STEADY-STATE DETECTION FOR MULTIVARIATE SYSTEMS BASED ON PCA AND WAVELETS

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Abstract: Steady-state detection has been an important tool in data processing, for nonlinear model identification, real time optimization, variability analysis, and so on. In this article, it is proposed a new methodology applied to multivariate systems for steady-state detection based on PCA and wavelets. The proposed approach is applied to an industrial distillation column. The combination of PCA and wavelets allows quantifying the steady-state considering a single variable generated by a PCA projection.

Keywords: waves, signal analysis, multivariate systems, Principal Component Analysis, steady-state.

1. INTRODUCTION

An efficient method for steady-state detection is of great importance for process analysis, optimization, model identification, and data reconciliation. These applications require data under steady-state or very close to it.

With this aim, several methods have been developed. Most methods are based on statistical tests. Narasimhan *et al.* (1986) presented a Composite Statistical Test - CST (1986) and a Mathematical Test of Evidence - MTE (1987). In CST method, successive time periods are defined and evaluated according to covariance matrices and sample mean. In MTE method, differences in averages are compared to the variability within the periods. More recently, Cao and Rhinehart (1995) proposed a method based on moving average or conventional first-order filter which is used to replace the sample mean.

But these approaches evaluate the process status over a period of time, instead of a point in time. This is an important detail for on-line applications. Besides these techniques consider only the presence of random errors, and it is known that nonrandom errors are present in form of spikes for example (Jiang *et al.*, 2003).

The wavelet transform (WT) has been widely applied, in signal and image processing, singularity detection, fractals, trend extraction, denoising, data suppression and compression, due to its simple mathematical application and because it provides time-frequency localization simultaneously.

The WT is a tool that cuts up data or functions into different frequency components, and then studies each component with a resolution matched to its scale (Daubechies, 1992). In other words, WT consists of scaled and shifted versions of a mother-wavelet (the original wavelet). The process of multiplying the signal by scaled and shifted wavelets over all time produces wavelet coefficients that are function of scale and position. It is like a resemblance or correlation index between the section of the analyzed signal and the wavelet. One advantage of wavelets is to work with global or local analysis. Other advantages are to denoise a signal without degradation of the original signal (without losing information), to choose the resolution level, to obtain signal derivatives and to process unsteady signals.

Hence, in this work wavelets are used as a tool for steady-state detection of process signals. The methodology is based on a fast algorithm of two channel subband coder using conjugate quadrature filters or quadrature mirror filters. Process trends are extracted from raw measurements via wavelet-based multi-scale processing by eliminating random noise and nonrandom errors. This "clean" signal still preserves the nuances of the original signal. Then the process status is measured using an index with value ranging from 0 to 1 according to the wavelet transform modulus of the extracted process signal and historical data. This index has a great application since it can be used for data compression and determination of optimal operating points for example.

Since most chemical processes are multivariable, it is necessary to have a procedure which makes possible to quantify how close it is to the steady-state. Therefore, it is necessary a way to deal with multivariable systems. Usually, a unique index for the whole process would be recommended, since it is easier to analyze. Jiang *et al.* (2003) suggest selecting key variables and combining them through the Dempster's balance rule. Thus, it is necessary to calculate a status index for each key variable and, by the balance rule, it is necessary to attribute a weight for each variable. Instead, in this work it is proposed to use the PCA (Principal Component Analysis) approach to combine all variables of a multivariable process into a single steady state measurement index, which would be representative of the whole process.

2. WAVELET TRANSFORM APPLIED TO STEADY-STATE DETECTION

2.1. Background of Wavelet Transform Concepts

Wavelet Transform (WT) is a tool for non-stationary signal analysis, and it is applied to steady-state detection in this work.

