Fan Beam Emission Tomography for Estimating Scalar Properties in Laminar Flames

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This report is a formal draft or working paper, intended to solicit comments and ideas from a technical peer group.

This report contains preliminary findings, subject to revision as analysis proceeds.

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FAN BEAM EMISSION TOMOGRAPHY FOR ESTIMATING SCALAR PROPERTIES IN LAMINAR FLAMES

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Abstract
A new method of estimating temperatures and gas species concentrations (CO$_2$ and H$_2$O) in a laminar flame is reported. The path-integrated, spectral radiation intensities emitted from a laminar flame at multiple wavelengths and view angles are calculated using a narrow band radiation model. Synthetic data, in the form of radial profiles of temperature and gas concentrations, are used in these calculations. The calculations mimic measurements that would theoretically be obtained using a mid-infrared spectrometer with a scanner. The path–integrated spectral radiation intensities are deconvoluted using a maximum likelihood estimation method in conjunction with an iterative scheme. The deconvolution algorithm accounts for the self-absorption of radiation by the intervening gases, and provides the local temperature and gas species concentrations. The deconvoluted temperatures and gas concentrations are compared with the synthetic data used for calculating the spectral radiation intensities. The deconvoluted temperatures and gas species concentrations are within 0.5 % of the synthetic data. The deconvolution algorithm is expected to provide combustion researchers with an easy method of obtaining the radial profiles of major gas species concentrations and temperatures in laminar flames non-intrusively using a mid-infrared spectrometer with a scanner.

Introduction
Obtaining information on the instantaneous structure of turbulent and transient flames is important in a wide variety of applications such as fire safety, pollution reduction, flame spread studies, and model validation. Durao et al. (1992) has reviewed the different methods of obtaining structure information in reacting flows. These include Tunable Laser Absorption Spectroscopy (Hanson et al., 1980), Laser Induced Fluorescence (Crosley and Smith, 1983), Coherent Anti-Raman Spectroscopy (Eckbreth et al., 1979), and Fourier Transform Infrared Spectroscopy (Best et al., 1991), Laser Induced Incandescence (Dasch, 1984), and Emission Spectroscopy (Sivathanu and Gore, 1991) to mention a few.

LIF and CARS can be used to measure temperatures and species concentrations with much higher spatial resolution than either absorption or emission spectroscopy (Durao et al., 1992). However, the accuracy of these two techniques in the presence of interference from soot radiation is an unknown factor. These techniques in addition require very expensive and bulky lasers, detectors and signal processing equipment. Therefore, they may not be suitable in drop tower or micro-gravity experiments, due to power, volume, and mass restrictions. LIF and CARS are ideally suited to measure concentrations of minor species and radicals, but for temperature and major gas species concentration measurements, absorption or emission spectroscopy is the more accurate and feasible technique.

Absorption spectroscopy using either tunable laser diodes (Hanson et al., 1980) or FTIR (Best et al., 1991) can be used with deconvolution to obtain local gas species concentrations, soot volume fractions and temperatures in laminar flames. However, absorption spectroscopy requires a source, with corresponding alignment problems. The biggest advantage of absorption spectroscopy is that it can be utilized even in low temperature flows. In addition, absorption spectroscopy is relatively insensitive to temperature variations and is ideally suited to measure gas species concentrations (Zhang and Cheng, 1986).

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Most flames emit significant radiation signatures that are used in various applications such as fire detection (Sivathanu and Tseng, 1996), light-off detection (Vaidya et al., 1982), flame diagnostics (Choi et al., 1995), etc. Radiation signatures can be utilized to maximum advantage for determining structural information in turbulent flows (Sivathanu and Faeth, 1990, Sivathanu and Gore, 1991, Sivathanu et al., 1991). Emission spectroscopy does not require a light source. In addition, alignment and data collection are relatively straightforward. Emission spectroscopy is most advantageous in the infrared regions of the spectra, principally because these emission lines arise from transitions in the fundamental bands of stable species such as CO$_2$ and H$_2$O. Near-Infrared (NIR) and visible emission typically arise from transitions in the overtones (forbidden transitions) and are from minor species that are not in thermodynamic equilibrium with the flow. Emission spectroscopy currently offers the most accurate method of temperature determination (Zhu et al., 1997).

Near-IR emission tomography has been utilized to measure the distribution of soot temperature in laminar flames (Correia et al., 2001). The deconvolution algorithm was based upon the Abel transform, and self-absorption by soot was incorporated.

**Objective**

The objective of this work is to develop a tomographic algorithm to obtain local scalar properties such as gas temperature and mole fractions of major gas species from path-integrated multi-wavelength infrared radiation measurements. The potential errors in the tomographic algorithm are also quantified.

