Mid-Infrared Laser Measurement of Diffusion Flame Temperature Field Postprint

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Full Text

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Temperature Field Measurement of Diffusion Flames Using Mid-Infrared Laser

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Abstract

This study measures the temperature field of an ethylene coaxial diffusion flame based on direct absorption spectroscopy of the v3 fundamental absorption band of carbon dioxide. The experiment employs a room-temperature interband cascade laser (ICL) with a wavelength of 4.17 µm to measure path-integrated absorption through the axisymmetric flame at multiple absorption peaks of this band. Through Abel inversion, the radial distribution of absorptivity at different flame heights is retrieved, and subsequently, referencing the HITRAN database and fitting the experimental data via least squares method yields the temperature field distribution of carbon dioxide in the flame. To improve the accuracy of Abel inversion, this paper adopts a regularized Abel inversion method and verifies its feasibility through numerical simulation.

Keywords: axisymmetric diffusion flame; quantum cascade laser; Abel inversion; temperature; carbon dioxide

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Laminar coflow diffusion flames serve as standard flames and are commonly used in studies of soot formation and combustion chemistry [1,2]. The temperature field and combustion product concentration are important flame parameters that determine the rates of soot formation, oxidation, and combustion reactions. Thermocouples are commonly used for gas temperature measurement. However, when applied to flames, radiative heat conduction around the thermocouple junction can cause thermal imbalance between the junction and surrounding gas, and the instability of materials used for high-temperature thermocouples in flame environments increases uncertainties associated with radiative heat transfer corrections [3].

Tunable diode laser absorption spectroscopy (TDLAS) enables in-situ measurement of temperature and gas concentration in flames [4-6]. Carbon dioxide in flames has strong absorption in the mid-infrared band at 4.17 µm. Near this wavelength, absorption interference from other atmospheric gases or other combustion products in the flame can be neglected, facilitating measurement with high precision [5,6]. Direct absorption spectroscopy measures path-integrated signals along the laser beam. For non-uniform flame parameters, tomographic methods are typically required to reconstruct the flame parameters at each location along the laser path [7].

For axisymmetric flames, such as laminar flat premixed flames [6] and laminar coflow diffusion flames, flame parameters like temperature and gas concentration exhibit axisymmetric radial distributions. Therefore, they can be reconstructed through Abel inversion of path-integrated signals measured at different distances from the flame center. Abel inversion finds wide application in science and engineering, and numerous inversion methods have been developed, among which the most commonly used are the Onion-Peeling (hereinafter referred to as OP) and Abel Three-Point (hereinafter referred to as ATP) methods [8]. However, due to the ill-conditioned nature of their corresponding matrix equations [9-11], small errors in experimental signals are amplified during the inversion process, causing the results to deviate significantly from true values.

Tikhonov regularization has proven effective in reducing errors in Abel inversion

[9-11]. The key to proper application of Tikhonov regularization lies in determining an appropriate regularization parameter, with the L-curve method being a commonly used approach for this purpose [9-11]. Previous work on reconstructing axisymmetric flame temperature fields using TDLAS combined with Abel inversion has primarily focused on flat flames [6,8]; no studies have applied this method to diffusion flame temperature fields. This paper verifies the applicability of the regularization method through numerical simulation and measures path-integrated absorption signals of carbon dioxide in an ethylene coflow diffusion flame using a room-temperature interband cascade laser (ICL) at 4.17 µm wavelength. Combining Abel inversion with HITRAN database fitting, the temperature distribution of the ethylene diffusion flame is obtained.

1 Fundamental Principles and Numerical Simulation

1.1 Direct Absorption Spectroscopy Principle

TDLAS technology is based on the Beer-Lambert absorption law. When a laser beam with frequency passes through a gas of length L, the transmittance T_ can be expressed by the absorption integral along the optical path. The absorption coefficient _ (l) at position l depends on the mole fraction (l) of the target gas, its line strength S_j for transition j, and the lineshape function (, _0j), where _0j is the center transition frequency.

The relationship between line strength S_j and temperature T is given by:

$$S_j(T) = S_j(T_0)\frac{Q(T_0)}{Q(T)}\exp\left(-\frac{hcE''}{kT}\right)\exp\left(\frac{hcE''}{kT_0}\right)\frac{1-\exp(-hc\nu_{0j}/kT)}{1-\exp(-hc\nu_{0j}/kT_0)}$$

where h is Planck' s constant, c is the speed of light, k is Boltzmann' s constant, T_0 is the reference temperature (typically 296 K), E'' is the lower energy level of the absorption transition, and Q(T) is the partition function [12]. As shown in this equation, line strength depends only on temperature.

