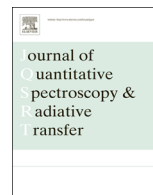


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Fitting narrow-band models to temperature-dependent, spectral absorption coefficients of fuel vapors

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ABSTRACT

Accurate modeling of infrared radiation transport through fuel rich cores of fires and other non-premixed combustion processes requires computationally efficient processing of temperature-dependent, spectral absorption coefficients for major fuel vapor species. Spectrally resolved transmissivity band measurements in the mid-infrared and near-infrared have been taken in recent years for numerous small fuel molecules including but not limited to ethane, ethylene, and propylene for a range of temperatures relevant for combustion environments. This paper compares the spectral transmissivity measurements using FTIR for both ethane and ethylene with the HITRAN 2012 edition. Narrow band absorption coefficients and overlap parameters are derived by fitting the spectral transmissivity measurements for ethane, ethylene, and propylene with narrow band models for temperatures up to 1000 K. The resulting fits provide a basis for calculating spectrally resolved infrared radiation transport in fuel rich cores of flames and other combustion processes where these species can be prevalent.

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1. Introduction

In combustion processes/events such as fires and boiler flames, radiation transport through gaseous regions containing significant fractions of fuel or hydrocarbon vapors can be important in determining heat transfer to structural surfaces or to the original fuel source if that source is a solid or liquid. This has been well documented for pool fires where radiation through the fuel rich core inside the flame dominates the heat transfer to the fuel surface and thus the burning rate of the fuel [1–4]. In addition to pool fires, combustion events with solid fuels such as polymers and wood rely on radiation feedback through a rich zone of gasified fuel species to control fuel supply to the surface [5–7].

The dominance of radiation feedback to the fuel surface in these non-premixed combustion processes suggests the importance of the radiation absorption properties of the dominant species in the fuel-rich core. Developing predictive models of these types of fires and combustion processes therefore requires quantitative radiation absorption properties of the gaseous fuel vapors as a function of temperature between the flames and the fuel surface as well as surrounding structures.

Mid-range infrared (mid-IR) and near visible infrared (NIR) are the dominant frequency ranges associated with thermal radiation transport in fires and flames [8]. Many vibrational bands and their overtones for fuel molecules as well as for fuel decomposition and combustion products absorb in the mid-IR and NIR spectral ranges. The spectral behavior of these bands varies with temperature, and this variation must be captured in the highly non-isothermal fuel vapor cores to assess radiation transport back to fuel surfaces. Temperatures in fuel vapor cores can vary

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significantly, with relatively low temperatures near the fuel source due to vaporization or volatilization of the liquid or solid fuel respectively, and higher temperatures reaching 1000 K or higher nearer the flame [2,9–11]. The impact of temperature on the absorption bands of the fuel species tends to be a flattening and broadening of peaks with temperature due to an increase in the fraction of higher energy state transitions [12–14]. The impact of the change in spectral absorption properties on overall radiation transport in flames has not been well understood and indicates the value in developing a spectrally resolved fuel species database for radiative heat transfer calculations for fire and large-scale combustion simulations.

The temperature variation in absorption bands for combustion products (H_2O , CO_2 , and CO) and at least one fuel (CH_4) is captured well in both the HITEMP database [15] and the Radcal database [16], but temperature-dependent measurements of mid-IR and NIR radiation absorption bands for other common fuel species and fuel decomposition species have been limited to a few studies. Tien and co-workers measured spectrally resolved absorption bands for hydrocarbon fuels and methyl-methacrylate [17–19]. Fuss et al., [20], measured IR absorption properties for light paraffin fuels for a range of relevant temperatures but only reported integrated absorption coefficients. More recent studies have used multi-wavelength, narrow-band absorption measurements of hydrocarbon fuels as a means of providing a diagnostic tool for species measurements in non-isothermal flames [21], but these studies have not provided the spectral breadth of measurements and the consistency of temperature coverage to provide a basis for developing a database for use in numerical modeling tools.