**Tomographic reconstruction algorithm**

Tomographic reconstruction of local scalar properties is based on the deconvolution of a finite number of two-dimensional path-integrated multi-wavelength radiation measurements that would typically be acquired by a mid-infrared spectrometer with a scanner. For an axisymmetrical flame, the domain of deconvolution is illustrated in Fig. 1. For each ring, unique scalars (temperature, mole fraction of CO$_2$ and H$_2$O) are defined. In the Fig.1, gas temperature, mole fraction of CO$_2$ and H$_2$O are denoted as $T_i$, $X_{i1}$ and $X_{i2}$, respectively. The spectral radiation intensity emitted from a homogeneous path is represented as

$$I_{\lambda} = I_{b\lambda}(1 - \tau_{\lambda})$$

where $I_{b\lambda}$ is the Planck function (dependent on the gas temperature), and $\tau_{\lambda}$ is the spectral transmittance of the homogeneous path. For a given temperature and mole fractions of CO$_2$ and H$_2$O, the spectral transmittance ($\tau_{\lambda}$) along the optical path can be calculated using a narrow band radiation model, RADCAL (Grosshandler, 1993). For the two representative homogeneous rings shown in Fig. 1, the measured path-integrated intensities are:

$$I_{1\lambda} = I_{1,b\lambda}(1 - \tau_{11})$$

$$I_{2\lambda} = I_{1,b\lambda}[(1 - \tau_{23}) \cdot \tau_{22} \cdot \tau_{21} + (1 - \tau_{21})] + I_{2,b\lambda}(1 - \tau_{22}) \cdot \tau_{21}.$$  

These two path-integrated intensities are calculated at several mid-infrared wavelengths. The iterative deconvolution algorithm used to obtain the local scalars from the path-integrated intensities involves two steps:

1. Calculate the local spectral radiation intensities for all homogeneous rings, given the value of the transmittances for all segments in the optical path. Therefore, the two unknown quantities in Eq. (2) and Eq. (3) are $I_{1,b\lambda}(1 - \tau_{21})$ and $I_{2,b\lambda}(1 - \tau_{22})$, the local spectral intensities. The two intensities on the left-hand side of Eq. (2) and Eq. (3) are the measured or given values. This linear system of equations is ill-posed. The solution must be obtained through an optimization process. The Maximum Likelihood Estimation (MLE) method (Vardi and Lee, 1993) is best suited for this problem because of its guaranteed convergence and ease of implementation. In Eq. (2) and Eq. (3), the transmittances for all segments are obtained from the previous iteration.

2. Estimate the gas temperature and mole fractions of CO$_2$ and H$_2$O from the local spectral intensities within each homogeneous ring. This process is essentially a curve fitting process to find three scalars using the multi-spectral radiation intensities using a narrow band radiation intensity database. RADCAL (Grosshandler, 1993) will be used in these calculations as the radiation intensity database. The estimated local temperatures and mole fractions are used to calculate the transmittances for all segments.
in the domain. These transmittances are then used in Step 1.

This two-step process is repeated until convergence is achieved. At the first iteration, local intensities are found only considering emission and neglecting self-absorption by intervening gaseous components.

**Results and Discussion**

The performance of the inversion algorithm was evaluated using a synthetic dataset. The synthetic dataset consists of a 13 point radial profile of gas temperatures and mole fractions of CO\textsubscript{2} and H\textsubscript{2}O. The radial profile is representative of measurements obtained in a laminar ethylene diffusion flame by Santoro et al. (1987). The major difference between the measurements (Santoro et al., 1987) and the synthetic data set is that soot is absent in synthetic data set. The path-integrated radiation intensities at 140 wavelengths (2.2-4.8 \(\mu\text{m}\)) are computed for 25 view angles using the RADCAL database. The diameter of the flame is 2 cm.

The path-integrated intensities at four representative view angles are shown in Fig. 2. These four view angles pass through the radial locations that are identified within the figure. The spectral radiation intensities were calculated for 140 wavelengths. The radiation in the 2.3 to 3.3 \(\mu\text{m}\) band has contributions from both H\textsubscript{2}O and CO\textsubscript{2}. The radiation in the 4.3 to 4.9 \(\mu\text{m}\) band has contributions only from CO\textsubscript{2}. Only a portion of these two gas bands (that have relatively high radiation intensities as shown in Fig. 4) is used by deconvolution algorithm. The CO\textsubscript{2} band from 4.1 to 4.35 \(\mu\text{m}\) is avoided because of interference by ambient CO\textsubscript{2}.

The temperatures and gas concentrations obtained from the deconvolution algorithm and the synthetic data are shown in Fig. 3. The lines represent the synthetic data and the symbols represent the deconvolved results. Since radiation intensities at 25 view angles were used in the deconvolution algorithm, it is possible to obtain temperatures and gas species concentrations for 13 rings. For all 13 rings, the deconvoluted scalars are within 0.1\% of the synthetic data. In general, it is more difficult to obtain the scalar property at the center accurately, since the volume of gas emitting radiation is the lowest in the innermost ring. However, the results obtained are accurate to within 0.1\%, even for the innermost ring.

The synthetic and deconvoluted path-integrated intensities, at the point of convergence, for the center of the flame are shown in Fig. 4.

