DOI 10.5162/sensor2015/P8.6

A New Mathematical Procedure for Simultaneous Analysis of Gases with Resistive Gas Sensors

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Abstract:

In many applications a multitude of different gases may occur which have to be identified and analyzed simultaneously, for example in detecting cable fire in a cable slot at a very early point of time but with high discrimination to other gases. But well introduced calibration and evaluation procedures are only designed to analyze only one gas or gas mixture. A new and efficient mathematical procedure called SimSens was developed to overcome this drawback. A short outline of SimSens and the validation with real data of four gases and one gas mixture is presented and the ability of simultaneous gas identification and reliability respective accuracy of analysis is discussed.

Key words: simultaneous analysis, substance identification, mathematical procedure, conduction over time profile, and thermo-cyclic operation

Background

In many applications a multitude of different gases may occur which have to be simultaneously identified and analyzed, for example in detecting cable fire in a cable slot at a very early point of time. Depending on the various coating materials of the cables, a variety of gases can escape which have to identified and analyzed for early detection of such a cable fire. Another field of potential application is the monitoring of storages of chemical substances with capability of evaporation like solvents, paints, etc. In this scenario a multitude of substances can be accidentally released to the environment and has to be simultaneously identified and analyzed. But well introduced evaluation procedures for data analysis like ProSens [1] are only designed to analyze one gas mixture.

Thermo-cyclic Operation

Thermo-cyclic operation means, that the working temperature of the sensor element is periodically increased and decreased over the time in a triangular shape. Simultaneous sampling of the conductance values over the time leads to so-called Conductance over Time Profiles (CTP) [2]. These profiles give a fingerprint of the surface processes with the gas and represent the gas mixture under consideration. The gas specific features of the CTPs can be used for component identification and concentration determination.

Figure 1 shows the CTPs of acetic acid at various concentration levels with the characteristic shape.

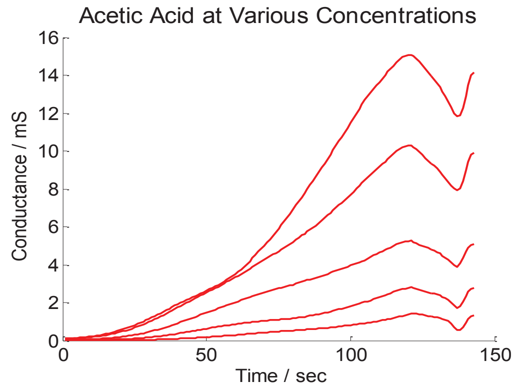

Fig. 1. CTPs of acetic acid at various concentrations.

The Procedure SimSens

A new and efficient mathematical procedure, called SimSens, was developed at the Karlsruhe Institute of Technology (KIT) which is able to meet requirements of simultaneous analysis of gases.

SimSens is an extension of the above mentioned program ProSens and consists like ProSens of a calibration part and an evaluation part.

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In a first step (calibration step) SimSens establishes for each gas under consideration which may occur the mathematical calibration model on the basis of calibration measurements.

When an unknown gas sample occurs, the evaluation part of SimSens is able to recognize whether this gas sample is one of the gases under consideration (identification) or not on the basis of the calibration models. Therefore, SimSens calculates theoretical CTPs for each calibrated gas and compares these CTPs with the measured CTP.

If measured CTP and one of the theoretical CTPs are close together, i.e. a difference value calculated from the sum of quadratic differences of every sample point of the measured CTP and the theoretical CTP is smaller than a predetermined decision value, SimSens identifies the unknown gas probe with the related calibrated gas.

Otherwise SimSens recognizes that the gas probe is none of the calibrated gases. This identification capability is very important to avoid misleading interpretations like false alarms. In the case of successful identification SimSens is able to analyze the gas probe, i.e. to determine the concentration of the sample.

Application and Results

To investigate the performance of SimSens, four mono gas applications (dimethyl sulfate (DMS), acetic acid, octane and methylfuran and a multi gas application (ternary acetic acid/hexane/octane-mixture, X111)) were considered as the gases under consideration. The gas samples, for calibration as well as for evaluation, were measured with only one gas sensor element operated by periodic variation of the sensor temperature and simultaneous sampling of the so called Conductance-over-Time-Profiles.

Fig. 2 shows, for example, that the measured CTP of a DMS sample is very close to the theoretical CTP based on the DMS calibration model. Therefore, the DMS sample can be identified.

