The Real Time Monitoring Platform for Urban Hazardous Chemical Gas based on Solar Occultation Flux -Fourier Transform Infrared

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With the development of industrialization, the surrounding areas of the city gradually become the important chemical industry bases, which have made important contributions to the economic development of the city. However, there are also some safety risks in the process of production, storage and transportation for chemical products. Once hazardous gas leaks, it will not only cause pollution of the environment, but also harm the health of people and animals. In order to deal with leakage incidents in time, many chemical enterprises have already built their own real-time monitoring system. However, most of these platforms are only for real-time monitoring within the enterprise, and cannot meet the needs of the city's overall monitoring for hazardous gases. Fourier Transform Infrared (FTIR) is a comprehensive monitoring technology developed rapidly in recent years, which is widely used in the emergency monitoring of pollution source gas. In this paper, a large area dangerous chemical gas monitoring platform is proposed by using the technology of Solar Occultation Flux (SOF-FTIR). First of all, this paper briefly introduces the gas monitoring technology. What is more, the principal component analysis (PCA) in FTIR technology is described in detail. Secondly, in view of the large amount of noise in the infrared spectrum data, an improved threshold denoising method is proposed by introducing the correction coefficient. Compared with traditional FTIR, SOF-FTIR can monitor hazardous chemical gas in a wider area, and has better mobility. Finally, the simulation results show that the improved denoising algorithm has better performance. Theoretically, the real-time monitoring platform for urban hazardous gas based on SOF-FTIR can effectively monitor the leakage of hazardous gas in cities.

1. Introduction

With the rapid development of petrochemical industry, many enterprises are trying to expand their production scale, which brings more and more risk sources. At the same time, more and more government departments began to pay attention to emergency treatment of hazardous chemicals leakage. Although we can prevent accidents effectively through safety design, standardized operation and safety inspection, it is impossible to achieve absolute security (Dong et al., 2015)). Therefore, timely monitoring of urban chemical leakage becomes very important.

FTIR is a comprehensive monitoring technology developed rapidly in recent years which has been widely used in air pollution monitoring. It is known that most of the trace gases in the atmosphere are infrared active gases, which have the ability of absorbing and emitting infrared characteristic spectra in the range of 2~30μm. Because this band is very useful for spectral measurements, the FTIR can be applied to the monitoring of hazardous chemical gases in large area (Zhai et al., 2015).

Many research institutions and teams are using this method for gas monitoring, some of which have achieved some success. Andria (2000) and his team in Italy establish a mathematical model for the concentration distribution of nitrogen oxides over the city, which is been applied to gas remote sensing and quantitative analysis system. The Jean-Marc (2004) and his colleagues in USA use FTIR and background subtraction technique to detect trace amounts of polluting gases at 1.5Km distance successfully. Santos (2005) and his colleagues use FTIR and Raman spectrometer to analyze the proportion of water in diesel fuel respectively. By contrast, it is found that the accuracy of Raman spectrometer combined with neural network analysis is the...
higher, which is close to 0.01%. Michael (2004) studies the spectral decomposition algorithm based on the sample absorption spectrum in the presence of background interference. This method overcomes the interference of carbon dioxide and volatile organic compounds on the measurement. Jin Ling (2010) puts forward the spectral acquisition model based on SOF-FTIR under the complex environment. This method has the advantages of simple operation and strong mobility, which has a good application prospect in the field of air pollution monitoring.

Nevertheless, FTIR is usually used to monitor a certain area, and there is a shortage of large area gas monitoring. In this paper, a real-time monitoring platform for urban hazardous gases based on SOF-FTIR is proposed, which solves the problem of gas monitoring in large areas. First of all, this paper briefly introduces the gas monitoring technology. What is more, the principal component analysis (PCA) in FTIR technology is described in detail. Secondly, in view of the large amount of noise in the infrared spectrum data, an improved threshold denoising method is proposed by introducing the correction coefficient. Compared with traditional FTIR, SOF-FTIR can monitor hazardous chemical gas in a wider area, and it has better mobility. Finally, the simulation results show that the improved denoising algorithm has better performance. Theoretically, the real-time monitoring platform of urban hazardous gas based on SOF-FTIR can effectively monitor the leakage of hazardous gas in cities.

2. Summary of gas monitoring technology

2.1 Commonly used gas monitoring technology

The commonly used gas monitoring methods mainly include three categories, and they are electrochemical method, electrical method and optical methods respectively (Yang et al., 2003).

(1) Electrochemical process method

Electrochemical method is a method for detecting gas based on the electrochemical properties of gases. When the gas reacts with the energized electrode, it will produce an electrical signal related to the concentration of the gas. The chemical sensor has the characteristics of small size, simple operation and easy to carry. Nevertheless, the sensor is also easily affected by the environment such as humidity, temperature and so on.

