Improvements of measurement technique for temperature and concentration fields using CT-TDLAS

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ABSTRACT

Recently, exhaustion of energy sources and environmental pollution are major issues. To solve these problems efficiently, we need to use fuel efficiently and reduce emissions. With the advent of the TDLAS (Tunable laser absorption spectroscopy) technique, the temperature and concentration of the gases can be measured simultaneously. To determine the actual behavior of the combustion process in a combustor of the engine, it is necessary to measure the temperature distribution in the state of high-temperature and high-pressure. To improve the TDLAS accuracy measuring of the combustion process of CH₄ and H₂O gases from the engine. This was measured temperature fields for the substance of CH₄ and H₂O at the same time. The laser wavelength of 1300nm and 1600nm was used at the same time. In this study to know the combustion state in the actual engine and detection of exhaust harmful gases. And practicality was expected to increase. Among them, CT-TDLAS (Computed tomography-tunable diode laser absorption spectroscopy) is the most important technique for measuring the distributions of temperature and concentration across the two-dimensional planes. This method has been developed to measure two-dimensional and three-dimensional temperature and concentration distributions. In CT-TDLAS, the accuracies of the measurement results are strongly dependent upon the reconstruction algorithms. In this study, four different reconstruction algorithms have been tested numerically using experimental data sets measured by thermocouples for combustion fields. Three reconstruction algorithms, MART (multiplicative algebraic reconstruction technique) algorithm, SART (simultaneous algebraic reconstruction technique) algorithm and SMART (simultaneous multiplicative algebraic reconstruction technique) algorithm, are newly proposed for CT-TDLAS in this study. The calculation results obtained by the three algorithms have been compared with previous algorithm, ART (algebraic reconstruction technique) algorithm. Virtual data sets have been generated by the use of thermocouples data obtained in an actual experiment. And we suggest a three-dimensional measurement to consider the irregular flow of flame or exhaust gases. Use the SMART algorithm among the CT algorithms. Virtual data sets have been generated by the use of thermocouples data obtained in an actual experiment. The HITRAN database in which the thermo-dynamical properties and the light spectrum of the H₂O are listed were used for
the numerical test. The reconstructed temperature and concentration fields were compared with the original HITRAN database, through which the constructed methods are validated. The performances of the four reconstruction algorithms were demonstrated. Furthermore, CT-TDLAS has been adopted for the measurements of temperature and concentration distribution at a cross-section of the exhaust gas of a burner. The absorption spectra of H$_2$O vapor near the wavelength 1388nm were used for signal reconstructions. SMART algorithm has been used for signal reconstructions, with which the temperature and concentration fields were obtained based on the HITRAN database. The temperatures obtained by the use of SMART algorithm were compared with those obtained by thermocouples, and their agreements revealed that the temperature and concentration distribution at a cross-section of the exhaust gas of a burner could be measured by the use of CT-TDLAS with a measurement accuracy of 5.27% relative errors. And we suggest a three-dimensional measurement to consider the irregular flow of flame or exhaust gases. Use the SMART algorithm among the CT algorithms. Virtual data sets have been generated by the use of Gaussian distribution for expected temperature and concentration. The data of the HITRAN database in which the thermo-dynamical properties and the light spectra of the H$_2$O are listed were used for the numerical test. Further, it is proposed a three-dimensional measurement to consider the irregular flow of fluid such as real flame and exhaust gas. In this study, CT-TDLAS technique was used to measure the three-dimensional temperature and concentration distribution of flame. The absorption spectra of the combustion product H$_2$O vapor near the wavelength 1388nm were used for signal reconstructions. The temperature and concentration fields were constructed using the SMART algorithm based on the HITRAN database. As a result of comparing the temperature of the high-temperature position using thermocouple and CT-TDLAS technique, it was possible to accurately measure with an average relative error of 0.7%. It can be shown three-dimensional temperature and concentration fields of the flame.

**KEY WORDS**: Computed tomography-tunable diode laser absorption spectroscopy, Temperature, Concentration, Data Reconstruction, Exhaust gas

**TYPE OF THESIS**: Laser diagnostic
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Chapter 1 Introduction

1.1 Background of the study

An International Convention for the Prevention of Marine Pollution from Ships (MARPOL, Tier III) will be effective from 2016, in which all ships navigating open seas should reduce NOx up to 80% compared to that of 2010. Certified Carbon Emission Reduction (CER) Exchange from industry is expected to be working from 2015, though markets are not still prepared enough. Behind the trend is the fact that increased carbon dioxide in the air causes global warming and adversely affects natural ecosystems. Further, the demands for lowering the burdens on the environment will continue to grow steadily. It is thus becoming more important to understand the emission characteristics to minimize environmental disruption and to improve the efficiency of engines. Considering the situation mentioned above, it is important to monitor controlling factors of engines in order to improve the engine combustion processes. Particularly, measurement techniques that can probe the temperature and species concentration are inevitable to elucidate the overall nature of engine systems. In engines, exhaust gas temperature distribution is an important factor in NOx, total hydrocarbon and particulate matter emissions. It is also a catalytically important parameter in both gasoline and diesel engines. Especially two-dimensional and three-dimensional temperature distribution plays an important role in the catalytic efficiency.

1.2 Previous research introduction and improving

The results of previous researchers are as follows. The measurement methods for the gases on ships are based upon pointwise sampling, in which a sensor is installed in a branch of the ship’s chimney. Stemhagen et al. [1] extended the wave sensor to measure the temperature and concentration of the emission gas. Fine et al. [2] constructed a metal oxide semiconductor sensors for the detection of a variety of gases (CO, NOX, NH3). For the measurements of the emission gas CO2, Wang et al. [3] used a SAW (surface acoustic wave) microsensor. Since all existing measurement methods are based on a single location, it is impossible to predict the harmful gases amount in the ship or vehicle. Meanwhile, experimental and theoretical studies are underway to develop two-dimensional temperature and concentration measurements. For
example, TDLAS (Tunable laser absorption spectroscopy) [4-13] showed a high speed and high response for the specific detection of the temperature and the concentration in the combustion of the actual combustion [14-25] apparatus. Transient phenomena such as engine load became clear under many conditions from this technology development. Further, CT-TDLAS [26-30] was applied to the two-dimensional temperature measurement of the engine exhaust gas. Deguchi et al. [31] measured two-dimensional concentrations and temperature distributions of NH₃ and CH₄ gases using CT-TDLAS. However, emission gas is not emitted uniformly, the necessity of two-dimensional or three-dimensional measurements has been emphasized. Selection of tomography method for three-dimensional measurement determines the speed and accuracy of the calculation. In the tomography method [32-51], Elsinga et al. [52] firstly adopted ART and MART algorithms for reconstructing the intensity signals of images obtained in tomographic PIV (particle image velocimetry), in which the light intensity distributions of the three-dimensional volume was reconstructed. Adopted ART and MART algorithms for reconstructing the two flow fields, ring vortex and tomographic jet flow using tomographic PIV [53-74]. Byrne [75] proposed the SMART algorithm in order to save the calculation time, especially for the large calculation load. Jeon et al. [76] suggest the SMART algorithm is best tomography algorithm in CT-TDLAS. In this study proposes a three-dimensional measurement to consider the complex flow of flame or exhaust gases. Using multiple two-dimensional measurements for three-dimensional measurements. It also proposes measuring devices that pass through a two-dimensional cell at the same time for each layer. The virtual dataset was created using Gaussian distributions for anticipated temperature and concentration. Specially proposes a three-dimensional method improve the temperature and concentration measurement of the H₂O gas. Furthermore, apply the SMART algorithm which shows the best performance in tomography calculation, and provides a measurement of three-dimensional temperature and concentration fields of actual flame. Furthermore, the Gaussian distribution was applied in the initial value setting. It is an important part of the tomography method. The temperature and concentration fields were constructed based on the Lambert Beer’s law.
Fig. 1.2.1 Application of CT-TDLAS method to industrial fields

Fig. 1.2.2 Two-dimensional and three-dimensional measuring method by CT-TDLAS
Chapter 2 Theory

2.1 Principle of TDLAS

TDLAS is a technique that measures the absorption spectra of the selected gas using fast response continuous lasers. The principle of TDLAS is based on Lambert Beer’s law. The main part of the TDLAS system is the diode laser of which working wavelengths are adjusted to the range of absorptive wavelengths of the target gas. When the incident laser beam passes through the target gas, the spectra of the transmitted laser beam at the opposite side have absorptive spectra at a certain wavelengths that are optically inherent characteristic of the gas. Accordingly, the number density ($n$) of the measured gas species is related to the absorbance of light as in the following Eq. (2.1.1):

$$\frac{I_i(\lambda)}{I_0(\lambda)} = \exp\{A_\lambda\} = \exp\{-\sum_i\left( P \cdot n_i \cdot L \sum_j S_{i,j}(T) G_{\nu_{i,j}}\right)\}$$  \hspace{1cm} (2.1.1)

Here, $I_0$ is the incident light intensity, $I_i$ is the transmitted light intensity, $A_\lambda$ is the absorbance, $P$ is the pressure, $n_i$ is the number density of species $i$, $L$ is the path length, $S_{i,j}$ is the temperature dependent absorption line strength of the absorption line $j$, and $G_{\nu_{i,j}}$ is the line broadening function.