The spectral lineshape for atmospheric pressure diffusion flame measurements in this study can be described by the Voigt profile, obtained through convolution of Gaussian and Lorentzian profiles:

$$\phi_V(u) = \int_{-\infty}^{\infty} \phi_G(u')\phi_L(u-u')du'$$

where u is the relative frequency (actual frequency minus center frequency), and and are the half-widths at half-maximum (HWHM) for Gaussian and Lorentzian profiles, respectively. The Gaussian and Lorentzian profiles are given by:

$$\phi_G(u) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{u^2}{2\sigma^2}\right)$$

$$\phi_L(u) = \frac{\gamma/\pi}{u^2 + \gamma^2}$$

The HWHM values and can be expressed as:

$$\sigma = \frac{\nu_0}{c}\sqrt{\frac{2kT\ln 2}{M}}$$

$$\gamma = \gamma_{\text{air}}\left(\frac{T_0}{T}\right)^{n_{\text{air}}} P$$

where N_A is Avogadro' s constant, M is molecular molar mass, _air is the air-broadened HWHM at normal temperature and pressure, and n_air is the temperature-dependent exponent. The HITRAN database provides relatively accurate data for _air and n_air for different transitions. Since this experiment is conducted at atmospheric pressure, absorptivity depends primarily on flame temperature and carbon dioxide concentration.

1.2 Abel Inversion Method

Figure 1 [Figure 1: see original paper] shows a horizontal cross-section of an axisymmetric flame at a certain height. According to the Beer-Lambert law and Abel integral equation, the relationship between path-integrated measurement P(x,) and radial distribution (r,) for a given frequency is:

$$P(x,\nu) = 2\int_x^R \frac{r\alpha(r,\nu)}{\sqrt{r^2 - x^2}}dr, \quad -R < x < R$$

where x is the distance from the flame center and R is the flame radius. The total path-integrated absorption signal is obtained by integrating over the laser scanning frequency range:

$$P(x) = \int_{\nu_1}^{\nu_2} P(x,\nu)d\nu$$

where _1 and _2 are the lower and upper limits of the continuous laser scanning frequency. The Abel equation has an analytical solution:

$$\alpha(r) = -\frac{1}{\pi}\int_r^R \frac{dP(x)/dx}{\sqrt{x^2 - r^2}}dx$$

However, in practical measurements, calculating derivatives of P(x) using finite differences amplifies experimental errors, making direct solution using this equation impractical [8,10,11].

Many alternative Abel algorithms have been proposed. The OP method divides the flame cross-section into N concentric rings of equal width, assuming uniform flame parameters within each ring, transforming Abel inversion into solving a linear system:

$$\mathbf{A}_{\mathrm{OP}}\alpha = \mathbf{P}$$

where { _1, _2, ···, _N} are absorption values in each ring, {P_1, P_2, ··· , P_N} are path-integrated signals at different distances from the center, and A_OP is an N×N geometric matrix. The ATP method offers higher accuracy by considering derivatives of adjacent paths [8] and transforms Abel inversion into a similar linear system:

$$\mathbf{A}_{\mathrm{ATP}}\alpha = \mathbf{P}$$

1.2.1 Ill-Conditioned Matrix Problem Due to the ill-conditioned nature of matrices constructed by OP and ATP methods, small noise in measured path-integrated signals leads to significant deviations between solutions and true values. In solving the equation A = P, singular value decomposition of matrix A yields [9]:

$$\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^T$$

where U and V contain N orthogonal column vectors, and Σ is a diagonal matrix containing singular values _i. Due to orthogonality of U and V, the solution can be written as:

$$\alpha = \sum_{i=1}^{N} \frac{\mathbf{u}_i^T\mathbf{p}}{\sigma_i}\mathbf{v}_i$$

where p is the experimentally measured path-integrated absorption signal, p_0 is the ideal signal without error, and = p - p_0 represents measurement error. This expression shows that small singular values amplify experimental errors, reducing Abel inversion accuracy.

1.2.2 Tikhonov Regularization Method For stable flames, temperature and concentration distributions should be continuous and smooth. An effective regularization approach adds a smoothness constraint to the matrix equation, modifying it for Abel inversion [7,10,11]:

$$\begin{bmatrix} \mathbf{A} \\ \lambda \mathbf{L} \end{bmatrix} \alpha = \begin{bmatrix} \mathbf{P} \\ \mathbf{0} \end{bmatrix}$$

where L is the Laplacian matrix imposing smoothness constraints and is the regularization parameter controlling constraint strength. Matrix L takes the form:

$$\mathbf{L} = \begin{bmatrix} 1 & -1 & 0 & \cdots & 0 \\ 0 & 1 & -1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 \end{bmatrix}_{k \times N}$$

Matrix L smooths transitions between adjacent terms in . The number of rows k can be adjusted based on the specific inversion object and matrix type. For the OP method, k = 1 yields good results, while for ATP, k selection has less influence. In the simulations below, k = N-1 is used for ATP. Since equation (15) is overdetermined, the optimal solution is obtained via least squares:

$$\alpha = (\mathbf{A}^T \mathbf{A} + \lambda^2 \mathbf{L}^T \mathbf{L})^{-1} \mathbf{A}^T \mathbf{P}$$

When using regularized Abel inversion, selection of is critical: too small yields insignificant regularization, while too large compromises accuracy despite smooth results. The L-curve method effectively determines the regularization parameter [9-11]. Figure 2 [Figure 2: see original paper] illustrates the L-curve principle: for various values, the curve connects points representing solution norm ‖Lx__ ‖ versus residual norm ‖Ax__ - P‖ . The ideal occurs at maximum curvature, where both norms are relatively small.