To provide consistent data for building an absorption coefficient database for many common fuel species, FTIR transmission measurements at the National Institute of Standards and Technology (NIST) were undertaken to provide highly resolved spectral absorption coefficients in the mid-IR and NIR as a function of temperature for many fuel species [14,22,23]. These measurements were performed over a range of temperatures from 300 to 1000 K for several fuel species, including paraffins (methane, n-propane, and n-heptane) and other fuels (methanol, propylene, toluene, and methyl-methacrylate). Previously unpublished measurements by the same authors, which followed the precise methodology of the published references [14,22], are presented here on ethane and ethylene. The uniform set of conditions and spectral resolution of these measurements has provided a set of data for developing calculation methodologies for absorption coefficients of these species in flame environments with non-uniform temperature and composition. Such calculations for integration with multi-dimensional fire or combustion simulation require computationally efficient algorithms with robust interpolation and efficient spectral integration. To that end, this paper presents the development of a narrow-band model fitting for three fuel species, ethane, ethylene, and propylene, as a function of temperature based upon the extensive FTIR measurements carried out at NIST. The resulting adaptation of the narrow-band models to the spectrally resolved fuel-vapor absorption bands in the mid-IR and NIR provides a

valuable tool for improving fire and combustion simulations where radiation through fuel-rich cores plays a major role in determining the rate of fuel consumption and/or the safety of solid structures inside flames.

2. Experimental measurements

2.1. Experiment

Wakatsuki et al. [23] presented spectrally resolved transmissivity measurements as a function of temperature for a wide array of fuels including methane, propane, n-heptane, methanol, propylene, toluene, and methyl-methacrylate. Additional measurements heretofore unpublished are presented in this paper for ethane and ethylene. In all the experimental tests, the spectral transmissivities of the gases diluted in high purity nitrogen were measured in the mid-IR and NIR wavenumbers from 700 to 4000 cm^{-1} (i.e., wavelengths from 2.5 to $14\text{ }\mu\text{m}$). Measurements were obtained using a Fourier transform infrared spectrometer (FTIR) in a transmission mode for temperatures ranging from ambient (near 300 K) up to 1000 K (for most gases) and only 800 K for gases like ethylene which readily decompose at higher temperatures. The experiment used a homogeneous flow cell of a heated nitrogen-fuel mixture. For each fuel and temperature, three different pathlengths (defined as the product of fuel partial pressure with the physical length) ranging from 0.07 to 0.5 atm cm were used to provide a basis for deriving concentration-independent absorption coefficients [14].

The spectral resolution of the FTIR measurements was set to 1.0 cm^{-1} over the entire measured spectrum. The experimental signal was averaged over 128 scans for each individual temperature and pathlength considered. The measurement process was repeated three times for each experimental condition to ensure reliability of the data. Additional details regarding the experimental apparatus and configuration can be found in relevant previous references [2,14,22,23].

Ethane data were obtained experimentally for the following temperatures: 296, 400, 450, 500, 600, 800, and 1000 K. For each temperature, three ethane pathlengths were tested: 0.3388, 0.2105, and 0.0812 atm cm. Similarly, ethylene experimental data were obtained for the following temperatures: 296, 400, 450, 500, 601, and 801 K. Attempts were made to obtain data at 1000 K but the chemical stability of ethylene at this temperature is questionable. The ethylene pathlengths tested were 0.304, 0.179, and 0.0782 atm cm. Propylene experimental data were obtained for the following temperatures: 296, 390, 444, 491, 594, 795, and 1003 K. The propylene pathlengths tested were 0.4761, 0.3174, and 0.1587 atm cm. Propylene data have previously been reported in Ref. [14]. The total pressure inside the measurement cell, set at a value of 101 kPa, was kept identical for all experimental conditions.

The experiments measured spectral transmissivity, denoted τ_ω , which is defined as the ratio of the transmitted radiant energy, I_ω , over the incident radiant energy, I_ω^0 :

$$\tau_\omega = \frac{I_\omega}{I_\omega^0}. \quad (1)$$

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