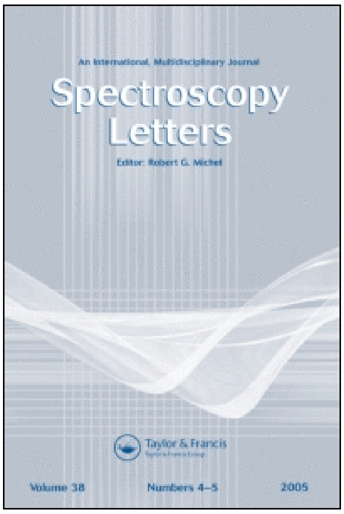

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Modern Spectral Estimation for Signal Processing in the Frequency Domain

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MODERN SPECTRAL ESTIMATION FOR SIGNAL PROCESSING IN THE FREQUENCY DOMAIN

Keywords: Modern spectral estimation, power spectral density, frequency domain, auto-regression model, ICP-AES

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ABSTRACT

Modern power spectral estimation technique was applied to the signal analysis of inductively coupled plasma atomic emission spectrometry (ICP-AES) in the present work. Two methods, Levinson-Durbin and Burg methods, were used to calculate auto-regression (AR) model parameters and the comparison was made. The influence of different AR model orders was studied to find the optimal order by calculating AR model parameters and power spectral density. Results showed that the Burg method gave higher resolution. Characteristics of real ICP-AES measurements were studied and compared by the two methods.

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INTRODUCTION

The power spectral estimation based on Fourier transform is now defined as classical spectral estimation. This technique had developed rapidly since fast Fourier transform (FFT) was invented. The spectral analysis technique, based on model parameters estimation, was proposed in 1940' and now is referred to modern spectral estimation. The modern spectral estimation technique can improve the resolution and variance comparing with the classical spectral estimation method[1]. Power spectral density estimation has been widely applied in many areas such as in engineering and communication.

Inductively coupled plasma atomic emission spectrometry (ICP-AES) is widely used in many fields. The ICP-AES is becoming a routine analytical means in life science, material science, food analysis, metallurgical process, pharmaceutical analysis, and many others. However, studies on characteristics of ICP-AES in the frequency domain are relatively much less reported than fundamental and application research of the technique. Goudzwaars and Loos-Vollebregt[2] studied frequency characteristics in ICP-AES analysis using Fourier transform technique. Van Borm and Broekaert[3] compared the noise performances of two different kinds of torches (Greenfield type and Fassel type) and noise characteristics using a GMK nebulizer for liquid and suspension solutions by using Fourier transformation. The above authors proved that the power spectral analysis is very useful in recognition of noise source in the ICP-AES measurement. Studies on ICP-AES by modern spectral estimation technique has not been reported so far.

In the present paper, two modern spectral estimation methods, Levinson-Durbin recursion and Burg methods, were used for the signal processing in inductively coupled plasma atomic emission spectrometry (ICP-AES). The resolution and performance of the two methods were compared using real ICP-AES measurement data and related issues were addressed.

THEORETICAL BASIS

The parametric modeling technique is the basis of the modern spectral estimation technique[4]. It presupposes that: (1) the studied procedure *x(n)* is the output of a linear processing system *H(z)*, by the input set *u(n)*; that (2) estimation of parameters of the system model *H(z)* can be made; and that (3) the estimated power spectral density is calculated by using the parameters. The input *u(n)* and output *x(n)* has following relations:

$$x(n) = -\sum_{k=1}^{p} a_k x(n-k) + \sum_{k=0}^{q} b_k u(n-k), \ b_0 = 1 \tag{1}$$

and

$$x(n) = \sum_{k=0}^{\infty} h(k) u(n-k) \tag{2}$$

performing Z-transform on the above equations, we can obtain

$$H(z) = \frac{B(z)}{A(z)} \tag{3}$$

in which

$$A(z) = 1 + \sum_{k=1}^{p} a_k z^{-k} \tag{4}$$

$$B(z) = 1 + \sum_{k=1}^{q} b_k z^{-k} \tag{5}$$

$$H(z) = \sum_{k=0}^{\infty} h(k) z^{-k} \tag{6}$$

suppose *u(n)* is a white noise series with variance σ^2 the power spectral density of the output can be estimated by

