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# Measurement of Gas Temperature and Concentration Based on TDLAS

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**Abstract.** The measurement of gas temperature and concentration in combustion process has always been an important part of research. Based on the application of tunable diode laser technology in gas detection, the molecular absorption spectroscopy system was established and the concentration and temperature of water vapor were measured. Based on the spectral parameters in the latest HITRAN 2016 database, a group of programs have been compiled, which adopt the form of VOIGT function and consider frequency shift caused by pressure and temperature and . The spectral absorbance of H<sub>2</sub>O was obtained by the computer program. Based on the scanning range of the laser, the spectral lines of water vapor molecule near 1392 nm were screened to obtain the suitable pairs of spectral lines for measuring temperature and concentration. The pairs of spectral lines were validated as gas temperature measurements at high temperature by numerical simulation. TDLAS system is built independently, and TDLAS technology is used to measure the gas concentration field and temperature field in an experimental way. It is of great significance for TDLAS technology in gas monitoring.

## 1. Introduction

The measurement of gas temperature and concentration is of great significance in aerospace, energy and chemical industry, environmental monitoring and other industries. With the development of molecular spectroscopy and semiconductor laser technology, tunable Diode Laser Absorption Spectroscopy (TDLAS) [1] technology is an optical diagnostic technology and can measure the concentration and temperature of gas components. It has the advantages of high sensitivity and is not easily affected by other gases [2]. It has become a research hotspot at home and abroad. At present, TDLAS technology has been applied in various aspects of industrial production and life, such as production of exhaust gas and flue gas, monitoring of production of toxic and combustible gases, diagnosis of combustion flow field such as engines, and monitoring of air pollutants [3-5]. As a spectral detection method with high sensitivity and resolution, TDLAS plays an important role in the fields of analysis chemistry and combustion diagnose [6-7].

Through the analysis of molecular spectra, molecular spectra can be obtained, which can be used as the application basis of TDLAS technology. At present, the spectral line data of TDLAS research at home and abroad are basically from HITRAN database. The spectral line parameters of 49 substances in HITRAN 2016, the seven main atmospheric absorbers in the initial infrared band, include spectral line position, linear intensity, several broadening coefficients and molecular cutting function, pressure frequency shift, Einstein coefficient and other molecular spectral parameters [8]. Existing tools for



molecular spectroscopy mapping, such as HITRAN 2012 and HITEMP 2010 databases used by Spectraplot, have not been updated in time, and many molecular spectroscopic maps, such as  $H_2$ ,  $SF_6$  and  $C_4H_2$ , are lacking. When calculating the absorbance, less attention is paid to the pressure frequency shift.

Water vapor, as a common hydrocarbon fuel combustion product, has a wide spectrum distribution and complete data parameters. It is suitable for measuring gas temperature and other aspects. It has important significance in gas diagnosis such as combustion field [9-10]. Because of many factors affecting the measurement results, the selection of water molecular spectral lines is diverse, and there is no standard for selecting spectral pairs. Generally, the selection depends on experiments according to the actual situation. In this paper, based on the HITRAN2016 spectral parameters of water, considering the influence of temperature, pressure and other factors, the absorbance of  $H_2O$  was simulated by using MATLAB. The absorption spectra of water at 1392 nm were taken as the object of study, and suitable spectral lines were selected to measure gas temperature and concentration. A TDLAS system platform based on THORLABS ITC4001 semiconductor laser with temperature control mode was built to measure gas temperature and water molecule concentration.

## 2. Measuring method of temperature and concentration based on TDLAS

Using TDLAS technology to measure gas concentration can be measured by direct absorption method. Direct absorption spectroscopy is to record incident and transmitted light intensity directly according to Lambert's law, and to retrieve gas concentration according to absorbance. According to Lambert Bill's formula:

$$PXS(T)L = \int_{-\infty}^{+\infty} -\ln\left(\frac{I}{I_0}\right)dv = A \quad (1)$$

$P$  [atm] is the partial pressure of the absorbing species;  $X$  is the concentration of gas; of the absorbing species;  $S$  [ $cm^{-2} \cdot atm^{-1}$ ] is the strength of the transition, which indicates the absorption intensity of the spectral line;  $L$  [cm] is the absorption path length;  $I_0$  is incident laser intensity or power, And  $I$  is transmitted intensity or power.

