 2D or 3D array, which means that they all require synchronization of all steps of the entire cycle to equal step and cycle durations. This can be done through different ways, including simple cut, interpolation, dynamic time warping (DTW), etc. However, all these pre-processing steps have their drawbacks, including trajectory distortion, information loss, etc. (He and Wang, 2007; Peter He and Wang, 2018). It is particularly undesirable for PSA process because the step and cycle durations are dynamically controlled. As shown in Fig. 3, there are significant variabilities in step and cycle durations in a PSA process under normal operations. Step durations are not shown due to limited space, however, about half of them follow similar trends as the cycle duration while the other half of the steps were maintained relatively constant. Therefore, the pre-processing steps mentioned above is highly undesirable for PSA process. To address these challenges, we propose a feature space monitoring (FSM) based fault detection method for PSA. In the next section, we first briefly review statistics pattern analysis (SPA), which is the predecessor of FSM, then introduce the FSM based framework for PSA process monitoring.

3. STATISTICS PATTERN ANALYSIS (SPA)

Statistics pattern analysis (SPA) was originally proposed for monitoring batch processes (He and Wang, 2011) and later extended to the monitoring of continuous processes and other applications such as soft sensor (Shah et al., 2019; Wang and He, 2010). Since then many variations and extensions have been proposed in the literature (He and Xu, 2016; Yang et al., 2018; Zhang et al., 2018; Zhou and Gu, 2019). Because cyclic or periodic continuous processes share many similarities with batch processes (e.g., they are usually highly nonlinear processes with multiple steps or phases and their behaviours somewhat repeat from cycle to cycle or batch to batch), batch-based SPA is reviewed here.

Batch-based SPA hypothesizes that the batch behaviour can be better characterized by the variance-covariance of batch statistics than by the variance-covariance of process variables. In SPA, a statistics pattern (SP) is a collection of various statistics calculated from a batch trajectory which capture the characteristics of each individual variable (e.g., mean and variance), the interactions among different variables (e.g., covariance), the dynamics (e.g., auto-, cross-correlations), as well as process nonlinearity and process data non-Gaussianity (e.g., skewness, kurtosis, and other higher order statistics or HOS). The basic idea of SPA is that the SPs of normal batches follow a similar pattern (i.e., normal pattern), while the SPs of abnormal or faulty batches must show some deviation from the normal pattern. More details on batch-based SPA can be found in (He and Wang, 2011).

4. THE PROPOSED FRAMEWORK

In this work, since only the pressure profile is monitored, only univariate statistics are calculated. However, to better capture the characteristics of pressure behavior in each step of the process, we include not only statistics, but also shape or morphological features. Therefore, the proposed approach falls into more general feature space monitoring (FCM) framework we proposed recently (Peter He and Wang, 2018). Specifically, the following statistical and morphological features have been evaluated in this work: mean (μ), standard deviation (σ), skewness (γ), kurtosis (κ), coefficient of variation (C_V), coefficient of quartile variation (C_{QV}), interquartile range (R_{IQ}), slope (S), slope of linear regression line (S_{LL}), mean absolute deviation (D_{Mean}), median absolute deviation (D_{Med}), and mean absolute error (MAE). Fig. 4 shows the flow diagram of the proposed FSM based fault detection approach. The first step is cycle feature generation where various statistical and morphological features are generated for each step of a cycle based on the raw data. These features are stacked row-wise to form a feature vector for each cycle and multiple cycle features are stacked column-wise to form a feature matrix. The second step is to perform fault detection based on the feature matrix, where a conventional fault detection method such as PCA can be applied.

