DOI 10.5162/17dss2024/7.3

Run-In Behaviour of MOS Sensors in Temperature Cycled Operation

Dennis Arendes, Johannes Amann, Andreas Schütze, Christian Bur

Saarland University, Lab for Measurement Technology, Saarbrücken, Germany
Contact: d.arendes@lmt.uni-saarland.de

Introduction

Metal oxide semiconductor (MOS) gas sensors are used in a wide spectrum of application [1],[2],[3]. Promising fields are especially the Indoor Air Quality (IAQ) [4], as well as the medicine field with drug monitoring [5]. In many cases an immediate evaluation out of the raw sensor data is impossible without a machine learning (ML) model. In order to train those ML models a proper individual calibration is necessary [6]. This calibration can be done by providing unique gas mixtures (UGMs) to the sensors in a gas mixing apparatus (GMA) [7]. When MOS sensors are operated for the first time, they show characteristic changes in their sensor responses, which do not correlate with the sensor environment. If this Run-In phase occurs during the calibration it will lead to invalid ML methods, for example incorrect predictions after the initial Run-In phase. Therefore, it is necessary to examine this phase to achieve stable and robust ML models. An easy method to compensate the Run-In phase is a pre-treatment before the actual calibration. This pre-treatment can be done by operating the sensor in a designated environment with a specific duration.

Material and Methods

There are several commercially available, digital MOS sensors on the market. In this work focuses on the four-layer multipixel MOS gas sensor SGP40 (Sensirion AG, Stäfa, Switzerland) but the results can be transferred to other sensors, too. To boost the sensitivity and selectivity of the MOS sensors, the heater temperature can be varied in a cyclic fashion, called temperature cycled operation (TCO). To study the impact of pre-treatment, several sensors are considered which differ in operation modes, the duration of the pre-treatment, and environments. Half of the sensors are operated in TCO with the temperature cycle, cf. Fig. 1. The other half is operated at a constant temperature of 400 °C. The environment is varied between a real office and an artificial environment consisting of relevant gases, cf. Tab. 1. The last examined parameter is the duration of the pre-treatment phase. The duration was varied between no pre-treatment phase at all, five days, and one day of pre-treatment. In total 20 SGP40 sensors were used in this experiment.

