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A New Method to Resolve Overlapped Voltammetric Peaks

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Abstract: A new method called spline convolution (SC) for resolving overlapped peaks was proposed in this paper. The differential pulse voltammetric overlapped peaks of mixtures of Pb(II) and Tl(I) were investigated by this method, and satisfactory results were obtained. The results show excellent correlation between peak areas of the processed signals and the concentrations.

Keywords: Spline convolution (SC), peak resolving function, overlapped voltammetric peaks

Chemometrics is a powerful tool in resolving overlapped peaks in analysis. We used spline wavelet self-convolution (SWSC) to resolve overlapped capillary electrophoresis peaks[4]. Based on that, we find that there is no need to use the filter of spline wavelet and the overlapped peaks without noise can be resolved by using a suitable peak resolving function to convolute with the original signal directly. Spline function is very flexible, which can flex and translate according to necessity[5]. So, in this work, the 3rd-order spline function was used to construct peak resolving function and a new method for resolving overlapped peaks called spline convolution (SC) is presented.

Function *f(t)* is supposed an analytical signal in time domain. A suitable peak resolving function is used to convolute with it. The discrete equation is:

$$F_j(x) = \sum_{j=1}^{n} \Omega_{n-j}(x) f_j(x) \qquad (1)$$

where, *f(x)* is the original signal, *F(x)* is the processed signal and $\Omega(x)$ is the peak resolving function. In this work, it is constructed by the 3rd-order spline function, $N_3(x)$. That is:

$$\Omega(x) = \sum_{k=1}^{m} N_3(x - x_k) \qquad (2)$$

where, m, x_k are the number and the peak position of the overlapped peaks respectively. They are determined with quadratic differential.

Spline convolution is used to resolve overlapped peaks simulated by computer directly in time domain. Compared with the original signals, the peak widths of processed signals are narrower while the peak positions and areas are scarcely affected. The resolution of the processed signals is improved. Baseline separation can be achieved in processed peaks. This method is simple and easy to carry out.

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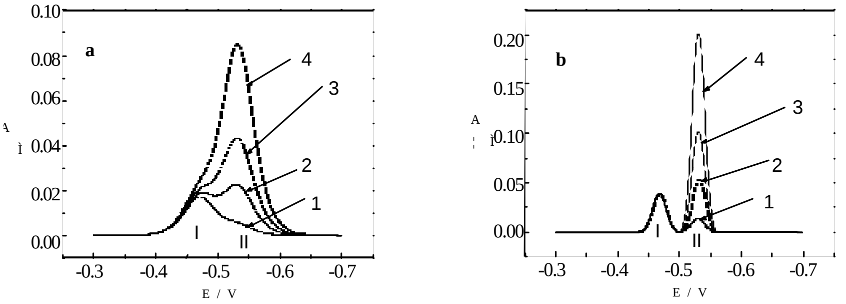
Figure 1(a) shows the voltammetric signals of mixtures of Pb(II)-Tl(I). In curves 1-4, the concentration of Pb(II) was kept constant (1.0×10^{-4} mol/L), the concentrations of Tl(I) were 2.0×10^{-5}, 1.0×10^{-4}, 2.0×10^{-4} and 4.0×10^{-4} mol/L respectively. It was impossible to get quantitative information from such original signals because of overlapping. **Figure 1(b)** shows the processed signal by spline convolution. The peak position and area of Pb(II) in processed curves are almost no changed. For Tl(I) with different concentrations, the correlation coefficient of calibration curve is 0.9999.

Figure 1 Processed results of Pb(II)-Tl(I)system by spline convolution
(a): original signals; (b): processed signals



I: peak of Pb(II); II: peak of Tl(I)
Curves 1-4: the concentration of Pb(II) was 1.0×10^{-4} mol/L, the concentrations of Tl(I) were 2.0×10^{-5}, 1.0×10^{-4}, 2.0×10^{-4} and 4.0×10^{-4} mol/L respectively.

In conclusion, the application of spline convolution (SC) to resolve overlapped peaks was proved to be efficient. Baseline separation can be achieved. It gives linearity between peak areas of the resolved voltammetric peaks and the concentrations, which ensures that quantitative results can be obtained from the resolved signals. The peak positions of resolved voltammetric peaks are scarcely changed, which shows that the results are also suitable for qualitative analysis. Besides, the algorithm of this method is simple and quick.

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