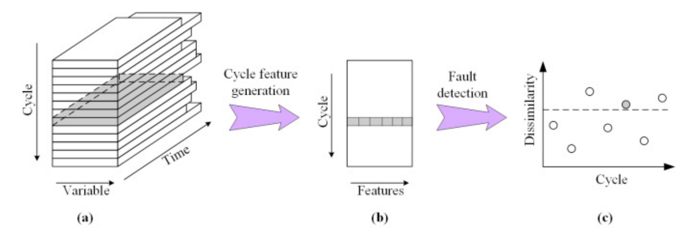


Fig. 4 Flow diagram of the proposed FSM method: (a) cycle trajectories with unequal cycle-times; (b) cycle features consists of various step features, which form the feature matrix when stacked column-wise; (c) fault detection based on the feature matrix.

Since features of a cycle consists of various statistical and morphological features calculated based on each step of the cycle, its dimension is independent of step durations as shown in Fig. 4. Therefore, FSM naturally handles unequal step durations and asynchronous cycle trajectories. In addition, FSM quantifies process dynamics and nonlinearity through various features as discussed previously. Therefore, FSM is well suited for the monitoring of PSA processes.

5. AN INDUSTRIAL CASE STUDY

In this section, we use an industrial PSA case study to demonstrate the performance of the proposed FSM method, and compare it to the traditional MPCA method. Because MPCA requires that each step across all cycles has the same duration, two different data preprocessing techniques are studied: one with simple cut denoted as $MPCA_{SC}$ and the other with dynamic time warping (DTW) denoted as $MPCA_{DTW}$. Totally 2070 cycles under normal operations were used as the training set. It is not necessary to use this many cycles as the training for the proposed FSM method. However, for

$MPCA_{DTW}$, the number of variables after unfolding is about 700. Therefore, we decided to use 2070 cycles, which is about three times the number of variables for $MPCA_{DTW}$. When simple cut is used, the shortest step duration across all cycles is used as the reference while the last measurements of any cycle with longer step duration were simply removed to match the shortest, which resulted in the number of variables to be about 440. While for FSM, 60 features were used. Six fault scenarios of a PSA process is studied in this work as listed in Table 1. The first four are simulated faults while the last two are from real industrial data. For each fault scenario, 16 cycles are used as the test set and among which 3 (cycle 4, 9 and 14) are faulty cycles. For the simulated faults, similar behaviours have been observed in actual operations, but the historical data for those types of faults are no longer available. In these cases, the faults were introduced by manipulating the real industrial data under normal operations. Details are provided later. It is worth noting that, it is only for better comparison that the faulty cycles were arrange in the same way for different fault scenarios, i.e., cycle 4, 9 and 14. For all methods, the number of principal component (PCs) is determined through 10-fold cross validation. The control limits on Hoteling's T^2 and squared prediction error (SPE) are calculated empirically using the training dataset at confidence level 99%. The number of PCs and other information discussed above are listed in Table 2.

Table 1. Fault scenarios studied in this work

Fault #	Description
1	During adsorption step, the faulty cycles have lower pressure than normal cycles.
2	During adsorption step, the faulty cycles have higher pressure variations than normal cycles
3	During a hold step, the pressure of the faulty cycles decreases instead of being held steady
4	During an equalization step, the pressure of the faulty cycles was held steady followed by a sudden drop instead of smooth decrease
5	During re-pressurization, the pressure of the faulty cycles does not follow the normal cycle trajectory
6	During an equalization step, the pressure of the faulty cycles follows a zig-zag or stair-like profile instead of a smooth increase

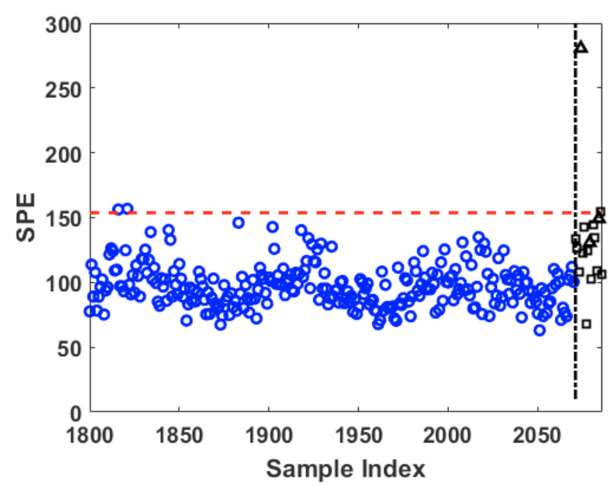
Table 2. Training, testing datasets and model parameters

