UNCERTAINTY QUANTIFICATION AND ROBUST LINE-PAIR SELECTION FOR H_2O-TUNABLE DIODE LASER ABSORPTION SPECTROSCOPY TEMPERATURE MEASUREMENTS UNDER GAS-TURBINE COMBUSTOR

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ABSTRACT

Tunable diode laser absorption spectroscopy (TDLAS) [1,2] provides a fast and non-intrusive approach for gas-temperature measurements in challenging combustion environments. However, its accuracy depends on both the selected absorption-line pair and uncertainties associated with spectroscopic modelling and the measurement system. This work develops an uncertainty-aware framework for H_2O two-line TDLAS thermometry under gas-turbine combustor conditions. Candidate line pairs are initially selected using conventional spectroscopic criteria and subsequently assessed by propagating model-form and measurement uncertainties through a synthetic temperature-retrieval chain. Model-form effects associated with line-shape representation and speed-dependent broadening are considered together with baseline, detector-noise, etalon, instrumental-broadening, digitization and spectral-axis uncertainties. The results show that measurement uncertainty dominates the combined error and can substantially alter the preferred line pair. Uncertainty-aware re-ranking reduces the conservative 95th-percentile temperature error from approximately 143 K to 71 K, demonstrating the importance of considering robustness during TDLAS line-pair selection.

INTRODUCTION

Accurate measurement of gas temperature at the exit of gas-turbine combustors is important for combustor development, numerical-model validation and the assessment of pollutant formation. In particular, NOx formation is strongly temperature dependent, while combustor-exit measurements are complicated by high temperatures, elevated pressures, spatial non-uniformities and turbulent flow. Optical techniques such as tunable diode laser absorption spectroscopy (TDLAS) are therefore attractive because they provide fast, non-intrusive measurements without introducing a physical probe into the hot-gas path [1,2].

In H_2O two-line thermometry, temperature is inferred from the ratio of the integrated absorbances of two spectral transitions having different temperature-dependent line strengths [1,2]. The common dependence on species concentration and optical path length is thereby removed. Nevertheless, the resulting temperature accuracy depends critically on the selected transitions and on the ability of the spectroscopic and measurement models to recover their integrated absorbances. Previous line-selection approaches typically emphasise properties such as absorption strength, thermometric sensitivity, lower-state-energy separation and spectral isolation [2]. Appropriate line-pair selection is recognised as a central element of TDLAS sensor design.

The present work investigates whether the line pair preferred under ideal spectroscopic conditions remains optimal when realistic uncertainty is considered. A numerical framework is developed to separately quantify model-form uncertainty associated with the absorption-line representation and measurement uncertainty associated with the TDLAS instrument. Both uncertainty branches are subsequently combined and used to reassess candidate H_2O line pairs. The objective is not only to quantify temperature-retrieval uncertainty, but also to use uncertainty information to identify more robust line pairs and measurement-system requirements for combustor-relevant TDLAS applications.

RESULTS AND DISCUSSION

The analysis used H_2O spectroscopic data from HITRAN [3] through HAPI [4] over a nine-point operating envelope of 700, 1300 and 1800 K and 1, 3 and 5 atm, with an H_2O mole fraction of 0.10 and a 10 cm optical path. Initial screening identified 161 candidate H_2O lines and 1375 valid line pairs, ranked according to

thermometric sensitivity, absorption strength, spectral isolation and lower-state-energy separation. Following additional inspection of line-strength balance, the original spectroscopic Rank-3 pair was selected as the reference pair for the uncertainty analysis.

Model-form uncertainty was investigated through speed-dependent Voigt broadening [5,6]. When both transitions exhibited similar speed dependence, the effect largely cancelled through the two-line ratio. However, differences in speed dependence between the two transitions introduced temperature bias that increased with temperature and pressure. Monte Carlo propagation resulted in a maximum 95th-percentile absolute temperature error of approximately 13.6 K at 1800 K and 5 atm.

Measurement uncertainty was assessed using a numerical measurement emulator incorporating instrumental broadening, baseline slope, etalon interference, detector noise, ADC quantisation, and spectral-axis calibration and jitter. Baseline slope and detector noise were the dominant uncertainty sources, while the remaining effects were comparatively small over the investigated ranges. Three instrument-quality scenarios were considered: optimistic, representing a high-fidelity measurement system; nominal, representing the baseline assumptions; and conservative, representing degraded measurement quality. For the reference pair, the corresponding global P95 temperature errors were 15.51, 67.08 and 145.03 K, respectively.

