



Optical determination of temperature and concentrations of homogeneous turbulent gas mixtures



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ABSTRACT

In this study, a previously developed inverse radiation model for a single gas species is extended to mixtures of the combustion gas species CO_2 , H_2O and CO . Time-averaged transmissivities and their root-mean-square (rms) values are successfully related to time-averaged temperatures, species concentrations and their rms values by considering interactions between turbulence and radiation (TRI). The sensitivity of the rms transmissivity spectra to all the parameters to be retrieved are examined and optimal wavenumber ranges for retrieving turbulent scalars of the gas mixtures are discussed. To validate the models, measured spectra are synthesized for different combinations of species concentrations, temperatures, turbulent intensities, pressure path length and turbulent length scales. Results show that mean and rms temperature and species concentrations and other turbulent scalars can be retrieved accurately from turbulent transmissivity measurements as long as the turbulent intensity is below 15% and the pressure path length for the gas mixture is less than 60 bar-cm.

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1. Introduction

As long as there has been research in the field of combustion and other applications involving heat transfer, researchers have attempted to measure temperature, reaction rates, species concentrations, heat fluxes, etc., in situ. Until recently, this meant using intrusive techniques that invariably alter the flow and heat transfer fields, such as thermocouples for temperature, gas chromatographs for concentrations, etc. During the past few decades many non-intrusive optical techniques have been developed. For example, single- and multi-color pyrometers have been employed to measure temperature [1,2], Rayleigh and Raman scattering are used as powerful combustion diagnostic tools for laboratory flames [3–9], laser-induced fluorescence (LIF) was used to determine concentration and/or temperature of certain gaseous species [10–13], extinction of a laser beam was employed to determine soot volume fractions [14–16], etc.

Among the numerous combustion diagnostic tools, infrared emission and transmission spectroscopy techniques are especially attractive due to: (1) strong rotational and vibrational transitions of combustion species in the infrared region, (2) separable and specific transitional bands for different species and (3) simplicity of emission and transmission measurements [17–19]. Spectra from

a flame or combustion chamber may be recorded with line-of-sight emission or transmission spectroscopy, and temperature and species concentrations can be retrieved along the line-of-sight. With proper tomography techniques, the entire combustion fields can also be reconstructed [20–23]. In order to evaluate temperature and species concentrations, the measured spectrum is fitted to a theoretical model, which involves information of molecular parameters, such as transitional line strengths, shapes and widths. A number of molecular spectroscopic databases [24–26] are available for infrared spectral predictions, which makes this method even more attractive. Work has been done to extract temperature and species concentration for laminar gaseous media containing a single emitting species [27–38] based on optical measurements of transmission or emission. To date, very few studies have been carried out for turbulent combustion diagnostics using infrared emission and transmission spectroscopy, partly due to the difficulty of predicting turbulent radiation accounting for nonlinear interactions between turbulence and radiation (TRI). Experimental investigations by Faeth and Gore [39–52] and probability density function (pdf) based calculations [53–57] have shown that TRI always increases the heat loss from a flame, and this additional heat loss can reach 60% of the total and more, leading to a reduction in the local gas temperature of 200 °C or more. Therefore, the radiative signal hitting a detector is influenced by the nonlinear interaction with turbulence. Reviews of experimental and numerical investigations on TRI effects can be found in [58].

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Nomenclature

C	correlation function, –
L	length of gas column, cm
P	total pressure, bar
s	distance along path, cm
t	total time interval, s
t_e	turbulence integral time scale, s
T	temperature, K
W	sensitivity coefficient, –
x	concentration by volume, –

\mathbf{z} vector of parameter scalars

Greek symbols

η	wavenumber, cm^{-1}
κ	absorption coefficient, cm^{-1}
τ	transmissivity, –
Γ	pixel response function (PRF), –
Λ	turbulence integral length scale, cm

In the present work, previously developed inverse radiation tools [58] for homogeneous turbulent single emitting gaseous media are extended to deduce temperature and concentrations for gas mixtures from measurements of line-of-sight transmissivities. By assuming the pdf shape of temperature and species concentration fluctuations, time-averaged transmissivity and its rms spectrum are successfully related to the time-averaged and rms values of temperature and mixture species concentrations. Optimal spectral ranges for retrieving turbulent scalars of the gas mixtures are discussed and identified for different combinations of species concentrations, different temperatures, different turbulent intensities, different turbulent length scale and different turbulent length scales.