	$MPCA_{SC}$	$MPCA_{DTW}$	FSM
# of features/variables	438	705	60
# of PC's	24	32	20
Training	2070 normal cycles		
Testing	16 cycles (13 normal, 3 faulty: cycle 4, 9, 16)		
Confidence level	99%		

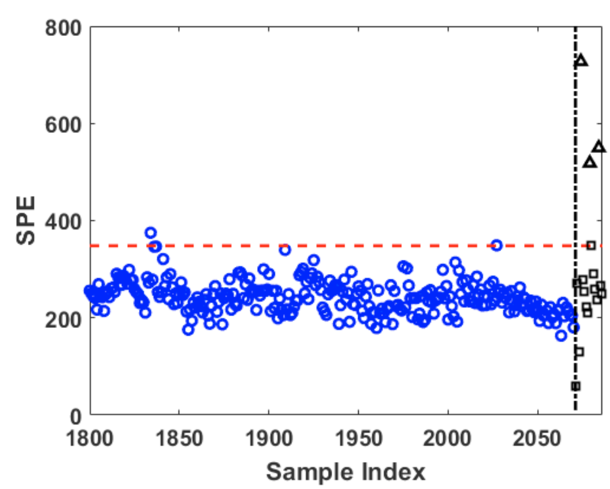
6. RESULTS

Due to limited space, only the fault detection results of fault scenario 1 and 5 in the residual subspace (i.e., using SPE index) are shown in Fig. 5 and Fig. 6. In both figures, (a) is the SEP plot based on $MPCA_{SC}$, (b) based on $MPCA_{DTW}$, and (c) based on FSM. Fig. 5 shows that for fault scenario 1, $MPCA_{SC}$ has difficulty in detecting Fault 1: missing two out of three faulty cycles. $MPCA_{DTW}$ detects all three faulty cycles but also generated a false alarm. Only FSM detects all three faulty cycles without generating false alarms. Fig. 6 shows that for fault scenario 5, $MPCA_{SC}$ detects all three faulty cycles while generating a false alarm. $MPCA_{DTW}$ failed to detect two out of three faulty cycles. Again, only FSM successfully detects all faulty cycles without generating false alarms.

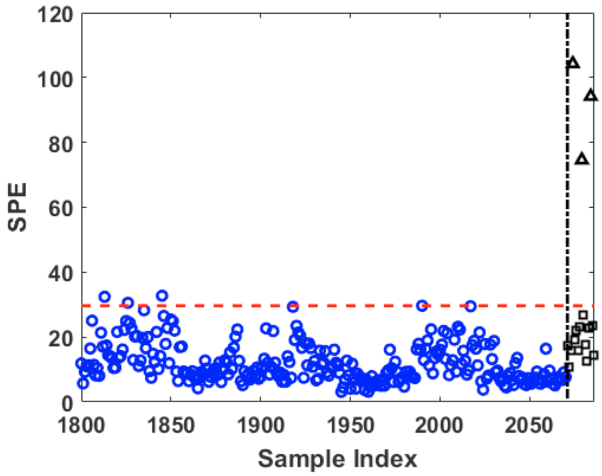
Further investigation is conducted to understand the reason for $MPCA_{DTW}$'s failure in detecting faulty cycles under fault scenario 5. Since $MPCA_{SC}$ was able to detect all faulty cycles, we suspect that the failure is related to data preprocessing by DTW. Therefore, we plotted the original pressure profiles of the 16 test cycles, which are shown in Fig. 7 (a), and compared to the pressure profiles after DTW as shown in Fig. 7 (b). The comparison clearly indicates that the irregular discrepancies of the faulty cycles shown in the original pressure profiles diminished after DTW. Therefore, it can be concluded that DTW caused severe information loss or distortion in the faulty cycles. This observation is consistent with our previous findings that data manipulations during preprocessing, including DTW, can cause information loss or distortion (He and Wang, 2011). This example further raise the alarm that the widely used DTW for batch trajectory warping or alignment in process monitoring applications is actually a problematic practice that can lead to missed detections of process faults.



