Machine learning-based prediction of global equivalence ratio from absorption spectra on a swirl combustor

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1 Abstracts

A new optical scheme that predicts a global fuel-air equivalence ratio of a swirl combustor from a limited set of absorption spectra is proposed in this study. Once the combustor is under normal operation, the temperature and concentration fields are determined by global equivalence ratio and total flow rate. Therefore, changes in absorption spectra of water vapor at wavelength ranges around 1343.34, 1391.6, and 1469.3 nm measured at three different downstream locations of the combustor were mapped to the global equivalence ratio, and since it is difficult to find analytical relationships between these values, a predictive model was acquired data-drivenly. The absorption spectra as an input were first feature-extracted through convolutional autoencoders (CAEs) and then a dense neural network (DNN) was used for regression prediction between the feature scores and the global equivalence ratio. The model was found to predict the equivalence ratio with an absolute error of ±0.025 with a probability of 96%.

2 Introduction

Continue your text here. Combustion is still the main energy conversion process for electricity generation. However, detrimental byproducts such as carbon particulate matters and nitrogen oxides were produced from the combustion process; thus, combustion diagnostics have been developed and studied to mitigate the production of these pollutants by optimizing combustors' operating conditions [1-2]. The global fuel-air equivalence ratio is one of the most important combustion parameters that determine the whole combustion process. The fuel-air equivalence ratio can be monitored through gas analyzers coupled with gas sampling and also optical methods such as flame chemiluminescence imaging, laser-induced breakdown spectroscopy, and a tunable diode laser spectroscopy (TDLAS). However, since intrusive measurements involving gas sampling inevitably perturb the flow field and combustion process, the optical methods are increasingly favored for the equivalence ratio measurement.

A flame chemiluminescence imaging used the ratio between the strengths of CH and C_2 emissions in the flame chemiluminescence to estimate the equivalence ratio. Although the technique has an advantage of measuring the map of local equivalence ratio, the change in this ratio becomes small for equivalence ratios less than 1. As swirl combustors are usually operated at fuel-lean conditions (e.g., equivalence ratio below 0.8) to minimize the pollutant emissions, it is still necessary to develop a new method to measure or monitor a wide range of equivalence ratio. TDLAS has been used to measure temperature and concentration of the combustion product in the swirl burners [3-4], Mckenna burners [5-6], scramjet combustors [7-8], as the absorption lines become functions of temperature and partial pressure of absorbing species. However, since the measurement is line-of-sight, tomographic reconstructions of temperature and concentration fields are often required from TDLAS signals obtained from various optical paths. In addition, simultaneous measurements on multiple major combustion products are needed for the equivalence ratio measurement.

We propose a new optical diagnostic scheme to measure or monitor the global equivalence ratio of a given swirl combustor based on a limited set of TDLAS spectra. We had paid attention to the fact that once the combustor is under normal operation, the detailed combustion fields are going to be governed by combustors' operation parameters that are fuel and air flow rates (i.e., equivalence ratio and total flow rate). Changes in these operation parameters will result in changes in the shape of the swirl flame, and subsequently temperature and concentration fields, and we speculate that although it is not trivial to find the analytical relationship between changes in absorption spectra and the changes in the temperature and concentration fields of the given combustor, the relationship can be acquired data-drivenly when there is a sufficient amount of relevant data. In this study, the absorption spectra of water vapor at 1343.34, 1391.6 and 1469.3 nm were exploited for prediction of global equivalence ratio, and the spectra were collected from three different downstream locations of the combustor. A model was composed of two parts: convolutional autoencoders (CAEs) and dense neural network (DNN). 9 absorption spectra as an input were first feature-extracted through the CAEs, and then the feature scores were mapped to the output global equivalence ratio through the DNN. Particularly, the CAEs were used for feature extraction to ensure we extract all the features in the spectra.

