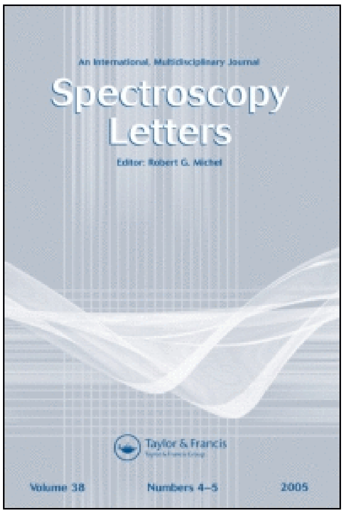

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Junde Wang[a]; Tianshu Wang[b]; Zourn Zhen[a]; Yunhua Luo[a]; Malcolm R. Clench[b]; David J. Mowthorpe[b]
[a] Laboratory of Advanced Spectroscopy, Nanjing University of Science & Technology, Nanjing, P. R. China [b] School of Science & Mathematics, Sheffield Hallam University, Sheffield, UK

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THE INFLUENCE OF THE TEMPERATURE OF BLACKBODY FOR CALIBRATING FTIR SYSTEM ON THE INSTRUMENT RESPONSE FUNCTION*

Key words: Instrument Response Function; Infrared Emission Spectroscopy; Remote Sensing; Fourier Transform Infrared Spectroscopy

Junde Wang [a], Tianshu Wang [b], Zouru Zhen [a], Yunhua Luo [a], Malcolm R. Clench [b], David J. Mowthorpe [b]**

[a)] Laboratory of Advanced Spectroscopy,
Nanjing University of Science & Technology, Nanjing 210014, P.R.China

[b)] School of Science & Mathematics,
Sheffield Hallam University, Sheffield S1 1WB, UK

Abstract

The instrument response function of Fourier transform infrared spectrometer is a very important parameter in infrared emission spectroscopy to obtain infrared spectral radiance distribution of the desired sample, the concentrations of the components of combustion products in the flame etc. This paper gives the effect of the temperature of the standard blackbody for calibrating Fourier transform infrared spectrometer on the instrument response function. The result illustrates that the values of the instrument response functions decrease as the blackbody temperature increased, and tends to a limit. The paper points out that the condition must be observed for using instrument response function correctly.

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** Auther to whom correspondence should be sent.

I. Introduction

With the rapid developments of applications of Fourier transform infrared (FTIR) spectroscopy to chemical systems, an increased number of the studies on FTIR emission spectroscopy had appeared. These studies include remote infrared emission spectral characterizations, spectral radiance distribution, determinations of the components of combustion products and the estimation of the temperature of the flame[1-7], the thermal fragmentation of the organic compounds in a hydrogen/air flame[8,9], remote infrared emission spectral quantitative determinations of the components of the exhaust plumes from the smokestacks[10-12], FTIR emission analytical studies of the solids, such as catalysts[13-15], thin polymer layers[16,17], minerals[18,19], jet fuel deposits[20], and pesticides[21], etc. All these studies relate to the intensity calibration of emission spectral intensity. In order to obtain the calibrated intensity of the emission spectrum the calibration of FTIR spectrometer is necessary for obtaining an instrument response function of the system. Hence, it is very important to calibrate FTIR emission system for obtaining correct instrument response function. In this paper, we will give measuring method of instrument response function at the different temperature of the standard blackbody used in the calibration of the FTIR emission system, and the influence of the temperature on the instrument response function.

II. Theory

1. The sample single-beam spectrum

For gaseous samples or condensed phase samples on a metallic support or in a non-absorbing matrix [where emissivity $\varepsilon(\nu)=0$ for both cases], the single-beam spectrum $S(\nu,T)$ of a sample at a temperature T has contributions from several sources and is given by[22,23]

$$S(\nu,T)=R(\nu)[\varepsilon(\nu)H(\nu,T)+B(\nu)+I(\nu)\rho(\nu)] \tag{1}$$

where $R(\nu)$ = instrument response function

$\varepsilon(\nu)$ = emittance of sample

$H(\nu,T)$ = Planck function

$B(\nu)$ = background radiation reaching the detector directly

$I(\nu)\rho(\nu)$ = radiation reflected from sample
$\rho(\nu)$ = reflectance of sample

