Measurement of Perceived Odor Intensity Using Gas-Sensor Systems

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SUMMARY

In the present study Multi gas-sensor systems (MGSS) are used to evaluate the odor intensity as it is perceived by humans. These systems measure volatile compounds in a holistic manner and present a signal pattern of the air sample. The model for the determination of the odor intensity consists of two major parts: discrimination into odor classes and subsequent quantification of the intensity. The discrimination is achieved by multivariate statistical methods or neural networks. The correlation to the intensity is done by odor class specific regression methods. The development of the data processing is based on calibration data consisting of simultaneously obtained MGSS responses and assessments of the perceived intensity by a trained human panel using a comparative scale. Different building materials were investigated. The study shows that MGSS have the potential to be used as a measurement device for perceived intensity using a data processing method on basis of an odor classification.

INTRODUCTION

Air quality in the indoor environment impacts the health and the wellbeing of the occupants. Studies showed that bad air quality has also a negative effect on the productivity of office workers [1]. Therefore there is a growing demand for technical devices to measure, maintain and control the indoor air quality. The air quality is determined by the volatile compounds in the air and mainly the provoked odor impression is the cause of discomfort. But so far no technical measurement technique for volatile compounds is able to measure the impact of the substances on the odor. Analytical chemical methods are able to detect the compounds in the air and their concentrations but the transfer to the human perception cannot be done and is still unknown. The concentrations of the interesting compounds are often below the detection thresholds of the measurement devices.

By now, the odor can only be assessed by human panels. Depending on the question formulation different aspects of the odor perception are evaluated, such as the acceptance or intensity of the odor. These methods are time consuming and cost-intensive due to the expenses for the panelists and in addition human panels cannot be used for continuous measurements for monitoring and control.

Since the analytical methods aren’t able to evaluate the perception of odors another approach is to measure gaseous substances in a holistic rather than analytical way. In recent years multi gas-sensor systems (MGSS) have been developed to evaluate mixtures of volatile compounds and odors. The fundamental idea behind these systems is to mimic the human sense of smell. Analogues to the human odor perception the systems evaluate the sample air as a whole. The sensor systems were often called electronic or artificial noses. Though the systems apply the principle of odor perception the performance (sensitivity and ability to recognize and
categorize odors) falls far behind the human sense of smell. The comparison with the human nose raises expectations which these systems cannot fulfill. Nevertheless these systems may be able to measure the odor intensity as it is perceived by a human panel for typical room air odors with adequate accuracy. The strength of MGSS is the recognition of differences in a mixture of gaseous compounds and deviations from a defined composition. The systems respond within seconds to a few minutes to changes in the mixture and can be used for online monitoring. Therefore the main areas of interest are the control and monitoring of product processes and quality control. They are widely used for applications and research in the food and nutrition industry as well as in the perfume and cosmetics industry [2]. In the last years in more and more areas of application the systems gain on interest and are discovered as useful instrument. In the field of indoor environment only few investigations have been done to assess the air quality [3]. The challenge for measuring the indoor air quality is the low concentrations of the volatile compounds and compared to the concentration the high intensity impression they invoke.

In the current study assessments of the perceived intensity of a trained panel were compared with measurements of a MGSS. On basis of these measurements it is tried to build up a model to correlate the measurements to the human perception of odor intensity.

MEASUREMENT APPROACH

Technical measurement devices are inherently not capable to measure the odor. To evaluate the odor intensity with multi gas-sensor systems the measured sensor responses must be correlated to human odor perception. A data processing model has to simulate the perception process in a simplified and abstract manner. In this study the focus is set on the odor intensity, which is a dimension of odor perception which is closely related to concentration and composition of the compounds and hence the measured sensor signals. As experience of odors made during the whole life is a main component of the odor perception and evaluation, a knowledge database consisting on measurements and associated odor assessments of a human panel will be the backbone of the data processing model.

Due to some preliminary measurements it was obvious, that it is very unlikely that one single mathematical algorithm is able to establish a relationship to the perceived intensity. Instead a theoretical data processing model was formulated which consists of two steps: a classification of the odors followed by a quantification using an odor class specific transfer function. The theoretical structure of the two-step data processing is illustrated in figure 1.

