SIGNAL EVALUATION OF GAS SENSORS WITH ARTIFICIAL NEURAL NETS

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ABSTRACT: Due to the lack in selectivity and separability of most common gas sensors, the use of sensor arrays together self adapting systems as artificial neural nets (ANN) is necessary. These systems can evaluate the gas concentration or deliver a binary signal (gas present or not, ventilation on or off, etc.), which gives a chance to solve measurement problems in gas mixtures. Also the estimation of indoor air quality, olfactometric measurements, etc. may be possible using ANN methods.
A promising new approach is the use of non-stationary (transient) signals of a single sensor after a certain stimulus (i.e. a temperature change, etc.). This additional information enhances the redundancy of such a system and a single sensor delivers further information (virtual sensor array).
Signal evaluation methods for chemical sensors are powerful tools, they are adaptable to specific applications and are compatible to customary micro controllers.

KEYWORDS: Gas Sensor, Semiconductor Sensor, Neural Networks, Signal Processing Algorithms, Air Quality, Process Control Olfactometry, Gas Warning

1 INTRODUCTION

The task of a gas sensing system is to measure one or more specified gases and to suppress any interference of other gases and humidity. A common method to suppress the interference is the use of multi-sensor systems together with a smart signal evaluation system. Foremost arrays of semiconductor sensors were used for such applications due to their easy availability and the possibility of easy modifications with several dopants for different gases [1]. In some applications (e.g. olfactometry) other sensor types (quartz micro balances, interdigitated capacitor with adsorptive coatings, conducting polymers, etc.) are also in common use [2].

The basic principles of the gas detection are similar for many sensors. Normally a gas molecule adsorbs and desorbes at the surface of the indicator material of the sensor, which can be measured with a transducer using a physical effect caused by this adsorption. Additionally a chemical reaction can occur, in the case of semiconductor sensor a reducing or oxidising reaction. These basic detection principles can be described with similar empirical formulas derived from first principles [3]. Anyway, a mature theory which describes sufficiently the operation of these sensors in „normal" field conditions with varying gases and disturbing substances (e.g. indoor air) is not available. Therefore, self-learning and interpolating systems like Artificial Neural Networks (ANN) are well-suited methods for the use in signal evaluation systems handling these highly non-linear problems. Evidently a pre- and post-processing of the raw data and the network output is recommended for reliable results.

In field applications the sensors are confronted with varying conditions and do not reach a stationary signal in all cases. Therefore, signal evaluation methods using stationary signals are obsolete.

Also the non stationary aspect of common operating conditions (transient modes) can be used for signal evaluation. Especially an artificial generation of such conditions after a certain stimulus may improve the signal processing. Examples of stimuli are temperature changes (used for pellistors or semiconductor sensor [4]), a sudden change in the gas combination (used in headspace methods for olfactometry), etc.. All these measurement methods increase the information delivered by the sensor. A thermal stimulus may deliver information about the adsorption and desorption properties of the species at the sensor surface. This transient signal can be used to discriminate between different gases or to shorten the response time. The stimulus-response method extends a single sensor to a virtual sensor array. For example micromachined sensors with small thermal time constants are best suited for temperature transient operating modes (figure 1).

A common disadvantage of fitting methods and self adapting systems is the necessity of an immense amount of training data for their calibration. The number of calibration measurements can be reduced with special techniques using a statistical and application related approach. This implies a sophisticated measurement technology to gather enough data and improved methods to handle the calibration data and the network training. Anyway, in a laboratory environment only a small number of gases can be blended for sensor calibration. The outlook is, that for more or less complicated applications as indoor air quality monitoring a combination of field tests and laboratory experiments will be the accomplished procedure.

2 SENSORS AND MEASUREMENT UNIT

The sensors used for the examples are classical conductivity sensors for CO, CH_4 and hydrocarbons on the basis of semiconducting metal oxides (taguchi type). At the surface of these metal oxide sensors oxidising or reducing gases react with oxygen at high temperatures (350 - 500°C) and thus change the oxygen concentration. Oxygen serves as an electron acceptor in metal-oxide semiconductors, as result of which the conductivity is changed noticeably under the occurrence of an oxidising or reducing gas. The space charge zones at the grain boundaries deliver the main contribution to this effect. Therefore, it is plausible that surface effects and grain growth are reasons for degradation effects. Figure 1 shows a typical micromachined sensor.