In this study, the intrinsic absorption wavelengths of H$_2$O, near 1388nm, was used for temperature sensitivity measurements of the combustion environments. Fig. 2.1.1 shows the absorption spectrum of H$_2$O in the near infrared region (1388nm), which has been calculated by HITRAN database [78]. Three absorption lines located at 1388.139 nm (#1), 1388.328 nm (#2) and 1388.454 nm (#3) have remarkable temperature dependence at three different temperatures (300K, 700K, 1500K), and they were utilized for temperature measurements.
Fig. 2.1.1 Relative intensity of theoretical H$_2$O absorption spectra (1388nm~1388.5nm)

Fig. 2.1.2 (a) shows the theoretical absorption intensity variations of three dominant wavelengths (#1, #2, #3) for temperature variations of H$_2$O. Fig. 2.1.2 (b) represents the temperature dependency of the ratios of the three dominant wavelengths. It can be said that the ratio of #1/#2 has strong linearity for temperature increments. In CT process, this linearity is utilized for temperature calculations, in which the calculation errors between the temperature obtained from the theoretical absorption spectra and the temperature obtained from the experimental absorption spectra.
(a) Temperature dependence of three absorption lines

(b) Intensity ratio of two absorption lines

Fig. 2.1.2 Theoretical temperature dependence H₂O absorption spectra
2.2 Line-strengths

In order to express the century of absorption transition by spectroscopic line-strength, it should become high energy due to absorption of light energy in low quantum energy state at the same type of molecule. And should know that spectroscopic transitions occur due to molecular motion. Furthermore, the line intensity of the molecules in low quantum energy states can be explained by the statistical Boltzmann distribution.

The fundamental unit of line intensity is shown in \( S \left[ \text{cm}^{-2} \text{atm}^{-1} \right] \) corresponding to pressure, and \( S^* \left[ \text{cm}^{-1} / \text{mol} \cdot \text{cm}^{-2} \right] \) as a unit of number density for each molecule provides wavelength in HITRAN database. It can be represented by the following Eq. (2.2.1).

\[
S \left[ \text{cm}^{-2} \text{atm}^{-1} \right] = \frac{S^* \left[ \text{cm}^{-1} / \text{mol} \cdot \text{cm}^{-2} \right] \times n \left[ \text{mol} / \text{cc} \right]}{P \left[ \text{atm} \right]} \tag{2.2.1}
\]

Applying an ideal gas state equation to Eq. (2.2.1) and switching the unit of pressure to \( \left[ \text{atm} \right] \) by \( \left[ \text{dynes} / \text{cm}^2 \right] \) makes it possible to obtain a relational expression like Eq. (2.2.2).

\[
S \left[ \text{cm}^{-2} \text{atm}^{-1} \right] = \frac{S^* \left[ \text{cm}^{-1} / \text{mol} \cdot \text{cm}^{-2} \right] \times 1013250 \left[ \text{dynes} / (\text{cm}^2 \cdot \text{atm}) \right]}{kT} \tag{2.2.2}
\]

Here, \( k \) is the Boltzmann constant \( \left( = 1.38054 \times 10^{-16} \left[ \text{erg} / \text{K} \right] \right) \), \( T[K] \) is the temperature of a target gas.
Considering the room temperature in Eq. (2.2.2), it can be obtained the following Eq. (2.2.3).

\[ S = S^* \times (2.488 \times 10^{19}) \text{[cm}^2\text{atm}^{-1}] \]  

(2.2.3)

The line-strength is a function of temperature it depends on the Boltzmann distribution of the molecule in the state where the molecule absorbs the light energy. It can be explained the following Eq. (2.2.4).

\[
S_{i,j}(T) \approx S_{i,j}(T_0) \frac{Q(T_0)}{Q(T)} \exp \left[ -\frac{\hbar c E_{\nu}''}{k} \left( \frac{1}{T} - \frac{1}{T_0} \right) \right] \frac{1 - \exp \left( \frac{-\hbar c v_{ij}}{k T} \right)}{1 - \exp \left( \frac{-\hbar c v_{ij}}{k T_0} \right)}
\]  

(2.2.4)

Here, \( T_0 \text{[K]} \) the reference temperature (296K), \( Q(T) \) the partition function of absorbing molecular at a particular temperature. \( Q(T) \) usually express as a fourth-degree polynomial function.
2.3 Broadening function

Broadening function $G_{vi,j}$ has been approximated by the general Voigt profile [25] represented by the following Eq. (2.3.1).

$$G_v(a,x) = \int_{-\infty}^{+\infty} G_D(u) G_L(V-u) du = G_D(v_0) \frac{a}{\pi} \int_{-\infty}^{+\infty} \frac{exp(-y^2)}{a^2 + (x-y)^2} dy$$

(2.3.1)

Here, a parameter $a$, $x$ and Voigt width $\Delta v_v$, follow Equations (2.3.2), (2.3.3) and (2.3.4)

$$a = \sqrt{ln 2} \frac{\Delta v_C}{\Delta v_D}$$

(2.3.2)

$$x = \sqrt{ln 2} \frac{(v-v_0)}{\Delta v_D}$$

(2.3.3)

$$\Delta v_v = \frac{\Delta v_C}{2} + \sqrt{\left(\frac{\Delta v_C^2}{4} + \Delta v_D^2\right)}$$

(2.3.4)

$G_C(v)$ and $G_D(v)$ are expressed as the following Eq. (2.3.5) and Eq. (2.3.6) representing the Lorentz function [14] and the function for the Doppler broadening.

$$G_C(v) = \frac{\Delta v_C}{2\pi} \frac{1}{(v-v_0)^2 + \left(\frac{\Delta v_C}{2}\right)^2}$$

(2.3.5)
Here, $v$ is the frequency of light, $v_0$ is the transition center frequency and $\Delta v$ is the transition full width at half maximum (FWHM). $\Delta v_D$ is FWHMs of the Doppler broadening, $c$ is the speed of light, $m$ is the atomic or molecular mass and $k$ is the Boltzmann constant. $\Delta v_C$ is FWHMs of the collision broadening. The collision broadening depends on species concentration and temperature [78]. In this study we assumed total collisional broadening of the measured field and each species dependence on collisional broadening parameters was not considered. The collisional broadening parameters were determined by measured spectra [77]. The natural broadening was not considered since the influence of the natural broadening was negligible in the conditions of this study.
2.4 Tomography reconstruction algorithms

The conventional reconstruction algorithm for CT calculation, the filtered back projection technique [80], has been widely used for medical image reconstructions, in which Fourier domain method is adopted. Since a large number of the transmitted lights from many angles should be considered for data reconstruction for Fourier transformation, this technique is restricted for delicate use such as medical use. This implies that the filtered back projection technique is not applicable for industrial use. To solve these difficulties, a method called ART algorithm was developed for easy use of industrial applications.

2.4.1 ART algorithm

ART algorithm is an iterative calculation algorithm used for tomographic reconstruction, in which the absorption coefficients, $\alpha$, at all grids, are renewed iteratively until all coefficients are close to converged values. That is, an iterative solution of linear equations is performed by using the feedback information of the deviation between the virtual experiment projection data and the calculated virtual projection data. ART algorithm is based on Eq. (2.4.1.1).

$$\alpha_{i,j}^{k+1} = \alpha_{i,j}^k + \omega \sum_{i=1}^{I} \frac{A_{i,j} - \sum_{j=1}^{J} \alpha_{i,j} \cdot L_{i,j}}{\sum_{j=1}^{J} L_{i,j}^2} \cdot L_{i,j}$$ \quad (2.4.1.1)

Here, $I$ is the total number of grid $j$ column direction. $\omega$ is a scalar relaxation parameter varied between 0 and 2. Large relaxation value produces slow convergence speed.

2.4.2 MART algorithm

MART algorithm was firstly adopted for Tomographic PIV (particle image velocimetry) by Elsinga et al. [52], since the scalar relaxation parameter, $\omega$, in Eq. (2.4.2.1) accelerates the convergence speed.
\[ \alpha_{i,j}^{k+1} = \alpha_{i,j}^k \left( \sum_{j=1}^{L} \frac{A_{i,j}}{\sum_{i=1}^{J} \alpha_{i,j} \cdot L_j} \right)^{\omega L_{i,j}} \]

\[ \sum_{i=1}^{J} \alpha_{i,j} \cdot L_j \neq 0 \]  

(2.4.2.1)

2.4.3 SART algorithm

Algebraic reconstruction technique SART algorithm [81] has been devised to purify the ART algorithm. It is used to reduce the error of the approximate value of the line integral of the soft image by a finite sum. Also it has been used for improving the quality of the reconstruction in the process of reasoning. SART algorithm is based on Eq. (2.3.3.1). Here, \( J \) is the total number of laser paths. \( \omega \) is a scalar relaxation parameter, and is less than 1 satisfying \((\omega \leq 1)\).

\[ \alpha_{i,j}^{k+1} = \alpha_{i,j}^k + \omega \frac{\sum_{j=1}^{J} \left( A_{i,j} - \sum_{i=1}^{J} \alpha_{i,j} \cdot L_j \right)}{\sum_{j=1}^{J} L_j} \cdot L_j \]  

(2.4.3.1)

2.4.4 SMART algorithm

SMART algorithm [75] is based on a combination product of the algebraic reconstruction, in which an iterative calculation is performed satisfying a cross entropy minimization. It has been used for accelerating the convergence speed for the calculation of large amount of image data. SMART algorithm is based on Eq. (2.4.4.1).