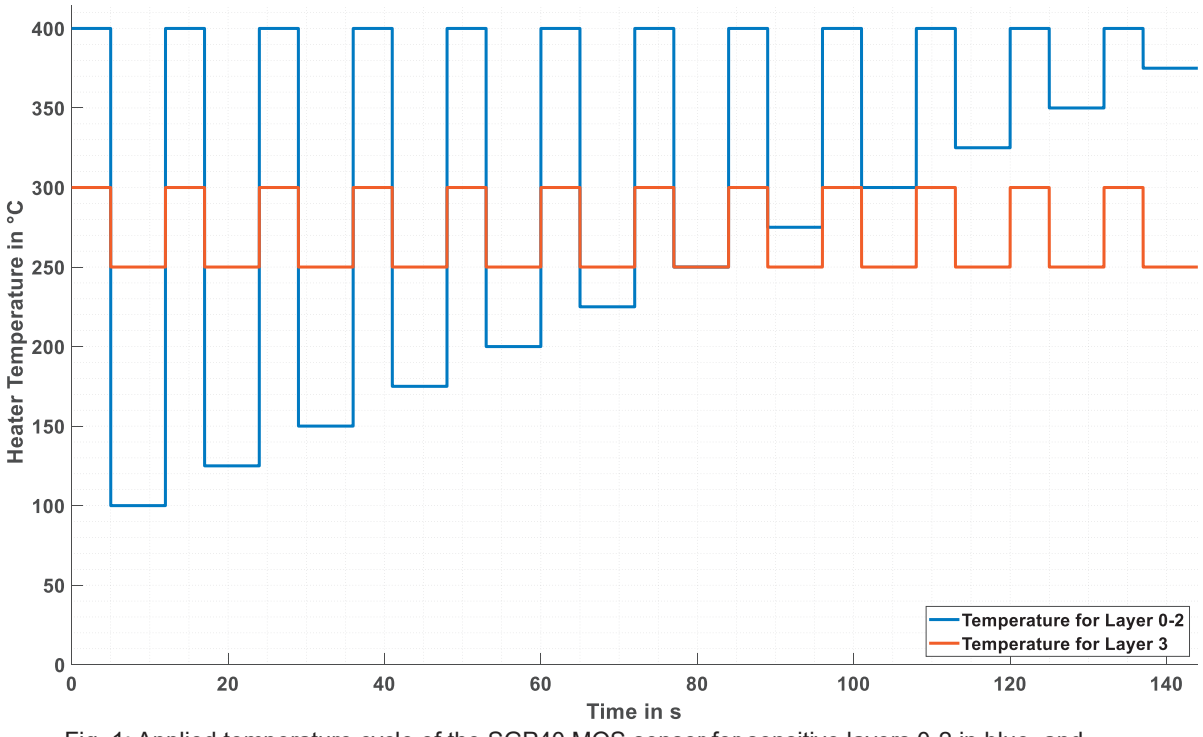

Fig. 1: Applied temperature cycle of the SGP40 MOS sensor for sensitive layers 0-2 in blue, and for layer 3 in orange.

Tab. 1: Concentration of the artificial environment during pre-treatment.

Gas	Concentration
Relative Humidity (20 °C)	50 %
Hydrogen	500 ppb
CO	150 ppb
Ethanol	50 ppb
Toluene	50 ppb
Acetone	50 ppb

After the pre-treatment phase, two calibrations were performed. Between both calibrations all sensors are operated for four weeks in an office environment. During the calibration, all sensors were operated in the same TCO, as in the pre-treatment phase. This allows for direct comparison between all sensors. Each calibration consisted of 200 UGMs, provided by the GMA. The concentration of each gas in the UGMs are randomly chosen by Latin Hypercube Sampling leading to an uncorrelated data basis, to minimizing the risk for overfitting of the ML algorithms. All relevant gases and ranges available for the LHS algorithm are listed in Tab. 2. Beside every gas, the relative humidity is also varied between suitable borders, to also compensate for the MOS sensor cross sensitivity to humidity.

Tab. 2: Relevant gases and concentration ranges for both calibrations.

Gas	Concentration
Relative Humidity (20 °C)	25 - 75 %
Hydrogen	400 - 1900 ppb
CO	100 - 2000 ppb
Ethanol	1 - 300 ppb
Toluene	1 - 300 ppb
Acetone	1 - 300 ppb
Formaldehyde	1 - 300 ppb
Ethyl Acetate	1 - 300 ppb

Each calibration has the same concentration ranges for the LHS algorithm, but is randomised newly, to prevent overfitting. For the same reason and to prevent the model to learn the run-in behaviour of the sensor, they are trained on the second calibration and are applied on the first calibration to compare the model quality.

Model building is done by extracting features first. The extracted features are the mean and the slope of one second intervals over the whole cycle for each layer. Thus, resulting into four times two times 144 = 1152 features. Afterwards a dimension reduction with a principal component analysis (PCA) is done, where the first 20 components were taken into account. The final regression is done by a partial least squares regression (PLSR).