Main detection principle is the (reversible) adsorption of a gas at the sensor's surface, in some cases followed by a chemical reaction. It is evident, that all these sensors follow the thermodynamic rules with temperature and (partial-)pressure as main influence parameters. Normally the detector material should be in thermodynamic equilibrium with the surrounding

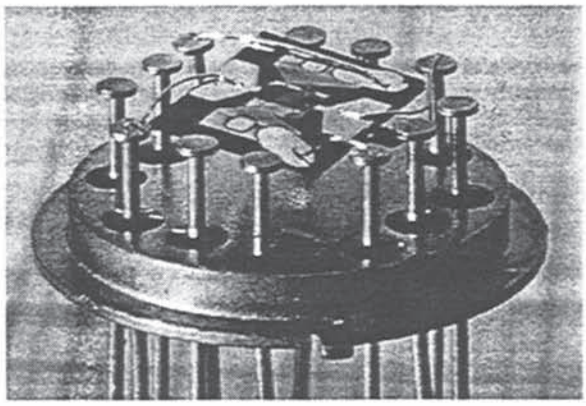

Fig. 1 Micromachined semiconductor gas sensor on a TO-socket

atmosphere. The adsorption energy rules the selectivity of the sensors and under the prerogative of a reversible sensor effect, all of these sensors show an interference to other gases than specified and to humidity. It is clear, that in case of fluctuating conditions a sensor never reaches a thermodynamically stable equilibrium. In the simplest case such conditions will be found in (indoor-, outdoor, etc.) air

The use of sensor arrays and signal evaluation techniques will suppress these imperfections and decrease the sensor's response time.

An important instrument in the development of gas sensor systems and pattern recognition methods is the test and measurement unit itself [5]. Whereas commercial gas sensors are often calibrated with prefabricated gas mixtures, research purposes require a more flexible system. The test system provides independent mixing of two test gases together with a humidification at a high dynamic range. Gas mixing is performed via volumetric method using an array of

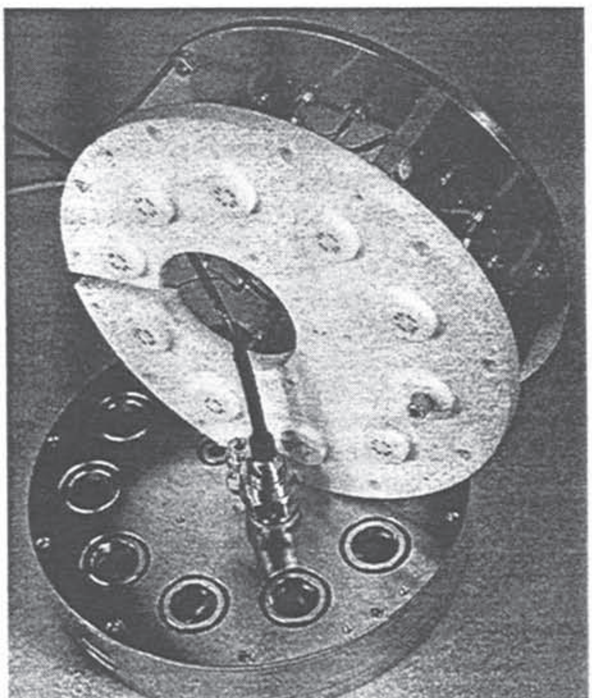

Fig. 2 Measurement chamber for 10 sensors

mass flow controllers. Several test chambers were developed and optimised with regard to a small volume and a precisely defined gas stream. These test chambers simultaneously contain up to ten sensors of different types (semiconductor, dielectric, microbalance, ...) and provide measurements of gas temperature and pressure. The exhaust gases are analysed by a dew point mirror to assure the accuracy of the adjusted gas concentrations.
For the electrical measurement commercial multimeter (Keithley) or A/D PC-Adapter (16 bit, PlugIn) together with some power sources and switching units were used. The sampling time differs among 20 seconds (Multimeter) and 1 second (A/D converter)

3 SIGNAL EVALUATION TECHNIQUES

For the use with gas sensors Artificial Neural Nets (ANN) are tools embedded in a signal processing environment. The main strategy for the processing techniques is indicated in figure 3. An appropriate pre-processing and measurement technology is essential for the success of the ANN calculations.

