

Hydroxyl radical measurement in atmospheric pressure dimethyl ether-air laminar premixed flat flame using tunable diode laser absorption spectroscopy

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INTRODUCTION

Spectroscopic detection of hydroxyl (OH) radical and determination of its concentration in flames have an elusive history and considerable influence on combustion research. Electronic transitions in ultraviolet spectral region were extensively studied in this context and until recent time chemiluminescence or laser induced fluorescence of excited hydroxyl (OH*) radical is broadly used for absolute concentration and temperature measurement in flames.

However, number densities of molecular species and population of relevant quantum levels in ground electronic state can be directly estimated from intensities of absorption lines observed by probing rovibrational transitions in infrared spectral region. Application of near-infrared tunable diode laser absorption spectroscopy (NIR-TDLAS) for the given purpose was demonstrated in an earlier work of Aizawa et al. [1]. Following his pioneering studies summarized in [2], we further explored feasibility of NIR-TDLAS (especially $2f$ -WMS technique) for monitoring minor species within combustion experiments particularly when dealing with dimethyl ether (DME) flames. Here we report our first results of NIR-TDLAS measurements focused on hydroxyl radical detection in laminar premixed flame burning DME-air mixture under fuel-lean conditions.

EXPERIMENTAL SETUP AND SIGNAL PROCESSING

Measurements were performed under atmospheric pressure using laminar premixed flat flame burner designed according to Hartung et al. [3]. Water cooled burner body was mounted on the manually driven vertical and horizontal translation stages (Manufacturer: Standa Ltd.) to enable its movement relative to optical path and to adjust appropriate height above burner (HAB). Two separate mass-flow controllers (Manufacturer: Bronkhorst High-Tech B.V.) were employed to prepare dimethyl ether-air mixture at desired equivalence ratio ($\Phi = 0.73$) and volumetric flow rate ($Q_v = 15$ l/min). Identical mixture was fed into central body of the burner and annular coflow, thus flat flame diameter of about 60 mm was achieved.

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Tuning range of distributed feedback (DFB) laser operating around $1.573 \mu\text{m}$ (Manufacturer: Eblano Photonics Ltd.) was periodically ($\tau_p = 10 \text{ s}$) scanned by ramping up electric current at constant diode temperature maintained by laser driver/controller (Manufacturer: Thorlabs Inc.). Sine wave ($f = 11 \text{ kHz}$) was superimposed electronically on repeating sawtooth wave to modulate the lasing wavelength. Signal from the amplified InGaAs photodetector (Manufacturer: Thorlabs Inc.) was demodulated at second harmonic ($2f$) frequency by analog lock-in amplifier (Manufacturer: Stanford Research Systems Inc.) and acquired on digital oscilloscope (Manufacturer: Teledyne LeCroy GmbH). Finally accumulation and averaging procedure (with $n = 10$ samples) was performed to increase the signal-to-noise ratio (SNR), thus each single measurement (averaged scan) was obtained during 100 s interval. Absorption path of the laser beam through the flame was doubled by its reflection on the planar mirror, which increase the effective optical path length to $L_p = 10 \text{ cm}$ mentioned above.

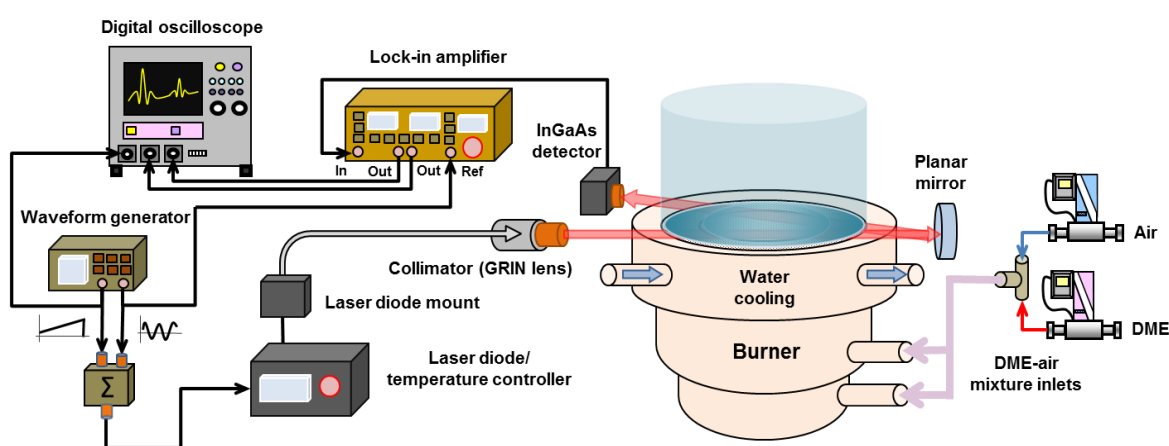


Fig. 1 Experimental setup employed for $2f$ -WMS measurement of OH radical in atmospheric pressure DME-air laminar premixed (burner-stabilized) flames.