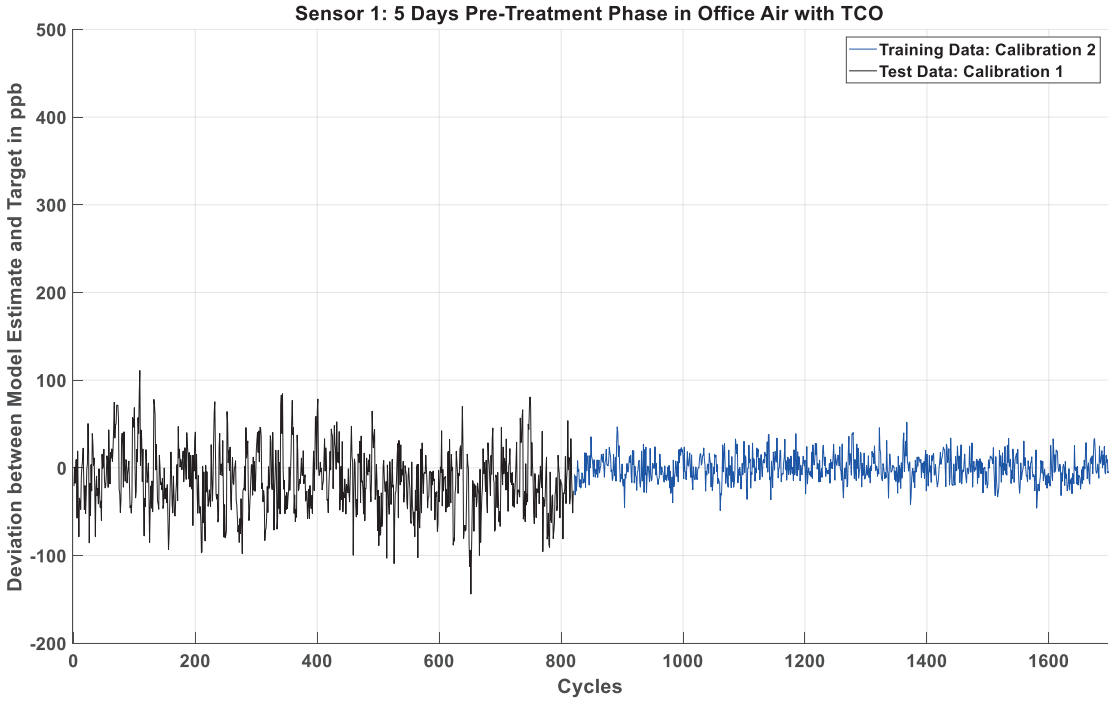

Fig. 2: Deviation between the POT and the target values for a sensor with five days pre-treatment phase in office air, operated in TCO for acetone as target gas.

