VACUUM PUMP DIAGNOSTIC ALGORITHM WITH LATENT VARIABLES

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Multivariate monitoring schemes based on latent variable have been shown to be a powerful monitoring tool in many industrial batch processes. Two techniques for analysis latent variable, principal component analysis (PCA) and independent component analysis (ICA), were applied to monitoring vacuum pump system. T^2 (or I^2) and SPE charts are proposed as diagnostic result, and contribution plot of these statistical quantities are also considered for fault identification. In this work, three types of state variables such as pressure, current and vibration acceleration are measured to monitoring vacuum pump system. According to the diagnostic result and its analysis, it should be focused not only individual variable but also relationship between variables. Especially, relationship between supply current and vibration acceleration well indicate the degradation of vacuum pump system.

1. Introduction

Demands on availability and reliability of vacuum pumps in modern semiconductor manufacturing process have been constantly increasing. It is the reason that the costs for failed wafer batches and lost production times are higher and higher as the size of the production wafer is larger and larger. In order to satisfy those demands, diagnostic algorithm is needed.

Multivariate monitoring schemes based on latent variable have been shown to be a powerful monitoring tool in many industrial batch processes. Two techniques for analysis latent variable, principal component analysis (PCA) and independent component analysis (ICA), were applied to monitoring vacuum pump system. Multiway principal component analysis (MPCA), a multivariate projection method, has been widely used to monitor batch and fed-batch processes. Methodology of PCA is briefly summarized in section II. In section III, another diagnostic algorithm (ICA) are introduced. In section IV, the measurement setup of multiple state variables and their statistical features are represented. In section V, diagnostic results (T^2 and I^2) are plotted. Finally, our conclusion are summarized in section VI.

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2. Principal Component Analysis (PCA)

2.1 Unfolding Method

Consider batch process, where J process variables are measured at K instances of time. So, raw data are arranged into a three-dimensional (3-D) array $X \in R^{I \times K \times J}$, where I is the number of batches, J is the number of variables and K is the number of sampling times in given batch.

For standard Principal Component analysis (PCA), three-dimensional array data are unfolded into two-dimensional matrix. The two primary unfolding methods preserve either the I direction (i.e. batches) or the J direction (i.e. variables) of the data. For variable-wise unfolding (i.e. $X \in R^{IK \times J}$), the nonlinear, time-varying trajectories of these data are preserved. These time-varying trajectories can provide the information for state of the vacuum pump system, but these time-varying trajectories can also provide more complications to the inexperienced user.

As variable-wise unfolded matrix provide one picture (chart) per one process while batch-wise unfolded matrix provide one value per one process, the diagnostic results from batch-wise unfolded matrix are familiar to the inexperienced user who monitor more than hundreds Vacuum pump systems. For this reason, batch-wise unfolding method was widely chosen for diagnostic research.

However, there is a critical shortcoming that all batch length (k) should be equal. In fact, the semiconductor manufacturing process are time varying, so k of each process are randomly determined. To overcome this problem, D. Sung[1] equalized all batch lengths with dynamic time warping (DTW) algorithm.

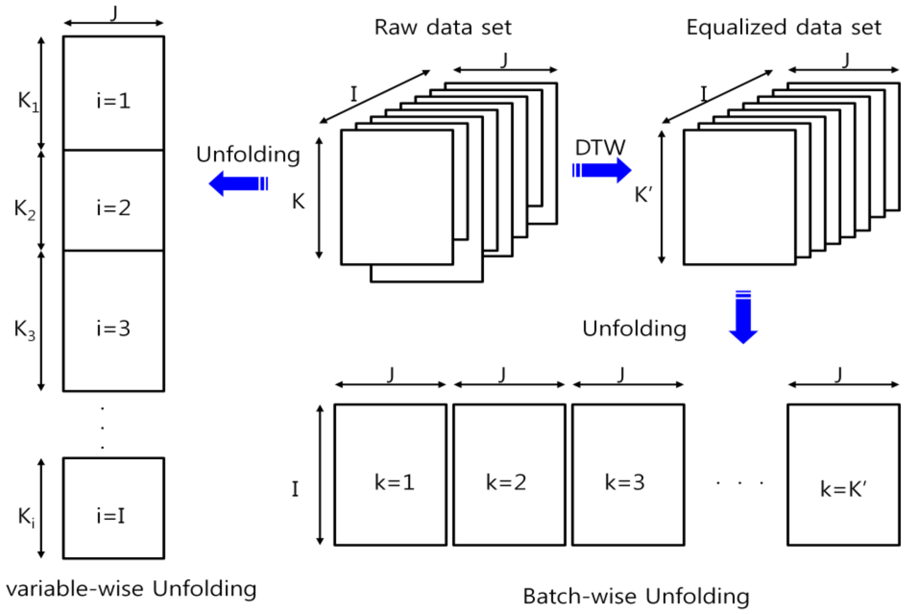

Figure 1. Unfolding methods.

