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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 to quantify 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 state-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 means 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 is used to replace the sample mean.

But these approaches evaluate the process status over a period of time, instead of a point of time. This is an important point 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, as in signal and image processing, singularity detection, fractals, trend extraction, denoising, data suppression and compression, due to its simple mathematical application and because provides a tool for 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 wavelet over all time produces wavelet coefficients that are a function of scale and position. It is like a resemblance or correlation index between the section of the analyzed signal and the wavelet. This mean one of the advantages is working with global or local analysis. Other advantages are denoising a signal without degradation of the original signal (without losing information), choosing the resolution level, obtaining signal derivatives and processing unsteady signals.

Hence, in this work wavelets are used as a tool for steady-state detection of process signals. The methodology is based in a fast algorithm based in 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. The process status is then 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 on data compression and determination of optimal operation points for example.

Since most chemical process 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) suggests selecting key variables and using the Dempster's ruler of combination. By this way, it's necessary to calculate a status index for each key variable and, by the combination rule, it is necessary to attribute a weight to each variable. Instead of these, in this work it is proposed the use of PCA, in order to avoid weighting attributions, and the estimation of only one status index, which would be representative of the whole process.

2. WAVELET TRANSFORM IN THE STEADY-STATE DETECTION

2.1. Background of Wavelet Transform Concepts

Wavelet Transform (WT) is a tool for analysis of non-stationary process or signals, and it is applied here to steady-state detection.

In the WT there are two important related concepts: scale and position. The scale is a parameter of compression or stretch of the wavelet. The higher the scale factor, the more stretched the wavelet. This implies working with lower frequencies. Hence, the scale factor is inversely related to the frequency. Another parameter is the position, related to the shifts of the wavelet, or delays. The scale and position are here represented by *a* and *b* respectively. Therefore, scaling a wavelet is equal to $\psi_a(t) = 1/\sqrt{a}\ \psi(t/a)$ and scaling and shifting is represented by $\psi_{a,b}(t) = 1/\sqrt{a}\ \psi((t-b)/a)$.

Then the Continuous Wavelet Transform (CWT) is a sum over all time of the signal multiplied by scaled and shifted versions of the wavelet function ψ. However, the Discrete Wavelet Transform (DWT) performs the analysis in a few scales and positions. When these follow a geometric sequence of ratio 2, we have a Dyadic Fast Wavelet Transform (DFWT). Hence, $a=2^j$ and $b=ka$. In practice, dyadic wavelets satisfy an additional scaling property, represented by a scaling function ϕ related to the low frequencies, allowing them to be implemented by filter banks.

The DWT can be then expressed as Eq. (1).

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

If ψ is the first-order wavelet, i.e., the first-order derivative of the scaling function $\psi(x) = d\phi(x)/dx$ then:

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

where $\phi_a(x) = 1/\sqrt{a}\ \phi(x/a)$.

When talking about DWT, the signals could be considered as a composition of approximations (identity or low-frequency content) and details (nuance). If an abnormal sudden change occurs in the signal, the detail coefficients will be affected. The extremum of the first derivative of a signal corresponds to its inflection point (Jiang *et al.*, 2000). For any $j \geq 0$,

$$a_j[n] = \left\langle f(x), \phi_{2^j}(x-n) \right\rangle \tag{3}$$

$$d_j[n] = Wf(n, 2^j) = \left\langle f(x), \psi_{2^j}(x-n) \right\rangle \tag{4}$$

where a_j are the approximation coefficients and d_j are the detail coefficients, or $W_{2^j}f$.

The "algorithme à trous" computes the DFWT in the following way:

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

The output a_{j+1} of an 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 zeroes between every x coefficient.

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

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 papers of 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 then 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 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. And the duration p_2-p_1 of the spike is determined from the average of WT modulus of historical data attribute a weight.

Latter the signal is reconstructed using the threshold coefficients a_j' and d_j', from scale $j=J$ to 2. Jiang *et al.* (2003) suggests 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 WT1 and WT2.

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 you are referred 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 considered basically for only 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 present some questions that must be take in account.

The first point to be considered is that choosing key variables (*i*) depends on the knowledge of the process. The key variables must be uncorrelated and should cover the whole system. Another point is that in the Dempster's combination rule some weights w_i must be established, as seen in Eq. (7).

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

Because of the before-mentioned points, it was developed a new methodology, based on the Principal Component Analysis (PCA).

