

SIMULATION AND EXPERIMENTAL STUDY OF DIESEL ENGINE EMISSION TEMPERATURE BASED ON TUNABLE DIODE LASER ABSORPTION SPECTROSCOPY

by

Xiaotao YANG*, Xiaonan LIU, Yanlong MU, Yanbo HE, Shaotian CHEN,
Zijian ZHANG, Ziyin JIANG, and Lele YANG

College of Power and Energy Engineering, Harbin Engineering University
Harbin, China

Original scientific paper
<https://doi.org/10.2298/TSCI190412461Y>

Based on the temperature measurement technology of tunable diode laser absorption spectroscopy, the simulation and experimental research on the temperature measurement of CO₂ gas emitted by D4114B Diesel engine is realized. The light source model, gas chamber model and data detection model were established by using SIMULINK, which is more general numerical simulation tool in MATLAB. Under the simulated Diesel engine emission environment, the measured CO₂ gas temperature was obtained by model simulation and analyzed. The simulation relative error was 0.077%. The marine D4114B Diesel engine was used as the test object, the visual window was reconstructed on the exhaust light path, and an optical path test system was established. The tunable diode laser was used as the detection light source to carry out on-line test research on the CO₂ gas temperature in the exhaust gas emission. The relative error was 4.4%. The results show that the model built by SIMULINK can reflect the actual laser modulation effect and CO₂ gas absorption. The simulation results have certain reference value for the research of tunable diode laser absorption spectroscopy temperature measurement system.

Key words: *tunable diode laser absorption spectroscopy, SIMULINK simulation, CO₂, Diesel engine emission*

Introduction

Diesel engines are compression ignition internal combustion engines, with combustion as their core function. Therefore, more in-depth and intuitive understanding of the combustion process of Diesel engines is required in the design process in order to improve and optimize emission control performance [1]. Diesel emissions contain important information on various parameters, for example temperature and pressure of exhaust gases. The above parameters are of great significance for evaluating the emission performance of Diesel engines and determining the operating state of Diesel engines. Transient emission data for closed-loop control of Diesel engines can be acquired by investigating Diesel engine emission components and combustion products. The closed-loop control of Diesel engines can provide strong support for in-depth study of the combustion process, optimization of the control strategy, and optimization of the performance of Diesel engines. In addition, the non-optical method has the shortcomings of short service life, easy aging and non-real time. The traditional contact measurement is easily

* Corresponding author, e-mail: yangxiaotao1985@163.com

affected by the bad temperature field environment caused by high temperature, which limits the instrument to obtain higher measurement accuracy and better spatial-temporal resolution. Therefore, temperature measurement technology based on tunable diode laser absorption spectroscopy (TDLAS) plays an increasingly important role in temperature field measurement due to its advantages of non-contact, real-time online, high sensitivity and high resolution.

Temperature can be measured using the direct temperature measurement technique of TDLAS on the basis of the relationship between the absorbed light intensity and the gas temperature under the absorption law [2-4]. Using this method, measurements can be taken over an extremely wide temperature range with high test accuracy, especially in high temperature field measurement, and intermediate products in the combustion process can be simultaneously detected, thus showing obvious advantages over the existing optical temperature measurement system [5]. The direct measurement method has a simple structure and does not require calibration. It is convenient for calculating the temperature of the gas to be measured. Based on the TDLAS technology, this study investigated on-line monitoring of the temperature characteristics of Diesel engine emissions, and selected CO₂ with a large volume concentration in the effluent for analysis. Firstly, the direct measurement method was used to establish the theoretical model of the diesel exhaust CO₂ emission online monitoring system in SIMULINK and the simulation analysis was performed. Then, the test system was built on a self-designed diesel exhaust light path to carry out experiments, and actual experimental results were obtained [6, 7].

