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Abstract. Spatial temperature and gas concentration distributions are crucial for combustion studies to characterize the combustion process and to evaluate the combustion regime and the released heat quantity. Optical computer tomography (CT) enables the reconstruction of temperature and gas concentration fields in a flame on the basis of line-of-sight tunable diode laser absorption spectroscopy (LOS-TDLAS). A pair of H2O absorption lines at wavelengths 1395.51 and 1395.69 nm is selected. Temperature and H2O concentration distributions for a flat flame furnace are calculated by superimposing two absorption peaks with a discrete algebraic iterative algorithm and a mathematical fitting algorithm. By comparison, direct absorption spectroscopy measurements agree well with the thermocouple measurements and yield a good correlation. The CT reconstruction data of different air-to-fuel ratio combustion conditions (incomplete combustion and full combustion) and three different types of burners (one, two, and three flat flame furnaces) demonstrate that TDLAS has the potential of short response time and enables real-time temperature and gas concentration distribution measurements for combustion diagnosis. © 2016 Society of Photo-Optical Instrumentation Engineers (SPIE) [DOI: 10.1117/1.OE.55.7.076107]

Keywords: line-of-sight tunable diode laser absorption spectroscopy; direct absorption spectroscopy; temperature field distribution; gas concentration field distribution; water vapor (H2O).

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1 Introduction

Combustion is the most common, typical, and direct energy conversion method. The spatial distributions of temperature and gas concentration play important roles in combustion research, optimization of combustion efficiency, and reduction of emission gases. These are crucial parameters to characterize the combustion process and to evaluate the combustion regime and the released heat quantity.1,2 For a long time, thermocouples have been widely used for temperature measurements, but, intrinsically, they permit only point measurements and do not enable noncontact temperature distribution and gas concentration monitoring. Recently, as a nonintrusive, noncontact, fast, and highly sensitive optical absorption scheme, light-of-sight tunable diode laser absorption spectroscopy (LOS-TDLAS) has been employed for accurate measurements of temperature and gas species concentrations.3–7 In general, traditional TDLAS is applied to monitor the average temperature and concentration along the laser path.8,9 However, in many practical applications, nonuniform temperature and concentration distributions are significant along the laser path due to heat transfer with the side walls, boundary layers, gas flow, and other effects.10,11 Hence, average measurements are no longer applicable for studies with nonuniform fields. At present, the absorption spectrum with image reconstruction technology and discrete grids to obtain the spatial distributions of temperature and gas concentration are developed.12–17

This work uses an alternative approach named optical computer tomography (CT) that employs conventional DFB diode lasers with narrow tuning range, as commonly used for LOS-TDLAS measurements. Specifically, the feasibility of performing limited-grid tomographic reconstruction for temperature and concentration of water vapor in a stationary flame is addressed. The H2O transitions at 1395.51 and 1395.69 nm are used for this work, in which spectroscopic parameters such as line-strengths and temperature dependency are taken from the HITRAN2012 database. Ratio thermometry from two selected absorption transitions is employed to infer local temperature and gas concentration in the furnace. The discrete algebraic iterative algorithm is chosen for the two distributions. In this paper, one, two, and four flat flame furnaces are applied to analyze the internal combustion parameters and reconstruct the image models.

2 Theory and Mathematical Algorithm

2.1 Direct Absorption Spectroscopy

If a collimated laser beam at frequency ν (cm–1) enters a gas sample with the total pathlength L (cm), the integrated
absorbance \( A \) (cm\(^{-1}\)) of the transition \( i \), which is defined as the area underneath the absorption line-shape function, can be described as

\[
A_i = \int_{-\infty}^{+\infty} \alpha_i dv = P \int_0^L X(x)S_i(T(x)) dx, \tag{1}
\]

where \( \alpha_i \) means gas absorption coefficient, \( P \) (atm) is the total pressure, \( X(x) \) is the local mole fraction of the absorbing species, \( S_i \) stands for the line strength at the temperature \( T \), \( T(x) \) is the local temperature and the \( L \) is the total laser path. If the laser path is divided into \( n \) parts \( L_j \) (\( j = 1 \ldots n \)), and each path is kept at a nearly uniform temperature \( T_j \) and gas concentration \( X_j \), Eq. (1) is rewritten as follows:

\[
\tilde{A}_i = \frac{A_i}{P} = \sum_{j=1}^{n} [S(T_j)X_jL_j]. \tag{2}
\]