The Discrete Wavelet Transform (DWT) represents a signal as successive approximations of the original signal and it can be considered as the convolution of the input signal f with a wavelet function ψ, as seen in Eq. (1), according to the decomposition level.

$$W_{2^j} f(x) = f * \psi_{2^j}(x) \qquad (1)$$

The wavelet function $\psi_{2^j}(x)$ is related to the high frequency components and so there is a scaling function $\phi_2{}^j$ related to the low frequency components at each scale j. Therefore, the signals could be considered as a composition of approximations (identity or low-frequency content) and details (nuances or high-frequency components). Thus, if an abnormal sudden change occurs in the signal, the detail coefficients will be affected (Jiang *et al.*, 2000). Then, for any j = 0,

$$a_j[n] = \left\langle f(x), \phi_{2^j}(x-n) \right\rangle \qquad (2)$$

$$d_j[n] = Wf(n, 2^j) = \left\langle f(x), \psi_{2^j}(x-n) \right\rangle \qquad (3)$$

where a_j are the approximation coefficients and d_j (or $W_2{}^j f$) are the detail coefficients or WT modulus.

It is specially attractive if the ψ is the first-order wavelet, i.e., the first-order derivative of the scaling function $\psi(x) = d\phi(x)/dx$, so thus Eq. (1) can be written as:

$$W_{2^j} f(x) = f\left(2^j \frac{d\phi_{2^j}}{dx}\right) = 2^j \frac{d}{dx}\left(f\phi_{2^j}\right)(x) \qquad (4)$$

where $\phi_{2^j}(x) = 1/\sqrt{2^j}\ \phi\left(x/2^j\right)$.

However, there is a fast algorithm to compute the DWT, computed as presented in Eq. (5).

$$a_{j+1}[n] = a_j * h_j[n], \quad d_{j+1}[n] = a_j * g_j[n] \qquad (5)$$

The output a_{j+1} of a FIR filter to any given input may be calculated by convolving the input signal a_j with the impulse response expressed by the coefficients of the filter h_j. For a given filter x with coefficients $x[n]$, $x_j[n]$ denotes the filter obtained by inserting 2^j-1 zeros between every x coefficient.

The process of synthesizing or reconstructing the signal is mathematically computed by the Inverse Discrete Wavelet Transform. Hence, the process of reconstruction can be expressed as the sum of the details, or modulus maxima, and the coarser approximations.

2.2. Procedure for steady-state detection

The proposed technique consists of a process trends extraction of raw data using wavelet-based multi-scale analysis and after detection of the process status with extracted process trends at various scales. The process status is measured using a status index with value ranging from 0 to 1 according to the WT modulus of the extracted process signal. This methodology is based on Jiang *et al.* (2000, 2003).

The process begins with a decomposition of the original signal (WT on process data) generating a_j and d_j at each scale j. The algorithm is based on two quadrature mirror filters h and g proposed by Mallat and Zhong (1992), where h_j and g_j are filters with 2^j-1 zeros interpolated between two successive coefficients of h and g respectively. The wavelet function used is a quadratic spline.

In the next step, soft-thresholding is applied on d_j for scales $1 < j < J$, obtaining d_j'. The threshold for the first scale is assigned as the average of the modulus maxima of historical data, because at scale j = 1 the WT modulus is completely dominated by noise.

Afterwards, abnormal peaks, such as spikes, are detected and treated with symmetric extension technique for scales $2 < j < J$, resulting in new d_j' and a_j'. Spikes are identified if a couple of maximum WT modulus with opposite sign occurs, which duration is less than a time interval t_p considered from historical data. This corresponds to a sudden change in the process data. The threshold for identification of a spike p is computed by the variance of WT modulus of historical data at a defined scale. The duration $p_2 - p_1$ of the spike is determined from the average of WT modulus of historical data attributed a weight.

Later the signal is reconstructed using the threshold coefficients a_j' and d_j', from scale $j = J$ to 2. Jiang *et al.* (2003) suggest reconstructing up to $j = 1$, but as level 1 is dominated by noise it was removed from the reconstruction step.

Another WT is applied on the reconstructed signal, and the extracted trend *f*s is obtained at the characteristic scale $j = s$, determined by the response time constant and the sample time. The detail coefficients of this last decomposition will indicate the process status.

The status index B is basically determined by the derivatives of the extracted trend *f*s, expressed as WT_1 and WT_2.

Equation (6) expresses the estimation of the status index, where T_s, T_w and T_u are thresholds estimated from historical data.

$$B(t) = \begin{cases} 0 & ,\theta(t) \geq T_u \\ \xi[\theta(t)] & ,T_s \leq \theta(t) \geq T_u \\ 1 & ,\theta(t) \leq T_s \end{cases} \quad (6)$$

For more details, refer to Jiang *et al.* (2003).