Methodology

For direct measurement based on TDLAS, the absorbed gas concentration can be obtained by measuring the spectral absorption signal [8]. From the obtained signal, interference between lines, various noises, etc. can be easily analyzed. The temperature can be calculated directly in a convenient and rapid manner because calibration using standard gas is not required. However, in the direct measurement process, the determination of the reference signal is critical to the concentration calculation process, especially in the case of low absorbance. Therefore, it is important to obtain the reference signal accurately [9].

Beer-Lambert law

According to the Beer-Lambert law [10], when a monochromatic laser passes through a gas medium, the intensity change can be expressed as:

$$I_t = I_0 \exp[-\alpha(\nu)] \quad (1)$$

where I_0 is the intensity of the reference laser when no laser light is absorbed, and I_t – the intensity of the absorbed laser. The definition $\alpha(\nu)$ is the spectral absorption rate obtained in the measurement, which can be expressed:

$$\alpha(\nu) = PS(T)\phi(\nu)XL \quad (2)$$

where P [atm] is the total pressure of the measured area, $S(T)$ [cm⁻²atm⁻¹] – the absorption line strength of the gas, $\phi(\nu)$ [cm] – the linear function used to characterize the shape and line width of the absorption line, which is related to temperature and pressure, X – the volume concentration of the gas, and L [cm] – the propagation distance of the laser through the gas.

Absorption line-strength

The absorption line strength indicates the degree of absorption of the incident light intensity by gas molecules. It is the combined effect of absorption and radiation for transition

at the molecular level. The value is related to the number of molecules corresponding to the transition level and the transition probability. For a particular molecular absorption line, the line strength depends only on the temperature and can be calculated from the molecular spectral database HITRAN. In actual use, a reference temperature, T_0 , is firstly selected, and the line-strength, $S(T_0)$, corresponding to the reference temperature, T_0 , is determined from the HITRAN database. Under certain temperature conditions, the line strength of the line can be calculated by:

$$S_i(T) = S_i(T_0) \frac{Q(T_0)}{Q(T)} \exp \left[-\frac{hcE_i''}{k} \left(\frac{1}{T} - \frac{1}{T_0} \right) \right] \times \frac{1 - \exp \frac{-hcv_{0,i}}{kT}}{1 - \exp \frac{-hcv_{0,i}}{kT_0}} \quad (3)$$

where Q is the total intramolecular partition function, E_i'' [cm^{-1}] – the low transition energy, h [Js] – the Planck constant, k [JK^{-1}] – the Boltzmann constant, c [cms^{-1}] – the speed of light, and $\nu_{0,i}$ [cm^{-1}] – the transition frequency. Where Q uses a polynomial fit to get an approximation:

$$Q(T) = a + bT + cT^2 + dT^3 \quad (4)$$

The coefficients a , b , c , and d have different values depending on the gas and temperature range and can be queried through the HITRAN database when performing calculations. It should be noted that for line strength obtained from HITRAN database queries, unit conversion must be performed before the calculation based on the Beer-Lambert law.

Linear function

The absorption line shape is a distribution state centered on the frequency of the molecular transition point, and the main considerations for causing such distribution are Doppler broadening (thermal action) and collision broadening (molecular collision action). The linear function reflects the relative change of the spectral absorption coefficient with frequency or wavelength and satisfies $\int_{-\infty}^{+\infty} \phi(\nu) d\nu \equiv 1$. Thus, $\alpha(\nu)$ can be obtained by integrating the whole linear function, which is a function of only temperature and component concentration. The line functions of the spectral line are mainly divided into three types: Gaussian line type, Lorentz line type, and Voith line type. Taking into account the actual situation of diesel exhaust emissions, the Lorentz line type function (5) was selected in this study:

$$\phi_C(\nu) = \frac{1}{2\pi} \frac{\Delta\nu_c}{(\nu - \nu_0)^2 + \left(\frac{\Delta\nu_c}{2} \right)^2} \quad (5)$$

where $\Delta\nu_c$ is the line width widened by the collision, proportional to pressure under conditions determined by ambient temperature:

$$\Delta\nu_c = P \sum X_B 2\gamma_{A-B} \quad (6)$$

where P is the total pressure of the environment, A – a certain gas, and X_B – the mole fraction of the collision gas B. The γ_{A-B} [$\text{cm}^{-1}\text{atm}^{-1}$] is the collision broadening coefficient, and its value can be obtained experimentally. The collision broadening coefficient of different gas molecules are available in the database.