2.2 Dynamic Time Warping (DTW)

The Multi-way principal component analysis has been shown to be powerful monitoring tool in many industrial batch processes. However, it has the shortcoming that all batch lengths (K) should be equal. To overcome this shortcoming, D. Sung[1] equalized all batch lengths with dynamic time warping (DTW) algorithm.

DTW synchronizes similar features in sets of signals using distance as a measure of similarity of signals. DTW non-linearly warps the two signals in such a way that similar events are aligned. One of these two signals is taken as a reference. If their roles are interchanged, a different path and minimum distance will be obtained. The application of DTW to the monitoring batch process was proposed by A. Kassidas[2].

2.3 Multi-Way Principal Component Analysis (MPCA)

The multi-way principal component analysis (MPCA) is used for analysis and monitoring of batch process data. The key idea of MPCA is to compress the normal batch data and extract the important information by projecting the data onto a low-dimensional space that summarizes both the variables and their time trajectories. So, MPCA can handle high dimensional and correlated data, by projecting the raw data onto a lower dimensional subspace which contains most of the variance of the original data. MPCA decomposed the normal operating condition (NOC) data matrix $X \in R^{I\times JK}$ as the sum of the outer product of vectors t_i and p_i plus the residual matrix $E \in R^{I\times JK}$.

$$X' = TP^T + E = \sum_{i=1}^{a} t_i p_i^T + E \tag{1}$$

Where T is a score matrix ($T \in R^{I\times M}$) and t_i is a score vector which contains information about relationship between batches, and P^T is a transposed loadings matrix ($P^T \in R^{M\times JK}$) and p_i is a loading vector which contains information about relationship between instant variables. M is the number of principal component retained in the model. Note that score vectors are orthogonal and loading vectors are ortho-normal.

A major advantage of MPCA modelling is its ability to compare new batch data, $X_{new} \in R^{1\times JK}$, to the NOC data in a systematic fashion. MPCA achieves this comparison by by projecting this new data set on the MPCA model generated from NOC data in order to determine the new batch scores, $t_{new} \in R^{1\times M}$:

$$t_{new} = X_{new} P (P^T P)^{-1} \tag{2}$$

After determining t_{new}, Eq. 3 can be used to calculate the new batch residual, $e_{new} \in R^{1\times JK}$

$$e_{new} = X_{new} - t_{new} P^T \tag{3}$$

The statistics used for a MPCA are Hotelling's T^2 and squared prediction error (SPE). Hotelling's T^2 can be used to measure the variation of systematic part of MPCA model. T^2 is the sum of the normalized squared scores, that is

$$T_i^2 = t_{new} (S_D)^{-1} t_{new}{}^T \tag{4}$$

$$S_D = \frac{T^T T}{I - 1} \tag{5}$$

Where $S_D \in R^{M\times M}$ is the covariance matrix of the model score matrix, T, and I is the number of NOC batches.

Singular values can be monitored by using SPE, also called Q statistics. The SPE is define as the sum of squares of each row of E; for example, for the i-th batch are calculated as

$$SPE_i = {e_{new}}^T e_{new} \tag{6}$$

3. Independent Component Analysis (ICA)

3.1 Basic concept of ICA

Independent component analysis (ICA) is originally developed for signal processing applications including speech signal processing, communications and so forth. ICA can be taken as an extension of PCA, however, the objectives for both algorithms are quite different. PCA extracts components by only considering variance–covariance matrix, and it aims at making the latent variables to be orthogonally uncorrelated. ICA has no orthogonality constraint which not only allows to decorrelate variables, but also to consider the higher order statistics for making latent variables to be independent. Therefore, ICA can be used to deal with a non-Gaussian process which is more practical in a real-world manufacturing environment, especially for the process industry.