(2) Electrical method

Electrical method is a method of detecting gas by using gas sensor based on the physical chemical properties. Electrical method includes many types, in which semiconductor method and catalytic combustion method are commonly used. Semiconductor method develops rapidly and widely in recent years. By contacting the gas to the semiconductor gas sensor, the nature of the semiconductor will change in accordance with the composition and concentration of the gas. The advantages of this method are simple structure, fast response, long life, less energy consumption and high sensitivity, while the disadvantages of this method are narrow measuring range and easy interference by ambient gas. Catalytic combustion method is used to obtain the information corresponding to gas concentration through the change of resistivity caused by combustion of combustible gas under the action of catalyst. However, because the corrosive gas can damage the sensor, this method can only be applied in a narrow range.

(3) Optical method

Optical method mainly includes optical interference method, non-dispersive infrared absorption method, tunable diode laser absorption spectroscopy and photochemical ionization method.

Optical interferometry is a method to deduce the concentration of gas by using the interference fringes produced by different gases with different interference rates. Non-dispersive infrared absorption refers to the method of obtaining gas concentration by using different absorption ability of different gas molecules to the specific wavelength of infrared light. This method has high precision, but it requires complex structure and high cost. Tunable diode laser absorption spectroscopy uses the wavelength tuning capability of the semiconductor laser to determine the type and concentration of the gas to be measured. In other words, the absorption spectrum information of the gas to be measured is obtained by scanning the output wavelength. The photochemical ionization method uses ultraviolet photo ionization molecules to detect volatile gas compounds. The core of this method is an ultraviolet lamp filled with low pressure inert gas. When the energy absorbed by the gas reaches their intrinsic frequency, resonance and ultraviolet spectrum will be produced.

2.2 FTIR

FTIR is a comprehensive monitoring technology developed rapidly in recent years, and it has been widely used in measurement, industrial automation, food manufacturing, military science and other fields. FTIR spectrometer mainly consists of optical system and computer, in which the optical system is the core part of
infrared spectrometer. The optical system is mainly composed of light source, detector, interferometer, sample room and all kinds of infrared mirrors. The schematic diagram of FTIR spectrometer is shown in figure 1.

![Schematic diagram of FTIR spectrometer](image)

**Figure 1: Schematic diagram of FTIR spectrometer**

PCA is a method of reconstructing original samples by linear combination of principal component which is a set of optimal orthogonal vector basis obtained by linear transformation. Despite the reconstruction, the mean square error between the sample processed by the PCA method and the original sample is very small. We use a $k$ dimensional random variable to represent the original spectrogram.

$$X = (x_1, x_2, \cdots, x_n)$$  \hspace{1cm} (1)

In the above formula, $x_i$ represents pixel $i$ of the image. When the mean value of the random vector is not zero, we need to do the centralized processing on the data. Let’s take the mean values for each column of vector $X$ by the following formula.

$$\mu = \frac{1}{n} \sum_{i=1}^{n} x_i$$  \hspace{1cm} (2)

Where, the variable $\mu$ means the mean value of all samples. Therefore, we can define the covariance matrix $S$ corresponding to $X$ according to the following formula.

$$S = \frac{1}{n} \sum (x_i - \mu)(x_i - \mu)^T$$  \hspace{1cm} (3)

Suppose there is a set of orthogonal bases, which make the new components of an $n$-dimensional vector orthogonal to each other.

$$y = P^T \cdot X$$  \hspace{1cm} (4)

Suppose that the rank of the covariance matrix $S$ is $m$, and the eigenvalue is $\lambda_i$ which satisfies the following conditions.

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_m$$  \hspace{1cm} (5)

We let $p_i$ represent the eigenvectors corresponding to $\lambda_i$, then $\lambda$ and $p_i$ satisfy the following formula.

$$S \cdot p_i = \lambda_i \cdot p_i$$  \hspace{1cm} (6)

We arrange the eigenvalues according to the order from large to small, and then select the eigenvalues whose cumulative contribution rate is greater than the threshold according to the following formula.
\[
\mu(l) = \frac{\sum_{i=1}^{\lambda} \lambda_i}{\sum_{i=1}^{\lambda}} \geq T
\]  
(7)

Then, the transformation matrix is constructed by using the eigenvectors corresponding to the eigenvalues.

\[
W = (w_1, w_2, \cdots w_l) \quad (l< m)
\]  
(8)

In order to reduce the dimension, we need to calculate the principal component of the previous m values to replace the original image \(X\). Since the projection coefficient is \(y\), the formula for reconstructing the original data is as follows.

\[
\hat{X} = WY + E
\]  
(9)

PCA is an optimization method to observe the information of data sets. It simplifies the complexity of data by reducing the dimensionality on the premise of maintaining the validity of the data, which is been used in many algorithms.