Temperature measurement

Temperature measurement using TDLAS is mainly based on the two-wire measurement approach. The basic principle is that the amplitude of the line intensity of different spectral lines changes with the change of temperature. Two relatively independent spectral lines are selected as the test object, and the relative values of their line strengths at different temperatures are calculated. The average temperature on the measured optical path is inverted by the relative ratios of the two absorption spectral lines.

Combining eqs. (1) and (2) to integrate the two sides of eq. (6) in the frequency domain, eq. (7) can be obtained:

$$A = \int_{-\infty}^{+\infty} -\ln\left(\frac{I_t}{I_0}\right) dv = PXS(T)L \tag{7}$$

where A represents the integrated area of the spectral absorption rate.

From the two-wire measurement approach:

$$\left(\frac{S_1}{S_2}\right)_T = \left[\frac{(SPLX)_1}{(SPLX)_2}\right]_T = \left(\frac{A_1}{A_2}\right)_T = R \tag{8}$$

Gas temperature can be obtained by the following formula:

$$T = \frac{\frac{hc}{k}(E_2'' - E_1'')}{\ln \frac{A_1}{A_2} + \ln \frac{S_2(T_0)}{S_1(T_0)} + \frac{hc}{k} \frac{(E_2'' - E_1'')}{T_0}} \tag{9}$$

Results and discussion

In order to complete the on-line monitoring of the temperature characteristics of the Diesel engine emissions, the test object can be abstracted into several parts, and then the software is used to build the model and run. The simulation system, as shown in fig. 1, consists of three parts: light source, air chamber absorption, and data detection.

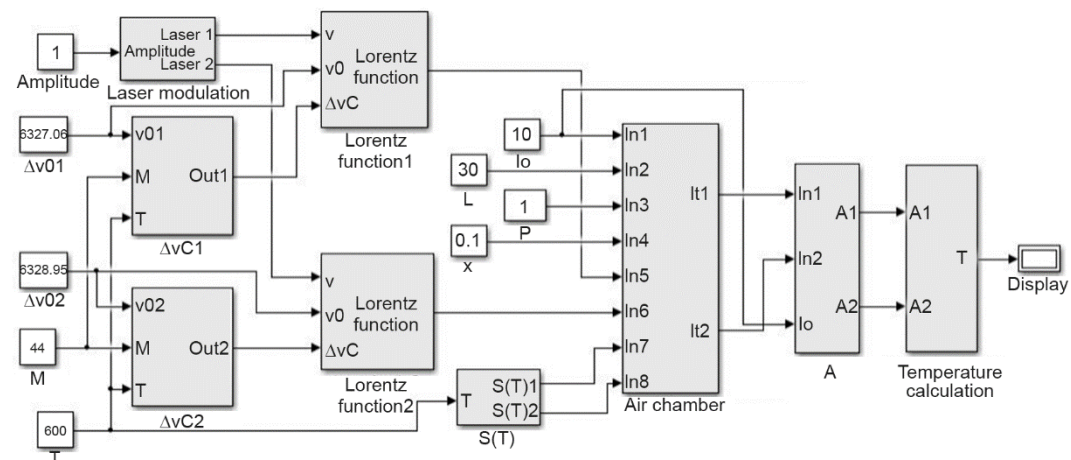


Figure 1. Schematic diagram of the SIMULINK simulation system model

Light source model

The source model is shown in fig. 2. The saw-tooth sweep signal provides the drive current for the DFB laser and periodically changes the output wavelength. The laser outputs light parameters to the gas absorption part.