2. Infrared spectral radiance

According to Eqn(1) the gas spectral radiance may be expressed as follows

$$W(\nu,T) = \{S(\nu,T) - [R(\nu)B(\nu) + R(\nu)I(\nu)]\} / R(\nu) \tag{2}$$

where $R(\nu)B(\nu)$ is the single-beam spectrum S_B of the atmospheric background radiation. $R(\nu)I(\nu)$ is single-beam spectrum S_I of the background radiation inside the instrument. We rewrite Eqn(2) in the following way

$$W(\nu,T) = \{S(\nu,T) - [S_B(\nu) + S_I(\nu)]\} / R(\nu)$$

$$= [S(\nu,T) - S_{B+I}(\nu)] / R(\nu) \tag{3}$$

where $S_{B+I}(\nu) = S_B(\nu) + S_I(\nu)$.

According to the above explanation, it is first necessary to measure the instrument response function $R(\nu)$ of Fourier transform infrared spectrometer.

3. The concentrations in combustion products in flame

The absorbance $A(\nu)$ or transmittance $\tau(\nu)$ of a gas sample at a given wavenumber ν is related to the concentration C' by Beer's law

$$A(\nu) = -\log \tau(\nu) = K(\nu)\, lC' \tag{4}$$

where $K(\nu)$ is the spectral absorption coefficient for a given wavenumber ν. l is the pathlength.

For any sample the sun of its transmittance $\tau(\nu)$, reflectance $\rho(\nu)$, and emissivity $\varepsilon(\nu)$ at any frequency ν is approximately equal to unity

$$\tau(\nu) + \rho(n) + \varepsilon(\nu) = 1 \tag{5}$$

Since the reflectance $\rho(\nu)$ of most gases with discrete emission spectra is low, the following approximation applies

$$\varepsilon(\nu) = 1 - \tau(\nu) \tag{6}$$

Thus the emissivity of the gas is related to the concentration C' by

$$C' = - \{\log[1-\varepsilon(\nu)\} / [K(\nu)l] \tag{7}$$

where the pathlength l is the flame diameter and C' is the concentration of gas neglecting the flame temperature T. The gas emissivity $\varepsilon(\nu)$ is related to the spectral radiance $W(\nu,T)$.

The actual gas concentration C at flame conditions is given by

$$C = C'T / 273 \tag{8}$$

4. The emissivity of the measured sample

The emissivity $\varepsilon(\nu)$ of the measured sample at the wavenumber ν and temperature T is given by

$$\varepsilon(\nu) = W(\nu,T) / W_{bb}(\nu,T) \tag{9}$$

where $W(\nu,T)$ is the spectral radiance of the measured sample at the temperature T. $W_{bb}(\nu,T)$ is the spectral radiance of a blackbody at the flame temperature T, i.e., theoretical Planck function in spectral radiance, which can be generated by the computer software for any temperature.

Thus, we can measure infrared spectral radiance distribution, spectral emissivity and the concentrations of the components of combustion product in the flame through the instrument response function. Hence, the instrument response function is a very important parameter for infrared emission spectroscopy.

In present many papers consider that the instrument response function is only a function of the frequency(wavenumber, cm^{-1}), and irrelative to the temperature of the blackbody used for the calibrating infrared spectrometer. But the instrument response function is often affected by the temperature of the blackbody for the instrument calibration from our experiments. Hence we will open discussion for the instrument response function $R(\nu)$.

III. Experimental

The FTIR spectrometer used in this work was a 170RS remote sensing FTIR spectrometer (NICOLET, Madison, Wisconsin, USA). The FTIR system has a ZnSe refracting telescope of 2 in. diam. to collect infrared emission and / or absorption from the infrared source to be located far apart the spectrometer. The system structure had been mentioned in detail in Refs.[1,24,25].

The main portion of remote sensing FTIR spectrometer is a Michelson interferometer. A ZnSe unhydroscopic beamsplitter is used. A liquid nitrogen cooled narrow band MCT (Mercury Cadmium Telluride) sandwich detector is utilized for obtaining maximize signal-to-noise ratios in the frequency region of 5200-700 cm^{-1}. There are two He-Ne lasers in this spectrometer. The two lasers are used as the reference wavelength laser and aiming remote object measured, respectively. The standard blackbody (Barnes Eng. Comp. USA) is used for calibrating FTIR system to get its instrument response function.