Therefore, a formula for calculating gas concentration can be obtained:

$$X = \frac{\int_{-\infty}^{+\infty} -\ln\left(\frac{I}{I_0}\right)dv}{PS(T)L} \quad (2)$$

TDLAS-based gas temperature measurement scheme is to obtain two spectral absorbances under different transition states at the same pressure, molar fraction and optical path in the wavelength scanning scheme. This method needs to scan two different characteristic absorption spectra of gases, and calculate the temperature by two spectra varying with temperature. It is also called bispectrum temperature measurement method. The ratio of spectral absorbance area measured can be expressed as the ratio of spectral line intensity, and the function related to temperature can be obtained.

$$R = \frac{A_1}{A_2} = \frac{S_1(T)}{S_2(T)} = f(T) \quad (3)$$

Therefore, the gas temperature can be calculated from the ratio of the spectral absorbance obtained. If the central wavelength of the two characteristic lines is close enough, and the intensity ratio of the two absorption lines can be expressed as follows:

$$R = \frac{A_1}{A_2} \approx \frac{S_1(T_0)}{S_2(T_0)} \exp\left[-\frac{hc}{k}(E_1^* - E_2^*)\left(\frac{1}{T} - \frac{1}{T_0}\right)\right] \quad (4)$$

From equation (4), the formula for calculating gas temperature can be obtained by measuring the ratio of absorption intensity of gas absorption line pairs. The sensitivity of temperature measurement is expressed by the differential of spectral intensity ratio to temperature.

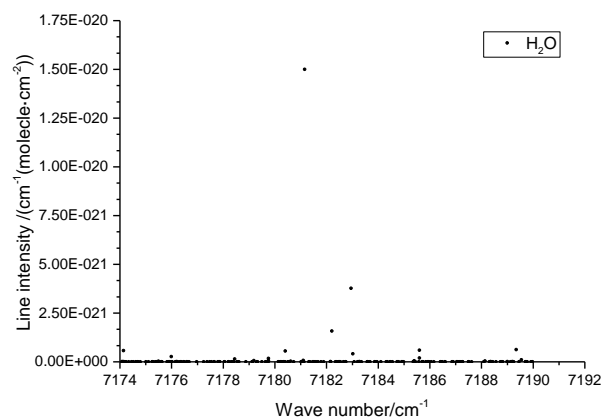
$$\frac{\partial R/R}{\partial T/T} = \left(\frac{hc}{k}\right) \frac{|E_1'' - E_2''|}{T} \quad (5)$$

At present, the output wavelength of commercial semiconductor lasers can be tuned by adjusting the magnitude of the current and the temperature of the laser. By changing the modulation current of the input laser, the single wavelength laser is driven to scan the gas absorption spectrum in frequency domain. The spectral absorption signal is determined by comparing the attenuated laser intensity with the reference laser intensity (baseline). Therefore, when the parameters such as pressure, linear intensity and laser traversing distance in gas medium are known, the integral value of spectral absorptivity in frequency domain can be brought into equation (2), and the gas concentration can be finally obtained.

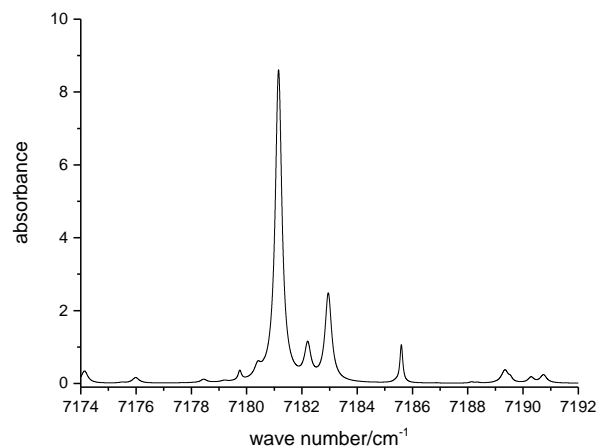
For TDLAS bispectrum temperature measurement, the key is to choose the right pair of lines. For direct absorption measurement, how to determine the reference signal of laser intensity is very important for the final calculation results. Especially for the measurement of weak absorption signal, the error caused by the baseline intensity would produce tremendous impact on concentration evaluation.