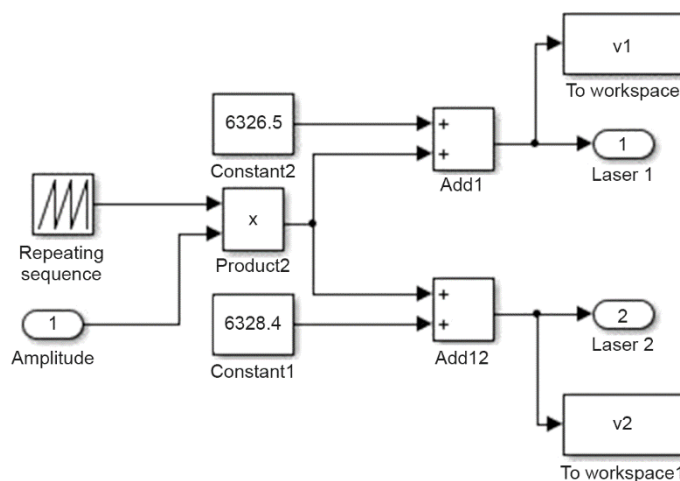


Figure 2. Schematic diagram of the light source model

Air chamber absorption model

The gas chamber absorption model is mainly constructed according to the line absorption function model of the gas to be measured at the center wavelength, and its function is to simulate the absorption of the laser in the gas chamber. At low pressure, the line type is determined by the Gaussian function, and the shape of the function is expressed by the Doppler line width, which is determined by temperature. As pressure increases, the collision broadening mechanism changes the spectral width of the line type, and the influence of the Lorentz function in the linear type becomes larger. In this study, the Lorentz linear function model was used. The gas chamber absorption model is shown in fig. 3.

Data detection model

The data detection model is mainly constructed on the basis of the absorption of the gas to be measured at a specified absorption line, as shown in fig. 4. SIMULINK and .m files are combined with the MATLAB Function module to simplify the temperature calculation process.

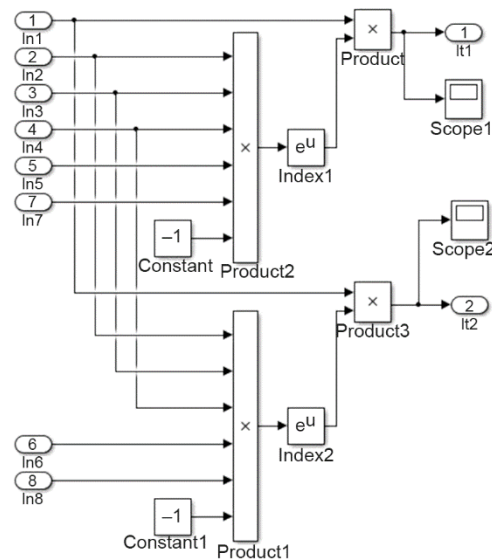


Figure 3. Schematic diagram of the gas chamber absorption model

Line selection

The intensity of gas absorption lines vary with temperature depending on the low-state transition energy of the molecule. First, it is necessary to make the spectral line pairs have a sufficiently low transition energy difference in order to ensure that the spectral lines intensity ratio, R , has high sensitivity to temperature. Then, according to the temperature range to be measured, two spectral lines having sufficiently large and relatively independent spectral lines will be selected to satisfy the TDLAS technical temperature measurement conditions. Finally, selecting the appropriate line width within the temperature range allows for better resolution of the line. According to the above requirements, two absorption lines with a frequency of 6327.06 cm^{-1} and 6238.95 cm^{-1} are used in the simulation model. In particular, both the spectral absorbance integral value ratio and the line intensity ratio obtained by the direct absorption method are equal. As shown in fig. 5(b), the line intensity ratio, R , decreases as the temperature increases, and when the experimental temperature is between 500 and 650, it can have a good response to the temperature measurement and meet the exhaust temperature range under normal operation of the Diesel engine.