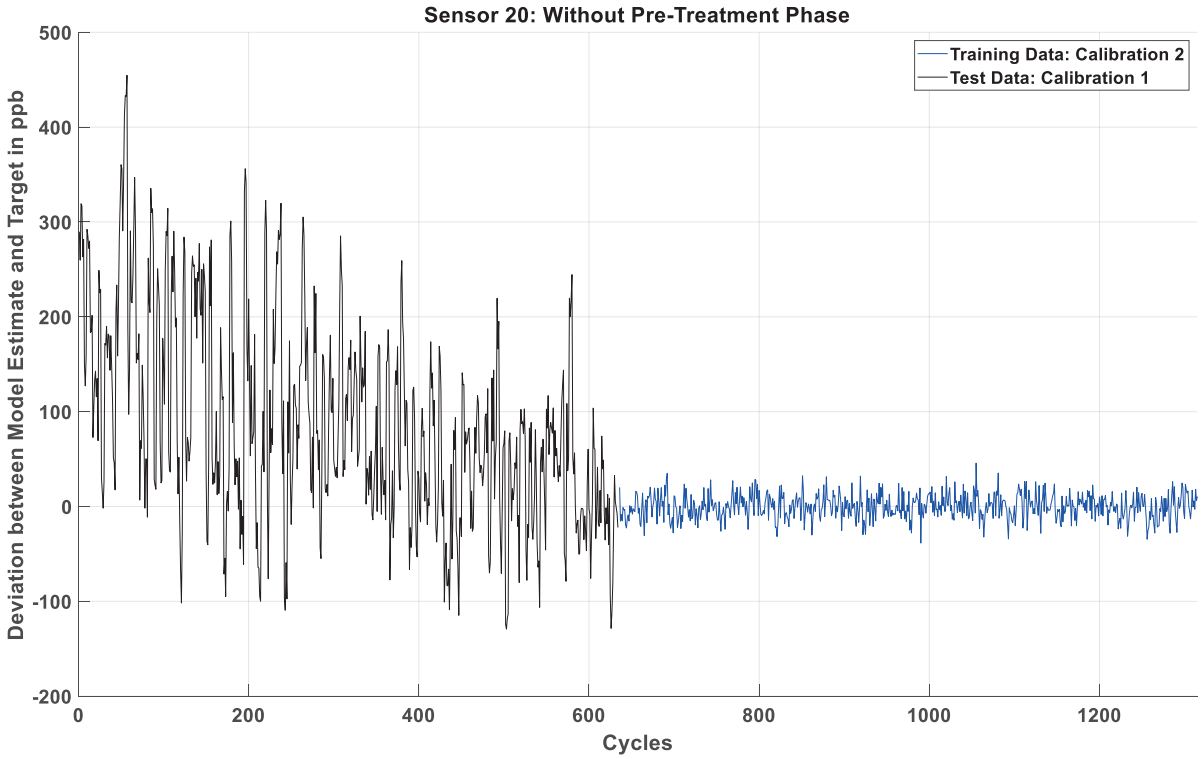

Fig. 3: Deviation between the POT and the target values for a sensor without pre-treatment phase for acetone as target gas.

The root mean square (RMSE) values of the test data do not correlate properly to the pre-treatment phases and is thus no valuable qualification index for the benefits of the pre-treatment phase. A more suitable approach is the model estimate itself, i.e. the prediction over time (POT). In order to highlight the effect, the difference between the POT for acetone and the corresponding targets for a sensor without five-day pre-treatment phase in an office environment, operated in TCO, are considered, cf. Fig. 2. In contrast, another sensor, operated without any pre-treatment phase is shown in Fig. 3. It is clearly visible, that the deviation is decreasing for the sensor without any pre-treatment in comparison to the one with pre-treatment. In order to compare all sensors with each other with a single scalar, the interquartile range between the 25 % and 75 % percentile of the deviation between target and POT are taken into account.

Results

The interquartile range for all sensors with acetone as target gas, cf. Fig. 4, prove that the five sensors without any pre-treatment phase have the highest value. This would result into ML models with poor quality. Comparing the other examined parameters suggest, that a longer pre-treatment phase with five days lead to a better result, compared to the sensors with only one day of pre-treatment. Furthermore, the artificial air has slightly worse results than the office air. Thus, the pre-treatment is more effective in an atmosphere of reducing gases, similar to the real-world application. As a side effect, this is more convenient, since no complex equipment, like a GMA is needed to perform effective pre-treatment. At least for the IAQ environment, using the sensors in their designated environment is an effective way to compensate for run-in behaviour, whereas the operation mode is negligible.

Fig. 5 summarizes the results for all other gases. The differences between all parameters are not yet remarkable, but the main findings still visible. Especially the benefits of any pre-treatment, compared to the sensors without. The differences can be explained by the overall ability of any ML model to differentiate between the gases. It also likely that the key features to quantify ethanol are based in slope features, instead of mean features. Therefore, the model is not that prone to differences due to the sensor Run-In.

Another relevant target gas is formaldehyde, cf. Fig. 6. For this gas the sensors with five-day pre-treatment still perform better than the others. The difference between no pre-treatment and one day of pre-treatment is not that distinct.