3.2 Steady-state detection based on principal components

This 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's no need of choosing key variables and weighting them. So the combination rule is different and more simple to be applied.

The steady-state detection based on principal components begins with the reduction of dimensionality by using PCA. Once the variables are chosen, they are transformed into independent variables which are linear combination 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 valves 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 Figure 1.

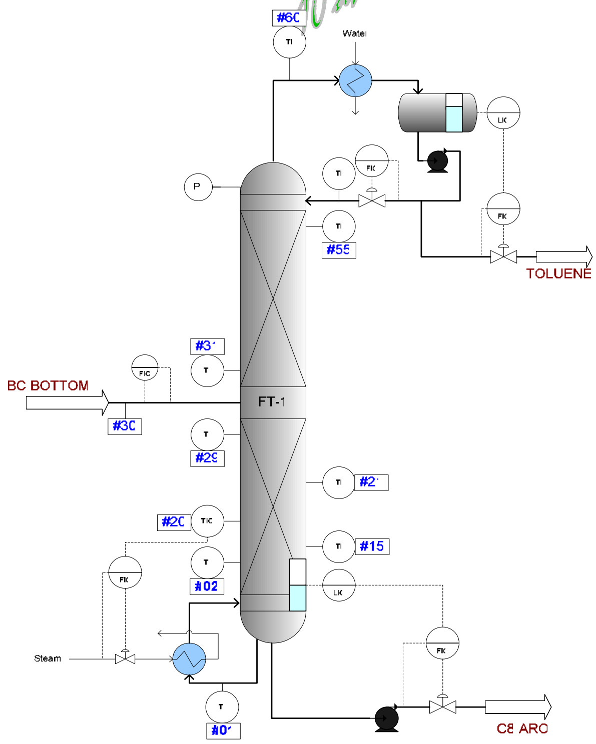

Fig. 1 – Measurements of the toluene column.

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

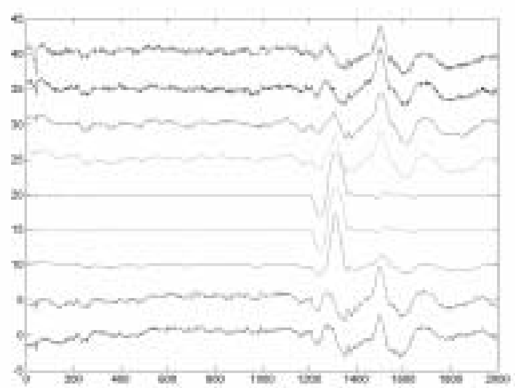

Fig. 2 – Temperature profile.

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:

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

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 set the algorithm, it is necessary to inform the typical process time constant τ. The time constant used in the case study is τ=30 min. This value was estimated through the approximation of the step response of a 10-order ARX identified model obtained by 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

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

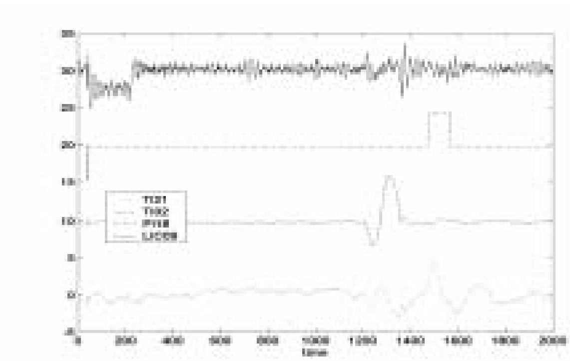

Fig. 3 – Selected key variables for determination of steady-state of the distillation column.

The results obtained for each key variable is presented in Fig. 4-7 respectively.

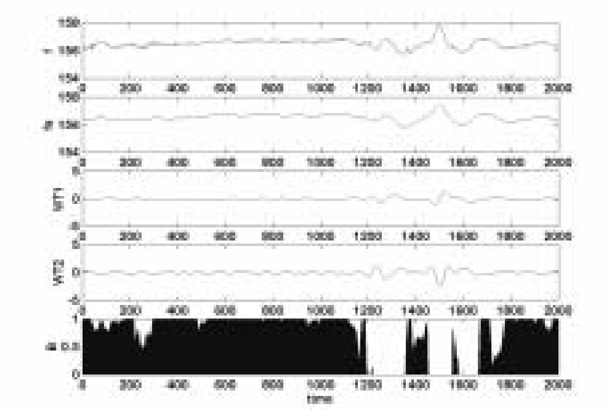

Fig. 4 – Representation of the steady-state detection using the WT for the temperature TI02.