At the point of convergence, the spectral radiation intensities obtained from deconvolution are within 0.1\% of those obtained from the synthetic data.
This indicates that the deconvolution algorithm provides scalars that can match the spectral radiation intensities provided by the synthetic data set very closely.

The diameters of laboratory-scale flames are relatively small. Therefore, they do not provide a true test of the deconvolution algorithm in the presence of strong self-absorption. The optical thickness of industrial flames is typically an order of magnitude larger than that of laboratory flames. An increase in optical thickness normally results in slower convergence and decreased accuracy for any optical tomographic method. The potential degradation in the estimated scalars due to increased optical thickness was examined by changing the diameter of the flame. The deconvoluted temperature profiles for three flames with different diameters are shown in Fig. 5.

![Figure 5. Effects of optical thickness on estimated gas temperatures obtained using deconvolution.](image)

For flames that are less than 5 cm in diameter, the deconvolution algorithm provides excellent results at all radial locations. When the diameter of the flame is 10 cm, there is some error in the deconvoluted temperatures near the center of the flame. The primary reason for this degradation is that only a small portion of the radiation that is emitted from the center of the flame reaches the outer surface, resulting in a greater degree of uncertainty in estimating the properties at the center of the flame. The transmittance at 4.35 µm along the diameter for 10 cm flame is approximately 0.2. One possible method of overcoming this degradation in performance could be to use only the portions of the band that are less absorbing. However, this was not investigated during this study.

All the results discussed so far utilized synthetic spectral radiation intensities. However, if these intensities were measured using a spectrometer, they are expected to have errors, both in the amplitude of the intensities and in the wavelengths. In order to better understand the sensitivity of the deconvolution algorithm to these measurement errors, a random noise was introduced in the synthetic path-integrated intensities.

A random 1% noise was added to the synthetic spectral radiation intensities, and then deconvoluted using the algorithm. The synthetic and deconvoluted gas temperatures are shown in Fig. 6.

![Figure 6. Sensitivity of the inversion algorithm to the random noise in radiation intensities.](image)

inversion error for the gas temperatures is less than 1 %. However, the inversion error increases toward the center of the flame. At the center of the flame, the deviation is about 20 %. The higher error at the center could be attributed to two reasons. The area of the center ring is approximately one tenth of the outermost ring, so the contribution of the center ring to the overall path-integrated intensities is much lower those of outer rings. Therefore, any error in the path-integrated spectral radiation intensities could lead to high deconvolution errors at the center of the flame. The second reason for the higher deviation is that the temperature of the center ring is lower than the peak temperature. Therefore, noise contribution to the local intensity of center ring is higher since the random noise 1 % is defined for peak intensities.

The measurement of infrared radiation using a spectrometer involves errors not only in intensity, but also in the wavelengths. The sensitivity of the deconvolution algorithm to the uncertainty in the wavelength was also evaluated by adding a random noise of 10 nm to each wavelength. The synthetic and deconvoluted gas temperatures are shown in Fig. 7. The error in the deconvoluted gas temperatures is less than 1.7 %. The results shown in Fig. 7 indicate that any measurement uncertainties in the wavelength of spectral radiation intensities do not affect the estimated temperatures significantly.
Figure 7. Sensitivity of the inversion algorithm to the random noise in the measured wavelengths.

Conclusions

A tomographic algorithm was developed to estimate local scalars from the multi-wavelength path-integrated spectral radiation intensities. The algorithm was evaluated using calculated spectral radiation intensities from a synthetic data set. The spectral radiation intensities were deconvoluted using the maximum likelihood estimation method in conjunction with an iterative scheme. The deconvolution accounts for the self-absorption of radiation by the intervening gases. The deconvolution algorithm successfully recovers the temperature and gas concentrations within 0.1% for a laboratory flame. The algorithm achieves reasonable results for flames up to 10 cm in diameter. The sensitivity of the algorithm to random errors in the amplitude and spectral location of the radiation intensities was also tested. The deconvolution error in gas temperatures, with the addition of 1% random error in the spectral radiation intensities, was less than 1%, except at the center of the flame. The error in the deconvoluted gas temperatures with the addition of a 10 nm random noise in the wavelength was found to be less than two percent (2%) at all locations within the flame.

References


A new method of estimating temperatures and gas species concentrations in a laminar flame is reported. The spectral radiation intensities emitted from a laminar flame is measured at multiple wavelengths using a mid infrared spectrometer. The spectrometer obtains the spectral radiation intensities from 1.3 to 4.8 microns with a scanner attached to the front of the spectrometer. The measurements are deconvoluted using a maximum likelihood estimation method in conjunction with an iterative scheme. The deconvolution accounts for the self-absorption of radiation by the intervening gases. The fan beam emission tomography (FBET) is validated using synthetic data created using a narrow band radiation model (RADCAL). The results obtained from the deconvolution successfully recovered the original synthetic data within 0.5 percent for the temperature and the concentrations of CO$_2$ and H$_2$O. The method is expected to provide combustion researchers an easy method of obtaining the major gas species concentrations, temperatures, and soot volume fractions in laminar flames non-intrusively with one instrument.