



A method for separation of overlapping absorption lines in intracavity gas detection



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ABSTRACT

We propose a novel method to separate overlapping absorption lines in gas detection based on fiber laser intracavity absorption spectroscopy. The method combines continuous wavelet transform, linear regression analysis and chaos particle swarm optimization together to retrieve the respective absorbance distributions of overlapping lines. The method's principle is outlined and the rules for parameter selection are given. The performance of the method is demonstrated by both the simulated and experimental data. When the method is applied to the mixed gas concentration calibration of CO and CO₂, high linearity is obtained with linear correlation coefficients of 0.9996 and 0.9997 respectively. The relative errors of CO and CO₂ concentration retrieval are no more than 0.93% and 1.13% respectively.

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1. Introduction

Gas sensors based on fiber laser intracavity absorption spectroscopy can detect multiple gases in wide wavelength coverage with high sensitivity [1,2]. Since each gas has multiple absorption lines whose linewidths are broadened by molecular collision, Doppler shift and measurement instrument [3], absorption spectrum overlap is likely to occur between adjacent lines. In previous reports only well-isolated lines with strong absorption were used for gas detection to avoid mutual interference and achieve sensitive measurement [4,5]. However, line selection is difficult when multiple absorption lines are required in gas detection to reduce the random error of concentration retrieval [6]. To obtain more usable lines and more accurate retrieved concentration, overlapping absorption spectrum separation is of great necessity especially when mixed gases are detected.

Although several chemometric methods based on multivariate curve resolution have been proposed for spectrum separation in analytical chemistry [7,8], they are mainly used to analyze the matrix data from an evolutionary process which contains both spectral and chromatographic information. Considering that the fiber-optic intracavity gas detection is a static process and only

contains the one-dimensional spectral information, these chemometric methods are not suitable for this application. To separate overlapping absorption lines into individual ones for intracavity gas sensors, multipeak fitting is the crucial step. Compared with the traditional gradient-based fitting algorithms, the particle swarm optimization algorithm has advantages of easy implementation and quick convergence [9–11]. The most important input parameters of multipeak fitting are the peaks' number and lineshape. Numerical derivative calculation is a common way to obtain the number and positions of overlapping peaks [12]. Although high order derivative can reduce peak width greatly, the resulting resolution improvement is often limited by the severely degraded signal to noise ratio. Continuous wavelet transform is another approach for derivative calculation and peak search [13,14]. The multiscale characteristic of wavelet transform can achieve a good balance between resolution enhancement and noise suppression. Although in essence the gas absorption lineshape coincides with Lorentzian profile well under atmospheric pressure [15], the practical lineshape in intracavity gas detection is usually distorted by the superposed spectral baseline. So baseline removal is essential for improvement of the fitting accuracy.

In this paper, we propose a method to separate overlapping gas absorption lines based on the above analysis. The method includes three steps, which are continuous wavelet transform for peak recognition, linear regression analysis for baseline extraction and chaos particle swarm optimization for multipeak fitting. The method's basic principle is outlined and the implementation steps

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are introduced in details by separation of three simulated overlapping absorption lines. Finally, the mixed gases of carbon monoxide (CO) and carbon dioxide (CO₂) are detected to demonstrate the method's performance in mixed gas concentration measurement.

2. Principle

Spectral absorbance is usually used to retrieve gas concentration for fiber-optical gas sensors. The total absorbance A at laser frequency ν is defined as the attenuation of laser intensity induced by gas absorption, which is expressed as

$$A(\nu) = \ln \frac{I_0(\nu)}{I(\nu)} \quad (1)$$

where I_0 is the incident laser light intensity and I is the transmitted laser light intensity. According to the Lambert Beer Law, the absorbance a of a single gas absorption line at laser frequency ν is the product of absorption line strength s , lineshape function g , molecule number density c and the effective absorption length l . In further detail, s is defined as the integrated absorption cross section across the whole lineshape and g is described by Lorentzian function. Thus a is written as

$$a(\nu) = sg(\nu)cl = \frac{sc l}{\pi} \frac{\gamma}{(\nu - \nu_0)^2 + \gamma^2} \quad (2)$$

where ν_0 and γ are the center frequency and half width at half maximum (HWHM) of absorption line respectively. The smaller the absorbance, the better the linear relation between the absorbance and gas molecule number density exists. When the absorbance is large enough, the Lambert Beer Law is not fulfilled and nonlinear effect occurs. Here we only relate to the linear condition due to the relatively weak absorption of gas absorption lines located in the near-infrared overtone region. So when multiple lines are overlapping, the total absorbance is expressed as the linear superposition of each line's absorbance [16], i.e., A can be further expressed as

$$A(\nu) = \sum_{i=1}^n \frac{s_i c l}{\pi} \frac{\gamma_i}{(\nu - \nu_{0i})^2 + \gamma_i^2} = \sum_{i=1}^n \frac{H_i \gamma_i}{(\nu - \nu_{0i})^2 + \gamma_i^2} \quad (3)$$

where i and n are the index and number of absorption lines respectively. As shown in Eq. (3), the essence of spectrum separation is to determine all the parameters including n , ν_{0i} , γ_i and H_i .

