Measurement of CO temperature and concentration in flat flame based on mid infrared wavelength modulation

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Abstract. CO in combustion products of aeroengine is a sign product of incomplete combustion. Real-time monitoring of CO can feedback combustion efficiency, which is of great significance to the design of combustion chamber and the optimization of fuel ratio of aeroengine. In this paper, based on the mid infrared absorption spectroscopy, a single optical path calibration-free wavelength modulation method is proposed to measure the temperature and concentration of CO in a flat flame. Firstly, the spectrum of light intensity signal and the amplitude frequency response of different frequencies are analysed, and the appropriate scanning frequency and modulation frequency are selected. Secondly, the equalization of Butterworth filter in DPLA is proposed to extract the first and second harmonics. The filter can effectively reduce the influence of nonlinear phase. Furthermore, calibration-free wavelength modulation method is simulated to measure CO at different temperature and concentration. Finally, CO in flat flame with different equivalence ratio at 5mm was measured for verification. The relative error between the measurement results of calibration-free wavelength modulation and that of thermocouple measurement is within 3.6% in the range of concentration 0.11% ~ 0.24%, which verified the feasibility and effectiveness of the measurement scheme, and provided a reference for the CO concentration measurement at the outlet of aeroengine.

1. Introduction

There are mainly gases such as carbon oxygen compounds, nitrogen oxides, unburned hydrocarbons and solid fine particles in the combustion of hydrocarbon fuel of aeroengine, in which CO is the landmark gas product of incomplete combustion and also a very important intermediate product [1-2]. At high temperature, CO has the characteristics of fast reaction rate and rapid concentration change. TDLAS (Tunable Diode Laser Absorption Spectroscopy, TDLAS) has the characteristics of high time resolution, high sensitivity and strong anti-interference ability. Therefore, it can monitor CO in high temperature combustion environment in real time and feedback combustion efficiency in time, which is of great significance to the optimization design of aeroengine combustion chamber and fuel ratio [3].

With the rapid development of photoelectric technology, TDLAS based on mid infrared absorption spectroscopy is gradually applied to CO measurement. Ronald K Hanson used 4.25 μm and 4.86 μm QCL on the supersonic combustion platform to monitor the mole fraction of CO and CO₂ in the combustion tail gas online [4] R M Wpearrin used QCL to simultaneously measure the temperature change and the concentration change of CO₂ and CO in the supersonic combustion flow field by direct absorption method and wavelength modulation method [5]. Kristin integrated near-infrared (1.39 μm) TDLAS and mid-infrared (2.7, 4.8μm) TDLAS into a light-path coaxial measurement system and measured the static temperature and H₂O, CO, CO₂ concentrations on the RC-22 scramjet at
wright-Patterson air force base [6]. In China, Tantu used QCL and new multi-channel pool to measure N₂O and CO in the atmosphere by wavelength modulation method [7]. Using quantum cascade laser, Tang Yuanyuan measured CO and NO in vehicle exhaust by direct absorption method [8].

A lot of researches have been carried out on the measurement of CO based on mid infrared absorption spectroscopy all over the world, while the research in this field in China mainly focuses on direct absorption method and traditional wavelength modulation method. The direct absorption method is simple and direct, but it is difficult to obtain the unabsorbed light intensity information when the environment of the measurement object is complex and the interference is serious. Traditional WMS (Wavelength Modulation Spectroscopy, WMS) needs to calibrate the application scenarios, and its application is greatly limited [9]. In this paper, based on the mid infrared absorption spectroscopy, the temperature and concentration of CO in the flat flame are measured simultaneously under the single optical path with calibration-free wavelength modulation. Generally, the measurement space of the ground bench test and flight test is limited, and it is difficult to arrange a complicated optical path to improve the measurement accuracy [10]. In addition to the advantages of high detection sensitivity and reduced impact of low-frequency noise, the mid-infrared calibration-free wavelength modulation measurement system can effectively reduce the impact of ground vibration on the measurement optical path, and has the advantages of simplicity, portability, and easy installation [11-12]. The research in this paper provides strong technical support for combustion efficiency evaluation, fuel ratio optimization and pollutant emission monitoring in aero engine bench test and flight test.