In this experiment, Abel inversion is required at multiple flame heights. Automated selection simplifies data processing. Curvature is calculated via finite differences to find the corresponding to maximum curvature, enabling automated regularized Abel inversion.

1.2.3 Numerical Simulation Verification At lower flame positions, radial absorptivity exhibits bimodal distribution, while at higher positions it shows unimodal distribution. To facilitate simulations, we constructed two representative distributions shown in Figure 3 [Figure 3: see original paper], where f (r) and f (r) are assumed single-peak and double-peak radial distribution functions, respectively, with normalized radius r.

Using equation (9) and integration by parts, the Abel path-integrated functions are:

$$P_1(x) = 2\int_x^1 \frac{rf_1(r)}{\sqrt{r^2 - x^2}}dr, \quad P_2(x) = 2\int_x^1 \frac{rf_2(r)}{\sqrt{r^2 - x^2}}dr$$

where P (x) and P (x) are Abel integrals for single-peak and double-peak distributions at distance x from the flame center. This experiment considers inversion using 20 equally spaced path-integrated values. Without experimental error, even the simple OP method achieves accurate results, as shown in Figure 3 [Figure 3: see original paper].

In the simulation, random noise with 2% amplitude was added to integrated values. Noisy data were inverted using OP, ATP, regularized OP (Tik-OP), and regularized ATP (Tik-ATP) methods, with results compared against original distributions to verify accuracy. Typical inversion results are shown in Figure 4 [Figure 4: see original paper].

For quantitative error analysis, 100 noisy numerical experiments were repeated. The averaged root-mean-square error (RMSE) from 100 trials compares method accuracy under noise:

$$E_{\mathrm{rms}} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(f_{\mathrm{inv},i} - f_{\mathrm{exact},i})^2}$$

where N = 20 is the number of terms, f_inv is the Abel inversion solution, and f_exact is the original distribution. Table 1 compares the mean RMSE values.

Table 1 Comparison of Mean Square Error

The methods rank in accuracy as: Tik-OP > Tik-ATP > ATP > OP. For the 20×20 OP matrix, regularization effectively improves accuracy, while for ATP matrices, improvement is limited. Based on these results, Tik-OP method is employed for experimental data processing.

2 Experimental Measurement

Figure 5 [Figure 5: see original paper] shows the experimental apparatus schematic. An ICL laser near 4.17 µm scans wavenumbers from 2396.9 cm ^{1} to 2397.4 cm ^{1} via a sine wave from a function generator. The laser splits into three beams: etalon for wavelength calibration, reference path, and coflow flame measurement path. To prevent beam steering in high-temperature regions from causing incomplete detection, focusing optics are placed before detectors.

A stepper motor controls burner position horizontally (from flame center to outer edge in 0.05 cm increments) and vertically (from flame base to tip in 0.1 cm increments). Detector 2 measures reference path signal I for baseline correction. The etalon signal has equally spaced peaks in wavenumber, enabling wavelength calibration within each scan period using known HITRAN absorption peaks.

Figure 6 [Figure 6: see original paper] shows raw data during half a sine scan period at one flame position, with corrected background signal. Strong CO absorption at 4.17 µm mid-infrared laser is evident at flame temperatures.

To compare reconstruction method accuracy for unimodal and bimodal distributions, absorption signals at Y = 50 mm and Y = 20 mm were inverted using the aforementioned methods. Results are shown in Figure 7 [Figure 7: see original paper]. Combining simulation conclusions with Figure 7 results, Tik-OP yields smooth, accurate results. Therefore, all horizontal path-integrated values at each height and wavenumber are processed using Tik-OP to obtain radial absorptivity distributions, which are least-squares fitted with HITRAN data to determine temperature distribution.

The experiment adopts conditions similar to Reference [2]: 60% ethylene, 40% nitrogen, 5 cm/s fuel exit velocity. Figures 8 [Figure 8: see original paper]-10 compare results with Reference [2]. At heights > 30 mm, temperature distributions are essentially consistent and smoother than literature data. At Y = 25 mm, temperatures differ by ~100 K but radial trends are similar. Differences in burner dimensions and air flow rates between experiments may account for discrepancies.

3 Conclusions

This study reconstructs the temperature field of an ethylene axisymmetric diffusion flame using TDLAS and Abel inversion. Tikhonov regularization constrains the inversion matrices (OP and ATP), with numerical simulation verification. Experiments under conditions similar to Reference [2] validate measurement and analysis reliability.

1) For the 20×20 OP matrix, Tikhonov regularization effectively reduces path-integrated noise impact, significantly improving Abel inversion accuracy.
2) The measured maximum temperature of the ethylene coflow diffusion flame is approximately 1850 K, with temperature distribution consistent with Reference [2].

Figure 8 [**Figure 8: see original paper**] Temperature distribution of vertical central section of flame

Figure 9 [**Figure 9: see original paper**] Radial distribution of flame temperature at several heights

Figure 10 [**Figure 10: see original paper**] Flame temperature profile along central vertical axis

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Note: Figure translations are in progress. See original paper for figures.