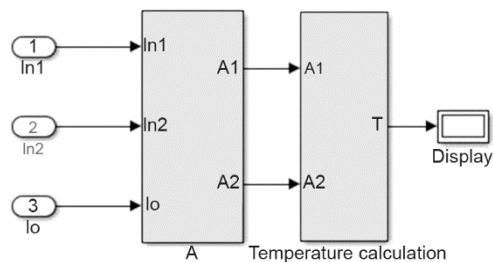


Figure 4. Data detection model

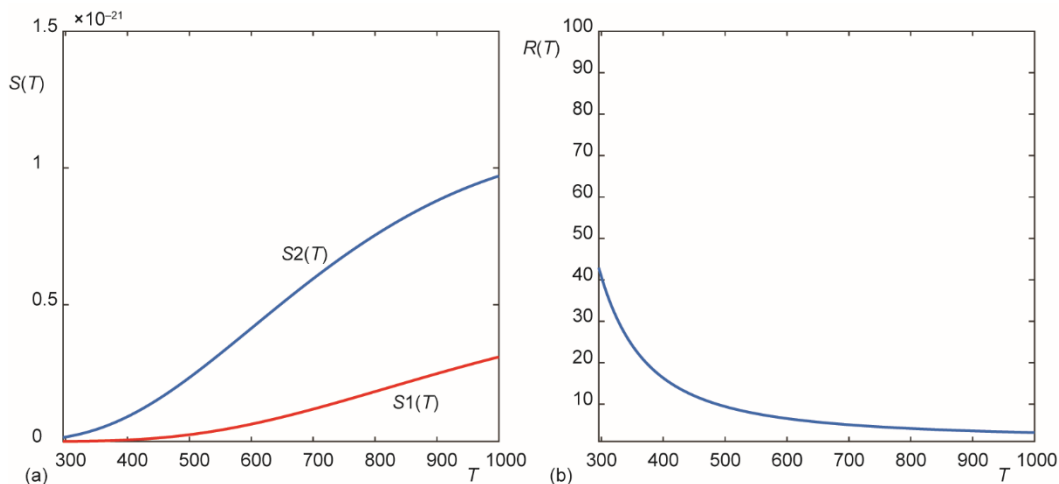


Figure 5. (a) Line strength-temperature curve, (b) $R(T)$ parameter variation curve

Analysis of simulation results

The two-wire temperature measurement approach was adopted in the simulation model. The frequency of spectral line 1 is 6327.06 cm^{-1} , the transition energy of low state is 234.08 cm^{-1} , the frequency of spectral line 2 is 6238.95 cm^{-1} , and the transition energy of low state is 197.41 cm^{-1} . The CO_2 concentration was set to 10%, the optical path was 30 cm, the total pressure was 1 atm, and the gas temperature was 600 K. The simulation process is as shown in fig. 6.

In the simulation process, the spectral absorption rate is collected to obtain a gas absorption curve. The simulation results are shown in fig. 7, which basically reflects the actual gas chamber absorption. The figure shows that the absorption peak of spectral line 1 is significantly larger than that of spectral line 2; in the simulation calculation, the gas absorption curve is integrated according to the spectral absorption rate data to obtain an integral ratio, R . The ratio is introduced into eq. (9) to obtain a simulation temperature of 599.54 K, with an error of 0.077%.