(a)

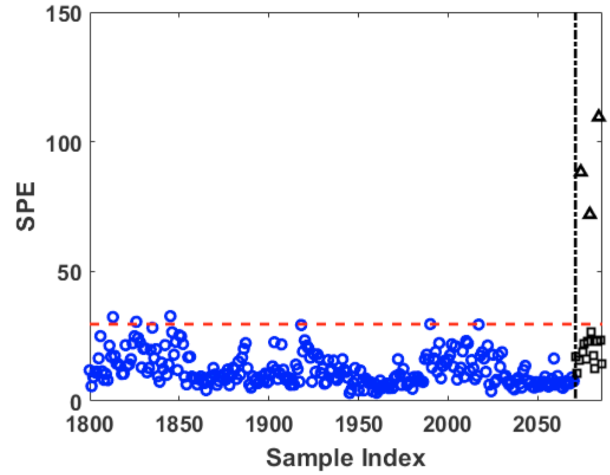


(b)



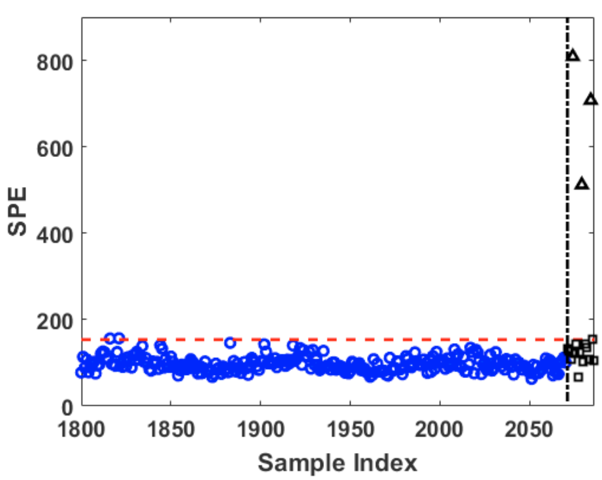
(c)

Fig. 5 Fault scenario 1: fault detection in residual subspace (SPE) from (a) $MPCA_{SC}$, (b) $MPCA_{DTW}$ and (c) FSM

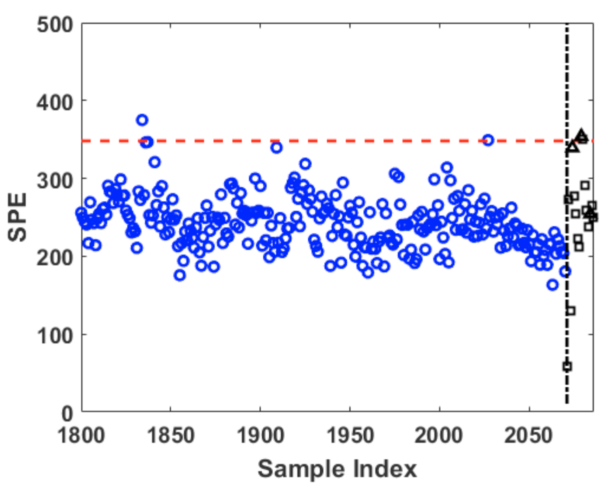


(c)

