Artificial Neural Network-assisted MIR gas spectroscopy to eliminate detrimental temperature-induced spectral shifts

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Abstract: We applied an artificial neural network to a mid-infrared trace gas sensing system to completely compensate the detrimental thermally-induced spectral shift of the spectrometer, improving the accuracy of the retrieved gas concentration.

1. Introduction

Air pollution is one of the major risk factors for premature death according to the statistics released by the World Health Organization. To address this concern, significant efforts have been made in developing accurate air quality monitoring systems, utilizing the molecular fingerprint region in the mid-IR (MIR) wavelength region of 2-10µm, to identify critical pollutants and greenhouse gases. To date, MIR light sources have been demonstrated, using various techniques such as quantum cascade lasers [1,2], optical parametric oscillators [3] and supercontinuum lasers [4,5]. Recently, we have implemented the novel high-brightness supercontinuum light source, associated with a high-resolution diffractive grating spectrometer, successfully proving the applicability of our system for highly accurate multi-gas monitoring with sub-ppm capabilities [5]. However, any presence of thermal fluctuation of the gaseous analyte leads to unwanted mechanical stresses on the optical components in the system, causing beam discrepancies. In turn unwanted spectral shifts occur in the measured absorption spectrum, which leads to a non-negligible amount of error for the gas concentration computation, traditionally performed by least squares calculation between the measured spectrum and database reference spectrum. In this paper, we successfully demonstrate that a multilayer perceptron (MLP) machine learning algorithm can overcome such a detrimental spectral shift imposed onto the measured absorption spectrum, making the sensing system more robust and immune to temperature variations.

2. Experiments and Results

An all-optical fiber-based supercontinuum (SC) that is spectrally broadened to ~4.5 µm was used as the light source to construct a MIR trace gas sensing system. The generated spectrum is passed through a 12 m-long multi-pass cell (MPC), where the light is interacting with the analyte and wavelength-specific absorption occurs. Then, the light exiting the MPC was collimated and directed to a blazed grating with 450 lines/mm. The 1st order diffracted light was focused on a single pixel detector. The spectrum of the SC light was readily resolved by mounting the grating on a motorized rotation stage and simply rotating the grating. Under the following conditions: a free space beam path length of 36 cm between the grating and the detector and the grating dispersion of 27.9 nm/m°, a grating rotation increment by 10 m° induced a rise in a geometrical beam steering of 60 µm. It corresponds to a spectral shift of 0.34 cm^{-1} in wavenumber. Based on these parameters, a 50 µm slit was placed in front of the detector to precisely record the spectral power density of the light source, resulting in a spectral resolution of 1.15 cm^{-1} for the sensing system. The grating was then scanned from 327° to 330° by steps of 10 m° to obtain the partial absorption spectrum of water vapor contained in the ambient air.

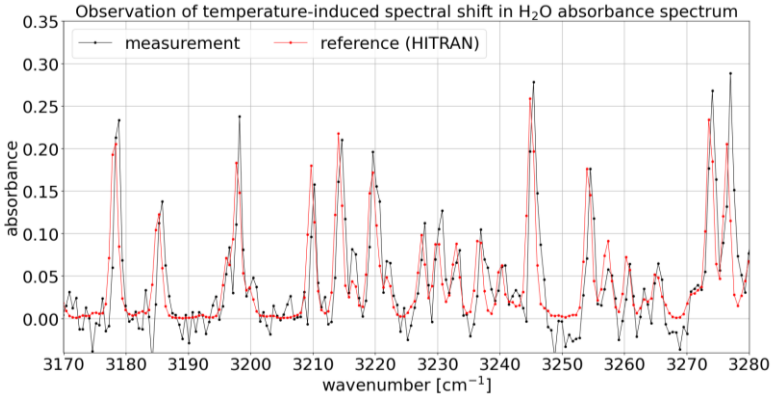

Figure 1. Spectral shift of 0.41cm^{-1} in the water vapor absorbance spectrum, caused by temperature change of 1°C inside the MPC.

As seen in Figure 1, a spectral shift of 0.41cm^{-1} was observed due to the temperature variation of 1°C inside the MPC, which leads to an error in the gas concentration computation based on least-square fitting, impairing the sensing system. The spectral shift was compared to the temperature change, measured by an electrical temperature sensor embedded inside the MPC. However, it turns out that the spectral shift has a complex response to the temperature change. By calculating the ratio between both, the slope coefficient was estimated to be in the order of 10 m°/K. The spectral shift imposed onto the measured spectrum was then manually compensated using different coefficients: 0, 7, 8, 9, 10 and 11 m°/K. Next, the temperature-compensated spectra were fitted to a reference spectrum calculated from the HITRAN database. To evaluate the reliability of such linear heat-compensation, the retrieved water concentration was compared to the normalized relative humidity (RH) measurement data, acquired by an electrical RH sensor built inside the MPC, as shown in Figure 2(a). We found that the 9 m°/K coefficient shows the best agreement to the RH profile, while the coefficients resulting in an underestimation or overestimation.