2. Basic principle

The basic principle of TDLAS technology is beer Lambert Law [13]. It describes the relationship between the intensity of light absorption, the concentration of light absorbing substance and the thickness of medium. The general expression is as follows:

$$I_t = I_0 \exp[S(T) \cdot \psi(\nu) \cdot P \cdot \chi \cdot L]$$

Where, $I_0$ and $I_t$ are the input and output light intensity, $\psi(\nu)$ is the integral area normalized absorption linear function, $P$ is the measurement environment pressure, $\chi$ is the molar concentration of the absorption component, $L$ is the absorption optical path, $S(T)$ is the line intensity of the absorption spectral line. The wavelength modulation method is to modulate the laser wavelength with high frequency signal. When the modulated signal is cosine signal, the change rule of the output optical wavelength is as follows:

$$\nu(t) = \nu_0 + a \cos(\omega t)$$

Where, $\nu_0$ is the central wavelength of the laser, $a$ is the modulation amplitude, and $\omega$ is the modulation angular frequency. The corresponding intensity modulation can be expressed as [14]:

$$I_0(t) = \bar{I}_0 [1 + i_0 \cos(\omega t + \psi_1) + i_2 \cos(2\omega t + \psi_2)]$$

Among them, $I_0(t)$ is the instantaneous laser intensity, $\bar{I}_0$ is the average laser intensity, $i_0$ and $i_2$ respectively are the linear and nonlinear modulation amplitudes of laser intensity, $\psi_1$ and $\psi_2$ respectively are the linear and nonlinear phase differences between frequency modulation and optical emphasis. The first harmonic X and Y components of the absorption signal can be obtained by digital phase-locked processing of $f_m$ and $2f_m$ sine and cosine reference signals respectively and low-pass filtering:

$$X_{1f} = \frac{G_{1f}}{2} [H_1 + \frac{i_0}{2} (H_0 + \frac{H_1}{2}) \cos \phi_1 + \frac{i_2}{2} (H_1 + H_2) \cos \phi_2]$$

$$Y_{1f} = \frac{-G_{1f}}{2} [i_0 (H_0 - \frac{H_1}{2}) \sin \phi_1 + \frac{i_2}{2} (H_1 + H_2) \sin \phi_2]$$

Similarly, the X and y components of the second harmonic signal:
In order to eliminate the influence of photoelectric amplification coefficient $G$ and average light intensity, $1f$ is used here to normalize $2f$ signal. The normalized harmonic signal can be free from the influence of particles, light intensity jitter and other noises or losses on the measurement \[15\], which can be expressed as:

\[
S_{ij} = \left( \frac{X_i + Y_i}{X_i} \right) \left( \frac{S_{ij}}{S_{jj}} \right)
\]

Because at the centre frequency, the odd term of $H_k$ is 0. When the case of weak absorption is considered ($\alpha < 0.05$), the above formula can be further simplified. The nonlinear term ($i_2 \approx 0$) can be ignored. The phase of frequency modulation and intensity modulation can be approximately opposite. The linear phase difference between them is $\pi$ [16, 17]. So, the above formula can be reduced to:

\[
S_{ij} (\nu_0) \approx -\frac{1}{i_1} H_2 (\nu_0) = -\frac{1}{i_1} \frac{S(T)P \chi L}{\pi} \int_{-\pi}^{\pi} \phi(\nu_0 + a \cos \theta) \cos(2\theta) d\theta
\]

From the above formula, the calculation formula of temperature and concentration can be obtained:

\[
T = \frac{h^2 c}{k} \left( E_2 - E_1 \right)
\]

\[
\ln R_{ij} / \ln i_1 + \ln \frac{A_i}{A_j} + \ln \frac{S_j(T_0)}{S_i(T_0)} + \frac{h^2 c}{k} \left( \frac{E_2 - E_1}{T_0} \right)
\]

Where, $i_1$ and $i_2$ are laser linear modulation amplitudes and they are the intrinsic parameters of the laser. In this paper, the same laser is used to scan two absorption lines at a time, so $i_{11} = i_{12}$. If the measured component concentration is small enough, the linear function is not sensitive to the component concentration, and the concentration can be expressed as follows:

\[
\chi = -\frac{\pi i_1 S_{ij}}{PS(T)LA}
\]

In the measurement of calibration-free wavelength modulation, $T$ and $\chi$ need to be iterated repeatedly. Finally, the temperature and concentration measurement results are obtained by iterative convergence. The iterative process is as follows in Figure 1.
### Figure 1. Iterative process of calibration-free algorithm.