For the selected \( m \) absorption transitions, the linear equation can be established as

\[
\begin{bmatrix}
S_1[T_1] & S_1[T_2] & \cdots & S_1[T_n] \\
S_2[T_1] & S_2[T_2] & \cdots & S_2[T_n] \\
\vdots & \vdots & \ddots & \vdots \\
S_m[T_1] & S_m[T_2] & \cdots & S_m[T_n]
\end{bmatrix}
\begin{bmatrix}
(PXL)_1 \\
(PXL)_2 \\
\vdots \\
(PXL)_n
\end{bmatrix} =
\begin{bmatrix}
\tilde{A}_1 \\
\tilde{A}_2 \\
\vdots \\
\tilde{A}_m
\end{bmatrix}
\]

simplified as

\[
SX = \tilde{A}, \tag{3}
\]

where \( m \) is the number of absorption lines probed in the measurement of the vector of measured data \( \mathbf{A,S} \) stands for an \( m \times n \) line strength matrix, \( \mathbf{X} \) is the vector of concentration distribution of the absorbing species at optical pathlength \( L \). Typically, the pressure \( P \) is uniform and a known quantity. Thus, it can be divided out from the vector \( \mathbf{X} \), leaving the solution \([ (XL)_1, (XL)_2, \ldots, (XL)_n ] \). In general, the divided pathlength \( L \) can be calculated with the averaged distribution, \( L_1 + L_2 + \cdots + L_n = L_{\text{total}} \).

### 2.2 Discrete Algebraic Iterative Algorithm

In order to acquire additional information on temperature and concentration distributions along the laser path, the number of discretized bins should be increased. As discussed in Eq. (3), \( 2 \times m \) unknown values of temperature and concentration can be deduced with a total of \( n \) measured integrated absorbances, where \( n \geq 2 \times m \). Figure 1 shows the \( m \times n \) discretization grid; \( L_{ij} \) is the path length of a laser beam \( j \) transmits \( i \) grid. Therefore, Eq. (2) can be rewritten as

\[
A_{sv1,j} = \sum_{i=1}^{j} [PS(T)X]_{i1,j}L_{ij} = \sum_{i=1}^{j} \alpha_{sv1,j}L_{ij} \tag{4}
\]

\( j = 1, 2, \ldots, J \).

Based on the number of laser source scanning wavelength and the optical path arrangement, the integrated coefficient can be obtained by the electrophotonic detector, named the projection data. Because of limited spectral parameter precision and various measurement errors, there will be certain differences in the integrated absorption coefficient value between experimental and theoretical data. The relative error \( e_{\text{relative}} \) between measurement and calculation can be expressed as

\[
e_{\text{relative}} = \sqrt{\sum_{j=1}^{J} \sum_{i=1}^{I} \left( A_{sv1,i}^{\text{mea}} - \sum_{m=1}^{M} \sum_{n=1}^{N} P[S(T)X]_{i,m,n}L_{ij,m,n} / A_{sv1,i}^{\text{mea}} \right)^2}, \tag{5}
\]

where \( J \) is the total number of light beams; \( I \) is the total number of using wavelength absorption, \( \text{mea} \) and \( \text{cal} \) stand for measurement and calculation identification, respectively; \( A_{sv1,i}^{\text{mea}} \) is the integrated absorption coefficient value at \( j \) path length. Equation (5) is thus the target equation for the reconstruction of the spatial distribution of gas temperature and concentration. The solution is found by minimizing \( e_{\text{relative}} \).