3. APPLICATION OF PCA

3.1. Steady-state detection based on key variables

As mentioned before, the original methodology for steady-state detection (Jiang *et al.*, 2003) is essentially developed for one process variable. For multivariate systems, the author suggests selecting key variables, calculating the status index for each one and then combining them using the Dempster's combination rule (Shafer, 1976). But this is an off-line methodology and it has some drawbacks considering its implementation.

The first drawback is related to the selection of the key variables (i), which requires good process knowledge. The key variables must be uncorrelated and should cover the whole system. Another drawback is that in the Dempster's combination rule some weights w_i must be established, as shown in Eq. (7).

$$B_m(t) = \prod_{i=1}^{N} [B_i(t)]^{w_i / \sum w_i} \quad (7)$$

In this work, we are proposing to eliminate these drawbacks through the Principal Component Analysis (PCA) discussed as follows.

3.2 Steady-state detection based on principal components

Principal Component Analysis (PCA) is a linear dimensionality reduction technique, optimal in terms of capturing the variability of the data. It determines a set of orthogonal vectors (loading vectors) ordered by the amount of variance explained in the loading vector directions (Chiang *et al.*, 2001). The loading vectors are calculated by solving the stationary points of the optimization problem shown in Eq. (8).

$$\max_{\mathbf{v} \neq 0} \frac{\mathbf{v}^T X^T X \mathbf{v}}{\mathbf{v}^T \mathbf{v}} \quad (8)$$

where $\mathbf{v}$ are the loading vectors and X is the data matrix. The stationary points are computed via singular value decomposition.

The proposed methodology based on PCA has some advantages. It can be easily applied to multivariate systems. The process variables are combined in a new orthogonal variable so that there is no need of choosing key variables and weighting them. So the combination rule is different and it is simpler to be applied.

The steady-state detection based on principal components begins with a dimensional reduction by using PCA. Once the variables are chosen, they are transformed into new variables which are linear combinations of the original variables.

These new variables are then individually computed with WT for steady-state identification, as described in section 2.

4. INDUSTRIAL APLICATION

The industrial plant consists of a toluene column which is fed by the bottom stream of a benzene column. The toluene column has 60 valve plates and the feed plates are 30 and 36. The temperature of stage 20 is controlled through the reboiler steam flow rate. There are 5 flow measurements, 9 temperature measurements throughout the column and a top pressure measurement, as shown in Fig. 1.

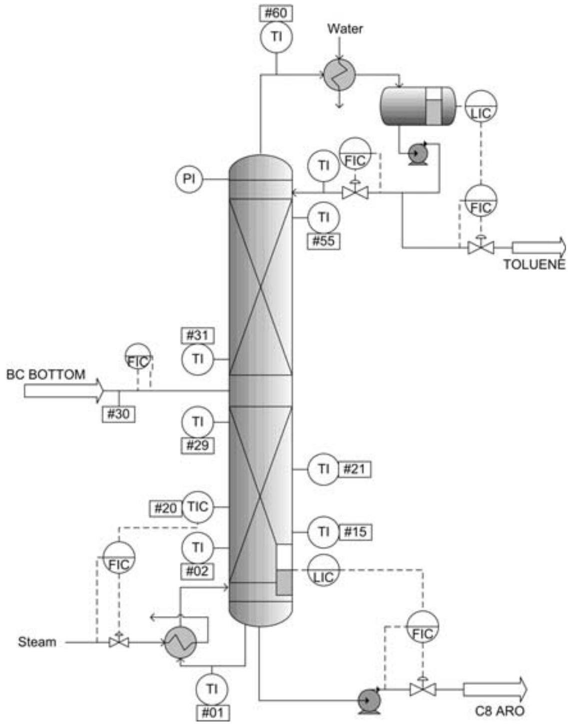

Fig. 1 – Measurements of the toluene column.

A time period was selected and its temperature profile is shown in Fig. 2.