$$P_x(e^{j\omega}) = \frac{\sigma^2 |B(e^{j\omega})|^2}{|A(e^{j\omega})|^2} \tag{7}$$

if $b_1, b_2, \ldots b_q$ in equation (1) are all zeros, then the equations (1), (3) and (7) become

$$x(n) = -\sum_{k=1}^{p} a_k x(n-k) + u(n) \qquad \textbf{(8)}$$

$$H(z) = \frac{1}{A(z)} = \frac{1}{1 + \sum_{k=1}^{p} a_k z^{-k}} \qquad \textbf{(9)}$$

$$P_x(e^{j\varpi}) = \frac{\sigma^2}{\left|1 + \sum_{k=1}^{p} a_k e^{-j\varpi k}\right|^2} \qquad \textbf{(10)}$$

This is the auto-regression (AR) model. This is an all-maximum model and is suitable for peak-shaped signal processing, such as in ICP-AES measurement. The "auto-regression" means that the present output of the model is the weighted sum of previous p outputs. The normal function of the AR model is a linear function group. This model has been received more attention and been applied widely because of its good variance performance.

The normal equation of AR model is as following

$$r_x(m) = \begin{cases} -\sum_{k=1}^{p} a_k r_x(m-k) & m \geq 1 \\ -\sum_{k=1}^{p} a_k r_x(k) + \sigma^2 & m = 0 \end{cases} \qquad \textbf{(11)}$$

The above equation can be written in matrix form as following

$$\begin{bmatrix} r_x(0) & r_x(1) & r_x(2) & \cdots & r_x(p) \\ r_x(1) & r_x(0) & r_x(1) & \cdots & r_x(p-1) \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ r_x(p) & r_x(p-1) & r_x(p-2) & \cdots & r_x(0) \end{bmatrix} \begin{bmatrix} 1 \\ a_1 \\ \vdots \\ a_p \end{bmatrix} = \begin{bmatrix} \sigma^2 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \qquad \textbf{(12)}$$

The above equation is also called the Yule-Walker equation. The coefficient matrix is symmetric and the elements referring to the main diagonal are equal. Such a matrix is called the Toeplitz matrix.

It can be seen that an AR model with p orders has $p+1$ parameters, i.e. $a_1, a_2, \ldots a_p, \sigma^2$ if we can know the $p+1$ self-correlation functions of $x(n)$, $r_x(0), r_x(1), \ldots, r_x(p)$, we can obtain the power spectral density using equation (10).

The Levinson-Durbin recursion and Burg methods were used to calculate the AR model parameters. Levinson-Durbin recursion can be obtained from the Toeplitz matrix:

$$k_m = -\left[\sum_{k=1}^{m-1} a_{m-1}(k) r_x(m-k) + r_x(m)\right] \Big/ \rho_{m-1} \qquad \textbf{(13)}$$

$$a_m(k) = a_{m-1}(k) + k_m a_{m-1}(m-k) \qquad \textbf{(14)}$$

$$\rho_m = \rho_{m-1}\left[1 - k_m^2\right] \qquad \textbf{(15)}$$

Levinson-Durbin recursion begins from low order to p order of the model and gives all the parameters at each order. In practice, we follow the procedures: (1) estimate self-correlation function $\hat{r}_x(m), m = 0,1,\cdots,p$ from discrete data $x_N(n)$. (2) using $\hat{r}_x(m)$ to replace the $r_x(m)$ in the equation to resolve the Yule-Walker equation, then we can obtain the estimated parameters $\hat{a}(1),\hat{a}(2),\cdots,\hat{a}(p),\hat{\rho}_p$; (3) to estimate the power spectral density of $x(n)$ using the parameters.

$$\hat{P}_{AR}(e^{j\omega}) = \frac{\hat{\rho}_p}{\left|1 + \sum_{k=1}^{p} \hat{a}_k e^{-j\omega k}\right|^2} \qquad \textbf{(16)}$$

The Burg method is based on maximum entropy estimation. Different from with the Levinson-Durbin recursion, it calculates reflectance coefficients first and then estimates the model parameters. The Burg method can obtain the AR parameters with higher precision.