By comparing with traditional methods, we found that the Levenberg-Marquardt (L–M) method is suitable to solve nonlinear least squares problems. However, the method can easily produce errors by falling into local optimum processes in the case of multiextreme value function. Therefore, in this paper, the simulated annealing, the genetic and simulated annealing algorithm (GSAA) and genetic algorithm are introduced. But this algorithm requires long computation times in ultimately determining the global optimal solution because its local search ability is not high. Fortunately, the L–M method can compensate for such problems. For these reasons, the GSAA is first used for global optimization to find the optimal solution region. Therefore, the L–M method is employed to reduce the computing time. Finally, “CT” models are used for the reconstruction of the spatial gas concentration and temperature distributions. Figure 2 illustrates the reconstruction process.
2.3 Absorption Wavelength Selection

In TDLAS monitoring, the DAS signal is generated by a rapid sawtooth modulation of the laser current around a central absorption wavelength. Accordingly, an important step in sensor design is the selection of the absorption wavelength. Sensor performance can be greatly improved by selecting optimum absorption transitions. Generally, several factors must be considered:

1. The two selected absorption lines should be free of significant interference from nearby other gas transitions.
2. The selected pair of wavelengths should exhibit strong peak absorption over the temperature range.
3. The influence of thermal boundary layers should be reduced.\(^\text{18}\)
4. The two lines should have a large difference $\Delta E$ in lower state energy $E'$.
5. The two lines should be close enough to be scanned by a single laser.

Water vapor is a common primary product among biomass fuel combustion, and it has several thousand absorption transitions in the near infrared. Compared with other species, it is more practical to choose absorption transitions of H$_2$O with appropriate line strengths and good temperature sensitivities. A pair of H$_2$O absorption wavelengths at 1395.51 and 1395.69 nm has been selected on the basis of their

![Fig. 2](image-url) The flow chart of the reconstruction of spatial temperature and concentration distributions.

![Fig. 3](image-url) (a) The line strength of the water vapor absorption lines in 1.3 to 1.6 $\mu$m region; (b) the temperature dependence of the lines strength of the selected two lines. All parameters are obtained from HITRAN2012 database.
suitable line-strength and the lack of significant interference from nearby transitions. Figure 3 and Table 1 present relative spectroscopic parameters of transitions obtained from the HITRAN2012 database. It is worth noting that the ratio does change much for high temperature range. If the measured temperature is above 1200 K, we should select another pair absorption wavelengths. In this paper, we emphasize the experimental methods and processes, rather than the highest measurement temperature.

### 3 Experimental Setup and Results

The diagram of the overall experimental apparatus is shown in Fig. 4. A fiber-coupled distributed feedback diode laser (NLK1E5EAAA, manufactured by NTT Electronics Company) with a wavelength of 1395.60 nm and a linewidth of 3 MHz is used as a laser source. The pair of H$_2$O absorption wavelengths at $\lambda_1 = 1395.51$ nm and $\lambda_2 = 1395.69$ nm has been selected on the basis of their suitable line-strength and the lack of significant interference from nearby transitions. The laser current and temperature are controlled by a homemade OEM board controller. The fiber-coupled diode laser is injection-current tuned over above two transitions with a linear sawtooth at 1 kHz. The laser beam is split into eight components with a 1:8 fiber splitter during the one-furnace experiment (1:16 fiber splitter for two- and four-furnace experiments), and each beam is directed into the corresponding collimator to form a freespace beam. The eight detector signals are recorded simultaneously by a data acquisition card. These data are calculated to transfer the integrated absorption for each transition. The baseline ($I_0$) is determined by a polynomial fitting with two-sided nonabsorption parts in the transmitted signal. The integrated absorbance also can be inferred with above method, simultaneously. In this paper, we used a different number of flat flame furnaces to design three systems (one, two, and four flat furnaces). Also, it’s important to note that all the following reconstruction processes are based on both assumptions: the temperature and concentration are the same value in each discrete grid, despite the influence of low-temperature boundary layer conditions.

#### 3.1 One Flat Flame Furnace

In this part, the eight crossed laser paths divide the combustion area into $4 \times 4$ grids and 16 crossing points for one furnace as seen in Fig. 5. In order to evaluate the precision of the laser absorption, a thermocouple is used to measure the different points along the second laser path [thick-dotted line in Fig. 5(a)]. Three kinds of combustion situations [incomplete combustion: Figs. 5(b) and 5(c) and full combustion: Fig. 5(d)] are presented. There are obvious differences among the corresponding three photos. According to the above measurement theories and the selected two absorption wavelengths, the direct absorption signals are shown in Fig. 6. The polynomial fitting method is used to obtain the absorption line shape based on the original detected signals. The left two plots [Fig. 6(a)] and the right two plots [Fig. 6(b)] are collected data for noncombustion process and full combustion state, simultaneously. The S1-7165.84 cm$^{-1}$ absorption signal amplitude becomes weaker than the low temperature. Instead, the S2-7164.91 cm$^{-1}$ signal amplitude is reversed at the initiation of the flat flame combustion furnace.