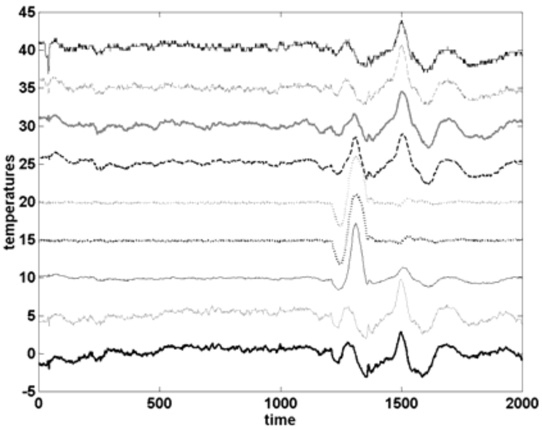

Fig. 2 – Temperature profile.

5. RESULTS

In this section, the PCA and Dempster's approaches are compared using the temperature profile of the industrial toluene distillation column. In this study, all selected variables are considered with same importance, what is translated into the following Dempster's combination rule:

$$B_m(t) = \prod_{i=1}^{N} B_i(t) \tag{8}$$

Equation (8) implies that the column will be considered in steady-state if all variables are in steady-state at the same instant of time.

5.1. Setting the algorithm parameters

To initialize the algorithm, it is necessary to inform the typical process time constant τ. The time constant used in the case study is $\tau = 30$ min. This value was estimated through the approximation of the step response of a 10-order ARX identified model obtained with the Matlab® System Identification Toolbox. The corresponding step responses were approximated through the SK method (Sundaresan and Hrishnaswamy, 1977), which delivered the time constant.

As a consequence, the parameter that represents the time interval over which a change usually persists, t_p, is estimated as 1/3-1/5 of τ. This parameter is used for identification of abnormal peaks, as cited in section 2.

5.2. Status index by key variables

In Dempster's approach, the decision variables should be non-correlated. For the case study, these variables were chosen through a correlation analysis, which selected the following variables: the temperatures TI02 and TI21, the top pressure PI18 and the bottom level LIC09. The plant data of these variables are shown in Fig. 3.

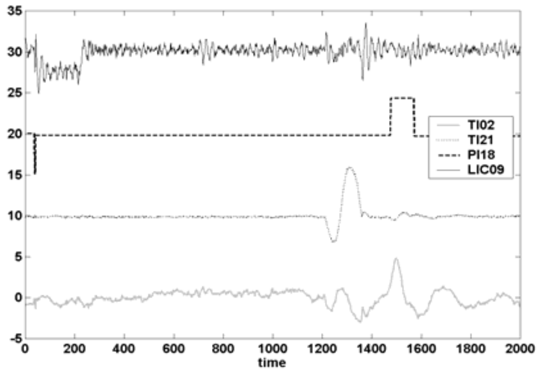

Fig. 3 – Selected key variables for the steady-state determination of the distillation column.

The results obtained for each key variable are presented in Figs. 4 to 7.

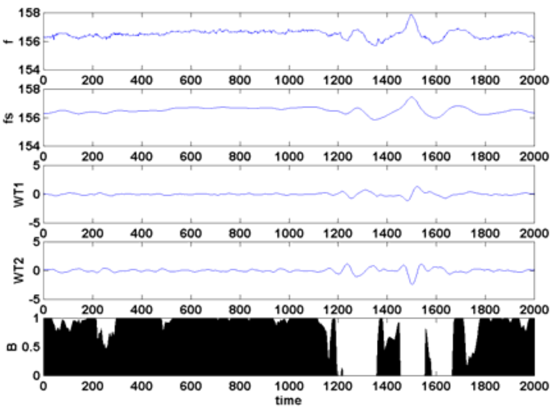

Fig. 4 – Representation of the steady-state detection using the WT for the temperature TI02.

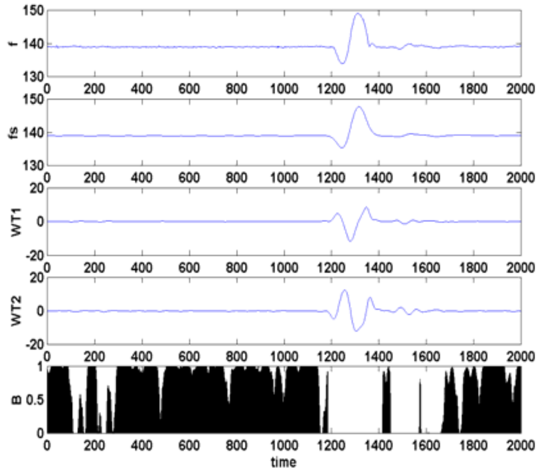

Fig. 5 – Representation of the steady-state detection using the WT for the temperature TI21.