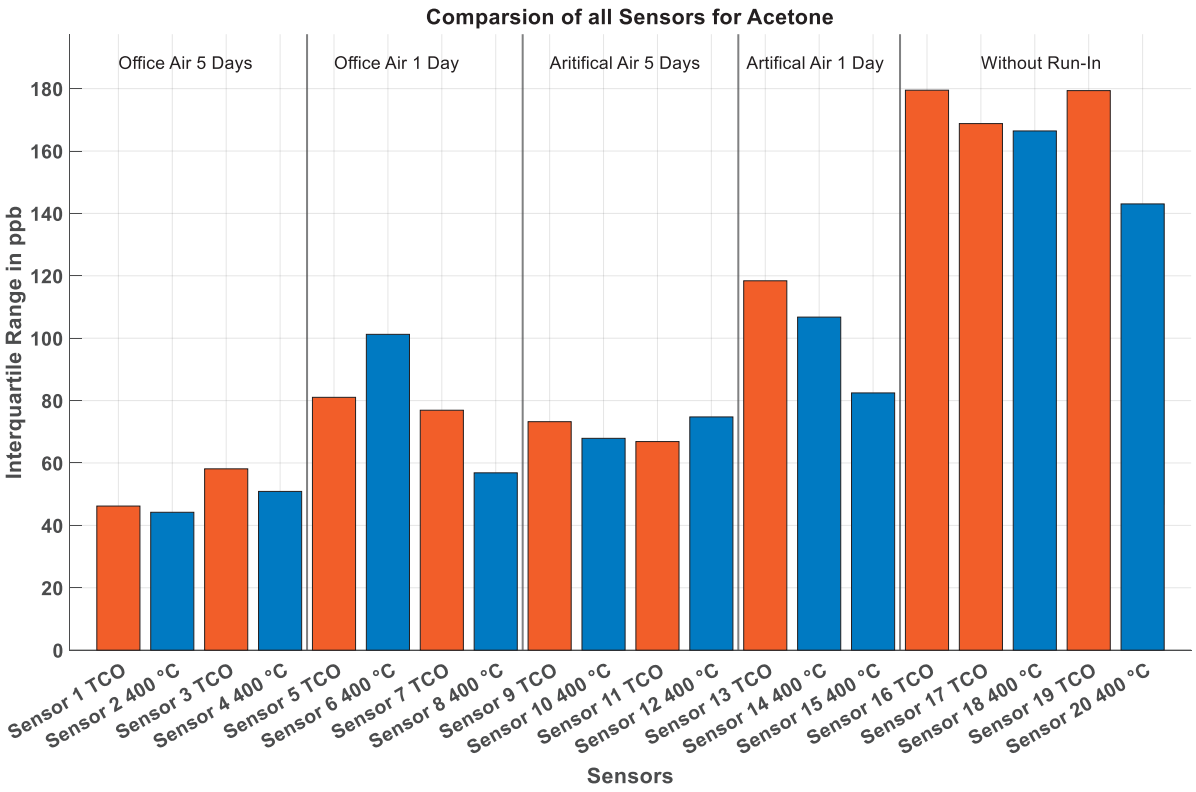

Fig. 4: Interquartile range for all sensors with acetone as target gas.