![Diagram of overall experimental apparatus](image1)

**Fig. 4** Schematic illustration of the TDLAS tomography experimental setup. The number 1, 2, . . . , 8 represent the fiber collimators, and the 1', 2', . . . , 8' are the uncooled InGaAs detectors, respectively.

<table>
<thead>
<tr>
<th>Wavelength number (cm$^{-1}$)</th>
<th>Wavelength (nm)</th>
<th>S (cm$^{-1}$/mol cm$^{-2}$ at 296 K)</th>
<th>$E^*$ (cm$^{-1}$)</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>7164.91</td>
<td>1395.51</td>
<td>5.893 $\times$ 10$^{-21}$</td>
</tr>
<tr>
<td>2</td>
<td>7165.84</td>
<td>1395.69</td>
<td>1.579 $\times$ 10$^{-22}$</td>
</tr>
</tbody>
</table>

**Table 1** Spectroscopic parameters of the two selected absorption transitions at 296 K.

![Analysis grids and laser beam paths](image2)

**Fig. 5** (a) Analysis grids and laser beam paths. The thermocouple is used to measure the different points along the second laser path (bold dashed line). The three kinds of combustion situations: (b) and (c) stand for incomplete combustion; (d) represents the full combustion.

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In order to validate the controllability and stability of the flame and the measurement precision of the DAS results, the thermocouple mounted on a movable two-dimensional (2-D) platform is employed to quantitatively measure the temperature distribution along the second path. The path that the laser beam passes through is identical to the one the thermocouple probe moves along. The thermocouple wires are supported by a ceramic tube with an outer diameter of 5 mm, and the thermocouple probe is beyond the end of the ceramic tube. It should be noted that the thermocouple is connected to a digital intelligent instrument, which is able to collect the temperature data in real time. The comparisons of measured temperatures by DAS and thermocouple, and the 3% error values 10 mm above the furnace surface are shown in Fig. 7. The $x$-axis stands for the measurement durations. The duration of each phase is about 200 s. The $y$-axis presents the measurement temperature and H$_2$O concentration.

Due to the nonuniform temperature and gas concentration distributions along the laser beam, the measured direct absorption line shapes cannot be fitted by a single Voigt function, and so the hybrid Voigt fitting procedure is employed to obtain the integrated absorbance areas. As is alluded to above, the discrete algebraic iterative algorithm is employed to solve the nonlinear equations for temperature and concentration for each grid. Because of the large analysis grids, the temperature and H$_2$O concentration become space averaged inside the grid. There are high temperatures and H$_2$O concentrations at the center of the combustion area in agreement with the thermocouple measurement results. Asymmetric temperature and H$_2$O concentration distribution models are created by the two absorption signal integrated areas, as depicted in Fig. 8. Each value for the corresponding region (like "1, 1 → 344 K," "3, 4 → 579 K"...) is illustrated in Table 2.

Figure 8 shows the 2-D discrete temperature and concentration measurement results in flame exhaust by LOS-TDLAS. The measurement spectral value in each grid is an averaged value, and it contains consistent. But in fact, the temperature and concentration images are not continuous in the combustion zone even though the reconstruction images are accurate. Therefore, we introduced the simple image fitting processing to smooth the grid interval data. The processed reconstruction images for temperature and H$_2$O concentration are shown in Figs. 9 and 10. Although the data acquisition
process is not fast enough for real-time sensing, this experiment can be used to evaluate the performance and feasibility of the DAS method. High-temperature region is detected at the combustion center and the measurement temperatures are slightly lower than the thermocouple data. Considering the space-averaged nature of this “umbrella-type” model, the two results nevertheless agree well with each other.

In order to verify the system’s temporal response and judge the flame position, small wind perturbations are applied in this part. The wind blows from detectors (1',2',3',4') to laser fiber collimators (1,2,3,4) high out of this plane 2 cm as seen in Fig. 4. The captured continuous flame signals and the 2-D TDLAS tomograms of the temperature are depicted in Figs. 11(a)–11(f). The central red region represents the high-temperature region; brighter colors correspond to higher temperatures. The intensity of the wind directly determines the height and size of the flame, and it also determines the distribution of the temperature field. The results demonstrate that due to the effect of wind direction, there are obvious differences in the high-temperature flame areas and positions. Therefore, the reconstructed temperature models prove that a fast scan modulation signal can reflect the changes of flame parameters.