\[ \alpha_{i,j}^{k+1} = \alpha_{i,j}^k \cdot \exp \left( \sum_{j=1}^{J} \frac{L_j}{\sum_{j=1}^{J} L_j} \cdot \log \frac{A_{i,j}}{\sum_{i=1}^{J} \alpha_{i,j} \cdot L_j} \right) \]  

(2.4.4.1)
2.5 Two-dimensional temperature and concentration measurement

In order to get two-dimensional temperature distribution via CT calculations, multiple laser beams produced in a form of mesh shown in Fig. 2.5.1 are constructed by multiple semiconductor lasers, and then all laser intensity information at the grid points of the mesh are reconstructed theoretically using the experimental absorption spectra. The signal intensity of the absorption lines of the laser pass $j$ is can be expressed in the following Eq. (2.5.1).

$$A_{\lambda,j} = -\sum_i n_i \cdot L_{i,j} \cdot \alpha_{\lambda,i}$$  \hspace{1cm} (2.5.1)

Here, $A_{\lambda,j}$ is the integrated absorbance of wavelength $\lambda$ in the path $j$, $\alpha_{\lambda,i}$ is the absorption coefficient of wavelength $\lambda$ inside a grid $i$ on the path and is dependent upon the temperature and the density of species. $L_{i,j}$ is the path length inside the grid $i$.

![Diagram of Calculation grids for tomographic reconstructions](image)

Fig. 2.5.1 Calculation grids for tomographic reconstructions
Fig. 2.5.2 shows how the temperatures and the concentrations at the grids of the mesh in Fig. 2.5.1 are obtained in CT calculations.

In CT process, it is important to adopt the initial values for the temperatures and the concentrations at all grids. In this study, SLOS (summation of line of sight) method [82] has been adopted. In this method, all absorption signals passing at a grid are added and they are used as the experimental spectra at all grids. The initial values of temperature and concentration at the grids have been installed considering the length and the location of the laser lines.

At the initial stages of CT calculation, the initial values obtained by the SLOS method are used for the calculation of SMART algorithm, in which Eq. (2.4.4.1) is used for the calculation of the absorption coefficients $\alpha_{\lambda,i}$.

Once the initial absorption spectra are obtained by the use of SLOS, the absorption
coefficients represented by Eq. (2.4.1) are calculated iteratively until the differences between the theoretical absorbance and the experimental absorbance using the MSE function as shown in Eq. (2.5.2) are minimized so that the final temperature and concentration are decided. During iterative calculations, all theoretical spectra were normalized with maximum intensity.

\[ Error = \sum \left( A_{\lambda,i}^{\text{theory}} - A_{\lambda,i}^{\text{experiment}} \right)^2 \]  

(2.5.2)

2.6 Three-dimensional temperature and concentration measurement

Tomography refers to imaging by sections using any kind of penetrating wave. It can be reconstructed information on the space via the three-dimensional coordinate system.

Initial value making method is important to provide the initial condition for the calculation of the measurement object in the tomography calculation. In order to achieve the data of initial temperature fields were constructed using SLOS method. This temperature distribution result is not uniform. This problem can be solved using smoothness shape by the Gaussian distribution [83]. The Gaussian distribution is can calculate as shown in Eq. (2.6.1).

\[ B_{xyz} = B_{Max} \cdot \exp \left[ \frac{-\left( x^2 + y^2 + z^2 \right)}{\sigma^2} \right] + B_{Min} \]  

(2.6.1)

Here, \( B_{Max} \) is the maximum value 2.3, \( B_{Min} \) is the minimum value 0.8 and using \( \sigma = 2 \).

The calculation spectra of \( \text{H}_2\text{O} \) applied to CT-TDLAS, the procedure for obtaining the temperature and concentration fields are as follows in Fig. 2.6.1.
Fig. 2.6.1 Calculation process of temperature and concentration at all grids in CT-TDLAS (three-dimensional)
Chapter 3 Experiment method

3.1 Target gas detecting method in high-temperature and high-pressure using TDLAS

To broadening the value of the theoretical absorption spectra of the actual absorption spectra for H_2O and CH_4 in the situation of high-temperature and high-pressure using a Fig. 3.1.1 system. The measuring device is composed of a heating cell, it is used to improve the accuracy of the temperature measurement in the state of high-temperature and high-pressure. An experiment was performed the pressure was increased from 0.1MPa to 1.0MPa at each temperature (from 293K to 773K). For absorption spectral analysis of the measurement gases using two kinds of lasers. Scan frequency for measurement of the absorption spectra of H_2O is 30 kHz, it was used a laser (Santec, HSL-200-30-TD) having a wavelength region of 1330-1370nm. A laser (Santec, HSL-1.7-ES) having a wavelength region of 1600-1740nm and scanning frequency 90 kHz was used for measurement of the CH_4 absorption spectra. Further, the laser is transmitted to the target gas through the collimator (Optizone, C-20-S-1-C-200-2-L-0.95-S) is divided by fiber splitter. The transmitted light is detected by two kinds of photodiodes (For the 1300 nm band and 1600nm band), it is recorded by the data storage device (HIOKI E.E. Co., 8861 Memory Highcoda HD Analog).

![Experimental apparatus for evaluation of temperature measurement accuracy (H_2O and CH_4)](image)

Fig. 3.1.1 Experimental apparatus for evaluation of temperature measurement accuracy (H_2O and CH_4)
Fig. 3.1.2 Experimental setup for high-temperature and high-pressure

Fig. 3.1.3 Absorption signal on room temperature by CH₄ gas
3.2 Two-dimensional measuring method using CT-TDLAS

Fig. 3.2.1 shows the experimental setup. The absorption spectra of H\textsubscript{2}O in a flame burner have been measured. The burner has a double-tube structure composed of a sintered bronze filter and an external piping. Methane (CH\textsubscript{4}) gas has been used as fuel and it has been mixed with air supplied through a sintered bronze filter. The 16 path CT-TDLAS measurement cells as shown in Fig. 3.2.2 have been set at the position 95mm above the burner. The experimental parameters are summarized in Table 3.2.1.

Table 3.2.1 Experimental parameters (two-dimensional)

<table>
<thead>
<tr>
<th>CH\textsubscript{4} (L/min)</th>
<th>Feeder dry air/ Mixed air (L/min)</th>
<th>Around air</th>
<th>All air: Mixed air + Around air (L/min)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH\textsubscript{4}-Air flame</td>
<td>0.74</td>
<td>3.4</td>
<td>-</td>
</tr>
</tbody>
</table>

A DFB (distributed feedback) diode laser (NTT Electronics Co., NLK1E5GAAA) of which working wavelength is 1388 nm with a scanning range of 0.6 nm was used to get H\textsubscript{2}O gas absorption spectra.

In order to measure simultaneous two-dimensional absorption spectra a 16-path cell as shown in Fig. 3.2.2 has been used.

The laser beam has been separated by the use of an optical fiber splitter (OPNETI CO., SMF-28e 1310 nm SWBC 1×16). Then, the separated 16 beams pass through 16 collimators (THORLABS Co., 50-1310-APC) to attain focused light intensity. The intensity of the transmitted light has been detected by 16 photodiodes (Hamamatsu Photonics and G8370-01), and they have scanned with 1 kHz and have been recorded onto the recorder (HIOKI E.E. Co., 8861 Memory Highcoda HD Analog16). The detected signals have been amplified using the amplifier (Stanford Research Systems, SR445A).
Fig. 3.2.1 Experimental apparatus for two-dimensional temperature measurement in flame burner using CT-TDLAS

Fig. 3.2.2 16-paths CT-TDLAS measurement cell (two-dimensional)
3.3 Three-dimensional measuring device design for CT-TDLAS

By extending the structure of the existing two-dimensional measurement cells to three-dimensional, three-dimensional measurements for temperature and concentration fields can be attained by the use of 96 collimators and photodiodes. As shown in Fig. 3.3.1, conventional two-dimensional measurement cells could be constructed. As shown in Fig. 3.3.2, two-dimensional measurement cells were stacked into five layers to construct a three-dimensional measurement space.

Fig. 3.3.3 shows three-dimensional laser paths to attain three-dimensional measurements. Fig. 3.3.4 shows calculation results for the diagonal paths. The lengths of the diagonal lines can be obtained, with which the absorption of z-axis direction can be calculated.

![Diagram](image-url)

**Fig. 3.3.1 CT measurement cell for 16 paths**
Fig. 3.3.2 Three-dimensional measuring device drawing

Fig. 3.3.3 The entire optical path diagram
Fig. 3.3.4 Diagonal path calculation (x-z plane)

Fig. 3.3.5 Blueprint of the two-dimensional cell for three-dimensional measurement (bottom)
Fig. 3.3.6 Blueprint of the two-dimensional cell for three-dimensional measurement (top)

Fig. 3.3.7 Blueprint of the diagonal path cell
3.4 Three-dimensional measuring method using CT-TDLAS

Fig. 3.4.1 shows the actual flame experimental setup. The burner has a double tube structure for surrounding air and flame fuel. Methane gas has been used as fuel and it has been mixed with dry air. The three-dimensional CT-TDLAS measurement cell as shown Fig. 3.4.1 have been set at the position 118mm above the burner. The experimental conditions are summarized in Table 3.4.1. The N₂ test is making a basic line for actual absorption line calculation, and using air test make an experimental broadening factor for calibration.

