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An inverse radiation model for optical determination of temperature and species concentration: Development and validation

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In this study, we present an inverse calculation model based on the Levenberg–Marquardt optimization method to reconstruct temperature and species concentration from measured line-of-sight spectral transmissivity data for homogeneous gaseous media. The high temperature gas property database HITEMP 2010 (Rothman et al. (2010) [1]), which contains line-by-line (LBL) information for several combustion gas species, such as CO_2 and H_2O, was used to predict gas spectral transmissivities. The model was validated by retrieving temperatures and species concentrations from experimental CO_2 and H_2O transmissivity measurements. Optimal wavenumber ranges for CO_2 and H_2O transmissivity measured across a wide range of temperatures and concentrations were determined according to the performance of inverse calculations. Results indicate that the inverse radiation model shows good feasibility for measurements of temperature and gas concentration.

1. Introduction

Advanced optical diagnostics and multi-scale simulation tools will play a central role in the development of next-generation clean and efficient combustion systems, as well as in upcoming high-temperature alternative energy applications. Combustion diagnostics have reached high levels of refinement, but it remains difficult to make quantitatively accurate nonintrusive measurements of temperature and species concentrations in realistic combustion environments. Griffith et al. [2,3] were the first to recognize that measurements of the transmissivity or emissivity of rotational spectral lines of a gas can reveal its temperature. In order to extract temperature, a nonlinear least-square method was used to fit the integrated transmission minima. In their experiments, transmissivities for CO_2 10.4 μm and 9.4 μm bands at a fine resolution of 0.29 cm^{-1} for pure CO_2 [3] were measured. Best et al. [4,5] combined tomography and Fourier transform infrared (FTIR) spectrometer transmission and emission spectra to extract temperature, concentration and soot volume fraction fields. Not much detail was given, except that low resolution (32 cm^{-1}) scans were used. Song et al. [6–9] developed a spectral remote sensing technique to reconstruct temperature profiles in CO_2 mixtures based on radiative intensity measurements. In their experiments, spectra from 1.3 μm to 4.8 μm were imaged onto a 160-element lead selenide array detector. Spectral information only for the CO_2 4.3 μm band was used to retrieve the temperature profile and the spectral resolution is coarse and not changeable.

A number of gas property databases are available for transmissivity predictions, such as HITRAN 2008 [10] and HITEMP 2010 [1], which contain line-by-line (LBL) information

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for many gas species. HITEMP 2010, which is limited to only four species (CO_2, H_2O, CO and OH), contains data for “hot lines,” which become active at high temperature. In the updated HITEMP 2010 CO_2 parameters were calculated from CDSD-1000 [11]. The database was extensively tested against measured medium-resolution spectra of CO_2 [12,13] for the 15, 4.3, 2.7, and 2.0 μm bands at temperatures of 300, 600, 1000, 1300, and 1550 K and measured high-resolution spectra of CO_2 in the 15, 4.3 and 2.7 μm bands at temperatures up to 1773 K [14]. The database was also tested against measured medium-resolution spectra of H_2O [15] for the 6.3, 2.7 and 1.8 μm bands at temperatures of 600, 1000, and 1550 K and measured high-resolution spectra of H_2O in the 2.7 and 1.8 μm bands at temperatures up to 1673 K [16]. Good agreement between measured and calculated spectra was found. In the present study, the predicted spectral transmissivities were calculated for different medium-to-coarse resolutions using rovibrational band spectra created from HITEMP 2010. Ideal FTIR instrument line shape (ILS) functions were used to convolve the high-resolution transmissivity spectra to generate different medium-to-coarse resolutions of FTIR transmissivity spectra for the CO_2 2.7 μm and 4.3 μm bands and H_2O 1.8 μm and 2.7 μm bands.

