



Abstract **Prediction of Atmospheric Ozone Concentrations with a Temperature-Modulated Gas Sensor Array**⁺

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⁺ Presented at the XXXV EUROSENSORS Conference, Lecce, Italy, 10–13 September 2023.

Abstract: Ozone is one of the most important pollutant gases. The excellent sensitivity and low limit of detection of gas sensors based on Semiconducting Metal Oxides (SMOXs) make them ideal candidates to accurately monitor outdoor air quality. We present a convolutional neural network (CNN) architecture that is trained on the resistance readout of a multi-pixel SMOX gas sensor array operated in temperature modulation. The trained model outperforms a ridge regressor in the quantification of ozone concentrations in real outdoor air.

Keywords: gas sensor; SMOX; temperature modulation; convolutional neural network; outdoor air quality

1. Introduction

Tropospheric ozone (O3) is a reactive trace gas that is tightly linked to other natural and anthropogenic pollutants that act as ozone precursors [1]. To monitor air pollution on a global scale and maintain guidelines, small, cheap, and reliable sensor solutions are needed. Thanks to their low cost, excellent sensitivity, and low limit of detection, sensors based on Semiconducting Metal Oxides (SMOXs) are among the most commonly used in a plethora of applications, such as automotive, medical, safety, and environmental contexts [2]. To quantify analyte gases in a complex matrix, gas sensor arrays have been turned to, combining multiple, ideally orthogonal, sensing materials or sensor types [3]. Additionally, temperature modulation and convolutional neural networks (CNNs) have been shown to be promising approaches for various analytical tasks [4]. In this work, we demonstrate the superior performance of a temperature-modulated SMOX sensor array in combination with CNNs in the prediction of ozone in real outdoor air.

2. Materials and Methods

An SGP30 (Sensirion AG, Stäfa, Switzerland) sensor array was operated outside of our laboratory on the Morgenstelle Campus in Tübingen, Germany. The operating temperature was cycled continuously, increasing from room temperature to 375 °C and decreasing again, with a dip of the temperature in the middle [4]. For calibration and testing, the ozone concentration, as published by the German Umweltbundesamt (UBA), from the closest air-quality monitoring station (Tübingen Derendingen—DEBW107) was used [5]. The approach is similar to the one described by Mueller et al. for the field calibration of sensor units in Zurich [6]. The complete data set covers two months, and the hourly mean concentration was interpolated using cubic splines to yield concentrations corresponding to the measurement time of the sensor array.

3. Results and Discussion

The predicted ozone concentrations of the test set are plotted against the real ones for the best-performing CNN and ridge regression model in Figure 1.



Citation: Kobald, A.; Weimar, U.; Bårsan, N. Prediction of Atmospheric Ozone Concentrations with a Temperature-Modulated Gas Sensor Array. *Proceedings* 2024, 97, 178. https://doi.org/10.3390/ proceedings2024097178

Academic Editors: Pietro Siciliano and Luca Francioso

Published: 11 April 2024



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Figure 1. Predicted vs. real concentrations of ozone for (**a**) the CNN model and (**b**) the ridge regression.

The CNN model outperforms the ridge regression with mean relative errors in the test set of 16.1% and 26.9%, respectively. There are significantly fewer outliers for the CNN prediction, and the trend line is closely followed, especially for concentrations above 30 ppm.

Author Contributions: Conceptualization, N.B. and A.K.; data analysis, A.K.; writing—original draft preparation, A.K.; writing—review and editing, N.B.; supervision, U.W. and N.B. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: The raw data supporting the conclusions of this article will be made available by the authors on request.

Conflicts of Interest: The authors declare no conflicts of interest.

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