3 Theory of TDLAS

TDLAS is based on the Beer-Lambert relation that describes the relation between the incident and transmitted laser intensities. When the light of laser passes through a homogeneous and uniform medium, the absorbance of monochromatic radiation is described as

$$A_v = -\ln\left(\frac{I_t}{I_0}\right) = k_v L \tag{1}$$

where I_0 and I_t are the incident and transmitted laser intensities, v is the optical frequency, L is the optical path length, and $k_v$is the absorption coefficient. The monochromatic absorption coefficient is defined as

$$k_v = S(T)XP\phi \tag{2}$$

where $S(T)$ is the line-strength of the transition line, X is the mole fraction of the absorbing species, P is the total pressure, and ϕ is the line shape function. The line shape function is described by a voigt profiles, which is a convolution of Doppler and collisional broadened line-shapes. The profile is defined as

$$\phi_V(v) = \phi_D(v_0)\frac{a}{\pi}\int_{-\infty}^{\infty}\frac{\exp(-y^2)}{a^2+(w-y)^2}dy \tag{3}$$

a is the voigt parameter, given by

$$a = \frac{\sqrt{ln2}\Delta v_C}{\Delta v_D} \tag{4}$$

Δv_D is Doppler full-width at half-maximum (FWHM), given by

$$\Delta v_D = 7.162 \times 10^{-7} v_0 \sqrt{T/M} \tag{5}$$

where v_0 is the line center frequency, T is the temperature, and M is the molecular weight.

Δv_c is the collisional FWHM, given by

$$\Delta v_C = P \sum_i 2\gamma_i X_i \tag{6}$$

where γ_i is the collisional coefficient of species i, and X_i is the mole fraction of species i. The collisional coefficient depends on the temperature and is defined as

$$\gamma_i(T) = \gamma_i(T_{ref})(\frac{T_{ref}}{T})^n \tag{7}$$

where T_{ref} and n are the reference temperature (i.e., 296 K) and the temperature coefficient, respectively. The coefficient is generally less than 1. $\phi_D(v_0)$ is the linecenter magnitude, given by

$$\phi_D(v_0) = \frac{2}{\Delta v_D}\sqrt{\frac{ln2}{\pi}} \tag{8}$$

y is an integral variable, given by

$$y = \frac{2u\sqrt{ln2}}{\Delta v_D} \tag{9}$$

w is the nondimensional line position, given by

$$w = \frac{2\sqrt{ln2}(v - v_{0)}}{\Delta v_D} \tag{10}$$

Therefore, it can be seen that not only the peak intensities of the lines in the spectra but also their line-widths or shapes change with the changes in temperature and concentration fields.

4 Experimental setup

Figure 1 shows the schematic of the experimental setup for TDLAS measurement on a swirl combustor at different downstream locations. The swirl combustor consists of a plate, a combustion chamber, an axial swirler, and a bluff body. The nozzle exit dimeter was set to be 34 mm while the bluff body diameter is set to be 17.2 mm to anchor the flame base near the nozzle. The combustion chamber was made of a quartz for an optical measurement, and it had a height of 165 mm and inner and outer diameters of 64 mm and 70 mm, respectively. The swirler had 12 vanes with a vane angle of 50 degrees. The diameter and hub of the swirler were 34 mm and 10 mm, respectively. A geometric swirl number was calculated as 0.91. Methane was used as a fuel, and air was used as an oxidizer. The flow rate of fuel and oxidizer was controlled by mass flow controllers (MFCs) that were calibrated using a dry gas meter (DC-2C-M, Shinagawa Corporation). The methane was supplied from the high-pressure cylinder and the air was supplied using air compressors equipped with an air dryer (TX15K, Jemaco). The air flow rate was varied from 60 to 140 slpm in 10 slpm increments, and the equivalence ratio was varied from 0.6 to 1 in 0.05 increments. Three tunable diode lasers were used to measure water vapor. Each of the diode lasers was mounted on a butterfly mount (LM14S2, Thorlabs). The current to each diode laser was modulated using a current controller (LDC202C, Thorlabs) that received the modulating signal from a function generator (AFG-2225, GW Instek), and the temperature of the diode laser was maintained constant using a temperature controller. The outputs of the diode lasers were combined using optical fiber couplers (F-CPL-B12355, F-CPL-B22355, Newport), and fiber collimators (TC12APC-1310, Thorlabs) were mounted at the coupler output to collimate the laser beam. A ramp signal with a