![Figure 1. Schematic representation of the data processing model](image)
The crucial part of the model is the knowledge database. It contains measurements of different mixtures and single compounds of emissions found indoors in several varying odor concentrations covering an intensity range. For each measurement a couple of sensor responses and panel assessments data were stored in the database. In the first step the measurements are combined and classified into classes with similar odor and sensor response data. For each determined odor class in a second step a class specific transfer algorithm to quantify the odor intensity is calculated. When measuring an unknown sample with the sensor system, the measurement is allocated to an odor class. The associated transfer algorithm for this odor class is selected and used to calculate the perceived intensity.

**METHODS**

Measurements of emissions from building materials and furnishing were used to construct the database. The objective was to investigate if the data processing model is principally applicable for the estimation of the perceived odor intensity with MGSS. Emissions from building materials and furnishing are main contributors to the indoor air contamination. They were chosen because the emissions can be easily and reliably produced and controlled in a laboratory environment.

Figure 2 shows the experimental setup to measure the odor emissions of building materials. The samples of building materials are placed in CLIMPAQ emission chambers [4]. These chambers were slightly advanced to optimize the air flow pattern and to connect them to an existing air ventilation system.

![Figure 1. Test facility to measure the odor emissions of building materials](image)

Figure 1. Test facility to measure the odor emissions of building materials

Clean air from the supply system flows through the CLIMPAQ and is loaded with the emissions of the building material sample. The sample air can be diluted by adding clean supply air before it is presented at a glass cone for the assessments. The dilution ratios can be adjusted continuously from pure air to 100% sample air from the CLIMPAQ. The tubes were
The perceived intensity was assessed by a trained panel of 8 to 12 subjects. The odor intensity of the sample was ranked in a reference scale made up by acetone samples of 5 different odor intensities. The perceived intensity was assessed in the unit “pi” (perceived intensity) which was introduced by Müller in 2004 [5]. A pi of 0 is defined to an acetone concentration of 20 mg/m³ which corresponds approximately to the odor threshold of acetone. The scale was constructed linear in respect of the concentration. A step of 1 pi is equivalent to a concentration step of 20 mg/m³ of the reference substance acetone.

The assessments of the panel for a measurement series with varying dilution rate, the so called exposure response curves, can be approximated by a logarithmic function which was shown by Böttcher in investigations on the perception of odors [6]. Since the concentrations of the emitted substances of the building materials in the current investigation are not known the concentration dependency can be expressed by the airflow specific area load [7]. Figure 3 shows the dilution characteristics of two different building materials, a carpet and a painted wallpaper. The approximation was done using the mean values of the assessments of the panel members. In the model for data processing the calculated perceived intensities by the dilution characteristic were used as the intensity reference values instead of the assessment means in order to minimize the uncertainties which are inherent within the subjective sensory assessments.

Figure 3. Panel assessments of the perceived intensity of 2 building materials
As a multi gas-sensor system the commercially available system KAMINA from the Forschungszentrum Karlsruhe is used in this study. It operates with 38 tin oxide sensors, which are placed on one single chip. The metal oxide surface is coated with a sensitive layer of SiO$_2$. The different sensitivity and selectivity of the sensor elements are achieved by a gradient of the sensitive layer and a temperature gradient from 250-300°C across the sensor-chip. The transport of the sample air to the sensors is done by a fan in the housing. The sensor sensitivity and selectivity and combination of sensors have a major impact on the performance of the intensity estimation. But it is not part of this study to investigate and optimize the sensor device.

For the measurement of the emissions of building material the KAMINA was placed on top of the glass cone according to location where also the panel assessments took place. The measurements were conducted directly after the assessments of the panel. The duration of the measurement was about 5 minutes until the stationary sensor signals were achieved. The stationary sensor responses further were used for the data processing.

**RESULTS**

For the classification of the measurements of seven building materials statistical multivariate methods can be applied. One method is the principal component analysis (PCA). This method reduces the relevant parameters and maximizes the variance between the measurements. The PCA describes a data transformation where the eigenvectors of the covariance matrix are the new coordinates. The advantage of this transformation is that the main difference of the sensor signals will be presented with a few new coordinates only. The other coordinates can be dropt with little loss of the information on the variance between the different measurements. The transformed results can be shown in a 2 or 3-dimensional diagram, see figure 4a. The diagram shows the result of a principal component analysis with measurements of seven building materials. Three of the materials form independent material groups. The other four materials cannot be separated properly and build a wide spread group. The measurements of the silicon sealant form a chain and don’t show a grouping effect. This is caused by a change in the emissions as the sealant was investigated during the first days after preparation and was still in the process of hardening.