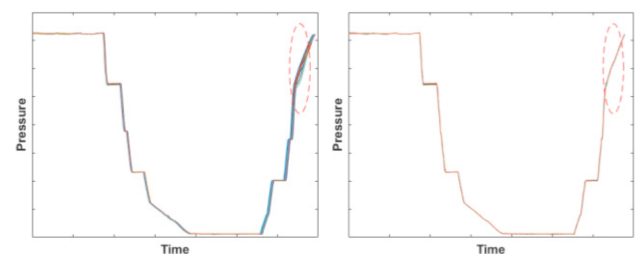
Fig. 6 Fault scenario 5: fault detection in residual subspace (SPE) from (a) $MPCA_{SC}$, (b) $MPCA_{DTW}$ and (c) FSM



(a)



(b)



(a) (b)

Fig. 7 Comparison between the pressure profiles of (a) the original 16 test cycles and (b) the test cycles after DTW. The irregular discrepancies among cycles shown in the original profiles (highlighted in the dashed ellipse) have diminished after DTW, indicating that DTW causes severe information loss or distortion.

By considering faults detected in both residual subspace using SPE and principal subspace using T^2, the overall fault detection results are shown in Table 3. Specifically, the table lists faulty cycles detected by either SPE, or T2, or both. These results are also summarized in fault detection rates shown in Table 4, and false alarm rates shown in Table 5. These tables show that FSM detects all faulty cycles under all fault scenarios without generating false alarms. In comparison, $MPCA_{SC}$ has missed detection under fault scenario 1, while $MPCA_{DTW}$ has missed detection under fault scenario 5. In addition, both $MPCA_{SC}$ and $MPCA_{DTW}$ have false alarms.

Table 3. Fault detection results (true fault cycles: 4, 9 & 14)

Fault	**FSM**	**$MPCA_{SC}$**	**$MPCA_{DTW}$**
1	4, 9, 14	4, 14, **15**	4, 9, **10**, 14
2	4, 9, 14	4, 9, 14, **15**	4, 9, **10**, 14
3	4, 9, 14	4, 9, 14, **15**	4, 9, **10**, 14
4	4, 9, 14	4, 9, 14, **15**	4, 9, **10**, 14
5	4, 9, 14	4, 9, 14, **15**	9, **10**
6	4, 9, 14	4, 9, 14, **15**	4, 9, **10**, 14

Table 4. Fault detection rate (out of 3 faulty test cycles)

Fault	FSM	$MPCA_{SC}$	$MPCA_{DTW}$
1	100%	66.7%	100%
2	100%	100%	100%
3	100%	100%	100%
4	100%	100%	100%
5	100%	100%	33.3%
6	100%	100%	100%

Table 5. False alarm rate (out of 13 normal test cycles)

Fault	FSM	$MPCA_{SC}$	$MPCA_{DTW}$
1	0%	7.7%	7.7%
2	0%	7.7%	7.7%
3	0%	7.7%	7.7%
4	0%	7.7%	7.7%
5	0%	7.7%	7.7%
6	0%	7.7%	7.7%

7. CONCLUSIONS

In this work, we proposed a simple yet effective fault detection method for pressure swing adsorption (PSA) processes. The proposed feature space monitoring (FSM) approach characterizes cycle behaviour with various statistical and shape/morphological features that are step-based. In this way, FSM naturally handles asynchronous cycle trajectories and variable step and cycle durations. We demonstrated that FSM outperforms MPCA with simple cut (SC) or dynamic time warping (DTW) data preprocessing in six PSA fault scenarios. Specifically, FSM successfully detected all three faulty cycles in each fault scenario without generating false alarms. In comparison, both $MPCA_{SC}$ and $MPCA_{DTW}$ had missed detections in some fault scenarios, and both had false alarms in all fault scenarios.

8. ACKNOLEDGEMENT

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REFERENCES

Arslan, E., Neogi, D., Li, X.J., Misra, P., 2014. Apparatus and methods to monitor and control cyclic process units in a steady plant environment.