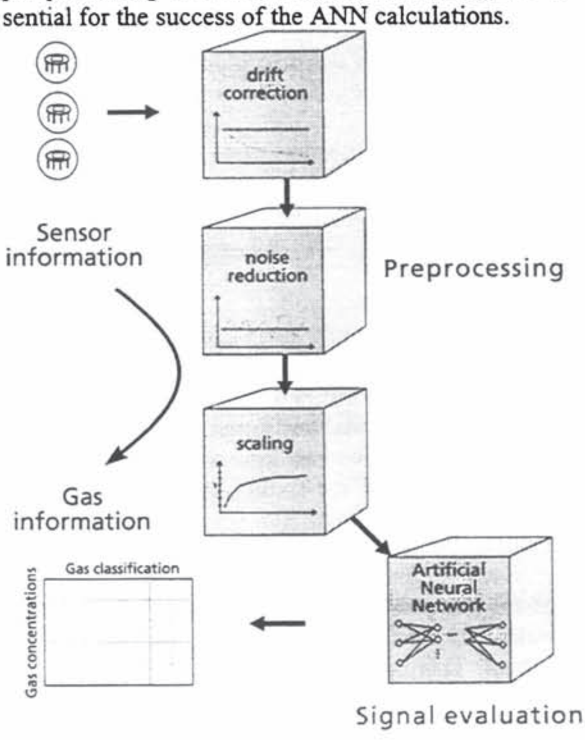

Fig. 3 Signal evaluation strategy

There are two main problems for the pre-processing tools: The rejection of drift effects and the proper scaling of the input. The drift processes are long term alterations in the indicator material, which are connected with diverse internal processes (i.e. grain growth) and external influences (i.e. aggressive gases). In general, the latter processes cannot be foreseen and demand for self-control methods [6].
A promising method is the use of non-stationary phenomena, e.g. the use of the so short time drift after a heating up phase necessary to initialise the semiconductor-sensor. This short time method can be empirically modelled with a double exponential decay function and provides a stable base line for about a week. The scaling is necessary for a numerical correct input of ANN's and implicates a calibration of the sensor with specified gases.
Base line stabilisation and scaling are alike a two point calibration of the sensor, which is necessary for an easy exchange of the sensors. A first survey gave an accuracy of about 10% after exchange of the sensors with the unchanged ANN. The other sets of sensors come from the same series and had a two-point calibration. Currently an industrial standard for such a calibration of gas sensors is missed.
Additionally an averaging of the data with a box car filtering reduces noise and other artefacts coming out of the measurement circuit. A width of three measurements (corresponding to circa one minute measurement time) seems the optimum, compared with the t_{90} time of a semiconductor sensor of about 1-2 minutes. Similar are the results for higher data acquisition rates, if the time dependence of the signal should not be smeared for time resolving applications. For the first time differentiation a simple algorithm, using only a few data points, was used.
The task of an ANN is twofold, it is possible to classificate and to quantificate the gases (quantification includes a classification). Result of a survey of different ANN architectures including Jordan, Elman and time delay networks gave a preference for classical perceptron networks with a single hidden layer. These networks have also the advantage of a modest numerical expense, which is important for the use of small processor chips. An example of such an ANN is shown in figure 4.