ICA is a statistical technique for revealing hidden factors that underlie set of multiple variables. The multiple data variables are assumed to be linear mixtures of some unknown latent variables, and the mixing system is also unknown. The latent variables, they are called the Independent Component(IC) of the observed data, are assumed non-Gaussian and mutually independent.

In the ICA algorithm, it is assumed that J measured variables $x_1,x_2,\cdots,x_j$ can be expressed as linear combinations of m unknown independent components $s_1,s_2, \cdots,s_m$ the independent components and the measured variables have means of zero. The relationship between them is given by

$$X = AS + E = \sum_{l=1}^{m} a_l s_l + E \tag{7}$$

Where X is the data matrix, A is the mixing matrix, S is the independent component matrix, E is residual matrix. The basic problem of ICA is to estimate the original components S or to estimate A from X without any knowledge of S or A. Therefore, the objective of ICA is to calculate a separating (de-mixing) matrix W so that the components of the reconstructed data matrix S, given as

$$S = WX \tag{8}$$

Become as independent of each other as possible. This formulation is not really different from the previous one, since after estimating A, its inverse gives W. Compared to the PCA, the S and W matrix in Eq. (8) may be considered as a loading matrix and a score matrix, i.e. S can be treated as a loading matrix T, while W can be regarded as loading matrix P..

3.2 Calculate de-mixing matrix

The initial step in ICA is centering, if mean values of the measured variable data $x_1,x_2,\cdots,x_j$ are not zero, by followings

$$x_j = x_j - E\{x_j\} \tag{9}$$

As Eq. (9), obtain the centered x_j, by subtracting the average value $E\{x_j\}$ from measured variables x_j. After centering, the next step is whitening which eliminates all the cross-correlation between variables. The whitened matrix, Z, have zero correlation and unit variance (i.e. $E\{zz^T\}=I$).

Consider a covariance matrix of X, Rx, the eigen-decomposition of Rx is given by

$$R_X = U \Lambda U^T \tag{10}$$

The whitening transformation is expressed as

$$Z = QX = QAS = BS \tag{11}$$

Where whitening matrix Q is $\Lambda^{-\frac{1}{2}}U^T$ and B is orthogonal matrix. According to Eq. 11, the ICA problem can be reduced from finding an arbitrary full-rank matrix A to finding an orthogonal matrix B. To calculate B, it is initialized and the updated so that the projection, $S=B^TZ$, has to maximize non-Gaussianity. Hyvärinen and Oja[3] showed that using the central limit theorem. There are two common measures of non-Gaussianity: kurtosis and negentropy. Kurtosis is sensitive to outlier and negentropy is based on the information-theoretic quantity of entropy. Based on the negentropy, Hyvärinen[4] introduced a fast fixed-point algorithm for ICA. This algorithm calculates on column of the matrix B by maximizing the negentropy under the constraint of $\|b_l\|=1$, which b_l is the l-th column of B. After finding A, the de-mixing matrix W can be obtain from $W=B^TQ$.

$$W = B^TQ \tag{12}$$

The selection of a small number of dominant components has at least two advantages, ‘robust performance’ and ‘reduction of analysis complexity’. In PCA, the order of the score vectors is determined by their variance. Therefore, data dimension can be reduced by selecting dominant score vectors. However, unlike PCA, there is no standard criterion for ordering of ICs, which complicates the ordering procedure. A number of methods have been suggested to determine the component order [5-7]. In this paper, we used the simple approach of sorting the rows fo the de-mixing matrix, W, on th basis of their Euclidean norm (L_2): $\arg_i \mathrm{Max}\|w_i\|_2$

After the ordering of the ICs, it is necessary to select the optimal number of ICs to be used for monitoring. The data dimension can be reduced by selecting the first few rows of the ordered W based upon the assumption that the rows with the largest Euclidean norm (L2) have greatest effect on the variation of S. This approach is based on the idea that the dominant variation in a process and be monitored by considering the cumulative sums of only the first few dominant ICs[7].

3.3 ICA based fault detection method

In MICA, three types of statistics are calculated from the process model in normal operation: the I^2 statistics for systematic part of the process variation, I_e^2 statistics based on excluded ICs and the SPE for the residual part of the process variation.