### 3. Selection of spectral pairs

According to the scanning center wavelength of the laser at 1392 nm and the HITRAN 2016 database, the absorption spectra of water molecules in the range of 7174-7192  $\text{cm}^{-1}$  are shown below.



**Figure 1.** Absorption spectra of water molecules in the range of 7174-7192  $\text{cm}^{-1}$ .



**Figure 2.** Absorbance of  $\text{H}_2\text{O}$  in the range of 7174-7192  $\text{cm}^{-1}$ .

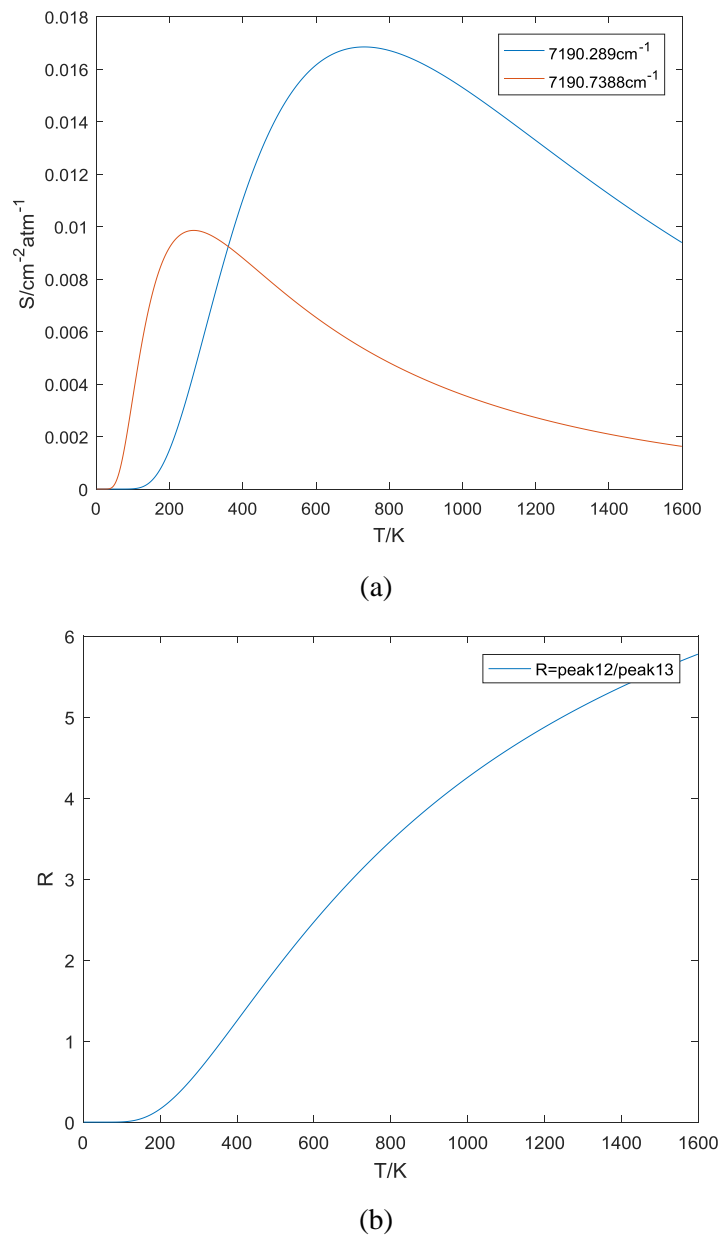
The spectral absorption map of this section can be calculated by a MATLAB program. Figure 2 shows the spectral absorbance at 296K and 1% concentration at 1atm and 100cm pathlength. There are 13 peaks in the absorption spectrum. The spectral data of this spectral position are derived from HITRAN 2016. Considering that temperature measurement requires a larger spectral intensity, the spectral lines with a spectral intensity more than  $4\text{E-}23$  ( $\text{cm}^{-1}/(\text{mol} \cdot \text{cm}^{-2})$ ) or  $0.001$  ( $\text{cm}^{-2}\cdot\text{atm}^{-1}$ ) are selected as the optional spectral lines. Table 1 shows the spectral parameters corresponding to the absorbance peaks of water molecules in  $7174\text{--}7192$   $\text{cm}^{-1}$ .