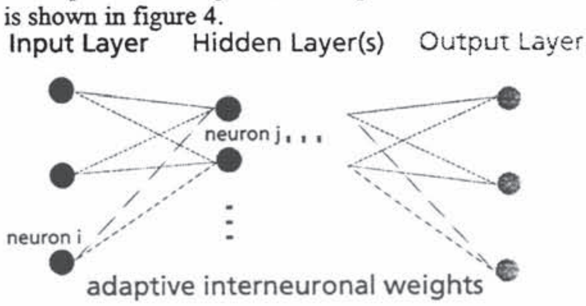

Fig. 4 Perceptron Network

Around the perceptron architecture toolbox of various methods have been developed to solve application problems. One of the first problems is the enormous amount of calibration data, necessary to train the networks. The gathering of calibration points needs a certain long time and the interpolation additional calibration point needs a minimum number of measurements. A satisfying limit of a laboratory calibration run is about one week in maximum. Similar to the statistical experiment planning is an application oriented method: The DTPD method (dynamic test point distribution).
From a combinatorial viewpoint a high density of calibration points should be equally distributed in the n-dimensional input space (concentration of n-gases), which causes an unacceptable long calibration time. The DTPD method proposes a different and application related distribution of calibration points:

- High density near regions of interest (e.g. TLV or LEL).

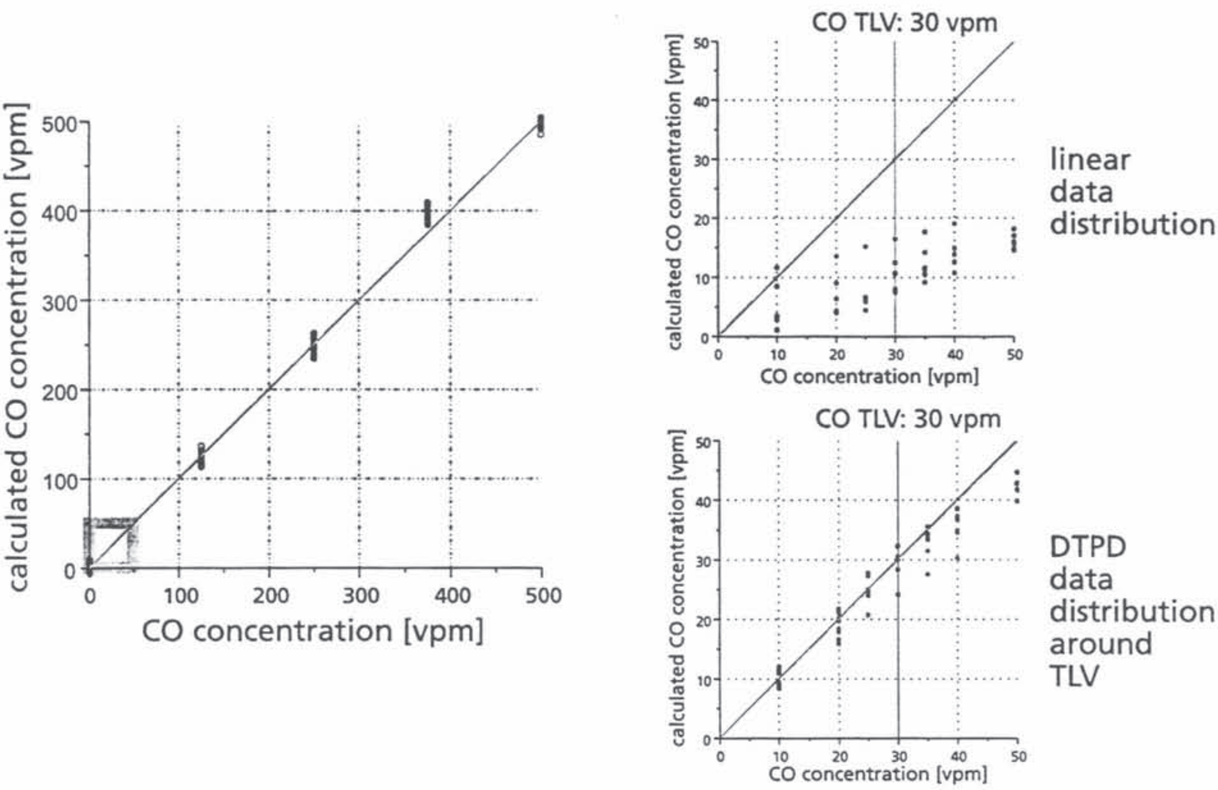

Fig. 5 Quantification of a gas mixture with a DTPD calibrated ANN

• Modest density elsewhere.