<table>
<thead>
<tr>
<th>Case</th>
<th>CH₄ (L/min)</th>
<th>Dry air (L/min)</th>
<th>Surrounding air (L/min)</th>
<th>Inside of 3D cell : N₂ (L/min)</th>
</tr>
</thead>
<tbody>
<tr>
<td>N₂ test</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>55.0</td>
</tr>
<tr>
<td>Air test</td>
<td>-</td>
<td>-</td>
<td>25.0</td>
<td>55.0</td>
</tr>
<tr>
<td>CH₄-Air flame</td>
<td>0.24</td>
<td>1.9</td>
<td>25.0</td>
<td>55.0</td>
</tr>
</tbody>
</table>

In order to measure the H₂O gas absorption spectra was used a DFB (distributed feedback) laser (NTT Electronics Co., NLK1E5GAAA) of which working wavelength is 1388nm with scanning range of 0.6nm. In addition, to measure simultaneous three-dimensional absorption spectra a 96-path cell as shown in Fig. 3.4.2 has been used.

The laser beam has been separated by the use of an optical fiber splitter (OPNETI CO., PLC-367020-0132-2, 1x32, 2ea, PLC-367020-0116-2, 1x16, 2ea). Then, the separated 96 beams pass through 96 collimators (THORLABS Co., C-20-S-1-C-200-2-S-2-S) to attain focused light intensity. The intensity of the transmitted light has been detected by 96 photodiodes (Hamamatsu Photonics, G12180-010A), and they have scanned with 4 kHz and have been recorded onto the recorder (HIOKI E.E. Co., 8826 Memory Highcoda, 2ea, MR8741 Memory Highcoda, 2ea). The detected signals have been amplified using the amplifier (COSMOWAVE, 30).
FP150MSA-10dB). In order to compare the thermocouple and CT-TDLAS, to measure the temperature for center position of each layer using a thermocouple (K type thermocouple, KMG-100-100-050).

Fig. 3.4.1 Experimental apparatus for three-dimensional temperature measurement in flame burner using CT-TDLAS

Fig. 3.4.2 96 path CT-TDLAS measurement cell (three-dimensional)
Fig. 3.4.3 Measurement setup for three-dimensional

Fig. 3.4.4 Function generator sets
Fig. 3.4.5 LD driver

Fig. 3.4.6 DFB laser sets
Fig. 3.4.7 Fiber splitter sets

Fig. 3.4.8 Absorption signal on room temperature by Air
Fig. 3.4.9 Measurement setup using a thermocouple

Fig. 3.4.10 Measurement setup for flame
Chapter 4 Results and discussion

4.1 Target gas detection in high-temperature and high-pressure using TDLAS

Numerical simulation was carried out using HITRAN database for H\textsubscript{2}O and CH\textsubscript{4} measurement to select the most suitable absorption lines (P=0.1Mpa, T=300K, n=5\%, L=10cm). Fig. 4.1.1 shows the absorption of other combustion components at the selected spectral lines is ignorable comparing with that of H\textsubscript{2}O. On the contrary, Fig. 4.1.2 shows the absorption of H\textsubscript{2}O components at the selected spectral lines is ignorable comparing with that of CH\textsubscript{4}. Fig. 4.1.3 shows the absorption spectra of the H\textsubscript{2}O gas in the region of 1300nm, Fig. 4.1.4 shows the absorption spectra of CH\textsubscript{4} gas in the region of 1600nm. It was calculated using the HITRAN database.

![Absorption spectra](image)

Fig. 4.1.1 Relative intensity of theoretical H\textsubscript{2}O & CH\textsubscript{4} absorption spectra (1364nm~1370nm)
Fig. 4.1.2 Relative intensity of theoretical H$_2$O & CH$_4$ absorption spectra (1630nm~1680nm)

Fig. 4.1.3 Relative intensity of theoretical H$_2$O absorption spectra (1364nm~1370nm)
Fig. 4.1.4 Relative intensity of theoretical CH$_4$ absorption spectra (1630nm~1680nm)

Fig. 4.1.5(a) is an absorption spectra of the H$_2$O gas for each representative wavelengths, it seems absorption intensity varies depending on the temperature change. Fig. 4.1.5(b) is shown the absorption intensity which varies according to temperature change. The correlation between another representative wavelength was obtained by expressing a ratio of the absorption intensity. Since the absorption intensity ratio shows linearity, it can be said that absorption intensity depends on temperature.

However, in the high-temperature and high-pressure situation, it is difficult to evaluate the absorption spectra by broadening phenomenon due to the pressure rise. To solve this problem, by using a laser having a wavelength sweep range of several tens nm. It is possible to evaluate broadening the absorption spectra.
Fig. 4.1.5 Theoretical temperature dependence H₂O absorption spectra

(a) Temperature dependence of different absorption lines

(b) Intensity ratio of different absorption lines
Fig. 4.1.6 and Fig. 4.1.7 show the can be confirmed changes in absorption spectra of H$_2$O and CH$_4$ at high-temperature and high-pressure conditions. Fig. 4.1.6 confirmed the absorption spectra gives a pressure change at a specific temperature to H$_2$O gas. Further, Fig. 4.1.7 confirmed the absorption spectra gives a pressure change at a specific temperature to CH$_4$ gas.

(a) Absorption spectra due to the pressure changing at 373K

(b) Absorption spectra due to the pressure changing at 573K

Fig. 4.1.6 Absorption spectra by pressure changing of H$_2$O gas at each temperature
When given pressure changes at specific temperatures to H₂O and CH₄ gases as shown in Fig. 4.1.8 and Fig. 4.1.9, the intensity of the absorption spectra for representative wavelength
was confirmed to vary linearly. By applying results of the experiments absorption spectra for the calculation of theoretical absorption spectra, the spectra fitting is possible with high accuracy.

![Graph](image1.png)

**Fig. 4.1.8** Normalized intensity on temperature dependence for H$_2$O by TDLAS (0.1MPa, 1364.69nm)

![Graph](image2.png)

**Fig. 4.1.9** Normalized intensity on temperature dependence for CH$_4$ by TDLAS (0.1Mpa, 1665.956nm)
4.2 Two-dimensional results by CT-TDLAS (Virtual data)

Fig. 4.2.1 shows the arrangement of the laser beams for numerical tests by [31], [57] and [64]. The total number of the laser paths was set to 16. The left half of the system is the detectors part while the right half is the 16 collimators by which the laser beams are adjusted for attaining best focusing. The diameter of the measurement space is 70mm, where the 16 lines are passing through. The temperature at the grids were obtained by actual thermocouple (KMT-100-100-120) measurements, and they were used as the test data for the four reconstruction algorithms.

Fig. 4.2.1 CT measurement cell for 16paths

Fig. 4.2.2 shows the initial distributions of the temperature measured by thermocouple experiments. The experimental conditions are summarized in Table 4.2.1. Fig. 4.2.2 is the original measured temperature distribution, and Fig. 4.2.3 shows the concentration field obtained by using the temperature values of Fig. 4.2.2. It has been regarded that the H₂O vapor passed through the measurement area. Representative wavelengths used for the measurement of the absorption spectra of H₂O are #1(1388.139nm), #2(1388.328nm) and #3(1388.454nm).
It has been regarded that the temperature field obtained in the actual measurement had been constructed virtually in the burner.

Fig. 4.2.2 Distribution of initial temperature used for reconstruction test

Fig. 4.2.3 Distribution of initial concentration used for reconstruction test
Since the concentration field can’t be obtained via thermocouple measurements, it has been generated virtually, and its value has been increased with temperature increments. The concentration of the H$_2$O has been assumed to be increased linearly as the temperature increases. Fig. 4.2.3 shows the initial distributions of the calculated virtual concentration. Fig. 4.2.4-5 shows the absorption spectra of each laser, which is generated virtually using Eq. (2.2.4) and Eq. (2.5.1).

The profiles have been used for calculating the temperature and concentration fields using the four reconstruction algorithms, ART, MART, SART and SMART. Two ratios of (#1/#2) and (#2/#3) of the representative absorption lines were used for the calculation of temperature. Evaluation for finishing iterative calculations adopted for data reconstruction is based on the MSE (mean square error) which is the error between the virtual experiment data (Fig. 4.2.2 and Fig. 4.2.3) and the reconstructed data at each iterative step.

Table 4.2.1 Experimental parameters

<table>
<thead>
<tr>
<th></th>
<th>CH$_4$ (L/min)</th>
<th>Feeder dry air / Mixed air (L/min)</th>
<th>Around air</th>
<th>All air: Mixed air + Surrounding air (L/min)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH$_4$-Air flame</td>
<td>0.74</td>
<td>3.4</td>
<td>-</td>
<td>100.0</td>
</tr>
</tbody>
</table>
Fig. 4.2.4 Recovered absorption spectra (H\textsubscript{2}O) for 16-path lasers (continued)
Fig. 4.2.5 Recovered absorption spectra (H$_2$O) for 16-path lasers
Fig. 4.2.6 Various initial temperature values for each algorithm test
Fig. 4.2.7 Comparisons between the results obtained by ART, MART, SMART and SART algorithms various initial values.