### 3.2 Two and Four Flat Flame Furnaces

Using the experimental setup illustrated in Figs. 4 and 5, we performed experiments to determine optically the temperature distributions in two and four flat flame furnaces. Similar concentration distribution is obtained as in the case of the one flat flame furnace discussed above. In order to distinguish the different flame regions, we took slightly different gas supplies for the different furnaces. Also, we make just a qualitative description instead of a

#### Table 2

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature/K</td>
<td>344</td>
<td>654</td>
<td>613</td>
<td>365</td>
</tr>
<tr>
<td></td>
<td>676</td>
<td>1157</td>
<td>1107</td>
<td>619</td>
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<td></td>
<td>360</td>
<td>600</td>
<td>559</td>
<td>376</td>
</tr>
<tr>
<td>H₂O volume fraction/%</td>
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<td>0.0089</td>
<td>0.0077</td>
<td>0.0035</td>
</tr>
<tr>
<td></td>
<td>0.0092</td>
<td>0.0271</td>
<td>0.0241</td>
<td>0.0079</td>
</tr>
<tr>
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<td>0.0239</td>
<td>0.0213</td>
<td>0.0071</td>
</tr>
<tr>
<td></td>
<td>0.0035</td>
<td>0.0079</td>
<td>0.0069</td>
<td>0.0039</td>
</tr>
</tbody>
</table>

![Fig. 8](image) (a) Unprocessed 4 × 4 grid temperature and (b) H₂O concentration distributions. Red area represents higher values, whereas blue stands for lower values. The temperature (K) and H₂O concentration (%) for each color is identified on the right of both graphs.

![Fig. 9](image) The processed reconstructed temperature distribution. [temperature (K), size (cm)].
quantitative expression. More detailed analysis and discussion will be carried out in future work. According to the theoretical analysis and traditional experience, the combustion temperature is in direct ratio relation with the gas supply in the case of sufficient oxygen. Therefore, Fig. 12 shows that the flame-T1 combustion area is the same as flame T2. But, the gas supply corresponding to T1 was slightly higher than that for T2, resulting in a slightly higher temperature T1 for flame 1 than T2 for flame 2. Similarly, Fig. 13 shows the temperature distributions for the four flat flame combustion furnaces. The T4 gas supply was the maximum; in contrast the T1 gas supply was the minimum, while T2 and T3 gas supplies were approximately equal. The theoretical analysis and measurement result simply in that the combustion zones are nearly equal in area, with different temperature data corresponding to T4 > T2 ≈ T3 > T1.

Different from the single furnace, 16 laser paths are selected for determining temperature and concentration based on TDLAS. But, there are small artifacts that can lead to large errors in the experiment process. As an example, ratio-thermometry uses the ratios of individual values from the two absorption line reconstructions to obtain temperatures and concentrations for an individual pixel. Based on temperature data, concentrations are then determined in an iterative fashion. It is important to note that some processing techniques, such as median filtering or three times interpolation fitting, only mitigate artifacts, but do not include any information that is inherent to its own data. Although the reconstruction of temperature and gas concentration of the...
core section of the flame with the discrete algebraic iterative image model may be discontinuous, it appears satisfactory for an experienced staff.

4 Conclusions

Compared with the traditional temperature measurements using many contact devices, the LOS-TDLAS scheme described here has great promise for tomographic reconstruction of temperature and gas concentrations of dynamic systems. The selection of initial values in the algorithm is important to reconstruct a meaningful set of temperatures and concentrations. The use of spectral polynomial fitting and image processing methods also plays an important role to stabilize the absorption profile and to smooth the discrete grid images. Computer tomographic reconstruction data of three different kinds of flat flame furnaces prove that TDLAS has the potential capability to real-time measure the temperature and concentration distributions in various engine combustion situations. In the future, we shall focus on issues such as accuracy, response, and automatic control of the air-to-fuel ratio in industrial areas.

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