Boukouvala, F., Hasan, M.M.F., Floudas, C.A., 2017. Global optimization of general constrained grey-box models: new method and its application to constrained PDEs for pressure swing adsorption. J. Glob. Optim. 67, 3–42.

Choi, C.-T., Wen-Chung, H., 1994. Incorporation of a valve equation into the simulation of a pressure swing adsorption process. Chem. Eng. Sci. 49, 75–84.

Choi, S.W., Lee, C., Lee, J.M., Park, J.H., Lee, I.B., 2005. Fault detection and identification of nonlinear processes based on kernel PCA. Chemom. Intell. Lab. Syst. 75, 55–67.

Chou, C., Huang, W.-C., 1994. Simulation of a four-bed pressure swing adsorption process for oxygen enrichment. Ind. Eng. Chem. Res. 33, 1250–1258.

He, F., Xu, J., 2016. A novel process monitoring and fault detection approach based on statistics locality preserving projections. J. Process Control 37, 46–57.

He, Q.P., Wang, J., 2011. Statistics pattern analysis: A new process monitoring framework and its application to semiconductor batch processes. AIChE J. 57, 107–121.

He, Q.P., Wang, J., 2007. Fault detection using the k-nearest neighbor rule for semiconductor manufacturing processes. Semicond. Manuf. IEEE Trans. 20, 345–354.

Jiang, L., Biegler, L.T., Fox, V.G., 2003. Simulation and optimization of pressure-swing adsorption systems for air separation. AIChE J. 49, 1140–1157.

Jiang, L., Fox, V.G., Biegler, L.T., 2004. Simulation and optimal design of multiple-bed pressure swing adsorption systems. AIChE J. 50, 2904–2917.

Nikolic, D., Giovanoglou, A., Georgiadis, M.C., Kikkinides, E.S., 2008. Generic modeling framework for gas separations using multibed pressure swing adsorption processes. Ind. Eng. Chem. Res. 47, 3156–3169.

Pan, Y., Yoo, C., Lee, J.H., Lee, I.-B., 2004. Process monitoring for continuous process with periodic characteristics. J. Chemom. 18, 69–75.

Peter He, Q., Wang, J., 2018. Statistics Pattern Analysis: A Statistical Process Monitoring Tool for Smart Manufacturing. Comput. Aided Chem. Eng. 44, 2071–2076.

Shah, D., Wang, J., He, Q.P., 2019. A feature-based soft sensor for spectroscopic data analysis. J. Process Control 78, 98–107.

Wang, J., He, Q.P., 2010. Multivariate Statistical Process Monitoring Based on Statistics Pattern Analysis. Ind. Eng. Chem. Res. 49, 7858–7869.

Wang, R., Edgar, T.F., Baldea, M., 2017. A geometric framework for monitoring and fault detection for periodic processes. AIChE J. 63, 2719–2730.

Wise, B.M., Gallagher, N.B., Butler, S.W., White, D.D., Barna, G.G., 1999. A comparison of principal component analysis, multiway principal component analysis, trilinear decomposition and parallel factor analysis for fault detection in a semiconductor etch process. J. Chemom. 13, 379–396.

Yang, J., Lv, Z., Shi, H., Tan, S., 2018. Performance monitoring method based on balanced partial least square and Statistics Pattern Analysis. ISA Trans. 81, 121–131.

Yoo, C.K., Lee, J.-M., Vanrolleghem, P.A., Lee, I.-B., 2004. On-line monitoring of batch processes using multiway independent component analysis. Chemom. Intell. Lab. Syst. 71, 151–163.

Zhang, H., Tian, X., Deng, X., Cao, Y., 2018. Multiphase batch process with transitions monitoring based on global preserving statistics slow feature analysis. Neurocomputing 293, 64–86.

Zhou, B., Gu, X., 2019. Multi-block statistics local kernel principal component analysis algorithm and its application in nonlinear process fault detection. Neurocomputing.