Using this method a significant reduction of the calibration time together with a higher accuracy in calculating the gas concentration in the regions of interest can be achieved compared with an equidistant distribution of calibration points[7]. The calibration points are statistically distributed in the calibration space. An example demonstrates the better result of a DTPD trained network to determine the TLV compared with a network calibrated with an equidistant spaced calibration set (figure 5).

The rise time and other time dependent properties of gas sensors are another main task for signal evaluation. To handle these time dependencies, a classification into three main time domains was proposed:

• Rise time of the sensor after a sudden concentration change or another stimulus.

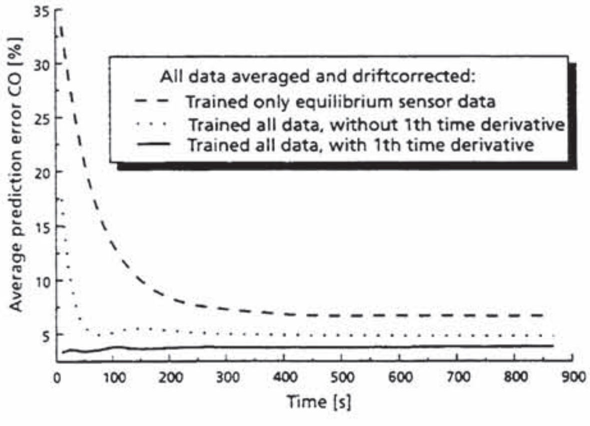

Fig. 6 Result of the ANN rise time reduction technique

• Short time drift after switching on of the sensor (used for base line correction as described before).

• Long time deterioration of the semiconductor material (determine service intervals).

An important improvement is the compensation of sensor's rise time. The sensor's rise time effects can be reduced by measuring the sensor signals with a high data acquisition rate and training ANN's with these signals. Here are some possibilities for a preprocessing of the data. The simplest method is to calculate the first time derivation of each sensor signal and to use it as second input node. Applying this method to a sensor signal, the rise time can be shortened up to 10% of the sensor's original time constant. This means also a significant reduction of the response time of the sensor system itself. Another possibility is the use of all signals (equilibrium and transient) to train the ANN's. Fig. 6 gives an overview about the performance of these methods. Differently trained ANN's (only equilibrium data, all data, all data with additional first time derivative as additional input node for each sensor) showed that the use of transient measurements reduces the prediction error shortly after the stimulus and the overall accuracy [8]. A main result is, that waiting for an equilibrium or an t_{90} time interval to achieve a reliable sensor signal is not necessary. It is interesting, that the use of the first time derivation and/or the use of all transient sensor data improves the quality of the ANN output over all data. It seems, that this effect leads to a general use of transient phenomena for improving the signal processing output.

The use of transient signals gives also the advantage to improve the selectivity of the system itself. A