The I^2 statistic is the sum of the squared independent scores and is defined as follows:

$$I_i^2 = s_{new}{}^T s_{new} \tag{13}$$

Also, we can calculate the I^2 metric of the excluded independent components, that is, I_e^2 metric. The I_e^2 metric has the further advantage that it can compensate for the error that results when an incorrect number of ICs is selected for the dominant part. The use of I^2 and I_e^2 statistics allows the entire space spanned by the original variables to be monitored through a new basis. The I_e^2 statistic is defined as follows:

$$(I_e^2)_i = s_{enew}{}^T s_{enew} \tag{14}$$

The SPE statistic for the nonsystematic part of the common cause variation of new data can be visualized in a chart with confidence limits. The SPE statistic is defined as the sum of the squares of e, the columns of E in Eq.7:

$$SPE_i = e_i^T e_i \tag{15}$$

4. Semiconductor manufacturing process

4.1 Measurement setup

Most of dry vacuum pump systems for semiconductor manufacturing processes are composed of booster pump parts and dry pump parts. In this study, Inlet pressure, exhaust pressure and the supply currents, acceleration for vibration are chosen as the state variables. Inlet pressure and exhaust pressure represent the condition of chemical reacting process and performance of vacuum pump. There are correlations between the supply current to dynamic behaviour of load torque of pump motor. Vibration accelerometers were proposed to monitor the dynamic running conditions of vacuum pump. The accelerometer signals measured from the body of the dry vacuum pump are vector-summed and converted into a scalar value. The signal sampling rate of 40.96 KHz was chosen, which is sufficient to cover the 10 kHz bandwidth of vibration signals. Collected digital signals are used to calculate in every 0.1 second the mean values of two pressure signals and the root mean squared (RMS) values of two supply current signals and two vibration signals. These six variables, which are installed and connected to the individual sensors, are listed in table 1.

Table 1. Measurement variables and selected sensors.

Measured State Variables		Selected Sensors and Instruments
pressure (mbar)	Inlet vacuum pressure	Pfeiffr Vacuum, CMR 362 (110 mbar) Gauge controller 256A
	Exhaust pressure	Trafag, 8489 model (1.6 bar, absolute, 0.2% F.S.)
Supply Current (A)	Booster pump	Taewa Trans., TZ84V/L (100A, 0.2%)
	Dry pump	Taewa Trans., TZ84V/L (100A, 0.2%)
Vibration Acceleration (m/s^2)	Booster pump	Endevco, model 7210-100 (Uni-axis,100g, 1%), Model 136 Amplifier
	Dry pump	Endevco, model 2230EM (3 axes, 500g, 1%) , Model 136 Amplifier

4.2 Characteristics of variables

As mentioned, PCA well works for Gaussian distributed variables and ICA is suitable for non-Gaussian distributed data. As seen, Fig. 2 shows typical batch trajectory profiles of semiconductor manufacturing processes. In semiconductor manufacturing processes, Gas-loaded state ($G_{1\sim4}$) and idle state ($I_{1\sim4}$) are repeated. At gas-loaded state, vacuum pump exhausted the purge gas from dome. We concentrated Gas-loaded state data, because vacuum pump actually works during these Gas-loaded state. During Gas-loaded state, three non-Gaussian distributed data (i.e. Inlet pressure, booster pump supply current and dry pump supply current) and three Gaussian distributed data (i.e. exhaust pressure and booster pump acceleration and dry pump acceleration) are measured. That is why we used PCA and ICA together in this paper.

For this research, measurements of vacuum pump stored for 20days (201 batch) until pump failed. There are variable failure reasons and selected data set is most frequently occurred case, ‘pumping speed decreased’.

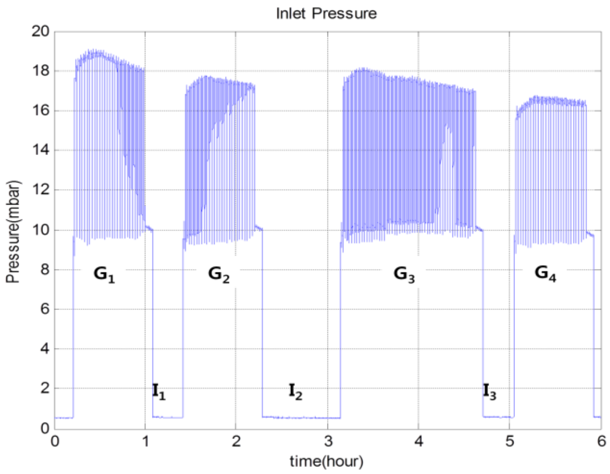

Figure 2. Typical trajectory of inlet pressure.