The spectra were recorded with a spectral resolution of 4 cm^{-1}. Each of them was the average of 32 scans.

IV. Results and discussion

1. System calibration

To measure the instrument response function $R(\nu)$ of the system, a blackbody operated at known temperature T is placed to fill field of view of receiver telescope. Thus spectrum collected $S'(\nu,T)$ will contain the background spectrum $S_b(\nu)$. The standard blackbody spectrum $S(\nu,T)$ equals the background spectrum $S_b(\nu)$ subtracted from $S'(\nu,T)$. In general CO_2 and H_2O absorptions in the atmosphere are removed from the standard blackbody spectrum $S(\nu,T)$ by the method generated a straight line in the portion of the spectrum between two specific frequencies. The standard blackbody spectrum $S(\nu,T)$ is divided by a computer generated Planck's blackbody radiation function $W_{bb}(\nu,T)$ to give the instrument response function $R(\nu)$:

$$R(\nu) = S(\nu,T) \,/\, W_{bb}(\nu,T) \tag{10}$$

2. Measured instrument response function

According to the method described in system calibration, a number of the curves of instrument response functions had been measured at eight different standard blackbody temperatures of 323, 423, 623, 723, 823, 823, 1023 and 1223 K, respectively. The results obtained are shown in Fig.1.

From Fig.1, we can see the instrument response function curves of the FTIR system are gradually moved downwards and moved separations decrease as the temperature increased , and these curves trend to a limit curve.

3. In the strict sense, when we measure the infrared spectral radiance of the measured sample, the instrument response function obtained at the temperature of the standard blackbody used in the system calibration to be the same with the temperature of the measured sample must be utilized. When the temperatures are more than 600K, their instrument response function curves are very near. For the convenience of the measurement, we can think similarly that the instrument response function bears irrelative to the temperature of the blackbody for FTIR system calibration. We can select one of the instrument response functions (T> 600K) used in the measurement. When the temperature of the measured sample is not more than 600 K, the temperature of the standard blackbody for calibrating system must be the same with the temperature of the desired sample.

V. Conclusion

Based on the result of the experiment, the following conclusion is appropriate. In general case, the instrument response function bears relation with the temperature of the standard blackbody for calibrating FTIR system. The effect of the temperature of the standard blackbody on the instrument response function decreases as the temperature of the standard blackbody increased. Thus, when we study high temperature flame combustion the instrument response function can be considered to be irrelative to the temperature of the standard blackbody. But the temperature is selected at higher temperature of the blackbody for calibrating FTIR system. In the general the blackbody temperature is

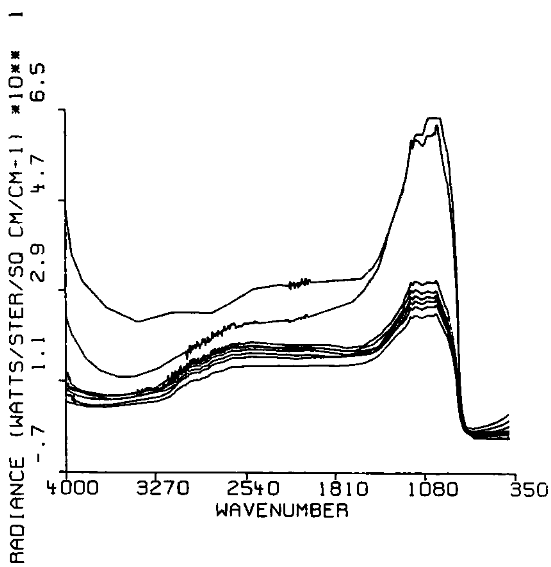

Fig. 1. Instrument response functions measured at the different standard blackbody temperatures

The temperatures corresponding from upper to under curves are 323, 423, 623, 723, 823, 923, 1023 and 1223 K, respectively.

more than 600 K. If we study infrared emission of the measured sample at lower temperature (<600K), the instrument response function that is obtained at the same the temperature of the blackbody for calibrating FTIR system as the temperature of the measured sample must be utilized.

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