Model-form and measurement uncertainties were then propagated simultaneously through the complete retrieval chain. Measurement-system effects dominated the combined uncertainty, demonstrating the strong influence of instrument quality on TDLAS performance. Importantly, uncertainty propagation also changed the preferred line pair, with the original spectroscopic Rank-4 pair emerging as the most robust candidate, replacing the Rank-3 reference pair.

Under identical combined-uncertainty conditions, the UQ-selected pair reduced the P95 temperature error from 16.33 to 14.26 K, 68.14 to 49.22 K, and 143.29 to 71.03 K for the optimistic, nominal and conservative scenarios, corresponding to reductions of approximately 13%, 28% and 50%, respectively. These results show that robust TDLAS line selection should account for both spectroscopic model uncertainty and expected measurement quality rather than relying solely on nominal spectroscopic performance.

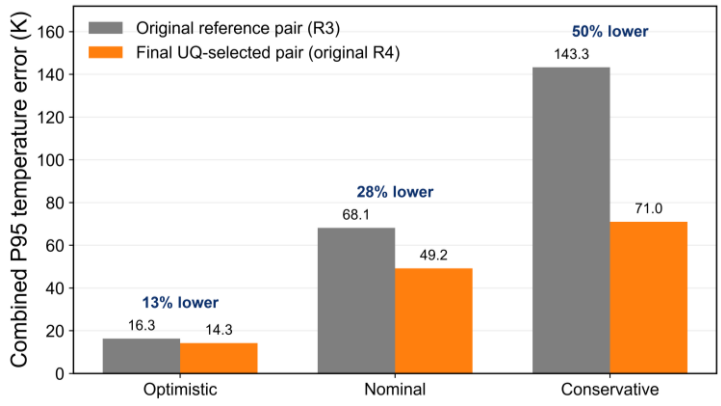

Figure 1. Impact of uncertainty-aware line-pair selection

REFERENCES

[1] X. Liu and Y. Ma, “Tunable Diode Laser Absorption Spectroscopy Based Temperature Measurement with a Single Diode Laser Near 1.4 μm,” Sensors, vol. 22, no. 16, 6095, 2022. doi: 10.3390/s22166095.

[2] X. Zhou, X. Liu, J. B. Jeffries, and R. K. Hanson, “Development of a sensor for temperature and water concentration in combustion gases using a single tunable diode laser,” Measurement Science and Technology, vol. 14, no. 8, pp. 1459–1468, 2003. doi: 10.1088/0957-0233/14/8/335.

[3] I. E. Gordon et al., “The HITRAN2020 molecular spectroscopic database,” Journal of Quantitative Spectroscopy and Radiative Transfer, vol. 277, 107949, 2022. doi: 10.1016/j.jqsrt.2021.107949.

[4] R. V. Kochanov, I. E. Gordon, L. S. Rothman, P. Wcisło, C. Hill, and J. S. Wilzewski, “HITRAN Application Programming Interface (HAPI): A comprehensive approach to working with spectroscopic data,” Journal of Quantitative Spectroscopy and Radiative Transfer, vol. 177, pp. 15–30, 2016. doi: 10.1016/j.jqsrt.2016.03.005.

[5] C. D. Boone, K. A. Walker, and P. F. Bernath, “Speed-dependent Voigt profile for water vapor in infrared remote sensing applications,” Journal of Quantitative Spectroscopy and Radiative Transfer, vol. 105, no. 3, pp. 525–532, 2007. doi: 10.1016/j.jqsrt.2006.11.015.

[6] S. C. Egbert, K. Sung, S. C. Coburn, B. J. Drouin, and G. B. Rieker, “Water-vapor absorption database using Dual Comb Spectroscopy from 300 to 1300 K Part II: Air-Broadened H_2O, 6600 to 7650 cm^{-1},” Journal of Quantitative Spectroscopy and Radiative Transfer, vol. 328, 109119, 2024. doi: 10.1016/j.jqsrt.2024.109119.