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Dynamic multi-sensor operation and read-out for highly selective gas sensor systems

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Abstract

We describe hardware and algorithms which enable highly selective and sensitive operation of the two gas sensor types used in the SENSIndoor project. The resistance of a metal-oxide semiconductor (MOS) type can rise above 1 GΩ in temperature cycled operation (TCO), which is measured using a logarithmic amplifier. A silicon-carbide based, gas-sensitive field-effect transistor (SiC-FET) driven with a combination of TCO and gate-bias cycled operation (GBCO) is used as second, complimentary sensor. The cyclic sensor signals exhibit distinct shape changes depending on the gas present which is captured by pattern recognition. In this study we use Linear Discriminant Analysis (LDA) for discrimination and Partial Least Squares Regression (PLSR) for quantification of ppb concentrations of target VOCs in changing ppm concentrations of interfering gases for indoor air quality assessment.

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Keywords: MOS; SiC-FET; pre-concentrator; temperature cycled operation; multivariate data analysis; regression

1. Introduction

People spend more than 80 % of their time indoors, rendering indoor air quality a high impact factor for human health. Hazardous volatile organic compounds (VOCs) are emitted from many solvents used in everyday products and, thus, accumulate indoors without ventilation. On the other hand, continuous ventilation is no viable solution

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either, as potentially higher pollution from outside can be carried inside, and air conditioning causes significant cost. Hence, a small and cheap system is desirable which is able to detect and quantify hazardous VOCs selectively and turn on the ventilation only when it is necessary. The total VOC (TVOC) value which is used in some systems on the market is no reliable indicator. This is easily seen for the example of ethanol, a VOC which can be present in large amounts (from perfume, cleaning agents or alcoholic drinks), but is not hazardous to human health in usual concentrations in the gas phase. Ethanol is thus treated as interfering gas in this study, i.e. its presence should not cause alarm up to ppm level. Benzene, naphthalene and formaldehyde have been identified as high-priority target VOCs because of their classification as carcinogens. The World Health Organization recommends no safe limit for benzene, and 5 ppb and 150 ppb for naphthalene and formaldehyde, respectively [1].

In the EU project SENSIndoor, two sensor technologies are combined in one system: a metal-oxide semiconductor (MOS) gas sensor and a silicon-carbide based, gas-sensitive field-effect transistor (SiC-FET) [2]. The MOS sensor is complemented with a micro-pre-concentrator [3]. All three devices are run with temperature cycled operation (TCO) to enhance sensitivity and selectivity. On the SiC-FET, TCO is complemented by gate-bias cycled operation (GBCO). All cycles must be synchronized precisely to achieve optimum system performance. The data from both sensor types are combined and fed to a model based on multivariate data analysis. Different models are applied for classification or quantification of the gas components present.

The following section will cover the hardware specifications with focus on the logarithmic amplifier, the applied cycles and their interplay, data processing approaches and preliminary results that have been achieved with the combination of the techniques described.

2. Methods and implementation

2.1. Hardware

TCO requires a reliable temperature control of the sensing element. Instead of power control or an integrated temperature sensor, heaters with well characterized R(T) dependency are used for all three devices as those allow for best accuracy in combination with a resistance control loop.

MOS-type sensors exhibit resistance values in the GΩ range in sections of their temperature cycle after a sudden cooldown [4]. To measure such values with low noise, the log amplifier LOG112 (Texas Instruments) is employed which converts a current signal to a logarithmic voltage signal. It is connected as closely as possible to the sensor in order to keep induced noise in the current signal low and enable tight guarding of this part of the system. The log amplifier then converts the small signals (~nA) into much larger signals (~V) which are easily transferred over longer distances, less influenced by induced noise, and can be measured with conventional hardware.

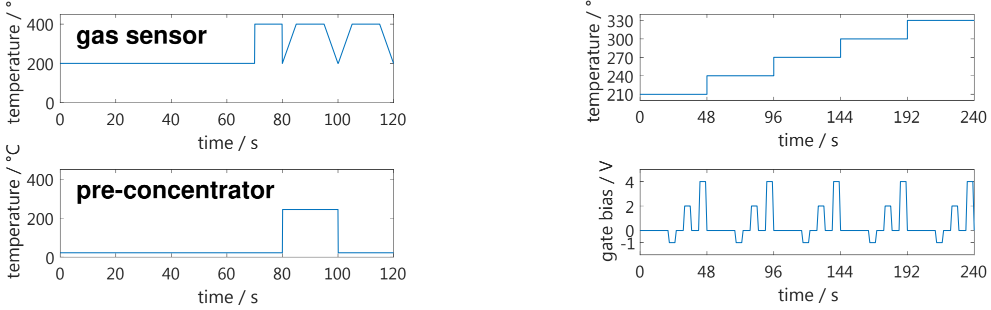
The hardware for both sensor types enables dynamic programming of temperature and gate bias cycles. While the board controlling the MOS/pre-concentrator system writes its data directly onto an SD card, the SiC-FET board is connected to a small PC running a LabVIEW program which saves the data as compressed HDF5, enabling continuous testing in the field for several weeks with both systems.

2.2. Operating modes

The MOS/pre-concentrator subsystem is driven with the cycles shown in Fig. 1a. For the first 70 s, the pre-concentrator is at room temperature allowing adsorption of gas molecules. The sensor temperature is 200 °C as a compromise between low energy consumption and preventing contamination of the surface. Ten seconds before release, the sensor is heated to 400 °C to clean the surface. The sensor then performs a ramp-plateau-ramp cycle twice (80-100 s, 100-120 s), of which the first one takes place during the release phase of the pre-concentrator, the second one during re-adsorption. The difference in the shape of these two cycles carries information about gases released from the pre-concentrator and their concentrations. Sensitivity is improved by the increased gas concentration available to the sensor [3], and selectivity both by the selective pre-concentrator and TCO [4,5].