Fig. 4.2.6 shows the initial temperature and concentration given to evaluate the performance of each algorithm. 5 different temperatures with 1% concentration were given to each case. Table 4.2.2 shows the temperature range given to each case. With each case, the most appropriate temperature range was found. Fig. 4.2.2 shows the original temperature distribution obtained from thermocouples measurements. This distribution was used as virtual...
data. Fig. 4.2.6 (e) shows calculation results, and the temperature distribution in this figure is the most closest to the results by thermocouples measurements than other cases. Fig. 4.2.8 shows the minimum MSE (mean squared errors) according to the 5 cases of the initial values, and the minimum value was $3.85 \times 10^{-5}$. Accordingly, case 5 has been chosen for virtual data tests. In the meantime, the convergence speed of calculation of MART algorithm was the fastest among four algorithms, while ART algorithm was the slowest for every cases (case 1-5). Further, it has been shown that the magnitudes of the iterative calculation errors by SMART algorithm are smaller than those by ART, MART and SART algorithms showing rapid calculation convergences. The results have been shown as Fig. 4.2.7.

Fig. 4.2.8 Comparisons between various initial values for SMART algorithm (MSE)

<table>
<thead>
<tr>
<th>Case</th>
<th>Temperature Range [K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>280–950</td>
</tr>
<tr>
<td>Case 2</td>
<td>255–925</td>
</tr>
<tr>
<td>Case 3</td>
<td>255–850</td>
</tr>
<tr>
<td>Case 4</td>
<td>260–855</td>
</tr>
<tr>
<td>Case 5</td>
<td>255–925</td>
</tr>
</tbody>
</table>
In tomography process, initial values for the iterative calculations play important role in obtaining the final converged values. Fig. 4.2.8 shows the error rates for the five different initial values. It seemed that the smallest error is the case 5, in which the highest temperature
region is at the center revealing that the pattern of the temperature distribution is very similar to that of Fig. 4.2.2. With this fact, the temperature distribution of case 5 was used to calculate the initial value of concentrations as shown as Fig. 4.2.9 (b).

Fig. 4.2.10 shows the reconstructed temperature and concentration fields obtained by SMART algorithm. The reconstructed temperature field as shown in Fig. 4.2.10 (a) is just the same as Fig. 4.2.9 (a), which reveals that the reconstruction process adopted in this study is appropriate. Fig. 4.2.10 (b) shows that the reconstructed concentration field using the initial concentration field (Fig. 4.2.9 (b)). The concentration field has some discrepancy from the original one as shown in Fig. 4.2.9 (b). This implies that the concentration fields should be obtained via other temperature case ranges not shown in Table 4.2.1 for more accurate calculations.

Fig. 4.2.11 shows the convergence speed of the iterative calculations for each algorithm up to 150 iteration. SMART algorithm was the fastest among four algorithms while ART algorithm is the slowest. Further, it has been shown that the error magnitudes calculated by SMART algorithm are smaller than those by ART, MART and SART algorithms showing rapid calculation convergences.

![Fig. 4.2.11 Comparisons of MSE (mean square error) between ART, MART, SMART and SART algorithms (MSE)](image-url)
The absorption spectra as shown in Fig. 4.2.4-5 have been used as an experimental signals to reconstruct the temperature and the concentration fields. Fig. 4.2.12 (a), (b), (c) and (d) show the error profiles along Y locations between the thermocouple temperatures (that were used for generating the theoretical absorption spectra, i.e., used as virtual data) and the temperatures reconstructed by four algorithms, ART, MART, SART and SMART, respectively.

The profile data are on the grid data that can be composed of the 16 laser paths in Fig. 4.2.1. Left figures in Fig. 4.2.12 (a), (b), (c) and (d) show the profiles obtained at the line of Y=14 mm, of which temperature is lower than the center region. Right figures in Fig. 4.2.12 (a), (b), (c) and (d) show the profiles obtained at the laser path of which region is the highest temperature.

It can be seen that the peak region of temperature is shifted to the edge. This is due to the fact that the location of the burner exit has been installed at off-center as shown in Fig. 4.2.1. Further, this implies that the temperature measured by thermocouples (chromel-alumel) at the exit of the nozzle is the highest.

At lower temperature regions (left figures), the temperature results calculated by ART and SART algorithms show good agreements with the reference data (virtual), while showing slight errors in the results calculated by MART and SMART algorithms.

On the contrary, the calculation results obtained by MART and SMART algorithms show good agreements with the reference data, while showing the results by ART and SART algorithms have large errors from the original reference data.

The calculation results obtained by SMART algorithm showed lowest errors for all temperature ranges. From this fact, SMART algorithm is the most appropriate one for reconstructing the multiple signals obtained in CT-TDLAS.

It could be said that the errors obtained by ART and SART algorithms show relatively large in high temperature region. This fact implies that ART and SART algorithms are not recommendable for CT-TDLAS calculation.

The maximum temperature calculated by SMART algorithm is 950K at the center, and this
value is the same as that of the virtual data. However, the average error by SMART algorithm for all temperature range obtained by SMART was about 1.4%. Table 4.2.3 shows MSE (mean squared errors) of temperature for every tomography algorithms.

Table 4.2.3 The average absolute temperature error

<table>
<thead>
<tr>
<th>Error[K]</th>
<th>ART algorithm</th>
<th>MART algorithm</th>
<th>SMART algorithm</th>
<th>SART algorithm</th>
</tr>
</thead>
<tbody>
<tr>
<td>35.2</td>
<td>9.1</td>
<td>8.5</td>
<td>31.5</td>
<td></td>
</tr>
</tbody>
</table>
Fig. 4.2.12 Comparisons between ART, MART, SMART and SART algorithms (Temperature)
4.3 Two-dimensional results by CT-TDLAS (Experimental data)

In this study, three absorption lines located at 1388.139 nm (#1), 1388.328 nm (#2) and 1388.454 nm (#3) have been chosen for the calculation of temperature and concentration of H$_2$O. Absorption spectra of H$_2$O at 1388-1388.6 nm in the 16-path cell have been measured by the CT-TDLAS system shown in Fig. 4.3.1.

![Graph showing comparisons between measured temperatures by TDLAS and thermocouple](image)

Fig. 4.3.1 Comparisons between the temperatures measured by TDLAS and thermocouple

The cause of the error in TDLAS is the disagreement between the theory and experimental. The discrepancies between the original virtual data and the TDLAS calculation data are not so large, and it would be also improved by revising the theoretical spectroscopic data [77]. In addition, important to evaluate CT algorithm errors [26, 85] together with the evaluation of these spectroscopic errors. The CT algorithm error is according to the shape of the temperature and concentration distributions, and the error tends to increase when the shape is complicated. In actual use of the optical experimental apparatus, the process of reducing the error between the theory and actual experiment is important. It is directly measured by changing the temperature and pressure of the target gas to be measured, and it can be corrected by contrast
with the theoretical value. Figure 8 shows the comparisons between the temperatures measured by the TDLAS and by the thermocouple. At the temperature range of 300K~800K, the absorption intensities obtained by a calibration process have been used, in which the concentration of H$_2$O, the temperature and the pressure could be controlled in a cell [86]. At the temperature range higher than 800K, the absorption intensities obtained by a flat flame burner test [77] performed under the temperature range from 1244K to 1264K have been used. Using these results, the HITRAN database over 800K have been modified for the actual TDLAS calculations. It can be said that the temperature measured by the thermocouple and the temperature calculated by the TDLAS shows a good agreement, revealing high accuracy.

The temperature distribution of a virtual flame was generated by the use of Gaussian function between 280K and 1200K. In order to evaluate the spatial resolution of the CT-TDLAS, three factors have been tested. The first one is FWHM (full width at half maximum). The virtual temperature profiles having three different FWHM values (10mm, 15mm, 20mm) have been generated, and the profiles have been reconstructed by CT-TDLAS using those virtual data. Then, the FWHM values of the reconstructed temperature profiles by CT-TDLAS have been compared with those of the virtual temperature profiles. The second one is SSD (sum of squared difference). The SSD value has been defined by Eq. (4.3.1). If the SSD value is close to “0”, the two profiles are almost same patterns. The third one is ZNCC (zero-mean normalized cross-correlation) value shown in Eq. (4.3.2). If this value close to 1, the virtual data and the data obtained by CT-TDLAS are similar patterns. That is, the correlation between the two values is very high.

$$SSD = \sqrt{\sum_{i=0}^{K-1} \sum_{j=0}^{M-1} \left( (T_{i,j})_{\text{virtual}} - (T_{i,j})_{\text{CT-TDLAS}} \right)^2 / NM} / T_R$$  \hspace{1cm} (4.3.1)
\[
ZNCC = \frac{\sum_{i=0}^{N-1} \sum_{j=0}^{M-1} (T_{i,j} - \bar{T})_{\text{virtual}} \times (T_{i,j} - \bar{T})_{\text{CT-TDLAS}}}{\sqrt{\sum_{i=0}^{N-1} \sum_{j=0}^{M-1} (T_{i,j} - \bar{T})_{\text{virtual}}^2 \times \sum_{i=0}^{N-1} \sum_{j=0}^{M-1} (T_{i,j} - \bar{T})_{\text{CT-TDLAS}}^2}}, \quad \bar{T} = \frac{\sum_{i=0}^{N-1} \sum_{j=0}^{M-1} T_{i,j}}{NM} \quad (4.3.2)
\]

Here, \( T_{i,j} \) is the temperature at each point in calculation area, \( T_g \) is the representing temperature (The max temperature of virtual data), \( N \) is the total number of meshes along the X-axis in the calculation area, and \( M \) is the total number of meshes along the Y-axis in the calculation.