EXPERIMENTAL

Instrumentation

An ICPS-1000 II spectrometer was used for spectral scans. The working conditions were as follows: 27.12 MHz working frequency; input forward power 1.2 kW; focal length 1 m; 3600 groves/mm grating; entrance slit 20 μm; exit slit 30 μm; coolant argon gas 14 L/min flow rate; carrier argon gas 1.0 L/min flow rate; observation height 17 mm above load coil; integration time 0.1second.

A Thermal Jarrel-Ash POEMS spectrometer (USA), in the atomic emission mode, was used for stability measurement. 63 groves/mm echelle grating; blazed at 19.5°; focal length 381 mm; wavelength range 190 ~ 900 nm; Charge injection detector (CID); input forward power 1.15 kW; coolant argon gas 14 L/min; carrier argon gas 0.55 L/min. Slits: 45 μm (wide) × 100 μm (high) for ultra violet range and 25 μm (wide) × 100 μm (high) for visible range; expose time: 15 sec. for ultra violet range and 5 sec. for visible range.

All the standards were prepared from high purity metals or oxides. Reagents used were above commercial AR grade. Water used was purified with Millipore (Millipore Inc.) high purity water equipment.

Procedure

In the spectral scans, measurement data were saved to floppy disk and then read and processed using a Pentium-based computer. The scan was in the range of 0.08 nm around the peak signals. Fifty data points were recorded, therefore, one scan step was equivalent to 0.0016 nm.

For the stability measurements, the AES mode of the Thermal Jarrel-Ash POEMS spectrometer was used and 50 normalized intensities were recorded. The measurement intensities were entered into a personal computer for calculation.

The program used for modern spectral estimation calculation was written with MATLAB (version 4.0, Mathworks Inc, USA). The internal functions of Levison-Durbin and Burg in the toolbox of the software package were used for simplify the programming.

In the power spectral density estimation, normalized frequency was used and the power spectral density was expressed by following:

$$A_{(dB)} = 10 \times \log_{10}\left(\frac{PSD(i)}{PSD(1)}\right) \qquad (17)$$

where *PSD (i)* is the *i* calculated power spectral density and *PSD (1)* is the first calculated power spectral density.

RESULTS AND DISCUSSION

Power spectral density of ICP-AES scans

Noise always exists in signal measurement. In ICP-AES measurement, there are mainly three kinds of noises: (1) shot noise, (2) flicker noise and (3) background noise. The information about frequency constitution and noise recognition can be obtained based on power spectral analysis. In the frequency domain, noises can be classified as (1) white noise, which is not related with frequency; (2) 1/f noise, which is inversely proportional to frequency; and (3) interference, which is derived from a certain interference source. We investigated the power spectra of simulated Gaussian signal, with different noises added, and then calculated the power spectral densities of ICP-AES spectral scans for seven rare earth elements (Tm 270.196 nm, Sm 359.260 nm,

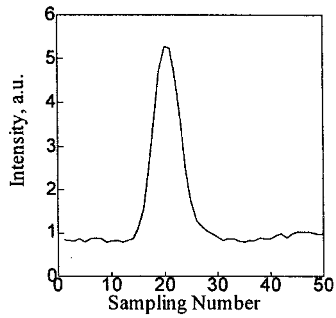

FIG. 1. Spectral scan of Sm 359.260 nm line

Ce 394.275 nm, Ce 413.765 nm, La 399.575 nm, Yb 328.931 nm, Y 377.433 nm, Eu 412.970 nm) using the auto-regression (AR) parametric models.

Due limited space, Sm 359.260 nm is discussed in detail as a representative example. The ICP-AES spectral scan of Sm 359.260 nm line is given in FIG. 1. The power spectral densities using the Levision-Durbin recursion, and Burg method for Sm 359.260 nm line are given in FIG. 2 and FIG. 3, respectively. It can be seen that the scan was composed of a two-part signal in the frequency domain; i. e. low frequency signal representing the atomic emission by Sm 359.260 nm line, and high frequency signal representing the noise in the measurement. The noise signals were spread throughout the entire frequency domain. This example showed that white noise is the main component in the ICP-AES measurement, while the other kinds of noise, such as flicker, and interferences, can be neglected.