5. Result and discussion

5.1 On-line monitoring and fault diagnosis

Two latent variables analysis techniques for on-line monitoring was developed from the historical data set of the selected 50 batches measured first five days to create a rather broad scope normal operating condition (NOC) batches. Four principal components were retained by the cross-validation method, approximately 95% of the total variability. Meanwhile, three independent components reduced by Euclidean norm (L_2). The newly measured data set that consisted of the remaining 150 batches were projected onto the reduced MPCA model space or ICA model space.

Each batch is converted to a value, T^2 with PCA or I^2 with ICA. These diagnostic results well represented at Fig. 3 and Fig.4. Diagnostic algorithm with MPCA detected fault at 187th batch, and ICA 186th batch.

5.2 Latent variables and contribution

If a fault was detected, the individual plot of latent variables (i.e. PCs and ICs) can be checked to get a better understanding of fault sources. As T^2 and I^2 are sum of normalized PC and IC, large score values result in large values of T^2 and I^2 values which are detected and the corresponding object isolated. In PCA, the variable contributions to the T^2 value of an object k are computed using the following equation[8]:

$$contribution = t(k)\sqrt{\Lambda^{-1}}P^T = x(k)P\sqrt{\Lambda^{-1}}P^T \quad (16)$$

Where Λ is a diagonal matrix with has diagonal elements equation to eigenvalues.

In ICA, the variable contribution of x(k) for $I^2(k)$ can be obtained using the following equation[9].

$$X_{cd}(k) = \frac{Q^{-1}B_d\hat{s}_{newd}(k)}{\left\|Q^{-1}B_d\hat{s}_{newd}(k)\right\|}\left\|\hat{s}_{newd}(k)\right\| \quad (16)$$

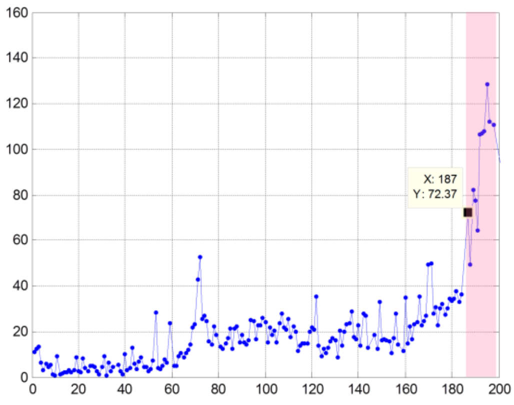

Figure 3. T^2 chart

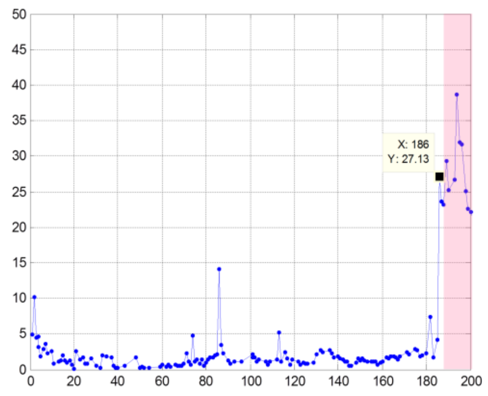

Figure 4. I^2 chart

6. Conclusions

We proposed two refinements to diagnose of vacuum pump, one is that two algorithms with latent variables detected a fault of vacuum pump; the other is that relationship between variables should be focused to analysis failure reason. Collected raw data converted to unfolded matrix with DTW algorithm, dimensional reduced by PCA or ICA, and calculated T^2 and I^2 statistics. The trend of these statistics well represented the performance state of vacuum pump, and detected fault point precisely. The introduction of variable contribution to the statistics means that the relationship of multivariable should be looked after. Especially, relation between supply current and vibration acceleration applies with special force in the case of vacuum pump diagnostics.

Acknowledgments

Results presented in this paper were partially attributed to a national projects (contract number 10031858) sponsored by the Korean Ministry of Knowledge Economy. This work was also supported by the New and Renewable Energy Program of the Korea Institute of Energy Technology Evaluation and Planning (KETEP) grant funded by the Korea government Ministry of Knowledge Economy (No.20104010100490).

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