To address the uncertainty of the slope coefficient, a neural network-based computational approach was devised to extract the gas concentration more precisely. An MLP composed of two hidden layers with 256 outputs and ReLU activation and an output layer was implemented. For the training and validation phases a synthetic dataset consisting of 10000 absorbance spectra with randomized concentrations of H_2O and CH_4 was generated, where the CH_4 is used as a perturbation for H_2O estimation. To mimic the practical signal noise and nonlinear spectral behavior, the dataset was formed by adding white Gaussian noise and a random spectral shift as well as a baseline. Finally, the measured absorbance spectra were fed to the neural network and the gas concentration was extracted by the trained algorithm, as shown in Figure 2(b). Remarkably, all temperature-compensated spectra with a different slope coefficient converged to predict an identical pattern of concentration variation in time, following the RH profile unlike the case of the typical fitting method. However, the current MLP architecture tends to overestimate the water concentration by ~11% while preserving the sensing sensitivity, which was determined by the standard deviation of the concentration fluctuation over the first half-day measurement. The error might be attributed to a bias in the RH data and/or the limit of the trained synthetic data. Nevertheless, the accuracy and precision of the sensing system can be further improved by an advanced neural network architecture including convolutional and pooling layers.

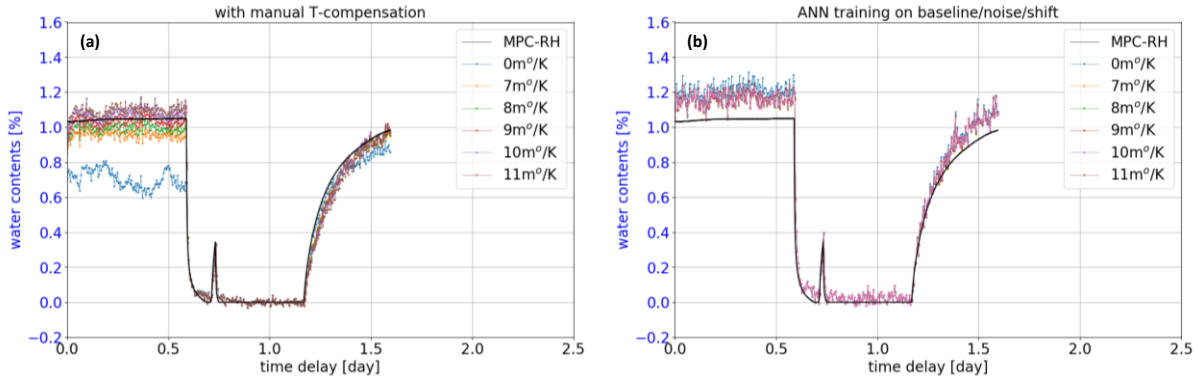

Figure 2. (a) Retrieved H_2O concentration resulting from the manual temperature compensation for different coefficients. (b) H_2O concentration estimated with an MLP.

3. Conclusions

An artificial neural network has been successfully applied to a MIR supercontinuum-based multi-gas sensing system to mitigate temperature induced instrument sensitivity. We believe that the proposed solution has a large potential to enhance the reliability of sensing systems and other instruments for field applications.

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4. References

[1] E. L. Normand *et al*, "Fast, real-time spectrometer based on a pulsed quantum-cascade laser", Opt. Lett. **28**, 16 (2003).

[2] S. Chin *et al*, "Electrically driven frequency blue-chirped emission in Fabry-Perot cavity quantum cascade laser at room temperature", Appl. Phys. Lett. **118**, 021108 (2021).

[3] D.D. Arslanov *et al*, "Continuous-wave optical parametric oscillator based infrared spectroscopy for sensitive molecular gas sensing", Laser Photonics Rev. **7**, 188-206 (2013).

[4] M.A. Abbas *et al*, "Fourier transform spectrometer based on high-repetition-rate mid-infrared supercontinuum sources for trace gas detection", Opt. Express **29**, 22315 (2021).

[5] K.E. Jahromi *et al*, "Sensitive multi-species trace gas sensor based on a high repetition rate mid-infrared supercontinuum source," Opt. Express 28, 26091-26101 (2020).