The power spectral density helps to analyze the frequency components by which the source of the noise can be recognized. Moreover, comparing the power spectral densities with Levison-Durbin recursion and Burg method, it can be seen that the Burg method gave higher resolution than the Levison-Durbin recursion method.

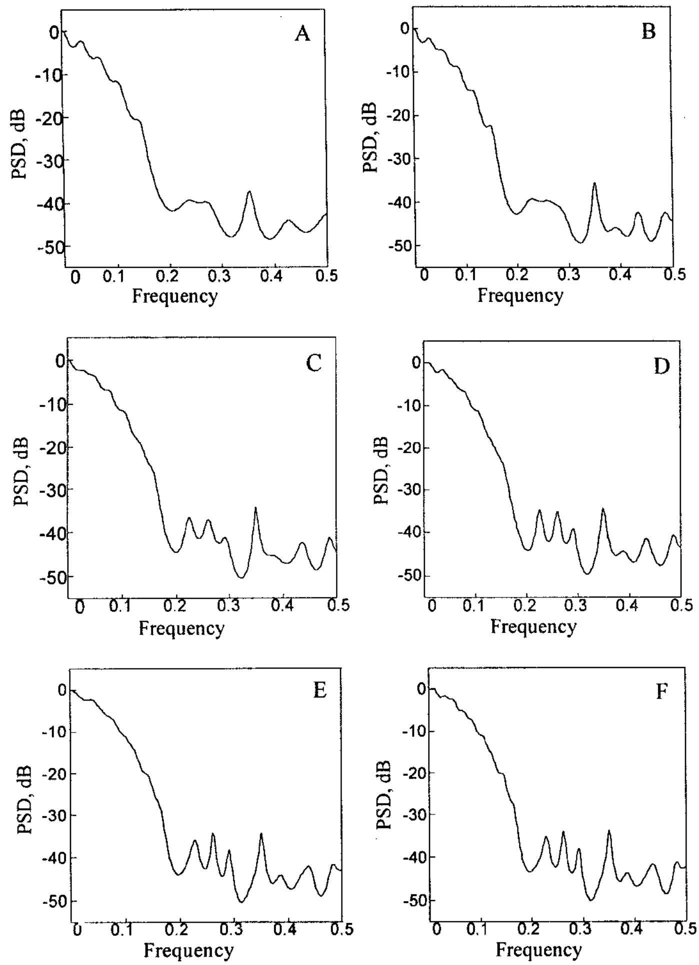

FIG. 2. Power spectral density of Sm 359.260 nm line with different orders (with Levinson–Durbin recursion) (A) order 20; (B) order 25; (C) order 30; (D) order 35; (E) order 40; (F) order 45□