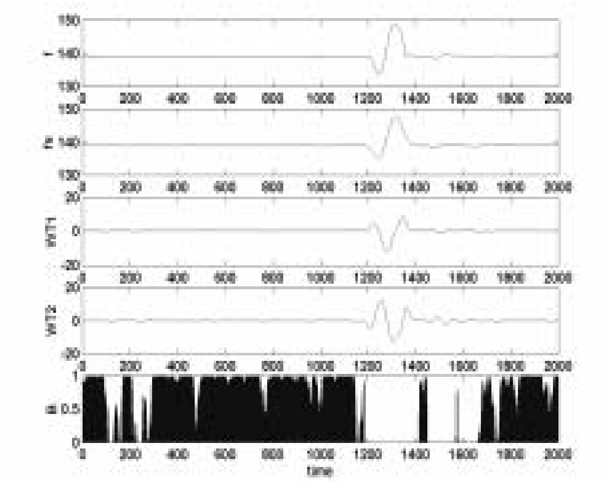

Fig. 5 – Representation of the steady-state detection using the WT for the temperature TI21.

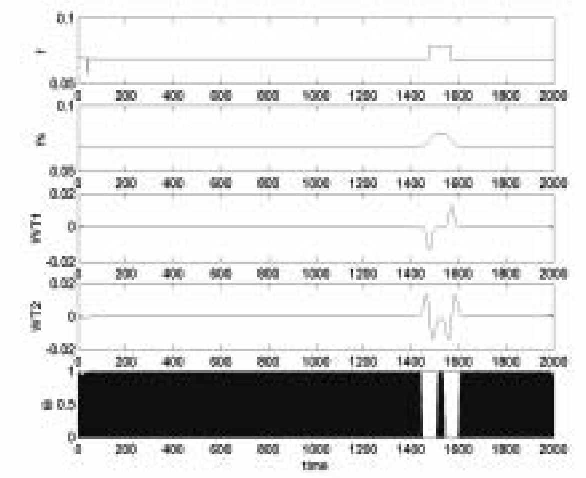

Fig. 6 – Representation of the steady-state detection using the WT for top pressure PI18.

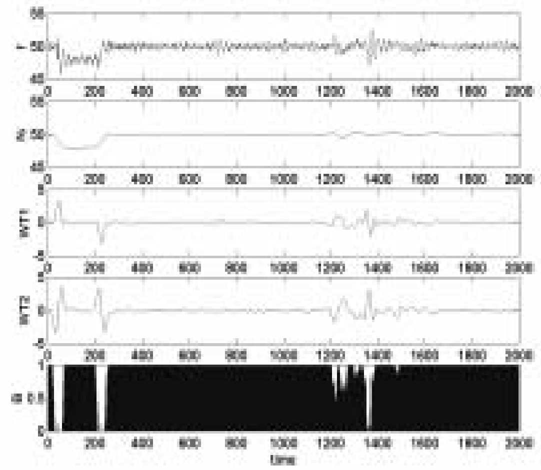

Fig. 7 – Representation of the steady-state detection using the WT for bottom level LIC09.

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

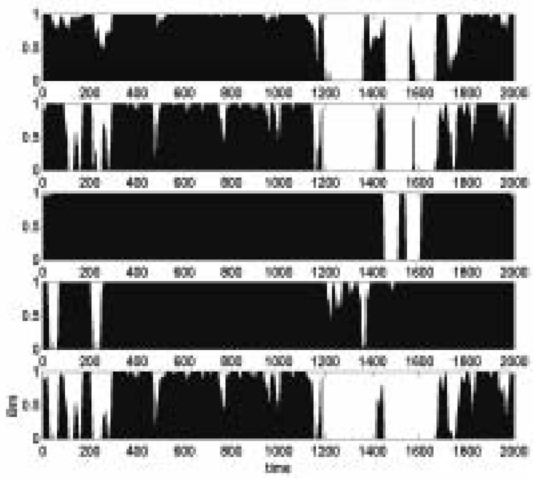

Fig. 8 – Combination of the status indexes of the key variables results in a unique status index Bm for the whole distillation column.