3. Simulation calculation

3.1. Digital dual channel phase lock technologies

In this paper, digital dual channel phase-locked technology is used to extract the first harmonics and the second harmonics of the original signal. In this method, the phase difference between the reference signal and the measured signal can be eliminated by using double channel phase lock [18]. However, Butterworth filter has phase nonlinearity and the group delay in the band-pass range is not constant, the original signal will be distorted in the filtering process. The all-pass filter is a filter with an amplitude frequency response of 0dB. In the full band range, the signal amplitude will not change, mainly changing the phase of the input signal [19]. Therefore, the influence of nonlinear phase and unfixed group delay can be improved by cascading Butterworth filter with all-pass filter [20]. The phase and group delay of low-pass filter before and after improvement are shown in Figure 2 and Figure 3. The processing flow of digital dual channel phase-locked technology is shown in Figure 4.

**Figure 2.** The phase of Butterworth filter before and after improvement.

**Figure 3.** The group delay of Butterworth filter before and after improvement.
3.2. Simulation of calibration-free wavelength modulation method

In order to study the method of wavelength modulation without calibration, the algorithm is simulated by MATLAB. The simulation conditions are as follows: the measurement optical path is 10cm, the pressure is 1atm, the temperature is 1200K, and the concentration is 0.05%. After the mixing signal collected by the detector is processed by the lock-in amplifier, the WMS-2f signal and WMS-1f signal of two spectral lines can be obtained, as shown in Figure 5.

According to formula (8), formula (11) and formula (12) are iterated to obtain the temperature and component concentration of CO. At the beginning of the iteration, the initial CO temperature $t_0 = 800K$, and the component concentration $x_0 = 0.35\%$. The iterative calculation process of temperature and concentration is shown in Figure 6. After 9 iterations, the results of temperature and concentration converged. The final calculated temperature value $T = 1184.5K$, the relative error is 1.29%; the component concentration value $x = 0.051\%$, the relative error is 2.66%. Simulate the measurement of different concentrations and temperatures, and the simulation results are shown in Table 1.
Table 1. Simulate the measurement of different concentrations and temperatures.

| Setting Temperature(K) | Setting Concentration | Calculated Temperature(K) | Calculated Concentration | Relative error of Temperature | Relative error of Concentration |
|------------------------|-----------------------|----------------------------|--------------------------|-------------------------------|---------------------------------|
| 1200                   | 0.6%                  | 1064.5                     | 0.521%                   | -11.26%                       | -13.3%                          |
| 1200                   | 0.4%                  | 1148.3                     | 0.384%                   | -4.3%                         | -4.1%                           |
| 1200                   | 0.1%                  | 1167.4                     | 0.102%                   | 2.6%                          | 2.3%                            |
| 1200                   | 0.05%                 | 1184.5                     | 0.051%                   | 1.28%                         | 2.6%                            |
| 1500                   | 0.05%                 | 1481.0                     | 0.051%                   | 1.26%                         | 1.4%                            |
| 1800                   | 0.05%                 | 1779.6                     | 0.052%                   | 1.13%                         | 0.45%                           |

From the simulation results can be obtained. At the same temperature, the relative error of temperature and concentration increases with the increase of concentration; at the same concentration, the relative error of calculated temperature and concentration decreases with the increase of temperature. This is because the theory of the algorithm is based on the assumption of weak absorption (α < 0.05). When the absorption coefficient α is large, the calculation error of the algorithm is large. Therefore, at the same temperature, the concentration and absorption coefficient increase gradually. When the temperature is 1200K and the concentration is increased to 0.6%, the absorption coefficient of one absorption peak is 0.06, which is too large and the approximation effect of weak absorption assumption is poor. When the concentration is constant and the temperature increases, the absorption coefficient decreases gradually. The better the approximation effect of weak absorption hypothesis is, the smaller the relative error is. Therefore, when the temperature is near 1200K and the concentration is greater than 0.6%, the measurement error of the calibration-free wavelength modulation algorithm is large.

