

Reliable TVOC Sensing: A Lab-to-Field Calibration Approach

Johannes Amann¹, Stefan Schumacher², Andreas Schütze¹, Christian Bur¹

¹ Lab for Measurement Technology, Saarland University, Campus A5 1, 66123 Saarbrücken, Germany

² Institute of Energy and Environmental Technology e.V. (IUTA), 47229 Duisburg, Germany
c.bur@imt.uni-saarland.de

Summary:

A methodology for reliable TVOC measurements of metal oxide semiconductor gas sensors in the example of indoor air quality is presented. It is based on representative lab calibration, dynamic operation, and field validation with release tests and air purifiers together. Volatile organic compounds are represented using substance groups derived from analytical studies. Calibration is performed using randomized gas mixtures and machine learning methods. The root means squared error of validation after the lab calibration was less than 10 %. In field tests, the system showed a high correlation to the PTR-MS used as a reference with deviations in the low parts-per-billion range. Thus, the approach enables robust and application-oriented TVOC measurement using cost-effective sensors.

Keywords: total volatile organic compounds (TVOC), calibration, metal oxide semiconductor (MOS) gas sensor, indoor air quality (IAQ), machine learning, validation

Motivation

Indoor air quality (IAQ) is becoming increasingly important, yet the focus remains on carbon dioxide (CO₂) and particulate matter, even though it has been known since Pettenkofer's time that CO₂ is merely a proxy and that volatile organic compounds (VOC) are the primary cause of poor air quality [1]. Unlike CO₂, the reliable and cost-effective measurement of VOC is a challenge, as VOC represent a complex multi-component problem due to the existence of hundreds of different VOC in indoor environments [2]. Therefore, the sum parameter total VOC (TVOC) is frequently used, although its definition depends heavily on the measurement method [3].

Metal oxide semiconductor (MOS) gas sensors are promising due to their low cost, high sensitivity, and real-time on-site capability, but they exhibit low selectivity and require application-specific calibration [4]. Furthermore, the transferability of laboratory conditions to real indoor environments has not yet been adequately addressed and remains one of the major challenges for chemical sensor systems.

The aim of this work is to develop a comprehensive methodology for reliable calibration of MOS sensors for field applications like indoor air quality (IAQ). This involves the definition of the measurement task, i.e., target and interfering gases, representative lab calibration of TVOC, and field

validation - a guideline from the laboratory to the application.

Method

The presented methodology is a unified approach consisting of four main steps: Defining the measurement task, selecting and adapting the sensor system, lab calibration of the system including model building, and field validation, see Fig. 1.

The first step is to understand the measurement task involving major target and interfering gases. Since any (lab) calibration is just a simplification of the real-world application, this step is outmost important. Here, literature research is suggested to identify dominating target and interfering gases including concentration ranges.

To simplify the complex task of, e.g., IAQ with hundreds of VOC, VOC are classified into chemical substance groups first. Each group is described by representative compounds with typical concentration ranges based on extensive studies [2, 5]. The goal of simplification is to reduce the complexity to a feasible number of compounds needed for lab calibration, yet representing the application well. Calibration of seven volatiles representing six substance groups plus hydrogen and carbon monoxide is performed using randomized gas mixtures to simulate realistic indoor air conditions [6].

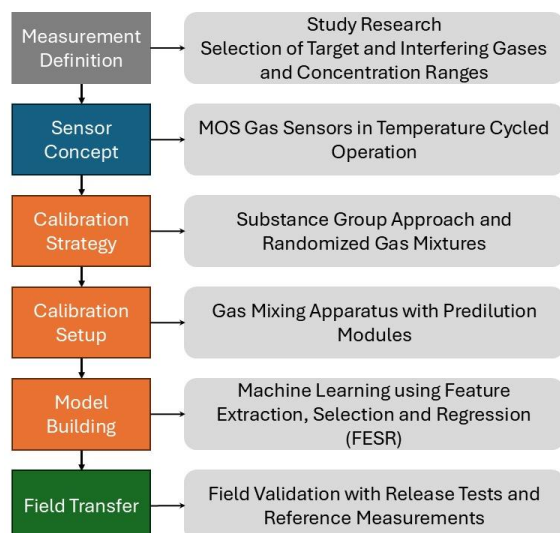


Fig 1. Flow Chart of the methodology showing the four main steps from defining the task to the field transfer.