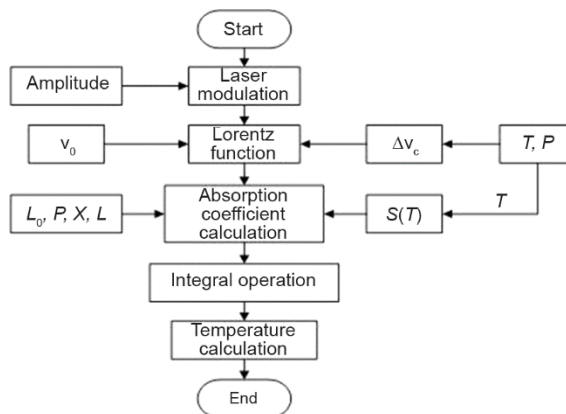


Figure 6. Flow chart of the simulation process

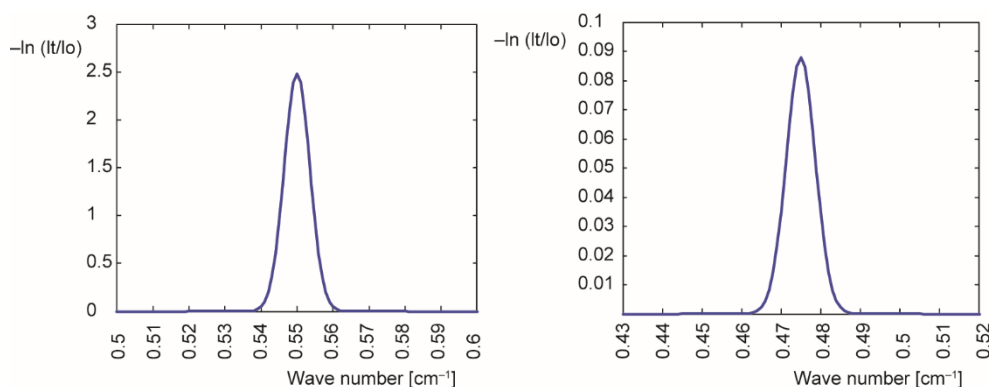


Figure 7. Gas absorption curves

Experimental study on discharge temperature of D4114B Diesel engine

In this study, the direct detection method was used to carry out online test of CO_2 gas temperature emitted by a Diesel engine. The direct test structure is shown in fig. 8.

In this experiment, a 4-cylinder D4114b Diesel engine was selected. Its rated power is 90 kW, rated speed is 1500 rpm, cylinder diameter is 114 mm, compression ratio is 17.3, and exhaust volume is 5.308 L. A DFB tunable semiconductor laser was selected as the light source. The center wavelength was 1508.387 nm and the maximum output power was 17 mW. In the experiment, the DFB tunable semiconductor laser was precisely controlled at a laser operating temperature of 28 °C using the ITC4001 Benchtop Laser Diode/TEC Controller (Thorlabs). The AFG2021 waveform generator (Tektronix) was used to provide a 200 Hz sawtooth signal as an external trigger signal. The PDA10JT thermal photodetector (Thorlabs) was used to convert optical signals into

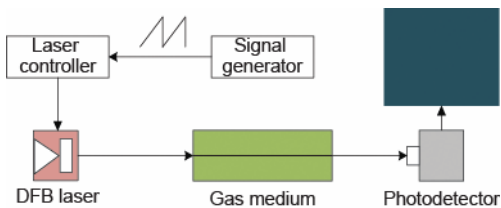


Figure 8. Direct test structure

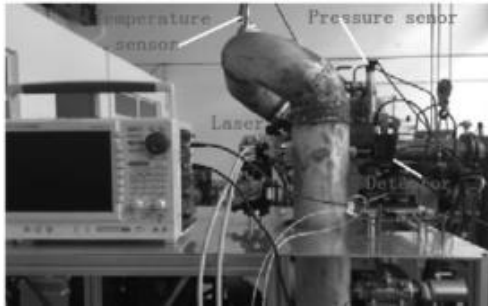


Figure 9. Set-up of the Diesel engine emission online test

electrical signals. A data acquisition card was used to obtain and upload the data to the computer for linear fitting and integral calculation. Then, the corresponding gas temperature information could be obtained. Figure 9 shows the built online test site.