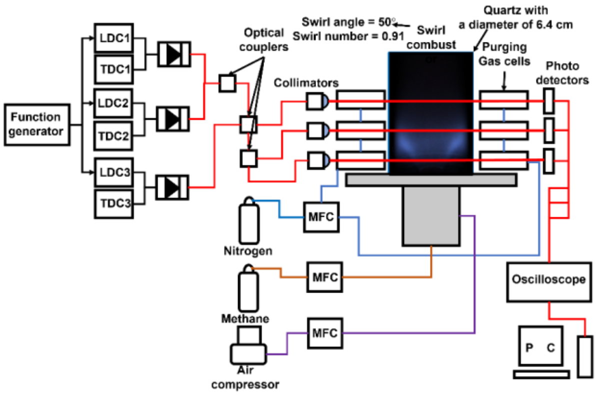

Figure 1: The schematic of the experimental setup for TDLAS measurement on the swirl combustor.

frequency of 1 kHz was provided as the modulating signal. In addition, the function generators were triggered using a pulse generator (Quantum 9520, Quantum composers) to ensure that the detector only receives signals from each laser at a given time. The laser signals were detected using photodiodes which were located at 10, 80, and 100 mm downstream locations from the combustor nozzle, respectively, and the stainless tubes with a diameter of 12.7 mm were placed between the fiber collimators and the photodiodes to be purged with nitrogen, ensuring that the signals could only originate from the combustion fields. Continue your text here.

5 Pre-processing

Absorption spectra were first obtained from raw signals using Eq. (1) and then normalized by their max and min intensities such that their max and min intensities can be ranged between 0 and 1.

6 Methodology

Once the combustor is under normal operation, the detailed combustion fields are going to be governed by their operation parameters that are total flow rate and equivalence ratio. Therefore, changes in these operation parameters result in changes in the shape of the swirl flame as well as the temperature and product concentration fields.

In this study, we particularly paid attention to changes in TDLAS signals and their quantification for changes in temperature and concentration fields caused by changes in these operating conditions. However, it is not trivial to analytically correlate these subtle changes in the absorption signals with changes in total flow rate and equivalence ratio for any given combustor. Therefore, in this study, as it is known that a predictive model can be successfully obtained data-drivenly when there is a sufficient amount of relevant data, we measured absorption spectra of water vapor at three different wavelengths at three different downstream locations of the combustor, and exploited a machine learning technique for signal quantification and finally (real-time) prediction of the global fuel-air equivalence ratio of a given operating combustor.

7 Model structure

Figure 2 shows the structure of the data-driven model used in the study. 9 absorption spectra as images have been used as the model input. Absorption spectra of different wavelengths were feature-extracted using different CAEs; as the absorption spectra used in the study were from wavelength ranges near 1343.34, 1391.6 and 1469.3 nm, three different CAEs were trained in the model. Each of the CAE is consisted of an encoder and a decoder. The encoder was set to have 4 convolutional layers and the