The overlapping lines can be effectively resolved by continuous wavelet transform (CWT). The peak positions of wavelet coefficients are almost the same as those of absorption lines but the HWHMs are greatly reduced after CWT. So the lines' number n can be obtained by counting the peaks of wavelet coefficients. The CWT of the overlapping gas absorption spectra is calculated as

$$WA(z, u) = \frac{1}{\sqrt{z}} \int_{-\infty}^{+\infty} A(\nu) \psi \left(\frac{\nu - u}{z} \right) d\nu \quad (4)$$

where WA represent wavelet coefficients, $\psi(\nu)$ is wavelet basic function, z is scale factor and u is translation factor. If $\psi(\nu)$ has m th-order vanishing moments, the m th-order derivative of $A(\nu)$ can be calculated and smoothed by Eq. (4). In other words, WA can be further expressed as [13]

$$WA(z, u) = z^m \frac{d^m}{d\nu^m} (A^* \theta_a)(u) \quad (5)$$

where θ_a is a smooth function determined by $\psi(\nu)$. The higher the vanishing moments' order, the sharper the peaks and hence the easier the identification of overlapping lines will be. The selection of wavelet basic function and scale factor is of great importance to get the proper analysis result. The lineshape of wavelet basic function should be similar with gas absorption lineshape and the scale factor should be moderate. Generally the smoothing effect

of CWT increases with decomposition scale. If scale factor is small, the resulting wavelet coefficients have small signal amplitudes and much high-frequency noise, which interfere with the recognition of weak peaks severely. On the contrary, large scale factor has strong smoothing ability which suppresses the improvement of resolution. The peaks may still overlap with each other after CWT and not be identified properly.

The center frequency ν_{0i} , HWHM γ_i and peak absorbance H_i/γ_i of each line can be obtained by multipeak fitting based on chaos particle swarm optimization (CPSO). The optimum solution is searched by calculating multiple particles' velocities and positions iteratively. The particle's position \mathbf{P} is defined as a vector whose value in each dimension denotes an unknown parameter in fitting, while velocity \mathbf{V} denotes the variation of each parameter. \mathbf{V} and \mathbf{P} are written as

$$\mathbf{V} = (\Delta\nu_{01}, \Delta\gamma_1, \Delta H_1, \dots, \Delta\nu_{0n}, \Delta\gamma_n, \Delta H_n) \quad (6)$$

$$\mathbf{P} = (\nu_{01}, \gamma_1, H_1, \dots, \nu_{0n}, \gamma_n, H_n)$$

The initial velocities and positions of the particles in the swarm are generated by the well-known logistic equation to exhibit chaotic dynamics [11]. Since the movement of each particle is guided by both its own historical best position \mathbf{Pb} and the whole swarm's historical best position \mathbf{Gb} , \mathbf{V} and \mathbf{P} are updated as follows [10]:

$$\begin{aligned} \mathbf{V}_j^{t+1} &= w\mathbf{V}_j^t + c_1 r_1 (\mathbf{Pb}_j^t - \mathbf{P}_j^t) + c_2 r_2 (\mathbf{Gb}^t - \mathbf{P}_j^t) \\ \mathbf{P}_j^{t+1} &= \mathbf{P}_j^t + \mathbf{V}_j^{t+1} \end{aligned} \quad (7)$$

where j and t are the index of particles and iterations respectively, w denotes the inertia weight, c_1 is cognitive learning rate, c_2 is social learning rate, r_1 and r_2 are two random variables uniformly distributed in the range from 0 to 1. \mathbf{Pb} and \mathbf{Gb} update only when better fitness are acquired for the corresponding particle and the whole particle swarm respectively. As for curve fitting problem, the particle's fitness F at position \mathbf{P} is evaluated by the fitting error. The smaller the fitness, the better it will be. The expression of fitness is written as

$$F(\mathbf{P}) = \sqrt{\frac{1}{M} \sum_{k=1}^M (A(\mathbf{P}, \nu_k) - A(\mathbf{P}^*, \nu_k))^2} \quad (8)$$

where M is the number of sampling points, ν_k is the frequency of the k th sampling point, $A(\mathbf{P}^*, \nu_k)$ and $A(\mathbf{P}, \nu_k)$ represent the absorbance at frequency ν_k of practical gas absorption spectrum and its fitted curve respectively. $A(\mathbf{P}^*, \nu_k)$ is calculated using Eq. (1) while $A(\mathbf{P}, \nu_k)$ is calculated using Eq. (3). To avoid being trapped in local optima and premature convergence, the chaos local search is applied to modify the particle swarm's best position \mathbf{Gb} by locally oriented search [11]. Iteration stops if the fitness at position \mathbf{Gb} does not improve or the number of iterations reaches the set upper limit. Then the respective absorbance distributions of overlapping lines are retrieved using the final value in each dimension of \mathbf{Gb} .

3. Simulation and analysis

Since the gas absorption lineshape satisfies Lorentzian profile, we simulate the separation of three overlapping Lorentzian profiles to demonstrate the general steps, parameter selection rules and performance of the proposed method. The three simulated Lorentzian profiles have center positions of 350, 375 and 410, HWHMs of 10, 15 and 20, and peak heights of 0.02, 0.03 and 0.04 respectively. Their width ratio and height ratio are both made 1:1.5:2. Since the spectral baseline in the narrow frequency range of several gas absorption lines is usually smooth and approximately linear, a linear baseline is employed in the simulation. Fig. 1(a)

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