First, the speed of the D4114B Diesel engine was set to 1400 rpm, and then multiple sets of data were obtained by changing the load at constant speed. The temperature sensor and the TDLAS test system simultaneously recorded data and averaged each group of data.

Comparison of temperature measurement values and simulated sensor values under different working conditions

The simulation system temperature measurement values under different working conditions and the Diesel engine emission on-line test sensor values are compared to verify the accuracy of the simulation model.

The test results under various working conditions are shown in tab. 1. From the table, the relative error of the test results was less than 3%, and the data fluctuation range was small, the maximum error was 18.8 K, indicating that the self-designed temperature measurement system can be applied to the online test of Diesel engine emissions. At the same time, the error of temperature calculation results increased with the increase of load power. The cause of the error may be due to an increase in temperature resulting in a decrease in sensitivity of the measurement.

Table 1. Test results under various working conditions

Load power [kW]	40	50	60	70	80
Sensor temperature [K]	532.6	558.3	585.1	611.1	638.3
TDLAS system temperature [K]	521.8	546.1	570.5	593.5	618.4
Relative error [%]	2.0	2.2	2.5	2.9	3.1

Comparison of temperature measurement value and sensor value under the same working condition

In order to further verify the accuracy of the simulation model, the experiment is based on the multiple measurements of the Diesel engine under different working conditions in different time periods. The temperature changes in the exhaust pipe are shown in tabs. 2-4.

Table 2. Temperature test results under 40kW working condition (the sampling interval is 5 minutes)

	1	2	3	4	5
Sensor temperature [K]	532.0	531.2	532.6	532.3	533.3
TDLAS system temperature [K]	521.6	519.3	521.8	520.0	521.2
Relative error [%]	2.0%	2.2%	2.0%	2.3%	2.3%

Table 3. Temperature test results under 60 kW working condition (the sampling interval is 5 minutes)

	1	2	3	4	5
Sensor temperature [K]	583.7	585.1	584.6	581.2	583.0
TDLAS system temperature [K]	568.5	572.2	572.0	566.7	566.1
Relative error [%]	2.6%	2.2%	2.2%	2.5%	2.9%

Table 4. Temperature test results under 80 kW working condition (the sampling interval is 5 minutes)

	1	2	3	4	5
Sensor temperature [K]	644.5	639.2	650.1	640.9	638.5
TDLAS system temperature [K]	622.6	619.4	629.9	621.7	620.7
Relative error [%]	3.4%	3.1%	3.1%	3.0%	2.8%

It can be seen from tables that the relative error between the temperature measurement values of the simulation model and the measured values of the exhaust gas temperature of the Diesel engine under the same working condition are within 4%, indicating that the self-designed temperature measurement system can meet the online test requirements for diesel exhaust emissions. The error of the actual measurement system was significantly larger than that of the simulation because errors in data collection and interference of signals occur in actual measurements.

Conclusions

In this study, the TDLAS direct measurement principle was used to build a model for simulating the gas absorption curve in SIMULINK. The model could realize the measurement of gas temperature and reflect the influence of concentration, pressure, optical path, and other parameters on the gas absorption curve. This has a certain reference value for the development of the software and hardware of an actual TDLAS measurement system. The measurement system was built on the exhaust pipe of marine D4114B Diesel engine to carry out on-line test on CO₂ gas temperature in exhaust gas emission. The test results are in good agreement with the actual results.

This model is suitable for simulating the on-line measurement of diesel exhaust, in various operating conditions, under the condition of satisfying the principle of two-wire temperature measurement. The absorption process of different concentration gases can be simulated by changing parameters of the gas chamber in the model and adjusting corresponding parameters of the light source module. The model introduced in this study mainly shows the research of TDLAS technology for real-time measurement of combustion field temperature, and promoted the application of TDLAS combustion temperature measurements in marine Diesel engines. A large number of simulation experiments based on SIMULINK model not only provide reference value for the on-line measurement of Diesel engines exhaust, but also verify the practicability of TDLAS technology. This study has reference significance for experiments on real-time temperature monitoring of marine Diesel engines.