The SiC-FET sensor cannot yet be implemented with a pre-concentrator. However, it provides the possibility to change gate bias in addition to temperature. As measurements do not have to be very quick for the intended purpose, we chose a cycle twice as long as for the MOS/pre-concentrator system. It is divided into five temperature plateaus

(210 °C, 240 °C, …, 330 °C) covering a range which has shown significant differences in sensitivity towards the target VOCs, so that the ratios of sensor signals during these plateaus should carry information about gas and concentration. On each plateau, the gate bias is varied to be 0 V, -1 V, 2 V and 4 V. Several publications have reported dependence between sensor response and gate bias [6,7], so that improved information gain is expected from this combination of cycles.



(a) (b)

Fig. 1. Cycles used for (a) the MOS/pre-concentrator system and the (b) SiC-FET sensor.

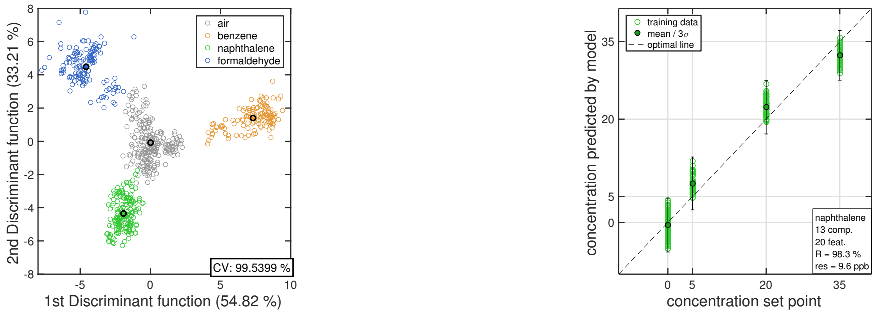
2.3. Data processing

For better sensitivity and selectivity, we interpret each cycle consisting of several hundred single measurements as just one measurement with several hundred dimensions. This procedure yields a signal very similar to what would be produced by a sensor array with several hundred sensors ("virtual multisensor") [5], however, with much redundant data. To reduce redundancy which would cause problems in the multivariate methods [8] applied later on, dimensionality must be reduced while keeping most of the important information. In a first step, this is achieved by manually selecting "relevant" parts in the cycle and computing features like, e.g., mean value or slope for each cycle. "Relevant" here refers to segments in the cycle where great differences between gases or concentrations are seen or expected (if a model is available). This step often reduces dimensionality by more than 90 %.

In a subsequent step, dimensionality reduction methods like PCA (principal component analysis, mainly for data exploration) or LDA (linear discriminant analysis, mainly for model building, Fig. 2a) can again reduce the dimensions [8], often to a number smaller or equal to three while still maintaining the important part of information contained in the original signal. Both methods produce a set of coefficients allowing the projection of new data points into the low-dimensional space using simple linear combinations. These new points must then be classified in order to find out which gas (or gas mixture) was present when the signal was recorded. Plenty of methods for classification are available. However, as SENSIndoor focusses on implementation of the algorithms on small, cheap systems, we chose to always reduce the data down to one dimension and use a classification threshold, i.e. a single number, to divide the data into two classes. As two classes will not be sufficient for the complex classification task at hand, a hierarchical approach will be employed where each point wanders down a tree and is classified into different categories at each fork. The resulting paths will eventually give a precise picture of the gases present. The tree can contain several forks where the same data point is once classified as, e.g., "benzene/no benzene" and as "naphthalene/no naphthalene". The classification threshold determines the "alarm value" for each gas specifically.

If a more precise quantification is required, Partial Least Squares Regression (PLSR, Fig. 2b) [8] can be performed with the same features that were used for PCA/LDA. PLSR builds a regression model and thus outputs a concentration estimate for each data point. Also here, different models for different gases will be built that can be employed for selective quantification of target VOCs while ignoring interfering gases.

Every model must be validated to show that it is not overfitted and produces meaningful results also for new data. This is done at the time of model creation on a regular PC (not the low-cost hardware) with 10-fold cross-validation (CV). In this method, the dataset used to fit the model is divided into ten parts, nine of which are used to build the model. The remaining part is then predicted using this model and the prediction result is compared with the known, true result. This is done ten times so that each part has been used for testing. Our framework DAV³E [9] provides an easy user interface and automatic processing abilities of large data collections to determine the best models.



(a) (b)

Fig. 2. (a) LDA discriminating benzene (1, 3, 5 ppb), naphthalene (5, 20, 35 ppb), and formaldehyde (50, 100, 150 ppb) from air and each other. The 20 underlying features, mean values and slopes, are taken from a SiC-FET with a one minute temperature cycle comprising three different temperatures. (b) PLSR quantifying different concentrations of naphthalene with the same features that were used for discrimination in (a).

3. Conclusion

We have presented hardware and signal processing algorithms used in the EU project SENSIndoor for selective detection and quantification of hazardous VOCs in indoor air. Sensitivity and selectivity are increased by TCO for both sensor technologies, and a selective pre-concentrator and GBCO for MOS and SiC-FET sensors, respectively. To enable quick and reliable measurements in the GΩ range for the MOS sensor, a log amplifier is used. The recorded data is processed with multivariate methods like LDA and reduced to one dimension so that it can be classified with a simple threshold value. For complex classification tasks, a decision tree of several specific LDA models and classifiers is built. Thus, the problem is divided into simple sub-problems easy to implement on cheap hardware, eventually enabling indoor air quality monitoring routinely in public buildings and private homes.

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