5.3. Status index by principal components

The temperature profile (Fig. 2) is composed by the 9 temperature measurements indicated in Fig. 1. Analyzing the temperature profile with PCA results in new two variables, expressed here as *t*1 and *t*2, as shown in Fig. 9.

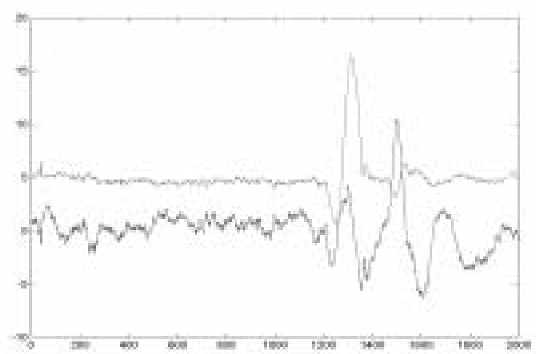

Fig. 9 – Resulting variables from PCA: t2 and t1, respectively.

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 are the response time constant and the historical data period. Here the 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.

The following Fig. 10 and 11 represent the analysis of steady-state, where *f* is the original signal (*t*1 or *t*2), *f*s is the extracted trend, WT1 is the first-order wavelet transform, WT2 is the second-order wavelet transform, and B is the status index.

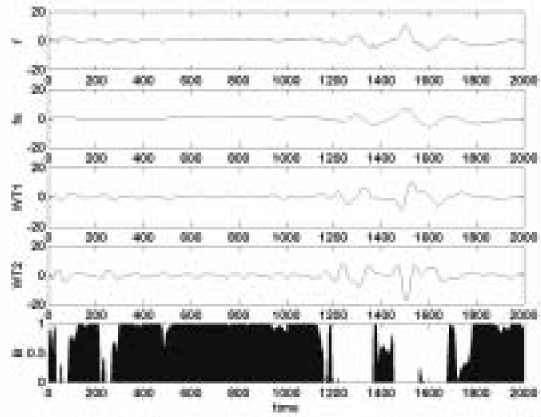

Fig. 10 – Representation of the steady-state detection using the WT for the first orthogonal variable *t*1.

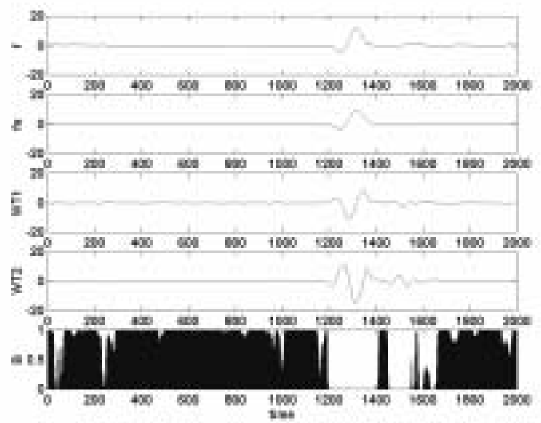

Fig. 11 – Representation of the steady-state detection using the WT for the variable *t*2.

The combination of the two indexes B according Eq. (8) results in a unique index Bm, 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 bring enough information for the column status determination.

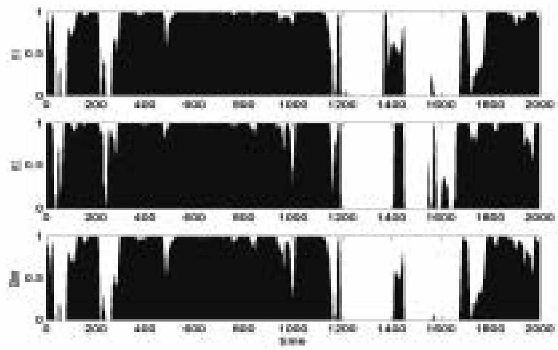

Fig. 12 – Combination of the status indexes B1 and B2 results in a unique status index Bm for the whole distillation column.

6. CONCLUSIONS

The results shown in Fig. 8 and 12 are very similar. Both show practically the same characteristics. However, using PCA provides an easier way of dealing with the variables and does not request weighting attribution. The variables are selected and linearly combined by PCA without the need of knowing what the principal variables are and what exactly their influences in the process are. This sometimes could be an important point of undesired sensibility. Another advantage is the status estimation of only one variable, and not for all key variables, reducing computational effort.

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