Diesel engine is a compression ignition internal combustion engine, with a complex internal working environment. When using TDLAS to test in-cylinder products, combustion temperature, and emission products, the influence of changes in test environment parameters on test results should be considered. Furthermore, avoiding interference between the gas

components is important. Therefore, it is necessary to consider the influence of the aforementioned factors on test results comprehensively, and when necessary, the corresponding correction algorithm should be introduced. In the future, the technology for testing pollutant emission from marine Diesel engines will be developed towards the direction of high precision, portable, and real-time on-line measurement of multiple components. Thus, research on on-line test technologies applicable to the emission of pollutants from marine Diesel engines is urgent.

Acknowledgement

This work is supported by National Natural Science Foundation of China (51709059).

Nomenclature

c	– speed of light [cms^{-1}]	$S(T)$	– absorption line strength, [$\text{cm}^{-2}\text{atm}^{-1}$]
E_i''	– low transition energy, [cm^{-1}]	T	– temperature, [K]
h	– Planck constant, [Js]	X	– concentration of the gas
k	– Boltzmann constant, [JK^{-1}]	$\nu_{0,i}$	– is the transition frequency [cm^{-1}]
L	– propagation distance of the laser through the gas, [cm]	<i>Greek symbols</i>	
P	– total pressure of the measured area, [atm]	γ_{A-B}	– collision broadening coefficient, [$\text{cm}^{-1}\text{atm}^{-1}$]
Q	– total intramolecular partition function	$\phi(\nu)$	– linear function, [cm]

References

- [1] Yang, X. T., The Research on Testing Technology for the Diesel Engine Emission Based on the Tunable Laser Absorption Spectroscopy Technology, Ph. D. thesis, Harbin Engineering University, Harbin, China, 2016
- [2] Yao, L., et al., Research on Open-Path Detection for Atmospheric Trace Gas CO Based on TDLAS, *Chin J. Las.*, 42 (2015), 2, pp. 313-320
- [3] Zhang, C. X., O₂ and CO sensing based on Tunable Diode Laser Absorption Spectroscopy, Ph. D. thesis, Zhejiang University, Zhejiang, China, 2016
- [4] Bernd, B., et al., Tunable Diode Laser Absorption Spectroscopy for Moisture Determination in Organic Solvents, *Chemie Ingenieur Technik*, 86 (2014), 1, pp. 136-143
- [5] Shu, X. W., et al., Research on Temperature Compensation Method for HCl Gas on-line Detection Based on TDLAS Technology, *Spectrosc. Spect. Anal.*, 30 (2010), 5, pp. 1352-1356
- [6] Werle, P., et al., Wideband Noise Characteristics of a Lead-Salt Diode Laser: Possibility of Quantum Noise Limited TLAS Performance, *Applied Optics*, 28 (1989), 9, pp. 1638-1642
- [7] Spearrin, R. M., et al., Multi-Band Infrared CO₂ Absorption Sensor for Sensitive Temperature and Species Measurements in High-Temperature Gases, *Applied Physics B*, 116 (2014), 4, pp. 855-865
- [8] Zhang, G. Y., et al., Reconstruction and Simulation of Temperature and CO₂ Concentration in an Axisymmetric Flame Based on TDLAS, *Optik*, 170 (2018)
- [9] Gabrysch, M., et al., Simultaneous Detection of CO and CO₂ Using a Semiconductor DFB Diode Laser at 1.578 μm , *Applied Physics B*, 65 (1997), 1, pp. 75-79
- [10] Cai, T. D., et al., High-Pressure Measurements of Temperature and CO₂ Concentration Using Tunable Diode Lasers at 2 μm , *Applied Spectroscopy*, 70 (2016), pp. 474-484