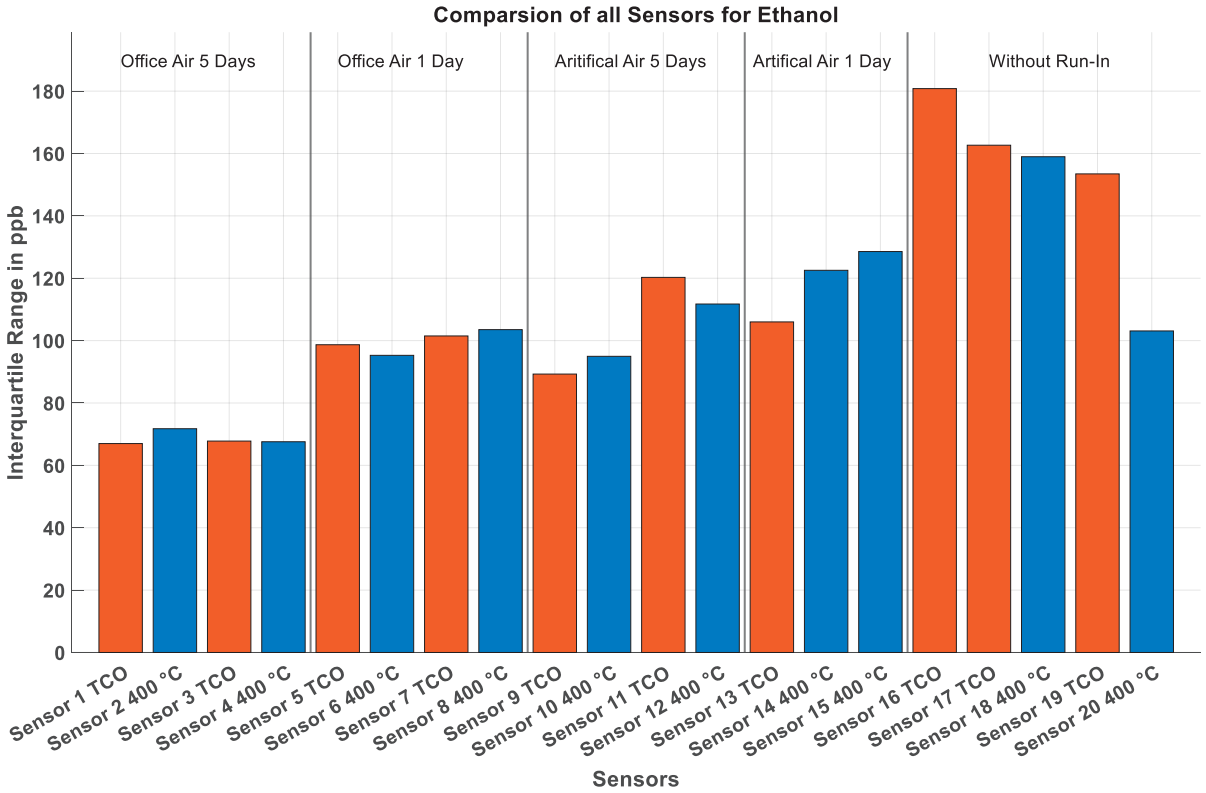

Fig. 5: Interquartile range for all sensors with ethanol as target gas.