Among the 13 absorption peaks in Table 1, peak5, 9, 10, 11 have overlapping spectral lines, which are not considered. Peak10 has been selected as available in many studies, but it is no longer applicable after the update of HITRAN 2016. It is necessary to re-select the more suitable spectral pairs. Although peak 1 laser can be scanned, it is not easy to control the temperature too high and cause damage to the instrument. It is not considered when there is a better choice. In the remaining spectral pairs, peak12( $7190.2890$   $\text{cm}^{-1}$ ) and peak13( $7190.7388$   $\text{cm}^{-1}$ ) were selected as the measurement line pairs considering various factors. The main reasons are as follows: the intensity of the two spectral lines is relatively high, and better spectral line measurement data can be obtained; the distance between the two spectral lines is  $0.4498$   $\text{cm}^{-1}$ , which ensures that the measurement results can be scanned by a laser beam, so that the measurement results can be separated under the same experimental conditions and at the same time have a certain wavenumber difference; within a certain range, the intensity of the two spectral lines varies with temperature, and the intensity ratio is different at different temperature. The ratio of absorbance area varies with temperature as a single valued function.

**Table 1.** Spectral parameters corresponding to absorbance peaks of water molecules in  $7174\text{--}7192$   $\text{cm}^{-1}$ .

peak	$\nu$ $\text{cm}^{-1}$	$\nu$ $\text{cm}^{-1}$	$S$ $\text{cm}^{-1}/(\text{molcm}^{-2})$	$E''$ $\text{cm}^{-1}$
1	7174.14	7174.13778	5.77E-22	95.1759
2	7175.987	7175.98676	2.68E-22	206.3014
3	7178.446	7178.44584	1.44E-22	602.7735
4	7179.19	7179.18718	5.76E-23	326.6255
5	7179.75	7179.7524	1.698E-22	1216.1944
		7179.7534	5.667E-23	1216.1897
6	7180.4	7180.39972	5.56E-22	224.8384
7	7181.154	7181.15578	1.50E-20	136.7617
8	7182.207	7182.209	1.58E-21	42.3717
9	7182.953	7182.94962	3.77E-21	142.2785
		7183.01579	4.07E-22	134.9016
10	7185.596	7185.596571	1.98E-22	1045.0583
		7185.5973	5.93E-22	1045.0578
11	7189.347	7189.34444	6.21E-22	142.2785
		7189.5420	1.07E-22	1255.1666
12	7190.29	7190.2890	2.41E-22	842.3565
13	7190.74	7190.7388	3.94E-22	275.4971

Figure 3 (a) (b) is linestrength of Peak 12 and Peak 13, and the ratio of line strength to peak 12 and peak 13. According to the sensitivity calculation formula, the energy difference between the low-state energy levels of the two lines is  $566.8594$ , and the temperature sensitivity is  $2.76 > 1$ .



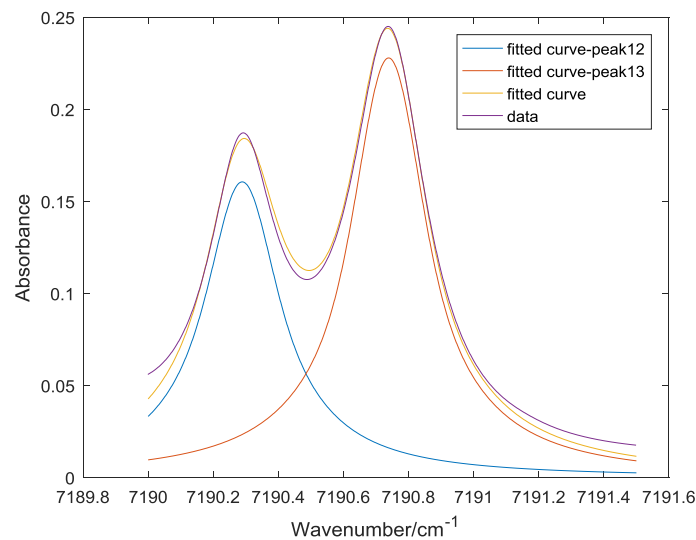
**Figure 3.** (a) Linestrength with temperature at  $\nu_{12}$  and  $\nu_{13}$ . (b) linestrength ratio with temperature at  $\nu_{12}$  and  $\nu_{13}$ .