Table 4.3.1 shows the comparison of the above three values between the virtual data and the data obtained by CT-TDLAS for three different cases, of which FWHM (full width at half maximum) are 10mm, 15mm and 20mm. It can be said that the SSD values for the three cases are less than 5% (13.155K/280K) at most. This implies that the discrepancy between the original virtual data and the data obtained by CT-TDLAS calculation is very small, showing that the present calculation approach is appropriate. Fig. 4.3.2 (a) and 4.3.2 (b) shows the results of the case 3. Fig. 4.3.2 (c) shows the temperature profiles at the center line of the calculation area for the virtual one and the CT-TDLAS calculation results.

<table>
<thead>
<tr>
<th></th>
<th>FWHM (Virtual) [mm]</th>
<th>FWHM (CT-TDLAS) [mm]</th>
<th>SSD</th>
<th>ZNCC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>10</td>
<td>16.9</td>
<td>0.14785</td>
<td>0.83801</td>
</tr>
<tr>
<td>Case 2</td>
<td>15</td>
<td>17.7</td>
<td>0.05381</td>
<td>0.97191</td>
</tr>
<tr>
<td>Case 3</td>
<td>20</td>
<td>18.1</td>
<td>0.01962</td>
<td>0.99907</td>
</tr>
</tbody>
</table>

Table 4.3.1 The spatial resolution evaluate for the virtual data
(a) Temperature distribution by virtual (Case 3)

(b) Reconstructed temperature distribution for the virtual data (Case 3)

(c) Comparisons of temperature distribution at Y=0mm (Case 3)

Fig. 4.3.2 The spatial resolution test of temperature distribution (Case 3)
The spatial resolution of CT is related to the spatial density of the calculation grid. The number of the grid in a CT calculation area and the distance between each grid is known as the sampling interval, which is a function of the accuracy of the CT calculation. In this study used a spatial resolution of the CT is about 17.6mm (FWHM) shown in Table 4.3.1. This result is due to the configuration of the CT calculation grid considering a position of laser path in the whole measurement area. The composition of CT grid used 10 x 10 for the measurement area with a diameter of 70mm. The larger the FWHM value of virtual temperature field is higher the estimation ability with respect to temperature, and the smaller the FWHM value is the lower the estimation ability of the temperature. It can be confirmed by SSD, ZNCC method.

Fig. 4.3.3 shows the two-dimensional temperature field measured by thermocouple experiments. This shows the reconstructed temperature calculated at the grids of 2mm intervals of the measurement cell. It can be seen that the temperature at the center area is relatively high temperature.

Fig. 4.3.3 Temperature distribution measured by thermocouple
Fig. 4.3.4 shows the minimum MSE of the absorption intensities on all grids when the SLOS initial values have been adopted. The minimum value was $3.26 \times 10^{-3}$.

![Graph showing MSE variations with iteration number](image)

**Fig. 4.3.4 Total MSE variations for the iteration number in case of adopting SMART algorithm**

Fig. 4.3.5-6 shows the reconstructed absorption spectra of H$_2$O obtained by the SMART algorithm and by the experiments for all laser path lines. It can be seen that the two profiles of the spectra substantially coincide with each other for all path lines. With these 16 profiles, the temperature and concentration fields have been calculated.
Fig. 4.3.5 Theoretical and experimental absorption spectra of H₂O gas at 1388nm and measured by DFB type laser diode (continued)
Fig. 4.3.6 Theoretical and experimental absorption spectra of $\text{H}_2\text{O}$ gas at 1388nm and measured by DFB type laser diode.
Fig. 4.3.7 (a) and (b) show the results obtained by the CT-TDLAS, in which the SMART algorithm has been adopted. It can be seen that the temperature distribution is similar to the distribution measured by the thermocouple as shown in Fig. 4.3.3, revealing that the temperature calculated by the current approach of CT-TDLAS is validated. However, there is some irregular distribution in concentration field. This is due to the influences of the boundary grids. This will be discussed in more details in the next reports.

(a) Temperature field

(b) Concentration field

Fig. 4.3.7 Temperature and concentration distributions reconstructed by SMART algorithm
Fig. 4.3.8 Comparisons of temperature distribution at \(Y=0\text{mm}, -7\text{mm}\) and \(-14\text{mm}\) calculated by the SMART algorithm of CT-TDLAS and measured by the thermocouple.
Fig. 4.3.8-10 shows the comparisons of the results measured by the thermocouple and calculated by the CT-TDLAS for three different Y locations at Y=0mm, Y=-7mm, and Y=-14mm. It can be seen that the discrepancies between the temperature measured by the thermocouple and the temperature calculated by the CT-TDLAS are quite small at higher locations. However, this discrepancy becomes relatively larger at center region (high-temperature area) at lower locations.

Table 4.3.2 shows the spatial resolution between thermocouple result and CT-TDLAS result in a temperature. It can confirm the reliability of CT-TDLAS results from these quantitative value.

Table 4.3.2 The spatial resolution evaluate for the real flame data

<table>
<thead>
<tr>
<th></th>
<th>SSD</th>
<th>ZNCC</th>
</tr>
</thead>
<tbody>
<tr>
<td>CT-TDLAS</td>
<td>0.05737</td>
<td>0.9480</td>
</tr>
</tbody>
</table>
4.4 Three-dimensional results by CT-TDLAS (Virtual data)

Fig. 4.4.1 shows the arrangement of the laser beams for numerical tests by CT-TDLAS. The total number of the laser paths for each layer was set to 16. And this shows the left half of the system is the detectors part while the right half is the 16 collimators by which the laser beams are adjusted for attaining best focusing. The diameter of the measurement space is 70mm, where the 16 lines are passing through in this cell.

As shown in Fig. 4.4.2, two-dimensional measurement cells were stacked into five layers to construct a three-dimensional measurement space. Fig. 4.4.3 shows three-dimensional laser paths to attain three-dimensional measurements.
Fig. 4.4.2 Three-dimensional measuring device drawing

Fig. 4.4.3 The entire optical path diagram
Fig. 4.4.4 Distribution of initial temperature used for reconstruction test
Fig. 4.4.5 Distribution of initial concentration used for reconstruction test.
Fig. 4.4.4 shows the initial distribution of temperature for the virtual measuring area generated by Gaussian distribution. The temperature variation is based on 280K-1080K. Fig. 4.4.5 shows the concentration field obtained using the temperature values in Fig. 4.4.4. It has been assumed that the H$_2$O vapor passed through the measuring area. Representative wavelengths used for the measurement of the absorption spectra of H$_2$O are #1 (1388.139nm), #2 (1388.328nm) and #3 (1388.454nm). This assumes the temperature and concentration field ranges of H$_2$O, which can be measured by combustion of the methane. The concentration (1%-5%) of H$_2$O increases linearly depend on the temperature increases. Fig. 4.4.5 shows the initial distribution of computational concentration. Fig. 4.4.6 represents the virtual absorption spectra of each laser, which is generated using the equations (2.2.4) and (2.5.1). The profiles has been used for calculating the temperature and concentration fields using the SMART reconstruction algorithms. Specially one ratios of (#1/#2) of the representative absorption lines were used for the calculation of temperature. Evaluation for finishing iterative calculations chosen for data reconstruction is based on the MSE (mean square error) which is the error between the virtual data (Fig. 4.4.4 and Fig. 4.4.5) and the reconstructed data at whole iterative step.
Fig. 4.4.6 Recovered absorption spectra (H$_2$O) for three-dimensional measurement cell
The parameter that causes the greatest change in the analysis of the absorption spectra is temperature. Therefore, the initial value is generated using the method of permutation with repetition in fixed concentration at 1%. This is obtained by using Eq. (2.2.4), (2.5.1) and (2.5.2). Next, the initial temperature at the obtained value is set. And the concentration value is set so that the concentration value rises according to the temperature increments. However, there are limits to what can be obtained via permutations, and the absorption spectra in the nearby region does not difference too much. Therefore, the initial value is corrected by comparing the ratio value for the virtual absorption spectra with the maximum value and the minimum value for each layer with relative values. As a result, the initial value given to the calculation of each layer shows a relative change. And this value as shown in Table 4.4.1.