To improve selectivity and sensitivity, the sensors run in temperature cycled operation (TCO), and the signals are evaluated using machine learning methods, i.e., applying the FESR (feature extraction and selection regression) method [5, 7]. Field phases are specifically integrated to account for drift and ensure transferability (merging lab calibration data and field data).

The novelty of the method lies in the overall approach, which consists of a combination of literature research, a substance-group-based calibration strategy, randomized gas mixtures, and continuous validation from the laboratory to real-world applications. The suggested method is universal and applicable to other use cases.

Results

The calibration provides an accurate prediction of TVOC across a wide concentration range (250 – 3400 ppb) with standardized errors of less than ten percent in the laboratory.

Field validation is demonstrated through release tests and measurements with air purifiers. Dynamic concentration profiles are reliably recorded and correlate well with reference measurements, i.e., a Proton Transfer Reaction – Mass Spectrometer (PTR-MS), see Fig. 2. Here, decay curves of a toluene release with and without an air purifier are compared. With the air purifier turned on, the toluene concentration decreases much faster than with the natural decay curve without an air purifier. The sensor results are identical to those of PTR-MS in relative terms and differ by only a few ppb in absolute terms.

Additionally, successful testing in accordance with VDI/VDE 3518 Part 4 is demonstrated, which allows VOC detectors to be tested for IAQ,

confirming their suitability for indoor air quality assessment.

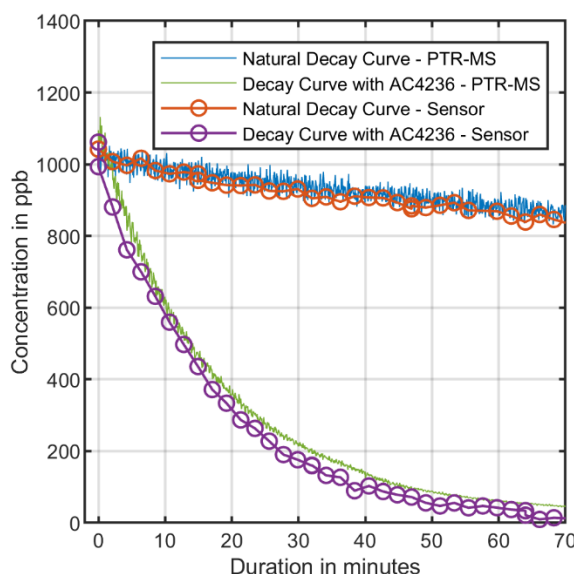


Fig 2. Natural decay curve vs decay curve during operation of an air purifier (Philips AC4236/10) recorded by a calibrated sensor (connected circles) and a PTR-MS during toluene releases (solid line).

References

- [1] M. Pettenkofer, Über den Luftwechsel in Wohngebäuden, *Literarisch-Artistische Anstalt der J.G. Cotta'schen Buchhandlung* (1858)
- [2] H. Hofmann, P. Plieninger, Bereitstellung einer Datenbank zum Vorkommen von flüchtigen organischen Verbindungen in der Raumluft, in *Wa-BoLu-Hefte, Umweltbundesamt* (2008); <https://www.umweltbundesamt.de/sites/default/files/medien/publikation/long/3637.pdf>
- [3] T. Salthammer, TVOC-revisited, *Environment international* 167, 107440 (2022); doi: 10.1016/j.envint.2022.107440
- [4] L. Spinelle, M. Gerboles, M. Aleixandre, Protocol of evaluation and calibration of low-cost gas sensors for the monitoring of air pollution, *Publications Office of the European Union, Luxembourg* (2013)
- [5] T. Baur, J. Amann, C. Schultealbert & A. Schütze, Field study of metal oxide semiconductor gas sensors in temperature cycled operation for selective VOC monitoring in indoor air, *Atmosphere* 12(5), 647 (2021); doi:
- [6] T. Baur, M. Bastuck, C. Schultealbert, T. Sauerwald & A. Schütze, Random gas mixtures for efficient gas sensor calibration. *Journal of Sensors and Sensor Systems* 9(2), 411-424 (2020); doi: 10.5194/jsss-9-411-2020
- [7] A. Schütze & T. Sauerwald, Dynamic operation of semiconductor sensors. In *Semiconductor gas sensors*, Woodhead Publishing, 385-412 (2020); doi: 10.1016/B978-0-08-102559-8.00012-4