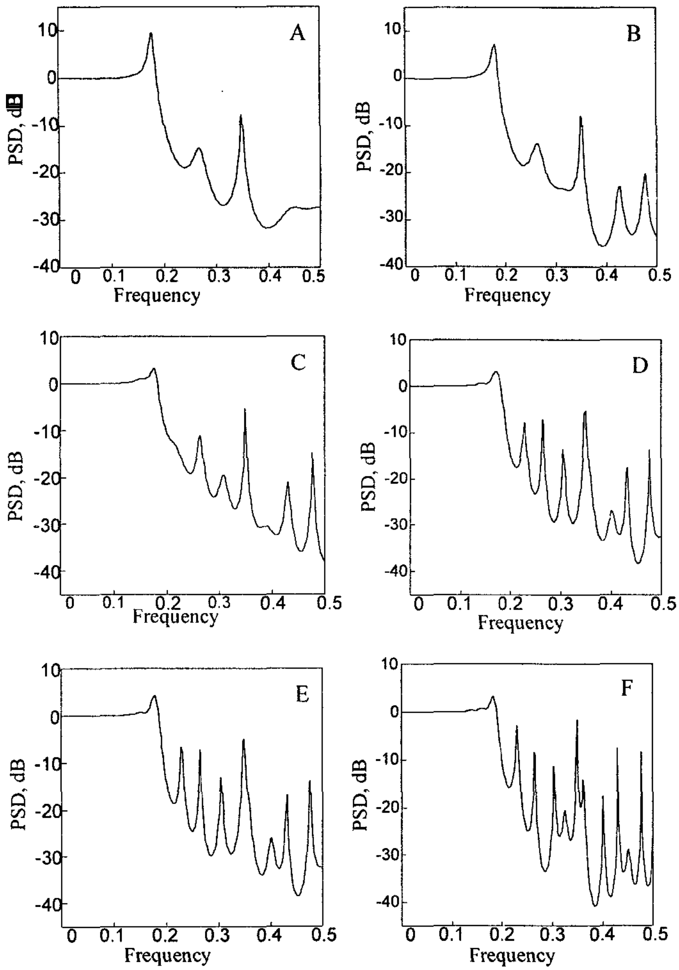

FIG. 3. Power spectral density of Sm 359.260 nm line with different orders (with Burg method) (A) order 20; (B) order 25; (C) order 30; (D) order 35; (E) order 40; (F) order 45.

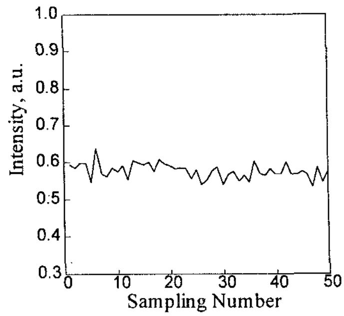

FIG. 4. Measurement intensities for As 189.042 nm line in about one hour

Signal shift recognition

For the stable random signals, it is not enough to describe the characteristics by using mathematical expectation and variance only. For example, two signals with quite different characteristics may have similar mean and variance. Therefore, a better method was needed in some cases to describe characteristics of signals. Self-correlation can be used to describe the differences between two signals. We can determine if the signal shifts based on the self-correlation are deviating from the δ-function. As an example, the measurement signals of As 189.042 nm line within about 1 hour were given in FIG. 4. The power spectral densities for the As 189.042 nm line with Levison-Durbin recursion and the Burg method were given in FIG. 5 and FIG. 6, respectively.

The self-correlation function obtained from the As 189.042 nm line measurement showed deviation from δ-function. This means that the shift exists in the measurement. It can be seen from FIG. 5 and FIG. 6 that there are interference signals relative frequency between 0.1 and 0.2 existing in the measurement. The results recommended further investigation on the source of the interference. The detail studies on the interference source are under investigation.

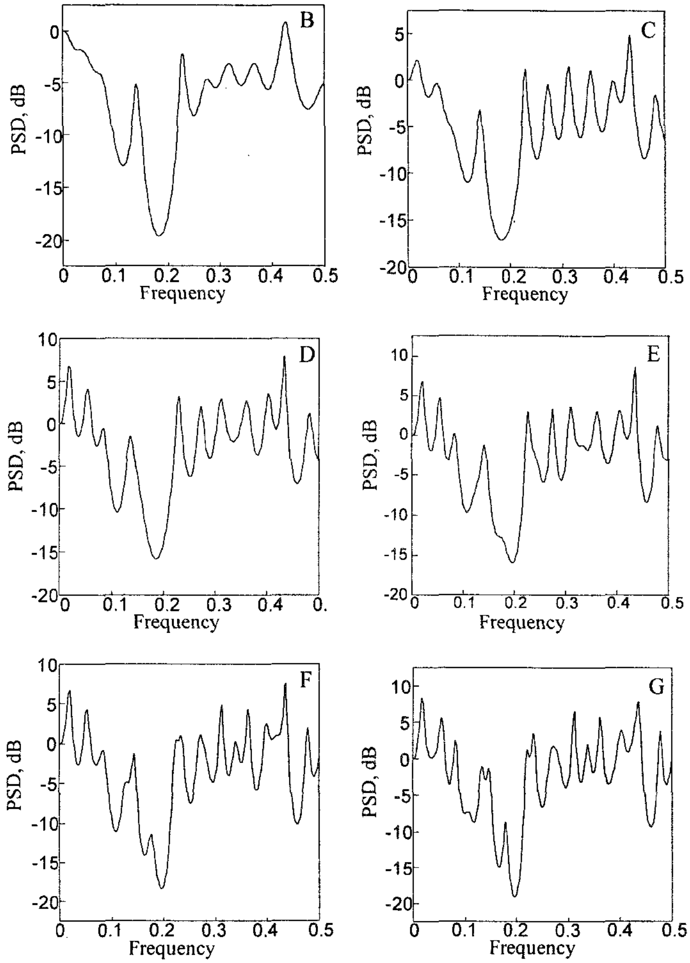

FIG. 5. Power spectral density of As 189.042 nm line with various order (with Levinson–Durbin recursion) (A) order 20; (B) order 25; (C) order 30; (D) order 35; (E) order 40; (F) order 45.