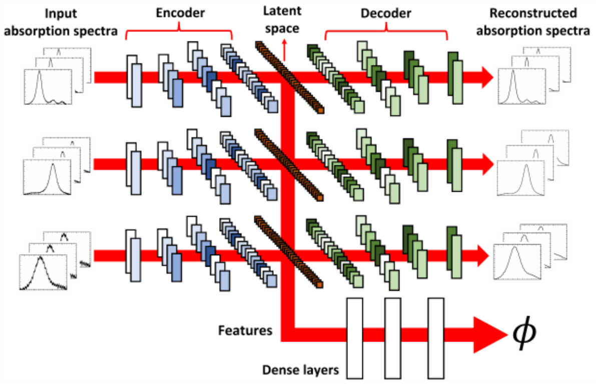

Figure 2: The structure of the data-driven model used in the study

decoder has 4 trans-convolutional layers. The 45 features extracted from CAEs were then mapped to global fuel-air equivalence ratio through the dense neural network for regression prediction. The DNN was set to have 3 hidden layers and 90 neurons in each hidden layer. In the model training, the CAEs were first trained such that each input absorption spectrum is dimensionally reduced to 5 features through the encoder and the reconstruction error from the 5 features through the decoder is minimized. Once the CAEs are trained, the weights and biases of the DNN were trained while fixing the weights and biases of the CAEs. Critical hyperparameters of an initial learning rate, latent space size of each CAE, and number of neurons in each hidden layer of DNN were searched and optimized by the simplest algorithm, grid-search [9], and the hyperparameters used in the study are summarized in Table 1.

Hyperparameters	Values
Initial learning rate	0.001
latent space size of each CAE	5
Number of neurons in each hidden layer of DNN	90

Table 1: Hyperparameters of the data-driven model.

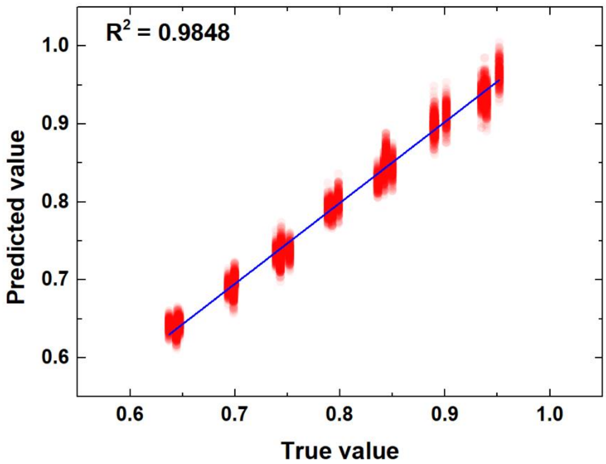

Figure 3: The comparison between the predicted values and actual values of the equivalence ratio.

8 Results

Figure 3 shows the comparison between the predicted values and actual values of the equivalence ratio. The actual values were calculated from the outputs of the MFCs. A linear fitting was conducted on the predicted values to evaluate the accuracy of the data-driven model. The coefficient of the determination

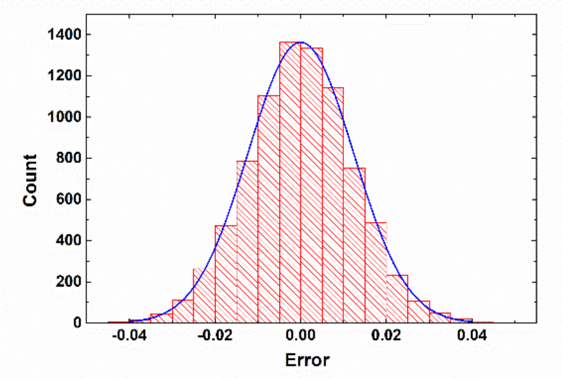

Figure 4: The error distribution of predicted values

was 0.9848 that is approximately close to 1. The result shows that the predictive model could predict the wide range of the equivalence ratio for a wide range of the total flow rate. The error distribution of predicted values with respect to their actual values was also obtained to estimate the prediction accuracy. Figure 4 shows an error distribution of predicted values and its gaussian fit. The distribution followed the normal distribution, and from that, the model was found to predict the equivalence ratio within ± 0.025 with 96% probability.

Acknowledgment

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (NRF-2021R1C1C1009607)

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