RESULTS AND DISCUSSION

At least one pair of spectral lines (doublet) from vibrational overtone ($\Delta\nu = 2$) band of OH radical were expected to be distinguishable according to custom wavelength specification of DFB laser diode and results of our preliminary simulations. Predictions of spectral features were carried out by the aid of SpectraPlot.com interactive tool [4] using HITEMP data [5]. Numerical simulation of one-dimensional burner-stabilized flame employing CANTERA software toolkit was used to estimate temperature and species concentration in the reaction zone. This calculation provided input values for prediction of absorption spectra, i.e. temperature ($T = 1500 \text{ K}$) and molar fractions, $X(\text{OH}) = 0.002$, $X(\text{H}_2\text{O}) = 0.11$. Appropriate atmospheric pressure ($p = 1 \text{ atm}$) and optical pathlength ($L_p = 10 \text{ cm}$) was assumed in relevance to above described experimental conditions. Complex spectral features of high-temperature water vapor absorption lines in the given region (around $1.57 \mu\text{m}$) is one of the main factors limiting straightforward determination of spatially resolved absolute concentrations of OH radicals in flames. Nevertheless, spectral lines belonging to hydroxyl radical can be unambiguously identified based on differences in spectra observed at various HAB in flame, as described more recently by Rutkowski et al. [6].

Three spectral lines showing significant difference between the $2f$ -WMS scans in various HAB were identified and assigned as rovibrational transitions of hydroxyl radical in its ground electronic (X^2II) state, see Fig. 2.

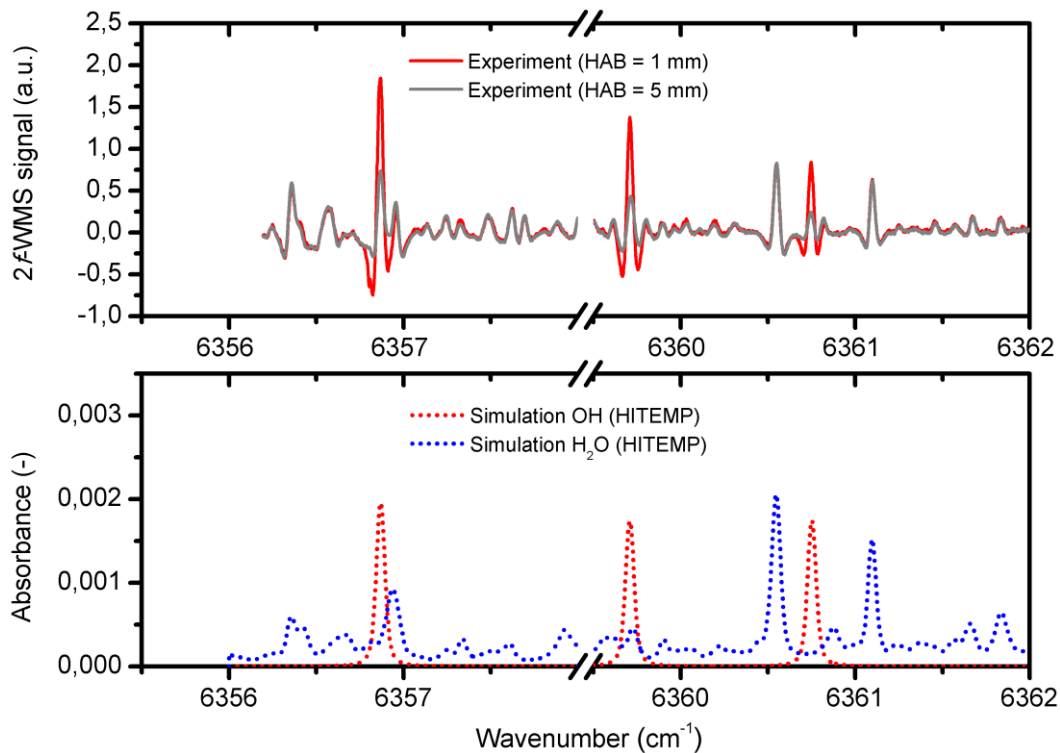


Fig. 2 Experimental $2f$ wavelength modulation spectra measured at different HAB (a). Two separate spectral scans at $T_{LD} = 25^{\circ}\text{C}$ and $T_{LD} = 29^{\circ}\text{C}$ (on the left and right side of the x-axis break) were performed in each HAB position. Predicted spectral absorption features of OH radical and hot water vapor are depicted below (b).

Qualitative agreement of predicted and experimental spectra indicates the ratio of molar fractions $X(\text{OH})/X(\text{H}_2\text{O}) \approx 1/50$ in the reaction zone (at HAB = 1 mm) which should coincide with the maxima of hydroxyl radical concentration according to calculated species profiles. When we compare experimental spectrum to results of similar studies (e.g. [2] or [7]) we can conclude satisfactory SNR and sufficient spectral resolution enabling us to estimate absolute OH concentrations in flame with minimal disturbing effect of H_2O absorption lines.

CONCLUSIONS

Absorption spectrum of the OH radical and high temperature water vapor around 6360 cm^{-1} was successfully measured in fuel-lean DME-air laminar premixed flame employing $2f$ -WMS technique. Improved spectral resolution and thus limited coincidence with hot water transitions in this region was achieved compared to other studies dealing with NIR spectroscopy of H_2O and OH radical in laminar flames. Broader applicability of $2f$ -WMS technique for laboratory scale optical diagnostics and monitoring of minor species within combustion experiments is therefore suggested.

ACKNOWLEDGEMENT

This research received funding from the Ministry of Education, Youth and Sport of the Czech Republic (Project No. LTC17071 supported in frame of the COST Action CM1404). Financial support from the Czech Science Foundation (Project No. 17-05167S) and from VSB-Technical University of Ostrava (Faculty of Safety Engineering) via the Project No. SP2017/127 and is also acknowledged.

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