### 3. Improved threshold denoising method

Compared with traditional FTIR, SOF-FTIR can monitor hazardous chemical gas in a wider area, and it has better mobility. When SOF-FTIR is used for sampling hazardous gas, noise will inevitably be introduced such as electrical noise, sample background and stray light. Because that the noise can affect the extraction of useful information, in order to increase the signal to noise-ratio and improve the resolution of the spectrum, we need to pre-process the infrared spectrum before pattern recognition. The commonly used denoising method is wavelet threshold denoising method, which Since that the noise is mainly concentrated in the higher frequency, we can use the threshold to deal with the wavelet coefficients, and then use the wavelet reconstruction method to achieve the purpose of denoising. There are two methods to deal with wavelet coefficients, and they are soft threshold method and hard threshold method.

The formula of soft threshold method is as follows:

\[
Y = f(x, T) = \begin{cases} 
    x - T, & x \geq T \\
    0, & |x| < T \\
    x + T, & x \leq T 
\end{cases}
\]  
(10)

The formula of hard threshold method is as follows.

\[
Y = f(x, T) = \begin{cases} 
    x, & |x| \geq T \\
    0, & |x| < T 
\end{cases}
\]  
(11)

The display of the two methods in coordinates is shown in figure 2.

![Figure 2: Soft threshold method and hard threshold method](image)

In this paper, in order to obtain better denoising effect, we introduce a correction coefficient, which makes the modified wavelet coefficients between soft threshold and hard threshold.
Since the value of the correction coefficient always varies with the signal to noise ratio, it is difficult to obtain the accurate value in the actual environment. So, when \( x > 0 \), we introduce the soft threshold method, and the formula 10 can be equivalent to the following formula.

\[
Y = f(x, T) = \begin{cases} 
\text{sgn}(x)(|x| - \alpha T), & |x| \geq T \\
0, & |x| < T 
\end{cases}
\]  \hspace{1cm} (12)

We define \( u \) as a global parameter whose formula is as follows.

\[
u = \frac{x}{T} \]  \hspace{1cm} (14)

When \( u \geq 1 \), we can consider that the signal contains useful information. Otherwise, it is considered as noise signal. Therefore, the formula can be modified to be the following formula.

\[
Y = f(x, T) = \begin{cases} 
T(\frac{x}{T} - 1), & \frac{x}{T} \geq 1 \\
0, & \frac{x}{T} < 1 
\end{cases}
\]  \hspace{1cm} (13)

Finally, an improved threshold denoising formula is obtained by transforming the above formulas.

\[
Y = f(x, T) = \begin{cases} 
\text{sgn}(x)(\sqrt{x^2 - T^2}), & |x| \geq T \\
0, & |x| < T 
\end{cases}
\]  \hspace{1cm} (16)

The graph of the improved threshold method is shown in figure 3.

![Graph of the improved threshold method](image)

Figure 3: The graph of the improved threshold method

It can be seen from figure 3 that the change curve of the improved threshold method is smoother. This method not only overcomes the problem of the signal oscillation caused by the discontinuity of the hard threshold, but also overcomes the problem of the deviation between the reconstructed signal and the real signal.

4. Simulation experiment and result analysis

In order to verify the effect of the improved threshold denoising algorithm, we selected ethane (C\(_2\)H\(_6\)) for experiments. In addition, the experiment is carried out under the ideal condition, which means that the influence of wind and humidity on the experimental results is not taken into consideration. In order to represent the performance of the new algorithm more intuitively, the original spectrogram and the denoised spectrogram are both recorded in the experiment. The spectrogram before and after denoising is shown in Figure 4.
From the graph above, we can see that the spectral curve of the improved denoising algorithm is much smoother than that of the original spectrogram. However, we can find in the spectrogram that some noise still exists, which indicates that the improved denoising algorithm is not perfect enough. Nevertheless, the improved algorithm can improve the application of SOF-FTIR technology in urban hazardous chemical gas monitoring greatly.

5. Conclusion

In this paper, a real-time monitoring platform based on SOF-FTIR for urban hazardous chemical gas is introduced. In order to solve the problem of high frequency noise in infrared spectrum, an improved threshold denoising method is proposed. Compared with the traditional monitoring method for dangerous chemical gas, the monitoring technology based on SOF-FTIR has a stronger mobility and lower cost, which is conducive to the realization of the monitoring of large area for dangerous gas in cities.

References

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