Empowering Optical Diagnostics with Image-Based Spectral Analysis via Multi-Objective Supervised Learning

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Abstract: Here, we demonstrate the application of a supervised learning-based deep neural network to extract plasma information from spectrum images, bypassing curve fitting. Utilizing a 2D-ResNet architecture, our model was trained on synthetic spectrum images designed for broadband ultraviolet-visible absorption spectroscopy, specifically targeting ozone–nitrogen oxides mixtures in air plasmas.

1. Introduction

Optical diagnostic methods have been pivotal in characterizing plasma across both basic science and industrial applications. However, spectral data analysis remains a significant challenge in plasma studies for both experts and novices due to its complexity and reliance on one's experience and intuition. Optical absorption spectroscopy (OAS) is one of the reliable spectroscopic techniques afflicted by these issues in spectral deconvolution. These issues have often necessitated manual fitting by human researchers, rendering OAS data analysis into a time and labor extensive task which has undermined the merits of OAS as a cost-effective and versatile diagnostic. Here, we introduce a sophisticated AI model which performs spectral deconvolution by taking both multidimensional spectral information into account.

2. Methods

In our demonstration, optical absorption spectroscopy was employed to quantify gaseous species such as ozone and nitrogen oxides produced in an air discharge reactor. Details on the reactor and a surface dielectric barrier discharge (sDBD) can be found in Ref. [1,2]. A sinusoidal voltage of 12 kV_{pp} at 2.5 kHz was applied to the source by using a waveform generator (Keysight 33512B) and a high voltage amplifier (Trek 20/20C). The optical absorption spectroscopy system comprised a deuterium–tungsten lamp (Ocean Insight DH-2000), collimating lenses (Ocean Insight 74-UV), optical fibers (Ocean Insight QP450-1-XSR), and a portable spectrometer (Ocean Insight Maya2000 Pro).

3. Results and Discussion

To deconvolute complex spectral data, we developed a hybrid experimental and AI-based analytical framework. Our AI model framework integrates a variational autoencoder[3] and ResNet-101[4] architecture, designed to process and analyze 2D spectral data. The encoder, based on a modified ResNet-101, extracts critical features from 2D spectral images while minimizing information loss during feature extraction. The decoder reconstructs spectral data according to the Beer–Lambert law to compute chemical densities directly. To enhance accuracy and robustness, the model employs Multi-Task Learning (MTL), which combines three key tasks: classification, regression, and reconstruction.

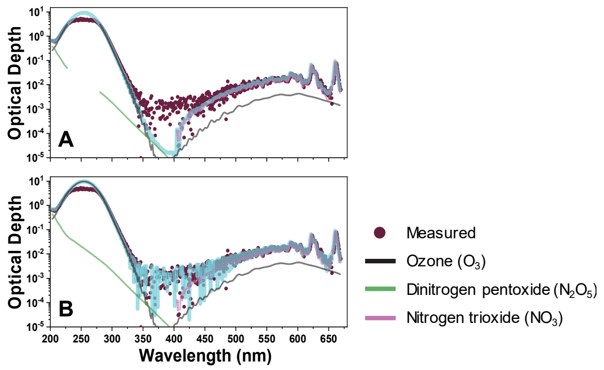

Fig. 1. **Comparison of spectral deconvolution methods.** Fitted spectra obtained by (A) linear regression with implicit regularization, and (B) the proposed AI-assisted method.

The AI model was tested using experimental absorption spectra from a complex gas mixture produced in the air discharge reactor. As shown in Figure 1, the proposed AI-based framework outperformed traditional methods (linear regression) across multiple metrics, particularly in handling noisy spectral regions such as 250–300 nm and 325–525 nm. Unlike conventional approaches, which often required noise masking, the AI model deconvoluted these regions automatically without manual intervention, preserving data integrity and reducing potential information loss. Our results reveal the remarkable ability of the model to analyze spectra following underpinning principles.

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