#### 4. Numerical simulation

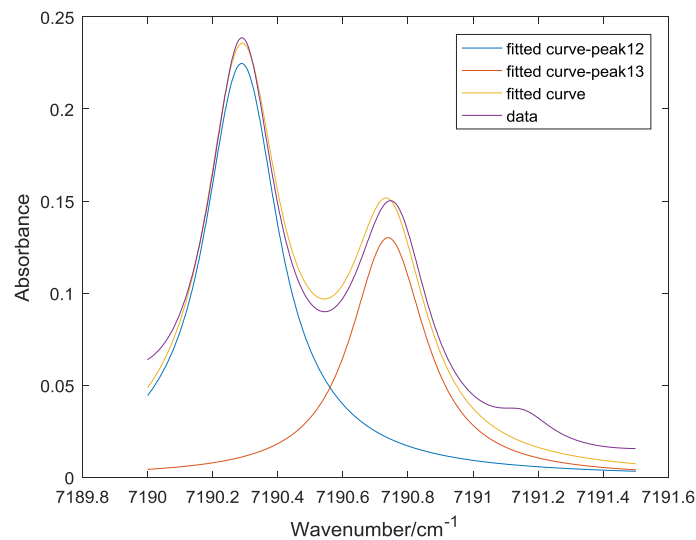
According to HITRAN 2016, peak12 and peak13 can be selected as spectral lines for temperature measurement. The absorbance data of 10% concentration, 100 cm optical path, 1 atm pressure and 300 K temperature were obtained by numerical simulation. The temperature and concentration were deduced from the data. According to the spectrum method, the absorbance area  $A_1$  ( $7190.2890\text{ cm}^{-1}$ ) and  $A_2$  ( $7190.7388\text{ cm}^{-1}$ ) need to be measured. In order to increase the accuracy of the experiment, this paper does not integrate the data directly, but fits the Voigt curve by bimodal fitting, and then carries out numerical integration to get the area ratio. The advantage of bimodal fitting is that the absorbance area of two spectral lines can be calculated separately by using the fitting Voigt curve of the two spectral lines. The following figure simulates the theoretical data as well as the spectrogram of the fitting curve based on the data. The numerical integration results are  $A_1 = 0.06067$  and  $A_2 =$

0.09514. The calculated temperature is  $T = 300.55\text{K}$ , the measurement error is  $0.55\text{K}$ , the calculated water molecule concentration is  $X1 = 9.89\%$ ,  $X2 = 9.89\%$ , and the calculation error is  $0.11\%$ .

Figure 5 is the data and fitting curve when the temperature is changed to  $500\text{K}$ . The numerical integration results are  $A1=0.09389$  and  $A2=0.05106$ . The calculated temperature is  $T = 492.88\text{K}$ , the measurement error is  $7.12\text{K}$ , the calculated water concentration is  $X1 = 10.9\%$ ,  $X2 = 10.9\%$ , and the calculation error is  $0.9\%$ .



**Figure 4.** Simulated data and spectrograms of fitting curves at  $300\text{K}$ .



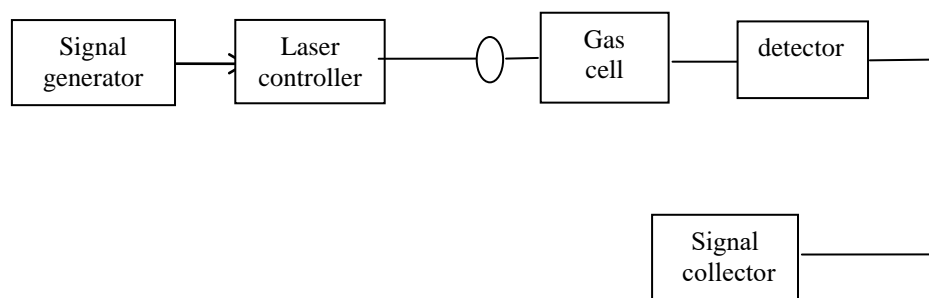
**Figure 5.** Simulated data and spectrograms of fitting curves at  $500\text{K}$ .