4. Experimental verification

4.1. Introductions to measurement system

Based on the technology of mid infrared absorption spectroscopy, an open single optical path calibration-free wavelength modulation measurement system is constructed in this paper. The light source of the system is a quantum cascade laser provided by Ningbo Haier Xin Optoelectronic Technology Co., Ltd. By tuning the wavelength to 2060 cm\(^{-1}\), it can be continuously tuned in the range of 2051 cm\(^{-1}\) ~ 2071 cm\(^{-1}\). It can be used for continuous and non-contact detection of flat flame CO. The flame furnace is McKenna flat flame furnace, the diameter of the middle furnace surface is 60mm, and nitrogen is introduced into the furnace surface to isolate air and stabilize the flame. High precision flow controller is used to control the equivalence ratio of fuel and air. The signal generator adopts ET 3325 dual channel function / arbitrary waveform generator provided by Beijing Henglong Shengda Technology Co., Ltd, which can provide the sawtooth wave signal with the frequency of 20Hz ~ 1MHz and cosine wave signal with frequency of 300Hz ~ 1MHz. The detector is a thermoelectric cooled optoelectronic detector produced by Ningbo Haier Xin Optoelectronic Technology Co., Ltd., which is sensitive to 2 ~ 10 μm mid infrared spectrum. Using NI USB-6361 signal acquisition card provided by National Instruments, the maximum sampling rate of the single channel is 2MS / s, and the resolution is 16 bits, which can ensure the effective acquisition of the absorption signal. The centre frequency of the optical filter provided by Thorlabs is 4.75 μm and the bandwidth is 400nm, which can effectively filter out the stray light of infrared radiation. The temperature verification adopts the S-type thermocouple measurement verification of Omega company, which can realize the temperature measurement within 1600 °C, and the measurement accuracy is 1 °C. The experimental device is shown in Figure 7.
4.2. Frequency selections

Appropriate scanning frequency and modulation frequency directly determine whether the harmonic signal can be obtained accurately. If the modulation frequency is too high, the output waveform will produce amplitude frequency distortion; if the modulation frequency is too low, the low-frequency noise cannot be effectively suppressed. Therefore, it is necessary to analyse the spectrum, amplitude frequency and integration step characteristics of the laser intensity signal, so as to select the appropriate scanning frequency and modulation frequency.

Firstly, the spectrum of laser intensity signal is analysed, as shown in Figure 8. From the spectrum, it is not hard to find that there is a relatively prominent 253kHz high-frequency noise in the high-frequency part. This noise is the inherent noise of the laser used for feedback control, which will reduce the signal to noise ratio of the second harmonic and lead to inaccurate peak value. Secondly, because of the existence of the reactance element of the amplifier in the laser and the detector, the gain of the signal with different frequency components is different, which will cause the amplitude frequency distortion of the output waveform. Therefore, it is necessary to input fixed amplitude signals of different frequencies to the laser to determine the frequency range of amplitude frequency distortion, as shown in Figure 9. When the input signal frequency is greater than 100kHz, the output signal amplitude will be seriously distorted. Finally, the harmonic coefficient is obtained by numerical integration. Only a small integration step can get the accurate value of the peak of the harmonic signal. Therefore, each integration period needs enough data points to reduce the error of numerical integration. Scanning frequency value should not be too large. Based on these reasons, it is determined that the scanning frequency is 100Hz and the modulation frequency is 100kHz.
4.3. Verification of flat flame CO measurement

In order to verify the calibration-free wavelength modulation method, the CO concentration and temperature of flat flame at 5mm under the equivalence ratio of 1.3 were measured at 100Hz scanning frequency and 100kHz modulation frequency. The collected light intensity signal is passed through the digital phase-locked low-pass filter to obtain 1f signal and 2f signal. The relationship between concentration and temperature with time is obtained by introducing it into the iterative formula. The temperature measurement result is 1230.9K + δ0.013. The concentration measurement result is 0.24% + δ0.048. The average response time of the system is 0.072s + δ0.012, as shown in Figure 10 and Figure 11. The thermocouple measures 1252k. The relative error between temperature measurement result and thermocouple measurement result is 1.6%. The temperature and concentration measurement results of equivalence ratio 1.1 ~ 1.4 are shown in the Figure 12 and Figure 13.

![Figure 10](image1.png)  
**Figure 10.** The temperature measurement results with calibration-free wavelength modulation when the equivalence ratio is 1.3.

![Figure 11](image2.png)  
**Figure 11.** The concentration measurement results with calibration-free wavelength modulation when the equivalence ratio is 1.3.

![Figure 12](image3.png)  
**Figure 12.** The comparison between the temperature measurement results of calibration-free wavelength modulation and that of thermocouple.

![Figure 13](image4.png)  
**Figure 13.** Concentration measurement results with equivalence ratio of 1.1-1.3.