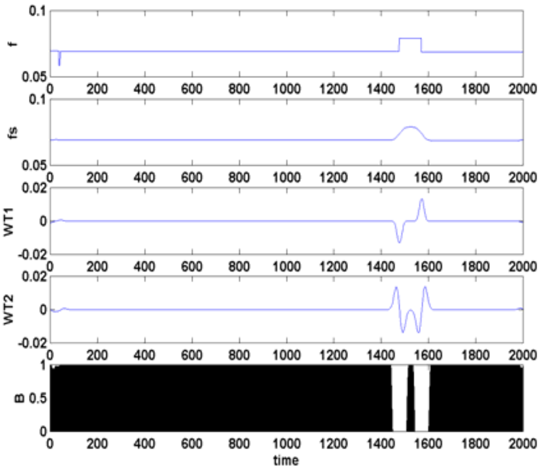

Fig. 6 – Representation of the steady-state detection using the WT for top pressure PI18.

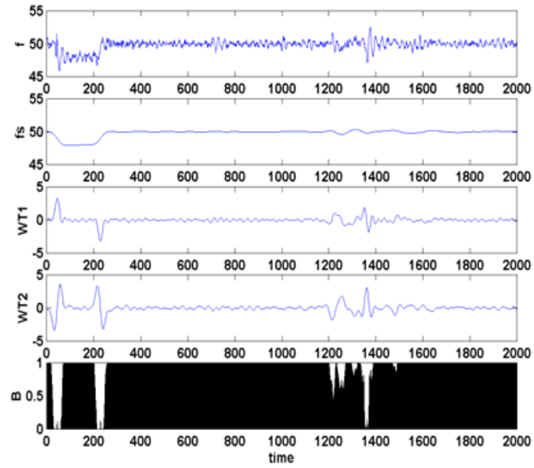

Fig. 7 – Representation of the steady-state detection using the WT for bottom level LIC09.

The status is computed for each variable and the overall status is computed by a combination as the one expressed in Eq. (8).

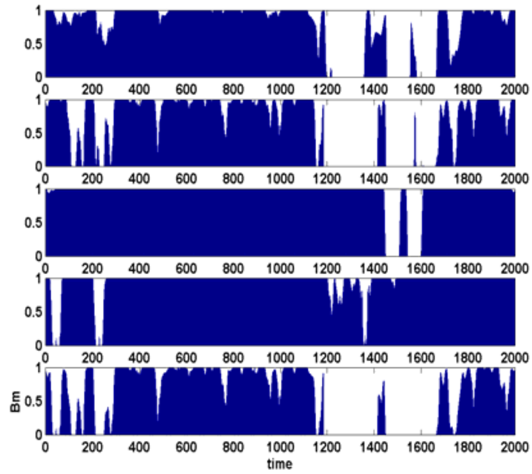

Fig. 8 – Combination of the status indexes of the key variables results in a unique status index B_m for the whole distillation column.

5.3. *Status index by principal component analysis*

The temperature profile (Fig. 2) is composed by the 9 temperature measurements indicated in Fig. 1. The analysis of the temperature profile by PCA results in two new variables, expressed here as t_1 and t_2, as shown in Fig. 9.

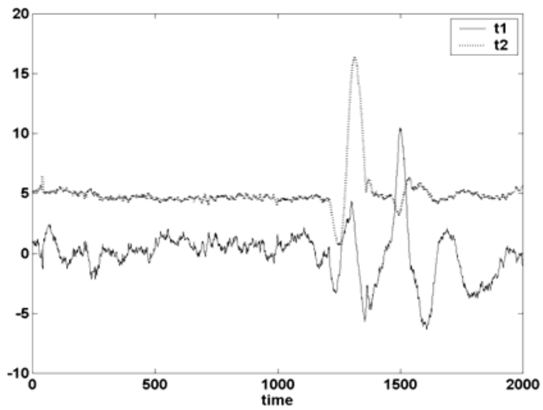

Fig. 9 – Resulting variables by PCA: t_2 and t_1.