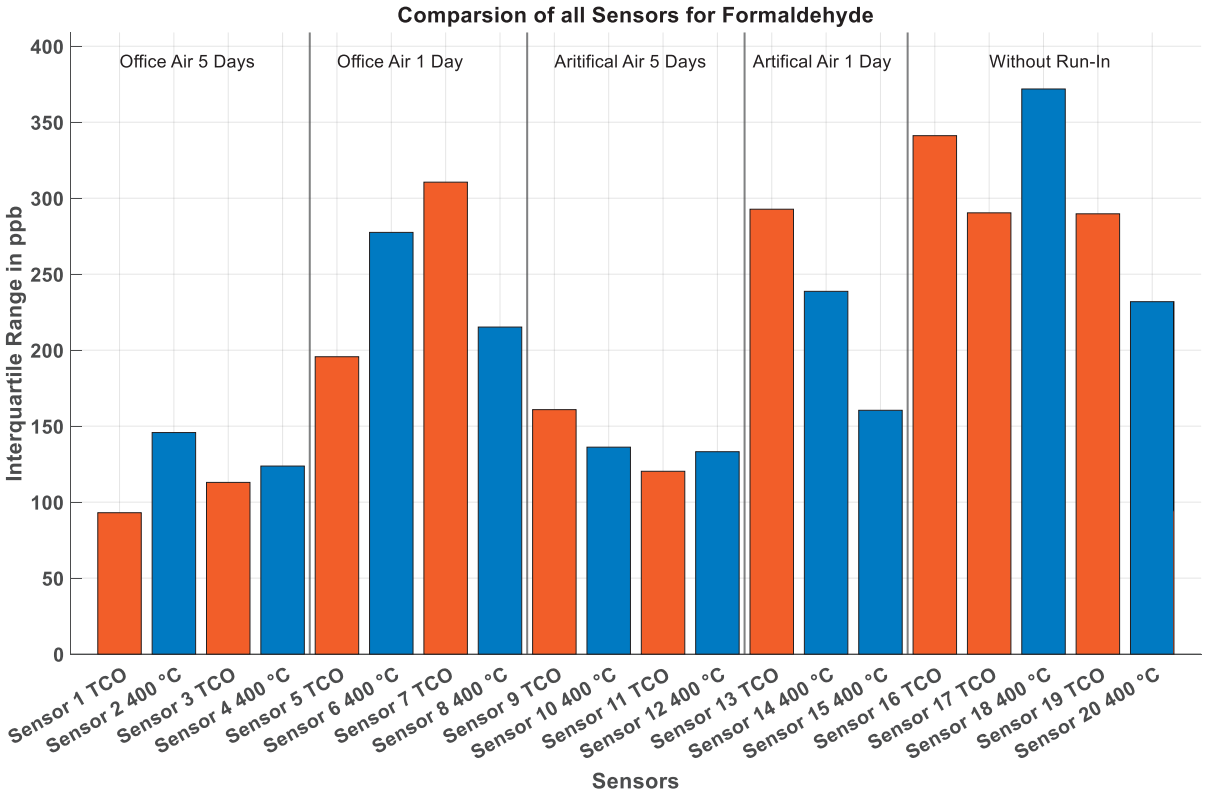

Fig. 6: Interquartile range for all sensors with formaldehyde as target gas.

In summary, sufficiently long pre-treatment time leads to significantly better results in a calibration. The operation mode in pre-treatment can be neglected, while the ambient atmosphere can be common office air.

Conclusion and Outlook

This work has shown that MOS gas sensors in fact show a run-in phase in the first operation time. Furthermore, this run-in phase can influence the performance of calibrations and thus, the quality of all ML models. However, these effects can be compensated by a previous pre-treatment phase, in which all sensors are operated for at least five days. The ambient sensor atmosphere can be common office air, therefore allowing pre-treatment without the use of expensive laboratory equipment. The operation mode of the sensors is minor important and does not affect the efficiency of the pre-treatment phase. Future work will address the optimal duration of pre-treatment, like three days or seven days. As a basic recommendation the sensors should be operated for a weekend, prior to any calibration, as a pre-treatment phase. Future work may also take a close look at other commercially available MOS sensors.

References

[1] CAPELLI, L.; SIRONI, S.; DEL ROSSO, R.: Electronic Noses for Environmental Monitoring Applications, Sensors 14 (2014), DOI: 10.3390/s141119979

[2] DE VITO, S.; PIGA, M.; MARTINOTTO, L.; FRANCIA, G.: CO, NO2 and NOx urban pollution monitoring with on-field calibrated electronic nose by automatic Bayesian regularization, Sensors and Actuators B: Chemical 143 (2009) Page 182-191 DOI: 10.1016/j.snb.2009.08.041

[3] BURGUES, J.; ESCLAPEZ M.D.; DONATE, S.; PASTOR, L.; MARCO, S.: Aerial Mapping of Odorous Gases in a Wastewater Treatment Plant Using a Small Drone, Remote Sensing 13-9 (2021), DOI: 10.3390/rs13091757

[4] BAUR, T.; AMANN, J.; SCHULTEALBERT, C.; SCHÜTZE, A.: Field Study of Metal Oxide Semiconductors Gas Sensors in Temperature Cycled Operation for Selective VOC Monitoring in Indoor Air, In: Atmosphere 21 (2021); Page 647, DOI: 10.3390/atmos12050647

[5] BUR, C.; LENSCH, H.; SCHÜTZE, A.: Propofol Detection with Metal Oxide Semiconductor Gas Sensors, Proceedings of the Dresdner Sensor Symposium (2022); DOI: 10.5162/16dss2022/P10

[6] BAUR, T.; BASTUCK, M.; SCHULTEALBERT, C.; SAUERWALD, T.; SCHÜTZE, A.: Random gas mixtures for efficient gas sensor calibration; In:

J.Sens.Sens.Syst 9 (2020); Page 411-424; DOI: 10.5194/jsss-9-411-2020

[7] ARENDES, D.; AMANN, J.; TESSIER, C.; BRIEGER, O.; SCHÜTZE, A.; BUR, C.: Qualification and Optimisation of a Gas Mixing Apparatus for Complex Trace Gas Mixtures", In: Technisches Messen vol.90 no.12 (2023); Page 822-834; DOI: 10.1515/teme-2023-0075