<table>
<thead>
<tr>
<th></th>
<th>Layer 1</th>
<th>Layer 2</th>
<th>Layer 3</th>
<th>Layer 4</th>
<th>Layer 5</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Max</strong></td>
<td>1</td>
<td>0.987835</td>
<td>0.948310</td>
<td>0.894724</td>
<td>0.805938</td>
</tr>
<tr>
<td><strong>Min</strong></td>
<td>1.031978</td>
<td>1.029369</td>
<td>1.021291</td>
<td>1.010583</td>
<td>1</td>
</tr>
</tbody>
</table>

It is placed in the initial value corresponding to the calculation on the 1-5 layers, the temperature and concentration fields are calculated by CT-TDLAS. The value representing the minimum error at this time is determined by the temperature field on each floor, the value between each layer is restored from the viewpoint of Fig. 4.4.7. However, an error occurs in relation to the actual temperature and concentration fields, since this method is a simple averaging method. In order to correct this, the value of the gradient laser absorption spectra is used. In the calculation principle as shown Fig. 4.4.8. The average value from the region calculated by 16 path cells is obtained, the 10×10×10 voxel region is simplified to the 9×9×9 voxel region. At this time, the diagonal laser beam will go through the area, use this part for CT-TDLAS to find the temperature and concentration value of the minimum error value. The minimum value of errors that will eventually be obtained is shown in Fig. 4.4.9.
Fig. 4.4.7 Simple averaging method for cell to cell area

Fig. 4.4.8 Average calculation principle for three-dimensional voxel
Fig. 4.4.9 The minimum value of errors for three dimensional calculation at final step (MSE)

Fig. 4.4.10 shows the temperature and concentration fields results for each layers (1, 3 and 5th layers). This CT calculation results is similar compare than virtual data. Fig. 4.4.11 (a), (b) and (c) shows a comparison of the virtual data and the CT-TDLAS result for each y location. Fig. 4.4.11 (a) shows a comparison result of the temperature profile passing through the center in the 1st and 3rd layer cell of y=0mm. Fig. 4.4.11 (b) and (c) shows a comparison result of the temperature profile passing through the 1st layer cell of y=14mm and y=28mm. We can know that each of the virtual data and CT-TDLAS results per location is fairly consistent. The maximum temperature difference was 86.8K and the minimum temperature difference was 0.03K from the comparison results of all absorption spectra.
(a) Reconstructed results of temperature and concentration field (1\textsuperscript{st} layer)

(b) Reconstructed results of temperature and concentration field (3\textsuperscript{rd} layer)

(c) Reconstructed results of temperature and concentration field (5\textsuperscript{th} layer)

Fig. 4.4.10 Temperature and concentration distributions recalculated by SMART algorithm
Fig. 4.4.11 Comparison of temperature distribution at $y=0$mm, 14mm and 28mm measured by CT measurement cell (1, 3 and 5 layer) and virtual data
Table 4.4.2 shows the spatial resolution between virtual data and CT-TDLAS results. It can confirm the reliability of CT-TDLAS results from these quantitative values. The first one is SSD (sum of squared difference). The SSD value has been defined by Eq. (4.4.1, 4.4.2). If the SSD value is close to “0”, the two profiles are almost same patterns.

The second one is ZNCC (zero-mean normalized cross-correlation) value shown in Eq. (4.4.3, 4.4.4). If this value close to 1, the virtual data and the data obtained by CT-TDLAS are similar patterns. That is, the correlation between the two values is very high.

\[
SSD_T = \sqrt{\frac{\sum_{i=0}^{N-1} \sum_{j=0}^{M-1} (T_{i,j}^{\text{virtual}} - T_{i,j}^{\text{CT-TDLAS}})^2}{NM}} / T_R
\]  
(4.4.1)

\[
SSD_C = \sqrt{\frac{\sum_{i=0}^{N-1} \sum_{j=0}^{M-1} (C_{i,j}^{\text{virtual}} - C_{i,j}^{CT-TDLAS})^2}{NM}} / C_R
\]  
(4.4.2)

\[
ZNCC_T = \frac{\sum_{i=0}^{N-1} \sum_{j=0}^{M-1} (T_{i,j}^{\text{virtual}} - \bar{T}_{CT-TDLAS}) \times (T_{i,j}^{\text{CT-TDLAS}} - \bar{T})}{\sqrt{\sum_{i=0}^{N-1} \sum_{j=0}^{M-1} (T_{i,j}^{\text{virtual}} - \bar{T}_T)^2} \times \sqrt{\sum_{i=0}^{N-1} \sum_{j=0}^{M-1} (T_{i,j}^{\text{CT-TDLAS}} - \bar{T})^2}} = \frac{\sum_{i=0}^{N-1} \sum_{j=0}^{M-1} T_{i,j}}{NM}
\]  
(4.4.3)

\[
ZNCC_C = \frac{\sum_{i=0}^{N-1} \sum_{j=0}^{M-1} (C_{i,j}^{\text{virtual}} - \bar{C}_{CT-TDLAS}) \times (C_{i,j}^{CT-TDLAS} - \bar{C})}{\sqrt{\sum_{i=0}^{N-1} \sum_{j=0}^{M-1} (C_{i,j}^{\text{virtual}} - \bar{C}_C)^2} \times \sqrt{\sum_{i=0}^{N-1} \sum_{j=0}^{M-1} (C_{i,j}^{CT-TDLAS} - \bar{C})^2}} = \frac{\sum_{i=0}^{N-1} \sum_{j=0}^{M-1} C_{i,j}}{NM}
\]  
(4.4.4)
Here, $T_{i,j}$ is the temperature at each point in calculation area, $T_R$ is the representing temperature (The max temperature of virtual data), $C_{i,j}$ is the concentration at each point in calculation area, $C_R$ is the representing concentration (The max concentration of virtual data), $N$ is the total number of meshes along the X-axis in the calculation area, and $M$ is the total number of meshes along the Y-axis in the calculation.

<table>
<thead>
<tr>
<th>Layer</th>
<th>$SSD_T$</th>
<th>$ZNCC_T$</th>
<th>$SSD_C$</th>
<th>$ZNCC_C$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1st Layer</td>
<td>0.03391</td>
<td>0.98031</td>
<td>0.04417</td>
<td>0.96574</td>
</tr>
<tr>
<td>2nd Layer</td>
<td>0.03401</td>
<td>0.98018</td>
<td>0.04397</td>
<td>0.96508</td>
</tr>
<tr>
<td>3rd Layer</td>
<td>0.03316</td>
<td>0.97974</td>
<td>0.04460</td>
<td>0.96127</td>
</tr>
<tr>
<td>4th Layer</td>
<td>0.03479</td>
<td>0.97949</td>
<td>0.04664</td>
<td>0.95532</td>
</tr>
<tr>
<td>5th Layer</td>
<td>0.03147</td>
<td>0.97752</td>
<td>0.05013</td>
<td>0.93883</td>
</tr>
</tbody>
</table>
4.5 Three-dimensional results by CT-TDLAS (Experimental data)

Fig. 7 shows the arrangement of the laser beams for numerical calculation using CT-TDLAS in each layer. The total number of laser paths for each layer was set 16-paths. Then, this system can divide the part for collimators and photo detectors. The diameter of measurement space is 70mm, and 16 laser lines are passing through in this cell.

![Diagram of laser beams arrangement](image)

Fig. 4.5.1 Temperature and concentration distributions recalculated by SMART algorithm

Fig. 4.5.2 shows the actual flame experimental setup. The burner has a double tube structure for surrounding air and flame fuel. Methane gas has been used as fuel and it has been mixed with dry air.
Fig. 4.5.2 Experimental apparatus for three-dimensional temperature measurement in flame burner using CT-TDLAS

Fig. 4.5.3 The entire optical path diagram
As shown in Fig. 4.5.3, two-dimensional measurement cells were stacked into five layers to construct a three-dimensional measurement space. And shows the three-dimensional laser paths to attain three-dimensional measurements.

In this study, absorption spectra of H$_2$O at 1388.0-1388.6nm in the 96-path cell have been measured by CT-TDLAS. Especially, three absorption lines located at 1388.139 nm (#1), 1388.328 nm (#2) and 1388.454 nm (#3) have been chosen for the calculation of temperature and concentration.

Important to evaluate TDLAS error together with the evaluation of CT algorithm error. The cause of the error in TDLAS is the disagreement between the experimental result and theoretical result. This discrepancy can be solved by revising the theoretical spectroscopic data [26, 65]. It can be corrected by contrast with the theoretical value by directly measured data.

Fig. 4.5.4 shows the comparisons between the changing temperatures measured by the thermocouple and by the TDLAS [77, 86]. It can be said that modified database shows a good agreement and high accuracy.

![Graph](image)

**Fig. 4.5.4 Comparisons between the temperatures measured by TDLAS and thermocouple**
The CT algorithm error can be explained by spatial resolution. The spatial resolution of CT is related to the spatial density of the calculation grid. The number of the grid in a CT calculation area and the distance between each grid is known as the sampling interval, which is a function of the accuracy of the CT calculation. In this study used a spatial resolution of the CT is about 17.6mm (FWHM) in each layer of the three-dimensional measurement device. It is most good performance value for CT calculation.

Fig. 4.5.5 show the two-dimensional temperature field measured by thermocouple experiments. This shows the reconstructed temperature calculated at the grids of 3.5mm intervals of the measurement cell. It can be seen that the temperature at the center area is a relatively high-temperature in whole layers.