Based on the absorbance data of the reconstructed spectral pairs under known conditions, the temperature error is less than  $1.5\%$  and the concentration error of water gas is less than  $10\%$ . It can be used as a spectral pair for gas temperature and concentration measurement.

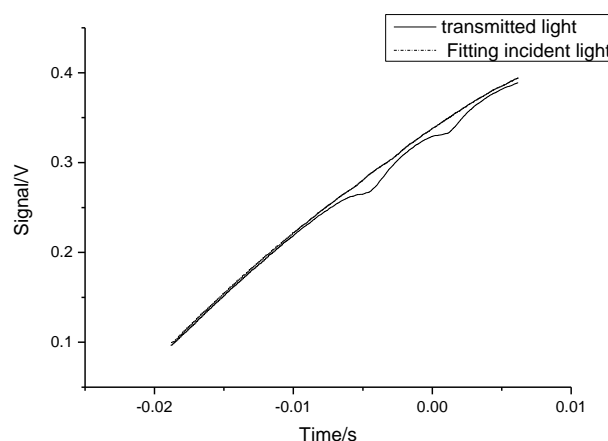
## 5. Experimental verification

The experimental scheme is shown in figure 6. The laser beam is passed through a etalon and a gas pipe containing water vapor, respectively. The etalon is used to obtain the variation of laser intensity

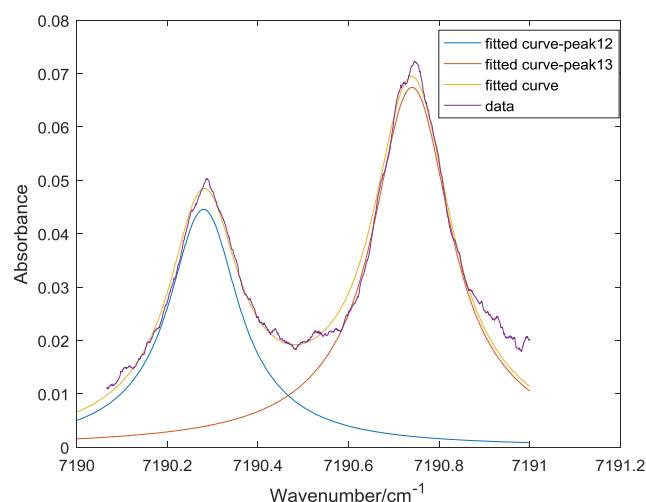
with wavelength. The laser emits a beam through a sample cell of 88 cm in length, and a certain concentration of water vapor is introduced into the tube. The gas temperature in the tube reaches 300 K by heating the tube. The laser intensity is collected after the laser beam is absorbed by the gas. The laser modulation condition is that the modulation frequency is 20 Hz, the central current is 65 mA, and the modulation depth is 8%. The heating pipe is 30.4°C and the concentration of water vapor is 2.5%. The transmission intensity under this condition is measured and Figure 7 is obtained.



**Figure 6.** Schematic of measuring device.



**Figure 7.** Transmission signals and fitting incident light.



**Figure 8.** Schematic of fitting curve.



## 6. Conclusion

In summary, TDLAS system can realize simultaneous measurement of temperature and gas concentration. It has important application prospects in energy and chemical industry, aerospace, environmental monitoring and other industries. Aiming at the application of TDLAS technology in gas temperature field and concentration field, based on the HITRAN 2016 database spectral line parameters, the spectrum lines at 1392 nm are selected through detailed theoretical and experimental analysis. The absorption lines of  $7190.2890\text{cm}^{-1}$  and  $7190.7388\text{cm}^{-1}$  spectral lines pairs are used as the absorption lines of spectrum temperature measurement method. The ratio of spectral line intensity to area is compared by numerical simulation, and it is proved that the spectral line meets the requirements of gas temperature and concentration measurement by back-stepping method. TDLAS experimental platform was built to verify that the spectral pair is suitable for gas temperature and concentration measurement.

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