The goals of our research are to develop new radiation tools to accurately deduce temperature and species concentration profiles from radiometric measurements in laminar and turbulent combustion systems. As a start, in the present work inverse radiation tools for homogeneous gas media were developed to deduce temperature and concentration from higher to lower-resolution measurements of line-of-sight transmissivities. A number of inverse techniques have been used for temperature or concentration inversion. Several inverse radiation algorithms like the Quasi-Newton method [17], the Conjugate Gradient Method [18] and the Levenberg–Marquardt method [19] have been applied. From many transmissivity inversions, we found the Levenberg–Marquardt inverse scheme to be relatively reliable to retrieve temperature and concentration along single lines-of-sight, and to be more accurate and requiring less computational effort. Therefore, only the Levenberg–Marquardt method was employed in the scheme described below. The inverse model was validated by retrieving temperatures and concentrations from experimental medium-resolution CO_2 and H_2O transmissivity data obtained previously [12–16] for a wide range of temperatures and species concentrations.

2. Transmissivity measurements for CO_2 and H_2O

Bharadwaj and Modest performed measurements of CO_2 and H_2O transmissivity at temperatures up to 1550 K and with a resolution of 4 cm^{-1} using a drop tube mechanism and FTIR spectrometer [12,13,15]. The gas temperature was measured by a thermocouple and a gas delivery system was used to supply mixtures of N_2+CO_2 and N_2+H_2O. By controlling the flow rate of N_2 and CO_2 or N_2 and H_2O, the desired mole fraction of CO_2 or H_2O in the test cell was obtained. CO_2 concentrations were measured by ball flow meters and H_2O concentrations were measured by an Agilent series micro-gas chromatograph. The reader is referred to [12,13,15] for more details on the experiment.

High-resolution transmissivity measurements have been made by Fateev and Clausen with an atmospheric-pressure high-temperature flow gas cell (HGC), Fig. 1, for CO_2 at temperatures up to 1773 K [14] and H_2O at temperatures up to 1673 K [16]. The gas cell was designed as a flow gas cell with a so-called “laminar flow window”, where care was taken to obtain a uniform gas temperature profile and a well-defined path length. “Laminar flow window” is not an actual window and it is not an aerodynamic lens. A laminar flow window is formed by two opposite gas flows that meet each other and escape the cell through a narrow gap between the left/right buffer and the central parts of the cell, Fig. 1. Arrows in Fig. 1 show directions of the gas flows.

It consists of three different parts: a high-temperature sample cell with a length of 0.533 m and two “buffer” cold gas parts on the left- and the right-hand sides of the hot sample cell. The buffer parts are filled with a UV/IR-transparent (purge) gas (e.g., N_2), whereas the central sample cell can be filled with the gas under investigation (e.g., N_2+H_2O/CO_2). The aperture of the sample cell is kept small (i.e., a diameter of 0.015 m) in order to reduce heat transfer by radiation from the sample cell and to reduce the risk of collapse of well-defined flows in the laminar flow windows. The laminar flow windows also function as a radiation shield. Similarly, apertures placed at the ends between the laminar flow windows and the cold windows reduce the heat losses by radiation and convection by breaking down the vortices created by the thermal gradient in the buffer sections. High-quality alumina ceramics were used in order to minimize hetero-phase reactions and to avoid contact of the sample gas with any hot metal parts. A uniform temperature profile is obtained by heating the gas cell with a dedicated three-zone furnace in order to compensate for the heat loss at the ends of the gas cell. The sample gas is preheated. Flows of the gases in the sample cell and in the buffer parts are kept at about the same flow rates. The outer windows placed at the ends of the buffer parts are replaceable. In all experiments, KBr-windows have been used. The gas flow through the HGC maintains a highly uniform and stable temperature in the range 23–1500 °C. The temperature uniformity over 0.45 m in the sample cell was found to be better than

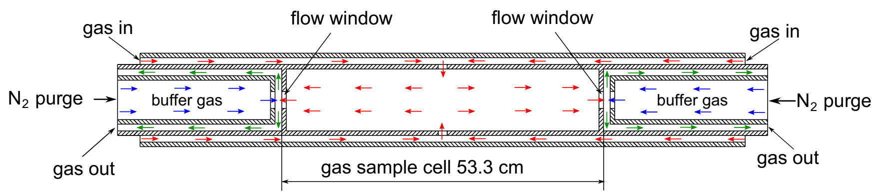

Fig. 1. High-temperature flow gas cell (HGC) used in the experiments [14,16]. Arrows show directions of the gas flows. See text for more explanation.