2. Turbulent transitivity calculation

Our preliminary work [58] for a homogeneous turbulent gas medium is limited to a single combustion species. However, combustion products usually are mixtures of several gas species. In this study, the model is extended to retrieve time-averaged and rms values for temperature, species concentrations as well as the turbulence length scale for a gas mixture containing three major combustion products, i.e., CO_2 , H_2O and CO . Here we define a parameter vector

$$\mathbf{z} = [T, x_{\text{CO}_2}, x_{\text{H}_2\text{O}}, x_{\text{CO}}] = [z_1, z_2, z_3, z_4] \quad (1)$$

which is a set consisting of temperature and species concentrations of CO_2 , H_2O and CO . In order to retrieve the scalars and their turbulent moments, it is important to have an accurate forward calculation model that can relate the measured lower-resolution time-averaged transmissivity $\langle \tau_{\eta c} \rangle$ and its variance $\langle \tau_{\eta c}^2 \rangle$ to the time-averaged temperature and concentrations $\langle z_j \rangle$ ($j = 1, 2, 3, 4$) and their variances $\langle z_j' z_j' \rangle$ ($j, k = 1, 2, 3, 4$). Where a prime denotes a fluctuation about the local mean and angle brackets denote time-averaged quantities.

2.1. LBL absorption coefficient

For moderate fluctuations, the spectral absorption coefficient for the gas mixture can be approximated by a linearized function as

$$\kappa_{\eta}(\mathbf{z}) \approx \kappa_{\eta}(\langle \mathbf{z} \rangle) + \sum_{j=1}^4 \frac{\partial \kappa_{\eta}(\langle \mathbf{z} \rangle)}{\partial z_j} z_j' \quad (2)$$

where temperature and concentrations fluctuations z_j' are assumed to be Gaussian random variables with zero mean. Taking the average of Eq. (2) leads to

$$\langle \kappa_{\eta} \rangle \approx \kappa_{\eta}(\langle \mathbf{z} \rangle) \quad (3)$$

where $\langle \mathbf{z} \rangle$ is a set consisting of time-averaged temperature and species concentrations. This basically means the time-averaged absorption coefficient can be calculated from time-averaged temperature and species concentrations. The variance of the absorption coefficient is defined as the mean-square fluctuation of the absorption coefficient. Combining Eqs. (2) and (3), the variance of κ_{η} can be deduced as

$$\begin{aligned} \langle \kappa_{\eta}^2 \rangle &= \langle (\kappa_{\eta} - \langle \kappa_{\eta} \rangle)^2 \rangle \\ &\approx \left\langle \left[\sum_{j=1}^4 \frac{\partial \langle \kappa_{\eta} \rangle}{\partial z_j} z_j' \right]^2 \right\rangle \\ &= \sum_{j=1}^4 \sum_{k=1}^4 \frac{\partial \langle \kappa_{\eta} \rangle}{\partial z_j} \frac{\partial \langle \kappa_{\eta} \rangle}{\partial z_k} \langle z_j' z_k' \rangle \end{aligned} \quad (4)$$

where $\langle \kappa_{\eta}^2 \rangle$ is the variance of the absorption coefficient, $\langle z_j' z_k' \rangle$ ($j, k = 1, 2, 3, 4$) are variances of temperature and species concentrations, which can be variances of temperature $\langle T'^2 \rangle$, variances of species concentrations $\langle x_j'^2 \rangle$, covariances of temperature and concentrations $\langle T' x_j' \rangle$ and covariances of different species concentrations $\langle x_j' x_k' \rangle$.

2.2. LBL transmissivity

Because of the approximately linear relation between absorption coefficients, temperature and species concentration, the absorption coefficient also varies temporally with a Gaussian distribution, which has a mean and variance of $\langle \kappa_{\eta} \rangle$ and $\langle \kappa_{\eta}^2 \rangle$, respectively. It is known that the transmissivity is

$$\tau_{\eta} = e^{-\int_0^L \kappa_{\eta}(s) ds} \quad (5)$$

Averaging over Eq. (5) yields the time-averaged LBL transmissivity

$$\langle \tau_{\eta} \rangle = \left\langle e^{-\int_0^L \kappa_{\eta}(s) ds} \right\rangle \quad (6)$$

and the covariance of the LBL transmissivity at two arbitrary wavenumber locations

$$\langle \tau_{\eta_1}' \tau_{\eta_2}' \rangle = \langle (\tau_{\eta_1} - \langle \tau_{\eta_1} \rangle) (\tau_{\eta_2} - \langle \tau_{\eta_2} \rangle) \rangle \quad (7)$$

where L is the length of the gas column. Detailed analysis for calculating these two terms can be found in [58] and the final expressions are presented here only. They are

$$\langle \tau_{\eta} \rangle = e^{-\langle \kappa_{\eta} \rangle L} e^{\frac{1}{2} \langle \kappa_{\eta}^2 \rangle L^2} \int_0^L \int_0^L C_s(|s_1 - s_2|) ds_1 ds_2 \quad (8)$$

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