![Figure 4](image.png)

Figure 4. Classification of measurements with a MGSS of seven different building materials using (a) Principal Component Analysis (PCA), and (b) Linear Discriminant Analysis (LDA). The percentage behind the axis title describes the fraction of the components on the total variance.
To improve the classification a linear discriminant analysis (LDA) was used. This method uses classifiers which were assigned to the measurement samples by the experimenter to build the discriminant functions. The discriminant functions are optimized to maximize the separation between the groups and to minimize the within group variance during a learning process. Figure 4b shows the results of the LDA. The four material classes which were inseparable with PCA are still near together but at least the silicon sealant and the floor adhesive build separate clusters.

The third classification approach was done using a self organizing map (SOM). SOM is a special type of neural networks which was developed by Kohonen [8]. As the PCA the SOM is an unsupervised method which uses only the sensor response data to classify the data. For each sample the SOM determines one single “wining neuron”, which fits best to the input data. During the learning phase the network weights of the winning neuron and the near by neurons were adjusted towards an optimized result. The Matlab neural network toolbox was used and a map of 7x9 neurons was used to classify the building materials, see figure 5. Each symbol characterizes a neuron. In the illustration the neurons are displayed equally distributed. The shading demonstrates the distance of the neurons (dark: near, white: far). With the selected SOM except the floor adhesive the building materials can be separated into groups. Some materials show some higher within group differences as can be seen for the acrylic sealant 1. Here the measurements are distributed on several neurons of light shading (bigger distances between neurons). The acrylic sealant 2, however, is spread over several neurons but these are located closer to each other.

A separation of the measurements of different building materials into classes seems to be possible, but some of the materials can not be separated perfectly. More sophisticated classification methods and an enhanced and modified sensor system with higher sensitivities might solve this problem. The classification was done in respect of building materials, which
means every material builds its own class. That might not be the best classification approach since this can lead to many different classes. Finding different classification criteria could optimize the separation of classes.

The second step of the data processing model is to find a correlation to the odor intensity. The data for a specific class is used to find a transformation algorithm to estimate the perceived intensity. For the correlation a principal component regression (PCR) was applied. A PCR is a combination of a principal component analysis and a multiple linear regression. The PCA reduces the dimension of data set and maximizes the variance for the first components. Since the later components contain only noise signals only the first three components were used for the multiple linear regression. The following diagram shows the deviation from the measured intensities from the assessments of the panel for all of the seven investigated materials, figure 6. It is assumed that an odor classification method is used which properly separates each material in its own class and the regression was done using measurements for one single material.

![Figure 6. Comparison of the measured intensities (calculated by PCR for each material separately using the “leave-one-out” method) with the intensities assessed by the human panel.](image)

The shown values were calculated with the “leave-one-out” method. In this method all except one (the tested) sample were used to estimate the regression parameters. The regression algorithm was then used to calculate the intensity for the left out sample. This is done n-times for all n samples of the odor class.

The diagram shows two ranges with 2 pi and 4 pi deviation from the ideal estimation. It should be mentioned here, that the reference value of the assessed perceived intensity is not an exact value itself and has also some uncertainties. Most of the estimations of the perceived intensity using the MGSS lie within the 2 pi range. Some calculated intensities for the acrylic sealant 1 and the floor adhesive are totally different from the assessed values. At a closer look it can be seen, that these values mark the edges of the range of intensities of this odor class. Near the edges of the intensity range the regression function is inaccurate.
DISCUSSION

MGSS have the potential to estimate the perceived odor intensity of building materials. It depends strongly from the sensitivity of the sensors and on the data processing model. A two-step-method for data processing is appropriate since a direct calculation method for a determination of the intensity cannot be found. A crucial point in the model is still the development of an odor space for the odor classification. It won’t be practical to have for each building material a different odor class with corresponding transfer algorithm. It is the aim to find a few primary classes which cover the relevant odors which occur in indoor environment.

In this study basic algorithms for classification and regression were used. More sophisticated methods may improve the results. An improvement of the sensors itself in optimizing the sensor combination and in increasing the sensitivity of the sensor elements would be a further step towards a measurement system for the intensity of the odor in the indoor environment - towards systems, that can be used for measuring, monitoring and controlling the indoor air quality. To reach this aim, the European project SysPAQ (Innovative Sensor System for Measuring Perceived Air Quality and Brand Specific Odors) has been started to develop an innovative system to measure the indoor air quality as it is perceived by humans.

The first investigations were done in a laboratory environment using single materials only. In real indoor environment the emissions of several materials were present at the same time. The additive behavior of the odorants must be investigated in further research work to transfer the laboratory results to real indoor environment.

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