The relative error between the temperature measurement results and the thermocouple measurement results is within 3.6%. However, when the ratio is 1.4, the relative error of temperature measurement results is large. This is because the CO concentration is relatively high, the absorption coefficient is 0.064, the approximation effect of weak absorption assumption is poor, and the measurement error is large, so the calibration-free wavelength modulation method is no longer applicable. The CO measurement of flat flame verifies the validity and reliability of calibration-free wavelength modulation method with the temperature of 1200 K and concentration of 0.11% ~ 0.24%.
5. Conclusions
In this paper, based on the mid infrared absorption spectrum technology, the single optical path calibration-free wavelength modulation method is used to measure the CO concentration of the flat flame from 0.11% ~ 0.24%. The relative error between the temperature measurement results and the thermocouple measurement results is within 3.6%. The validity and reliability of the scheme are verified. The research in this paper provides a timely, accurate and effective reference scheme for the combustion efficiency evaluation, fuel ratio optimization and pollutant emission monitoring in the aircraft engine bench test and flight test.

Reference
[1] Wu S T 2019 A review of research and development process of aeroengine combustion chamber design [J]. Shanghai Energy Conservation 07 584-588
[2] Liu T 2014 Basic research and progress of advanced engine combustion and key scientific issues[J]. China Science Foundation 92 20-25
[3] Hu Z Y 2018 Advances in diagnostic technology of laser combustion in Aeroengine ground test. Experimental Fluid Dynamics 32 33-42
[4] Hanson R K, Kunts P A and Kruger C H 1997 High-resolution spectroscopy of combustion gases using a tunable diode laser[J]. Applied Optics 16 2045-2048
[5] Jeffries J B and Hanson Spearrin R M 2014 Mid-infrared Absorption Sensor for Measurements of CO and CO2 in Propulsion Flows 52nd Aerospace, in American Institute of Aeronautics and Astronautics
[6] Michael S B and Mark Kristin M B 2016 Common-path measurement of H2O, CO, and CO2 via TDLAS for combustion progress in a hydrocarbon-fueled scramjet, in 54th AIAA Aerospace Sciences Meeting, American Institute of Aeronautics and Astronautics
[7] Tan T, Liu K, Wang G S, Wang L, Chen W D and Gao X M 2015 Research on high sensitivity measurement of CO and N\textsubscript{2}O based on mid infrared QCL laser and new multi pass cell [J]. Acta Optica Sinica 35 358-364
[8] Tang Y Y, Liu W Q, Yi R F, Zhang Y J, Zhang S, Xu Z Y and Ruan J 2011 based on quantum cascade laser, high sensitivity and fast detection of vehicle exhaust gas concentration [J]. China Laser 38 226-231
[9] Pan H, Wang G Y, Song J L and Yu X H 2014 Application of uncalibrated wavelength modulation spectroscopy in gas temperature and concentration measurement [J]. Infrared and Laser Engineering 43 956-960
[10] Zhao R and Cai W Z 2018 Research on temperature distribution debugging and testing technology of aeroengine combustor exit [J]. Tactical Missile Technology (05) 84-89
[11] Nie W, Yi R F and Yang C G 2018 [J]. China Laser 45 9-29
[12] Cheng H Y 2017 Research and optimization of calibration free gas detection method in wavelength modulation spectroscopy [D]. Southeast University 72
[13] Lambert J H 1760 Photometria sive de mensura et gradibus luminis, colorum et umbrae [Photometry, or, On the measure and gradations of light, colors, and shade] (in Latin). Augsburg, (Germany): Eberhardt Klett
[14] Rieker G B, Jeffries J B and Hanson R K 2009 [J]. Applied Optics 48 5546-5560
[15] Hu Y J, Zhao X Y and Zhang R 2013 [J]. Acta Optica Sinica 33 113000
[16] Qu D S, Hong Y J, Wang G Y and Hu P 2013 [J]. Acta Optica Sinica 33 338-343
[17] Yang B 2012 Research on near infrared TDLAS technology for RBCC parameter measurement [D]. Xi'an: Northwest University of technology 68-71
[18] Hu S M and Zhang G F 2000 [J]. Journal of Data Acquisition & Processing 15 222-225
[19] Han J C 2015 [J]. Electroacoustic Technology 39 35-39
[20] He L L 2019 Group delay optimization of IIR digital filter [D]: Xi'an University of Posts and telecommunications 83