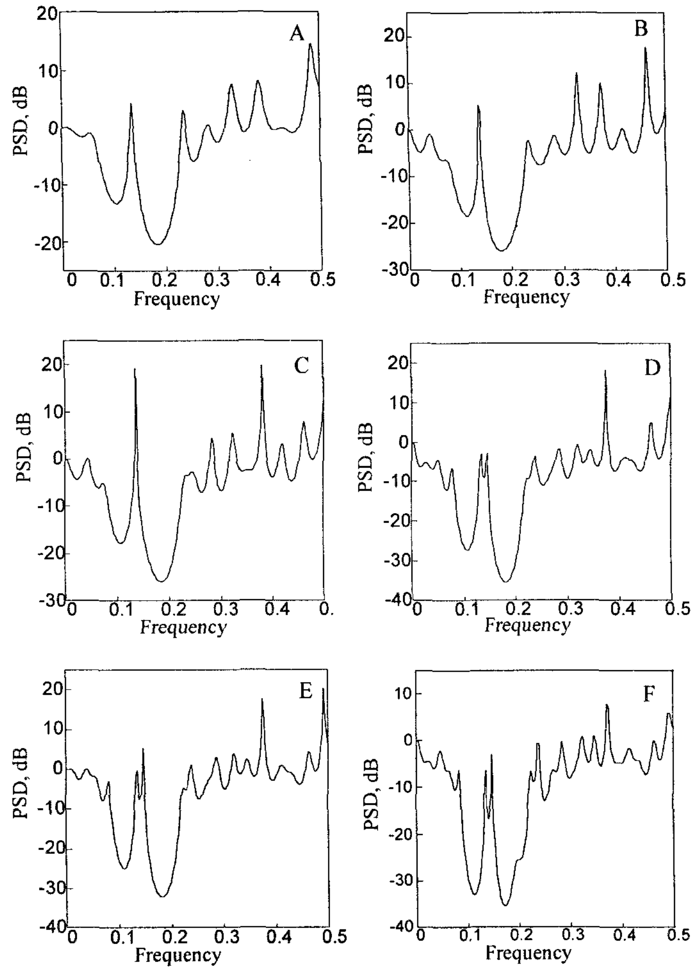

FIG. 6. Power spectral density of As 189.042 nm line with various order (with Burg method) (A) order 20; (B) order 25; (C) order 30; (D) order 35; (E) order 40; (F) order 45.

CONCLUSION

Modern power spectral estimation technique is a useful tool to signal processing the characteristics in frequency domain. Power spectral density can be used for recognition of the source of noises in the ICP-AES measurement. Results showed that white noise is the main source in ICP-AES peak profile measurement while other sources of noises can be neglected. In the stability study of measurement, the power spectral density suggested that there may be possible interferences in the measurements. The sources of the interferences need further investigation.

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REFERENCES

1. S. M. Kay, Modern Spectral Estimation---Theory and Application, Englewood Cliffs: Prentice Hall, 1988.

2. M. P. Goudwaard and M. T. C. de Loos-Vollebregt, Characterization of Noise in Inductively Coupled Plasma-Atomic Emission Spectrometry, Spectrochim. Acta 1990, 45B:887.

3. W. A. Van Borm and J. A. C. Broekaert, Noise Characteristics in Inductively Coupled Plasma Optical Emission Spectrometry Using Slurry Nebulization and Direct Powder Introduction Techniques, Anal. Chem. 1990, 62:2527.

4. Guangshu Hu, Digital Signal Processing---Theory, Algorithm and Realization, Tsinghua University Press, 1997.

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