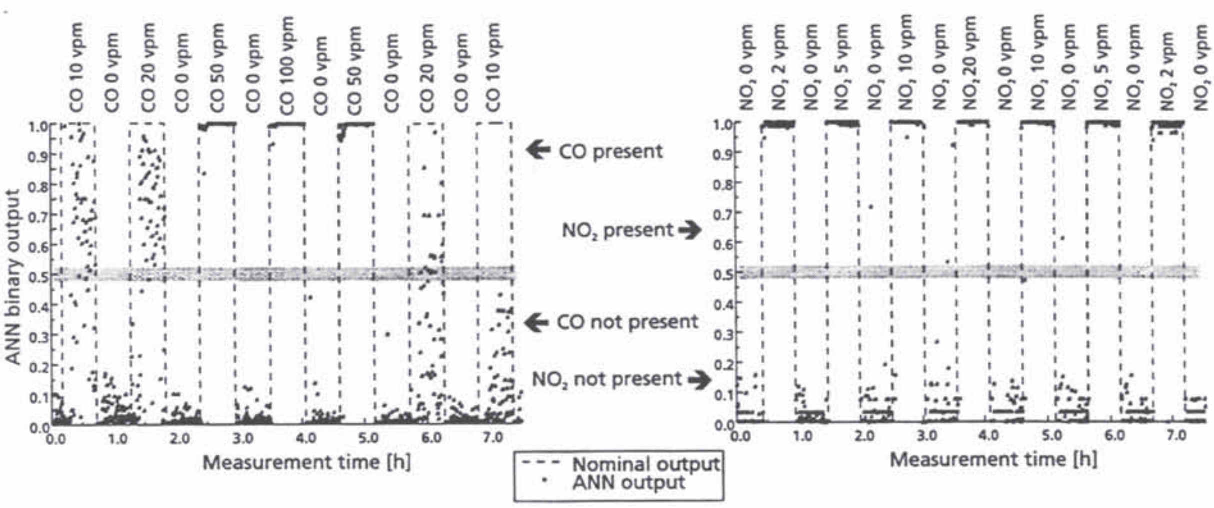

Fig. 7 ANN output of a network for classification of NO_2 - CO Mixtures (left drawing: 20 vpm, NO_2, variing humidity, right drawing. 100 vpm CO, variing humidity

similar technique was used to demonstrate a fast sensor system for the simultaneous recognition of CO and NO_2, i.e. for ventilation applications. The simultaneous detection of these two gases is a problem, because the oxidising NO_2 and the reducing CO result in a near zero signal with semiconductor signals. This system uses two different sensor types, different temperatures and the transient gas concentration for gas recognition [9] (figure 7).

Another approach to classificate different gases in a mixture is the moving window method together with a perceptron network, first suggested from Rebiere et al. [10]. This architecture uses a perceptron architecture together with a time-window for the sensor signals, which corresponds to a time-array of 10 to 500 input nodes for each sensor.. Therefore, a time dependence of the sensor signals will be introduced into the net-

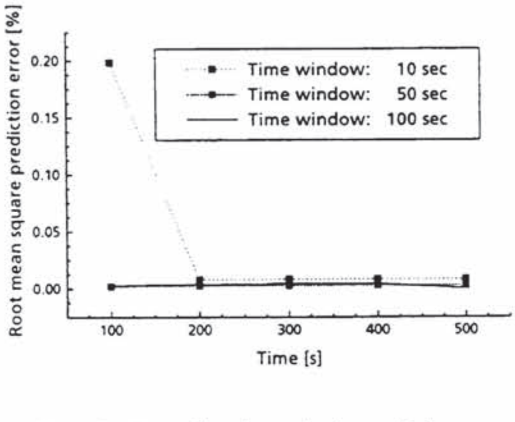

Fig. 8 Classification with a time-window technique

work, but the time dependence will be smoothed due to the special shape of the input. The width of the window varies among 50 and 500 data points corresponding to a sample time among 10 and 100 seconds. A medium window, which is small enough compared with the t_{90} time of the sensors and large enough to achieve an appreciable averaging. This approach is similar to a neural network with an averaging pre-processing step and has advantages for classification of gases. It provides a high quality classification result but a small time resolution (figure 8).

Transient methods are also prerequisite for the use of these sensors in olfactometry. The well Known head-space method is a good tool to discriminate between different odours. An example is the discrimination between different coffee flavours described by Gardner et. al. [11].

A CO_2 sensor demonstrates the extraction of additional information using temperature transient methods to reduce drift effects elsewhere in this booklet [12].

4 CONCLUSION

The use of advanced signal evaluation techniques is necessary for a reliable operation of gas sensors in industrial and home applications. A prerequisite for an effective use of these techniques is the knowledge about transient phenomena and their use for processing algorithms. Some technological and numerically skills were presented in the current paper and form a toolbox for application oriented system development. The signal processing algorithms are compatible to the wide spread μP and μC, for example the well known 8051 family.

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