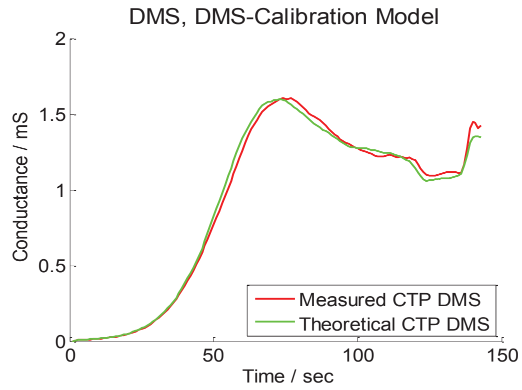

Fig. 2. Comparison of measured CTP of DMS with theoretical CTP of DMS based on the calibration model of DMS.

On the other hand Fig. 3 shows that the measured CTP of the DMS sample is quite different to the theoretical CTP based on the acetic acid calibration model. That means that SimSens recognizes that the DMS sample is not an acetic acid gas.

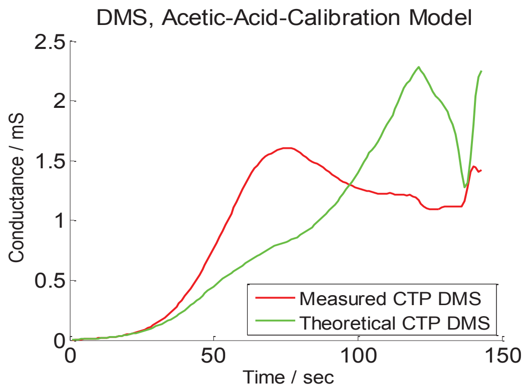

Fig. 3. Comparison of measured CTP of DMS with theoretical CTP of DMS based on the calibration model of acetic acid.

This is true for all the calibrated gases. Each of them could be recognized as the related gas and not as one of the other calibrated gases

Otherwise, Fig. 4 shows that the measured CTP of a hexanal sample is quite different to the theoretical CTP based on the DMS calibration model. This is also true for the comparison of the measured CTP of the hexanal sample with the theoretical CTPs on the basis of the calibration models of all gases included in the field of gas components to be analyzed. That means that SimSens is capable to recognize hexanal as a not calibrated gas.

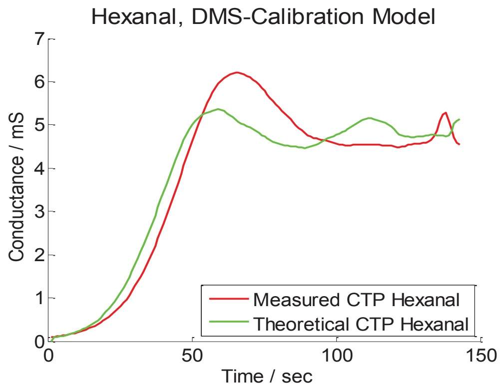

Fig. 4. Comparison of measured CTP of hexanal with theoretical CTP of hexanal based on the calibration model of DMS.

Table 1 shows the analysis results comparing dosed values and analyzed values and the relative deviations. It can be seen that in all cases the relative errors are smaller than 8% which is a very good analysis result.

Tab. 1: Comparison of dosed and analyzed values and relative deviation

	Dos	Anal	Rel	Dos	Ana	Rel	Dos	Anal	Rel
DMS	2981	2784	6,6	8821	8760	0,7	31455	32477	3,3
Acetic Acid	91	97,7	7,3	268	249	7,3	955	995	4,2
Octane	79	74	6,6	234	230	1,5	836	837	0,1
Methylfuran	786	749	4,7	2320	2275	1,9	8297	8523	2,7
X111	79	80	1,1	234	219	6,2	836	862	3,1

Dos: dosed values in ppm, Anal: analyzed values in ppm, Rel: relative deviation in %

Conclusion

The application with four mono gases (dimethyl sulfate (DMS), acetic acid, octane and methylfuran and a multi gas application (ternary acetic acid/hexane/octane-mixture, X111)) demonstrates that SimSens fulfills the requirements of simultaneous analysis. All the calibrated gases could be identified in a correct manner. On the other hand, a hexanal sample could be recognized as a not calibrated gas.

Also the analysis results of the concentration determination are very good. All the samples of the calibrated gases with various dosed concentrations could be analyzed and determined with a relative estimation error less than 8%.

References

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