The burner was placed middle and under the position of three-dimensional measurement cell, the temperature of each layer was measured using a thermocouple and compared with a result of CT-TDLAS. Fig. 4.5.6-10 shows the comparisons of the results measured by the thermocouple and calculated by the CT-TDLAS for three different Y locations at Y= 0mm, and Y= -10.5mm in each layers.
Fig. 4.5.5 Temperature distribution measured by thermocouple
Fig. 4.5.6 Comparisons of temperature distribution at Y=0mm and -10.5mm calculated by the SMART algorithm of CT-TDLAS and measured by the thermocouple (1st layer, Z=28mm)

Fig. 4.5.7 Comparisons of temperature distribution at Y=0mm and -10.5mm calculated by the SMART algorithm of CT-TDLAS and measured by the thermocouple (2nd layer, Z=14mm)
Fig. 4.5.8 Comparisons of temperature distribution at Y=0mm and -10.5mm calculated by the SMART algorithm of CT-TDLAS and measured by the thermocouple (3rd layer, Z=0mm)

Fig. 4.5.9 Comparisons of temperature distribution at Y=0mm and -10.5mm calculated by the SMART algorithm of CT-TDLAS and measured by the thermocouple (4th layer, Z=-14mm)
Fig. 4.5.10 Comparisons of temperature distribution at Y=0mm and -10.5mm calculated by the SMART algorithm of CT-TDLAS and measured by the thermocouple (5th layer, Z= -28mm)

The temperature difference in the first layer was the largest, and the average relative error in the entire layer was 0.6% in the center point each layer. It can be shown Fig. 4.5.11.

Fig. 4.5.11 Comparison result with thermocouple and CT-TDLAS (1-5th layers)
Fig. 4.5.12 shows the minimum MSE (mean square errors) of the absorption intensities on all grids when the SLOS method and Gaussian distribution initial values has been adopted. The minimum value was $5.55 \times 10^{-3}$.

![Graph showing Total MSE variations for the iteration number in case of adopting SMART algorithm](image)

In order to evaluate the spatial resolution of the CT-TDLAS, two factors have been tested between thermocouple temperature data and CT-TDLAS data.

The first one is SSD (sum of squared difference). The second one is ZNCC (zero-mean normalized cross-correlation). The SSD value has be defined by Eq. (4.4.1). If the SSD value is close to “0”, the two profiles are almost same patterns. The ZNCC (zero-mean normalized cross-correlation) value shown in Eq. (4.4.3). If this value close to “1”, the thermocouple temperature data and the calculated data obtained by CT-TDLAS are similar pattern. That is, the correlation between the two result values is very high.
Table 4.5.1 shows the spatial resolution between thermocouple result and CT-TDLAS result for a temperature. It can confirm the reliability of CT-TDLAS results from these quantitative value in each layers. Whole layer results show to similar results, SSD is about 0.1 and ZNCC is about 0.98. It can be said that has a good performance for CT-TDLAS about whole layers.

Table 4.5.1 The spatial resolution evaluate for the real flame data

<table>
<thead>
<tr>
<th>Layer</th>
<th>SSD</th>
<th>ZNCC</th>
</tr>
</thead>
<tbody>
<tr>
<td>1st</td>
<td>0.13574</td>
<td>0.86357</td>
</tr>
<tr>
<td>2nd</td>
<td>0.14520</td>
<td>0.85115</td>
</tr>
<tr>
<td>3rd</td>
<td>0.14561</td>
<td>0.84293</td>
</tr>
<tr>
<td>4th</td>
<td>0.13933</td>
<td>0.84933</td>
</tr>
<tr>
<td>5th</td>
<td>0.13815</td>
<td>0.84454</td>
</tr>
</tbody>
</table>

Fig. 4.5.13-17 shows the each layer (1st to 5th layer) results obtained by three-dimensional CT-TDLAS using SMART algorithm. The temperature and concentration were decreased with increasing distance from the center position in each layer. Fig. 4.5.18 shows the temperature distribution at YZ surface at x=0mm. The temperature was high at the center of the layer near the burner.
Fig. 4.5.13 Temperature and concentration distributions recalculated by SMART algorithm (1st layer)
(a) Reconstructed results of temperature field (2nd layer)

(b) Reconstructed results of concentration field (2nd layer)

Fig. 4.5.14 Temperature and concentration distributions recalculated by SMART algorithm (2nd layer)
Fig. 4.5.15 Temperature and concentration distributions recalculated by SMART algorithm (3rd layer)

(a) Reconstructed results of temperature field (3rd layer)

(b) Reconstructed results of concentration field (3rd layer)
Fig. 4.5.16 Temperature and concentration distributions recalculated by SMART algorithm

(a) Reconstructed results of temperature field (4th layer)

(b) Reconstructed results of concentration field (4th layer)
Fig. 4.5.17 Temperature and concentration distributions recalculated by SMART algorithm (5th layer)
Fig. 4.5.18 The temperature distribution of three-dimensional CT-TDLAS result (YZ plane, X=0mm)
Chapter 5 Conclusion

5.1 Target gas detection in high-temperature and high-pressure using TDLAS

CT-TDLAS experiments were carried out in a state of high-temperature and high-pressure (for H₂O and CH₄ gas). The measurement target gas, by applying the value of the change in high-temperature and high-pressure conditions in the calculation of the theoretical absorption spectra, it became possible to accurately evaluate the broader experimental conditions. The patterns of absorption spectra in the low temperature and high-temperature regions differ according to the target substance. In this study, it is expected that the accuracy of measurement can be improved by simultaneously measuring the absorption spectra of two substances.

5.2 Two-dimensional results by CT-TDLAS (Virtual data)

Four different reconstruction algorithms have been tested numerically using experimental data sets measured by thermocouples for combustion fields. The measurement data obtained by thermocouples were successfully used as the virtual reference data for generating the absorption spectra for the evaluations of four different reconstruction algorithms, ART, MART, SART, and SMART. The calculation results by all algorithms showed small error within 20K at low temperature region (280K~590K). Thus, the relative errors by all algorithms were 3% ~ 14% at lower temperature regions. However, at high temperature regions, ART and SART algorithm showed the maximum error of 350K at 950K, and 330K at 1280K, respectively. However, MART algorithm showed the maximum errors within 1K at high temperature regions. This implies that MART algorithm is recommendable rather than ART and SART algorithms for CT-TDLAS calculations. The calculation time for convergence to the minimum error by SMART algorithm was the shortest among four algorithms, while the convergence time to the minimum error by SART algorithm showed shorter than by those by ART and MART algorithms. Further, the magnitude of the MSE (mean squared errors) by SMART algorithm was the smallest, and the iterative number was only within 50 for reaching to the convergences. It has been proven numerically that SMART algorithm was the most reliable approach for reconstructing the multiple signals of CT-TDLAS. The relative error ratio in the result obtained by SMART algorithm was about 1.4%.
5.3 Two-dimensional results by CT-TDLAS (Experimental data)

Measurements for temperature distribution have been performed by a thermocouple. The temperature distribution has been reconstructed by the SMART algorithm and the results have been compared with those by the thermocouple giving the following summary. A SLOS method has been adopted to get initial values. It has been experimentally shown that this approach is appropriate for choosing the initial values for performing iterative calculations with experimental absorption spectra of the CT-TDLAS. In order to evaluate the performance of the adopted CT-TDLAS algorithm, three parameters, FWHM (full width at half maximum), SSD (sum of squared difference), and ZNCC (zero-mean normalized cross-correlation), have been adopted, by which the adopted CT-TDLAS algorithm is capable of reconstructing the temperature distribution and the concentration distribution with relatively high accuracy. The discrepancies between the spectra profiles calculated by theoretically and measured by experimentally were about 5.27%. This implies that a SMART algorithm is a reliable approach for reconstructing the multiple signals of the CT-TDLAS. The discrepancies between the temperature measured by the thermocouple and the temperature calculated by the CT-TDLAS were quite small at higher locations of the flame burner. However, these discrepancies were relatively larger at center region (high-temperature area) at lower locations of the burner. This would be improved by revising the theoretical spectroscopic data.

5.4 Three-dimensional results by CT-TDLAS (Virtual data)

CT-TDLAS calculation for the virtual three-dimensional measurement space was performed. The results of this study are summarized as follows. In order to three-dimensional CT calculation of the virtual H$_2$O absorption spectra, we adopted to Gaussian distribution to construct the initial temperature and concentration fields by three-dimensionally. In order to CT calculate for the absorption spectra of the virtual H$_2$O, we used the permutation method and the simple average method in the implementation method of the initial temperature field. As a result, we were able to differently input the initial temperature conditions based on the absorption spectra of each layer. By virtual and three-dimensional CT-TDLAS results was
match significantly, the application of the SMART algorithm for TDLAS is also assessed to be suitable. The calculation results of virtual and CT-TDLAS was almost matched for all absorption spectra. The relative average error ratio in the results obtained by SMART algorithm was about 3.2%. The maximum error was 86.8K and the lowest error was 0.03K. It has been proven numerically that SMART algorithm was reliable approach for reconstructing the multiple signals of CT-TDLAS.

5.5 Three-dimensional results by CT-TDLAS (Experimental data)

CT-TDLAS calculation for the three-dimensional measurement space was performed about the actual flame. The results of this study are summarized as follows. In order to three-dimensional CT-TDLAS calculate of the actual flame absorption spectra using special initial value. It was used SLOS method and Gaussian distribution. It has been shown that this method is appropriate for choosing the initial values for CT-TDLAS calculation. The temperature comparison result of the center in each layer about thermocouple and CT-TDLAS has an average relative error about 0.6%. The thermocouple measurement data and CT-TDLAS calculated results substantially match with each other for all area. In order to evaluate the performance of the adopted CT-TDLAS algorithm used two parameters. Have been adopted SSD (sum of squared difference) and ZNCC (zero-mean normalized cross-correlation) is capable of reconstructing the temperature and concentration distributions with relative high accuracy. In this study, we confirmed that it is possible to three-dimensional measure the temperature and concentration for the actual flame.
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