For each variable t_1 and t_2, it was made a steady-state analysis and a status index was computed for each one. The input parameters were the response time constant and the historical data period. This period was considered as the first 600 points of t_1 and t_2. It is important here to emphasize the adequate historical period selection. This is an important point for the correct status index estimation. Historical data must bring representative features of the process variable, but without periods of unsteady conditions.

Figures 10 and 11 show the steady-state analysis, where *f* is the original signal (for t_1 or t_2), *fs* is the extracted trend, WT_1 is the first-order wavelet transform, WT_2 is the second-order wavelet transform, and *B* is the status index.

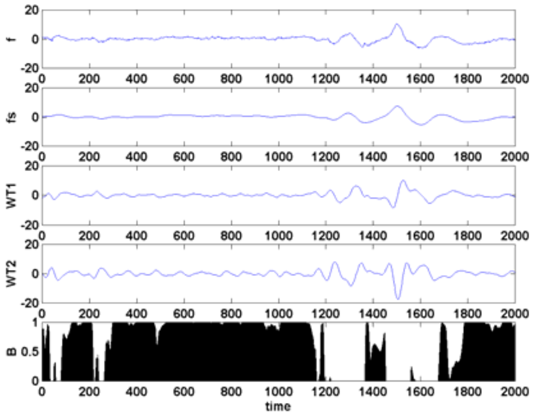

Fig. 10 – Representation of the steady-state detection using the WT for the first orthogonal variable t_1.

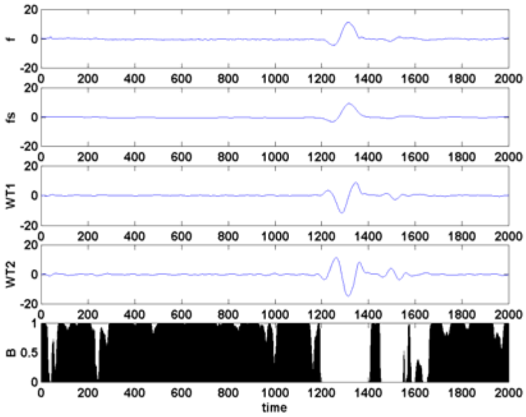

Fig. 11 – Representation of the steady-state detection using the WT for the variable t_2.

The combination of the two indexes B according Eq. (8) results in a unique index B_m, shown in Fig. 12, which represents the column status.

As seen in Fig. 12, the variables t_1 and t_2 have the same results, i.e., the same steady and non-steady time periods. This is a general observation that indicates it is not necessary to analyze the status of all orthogonal variables. Analyzing only the first variable, t_1 in this example, already brings enough information for the column status determination.

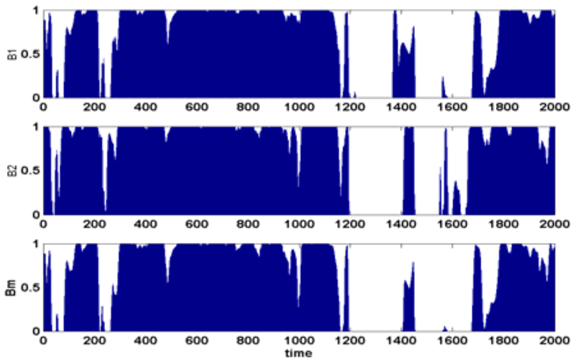

Fig. 12 – Combination of the status indexes B_1 and B_2 results in a unique status index B_m for the whole distillation column.

6. CONCLUSIONS

The results shown in Fig. 8 and 12 are very similar for the discussed industrial case study. Both approaches practically lead the same conclusion. However, the PCA approach is much easier and simpler for dealing with variables and does not require weighting attribution. The variables are selected and linearly combined by PCA without need of knowing what are the principal variables and what are exactly their influences in the process. This is an important point for practical applications. Another advantage is the status estimation of only one variable instead of all key variables, what considerably reduces computational effort.

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