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Gas sensing evaluation for the quantification of natural oil diffusion

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Recent clinical studies show the beneficial effects due to the inhalation of appropriate concentrations of certain natural oils on mental diseases like phobia, stress or Alzheimer. To demonstrate these effects, medical staff needs a system which permits an automatic control of the essential oil diffusion in a closed chamber. For this purpose, our work demonstrates the ability of chosen chemical gas sensors to identify the concentration of an essential oil evaporated in a neutral atmosphere. Sensor responses are studied using a selection of parameters which are tested for their performance to detect the oil concentrations and minimizing the drift effect of the sensors. Our system can detect various quantity of evaporated oil (pin and lavender) in the range of pleasant concentrations for humans.

1. Introduction

Inhalation of essential oils (EO) can be used in aromatherapy due to their activating and relaxing effects, and considerable investigations have already been carried out to evaluate the sedative properties of the odorous stimuli. These studies are based on neurophysiological as well as behavioral measures in both animal and human subjects [Lehrner et al., 2000; Heuberger et al., 2004; Gartner-Schmidt et al., 2006; Knasko, 1992] after the inhalation of a variety of essential oils and odorant sources. For example, successful experiments were carried out with oils of citrus fruits on patients affected with hysteria or depression [Komoro et al., 1995]. However, the scientific proof of such applications requires to realize behavioral measurements by varying not only the nature but also the quantity of the volatile substances inhaled by the patient. In our knowledge, there are no such quantitative studies reported in the literature. The main difficulty in this study is due to the impossibility to measure the inhaled quantity. To pass around this problem, it is necessary to carry out the behavioral experimentations in a chamber where the physical and chemical parameters (natural oil concentration, temperature, humidity,…) of the ambient atmosphere are closely controlled. So, we propose the conception of a system which creates a chosen atmosphere with a constant concentration of selected natural oil. This automatic diffusion/detection experimental set-up can be used by biologists to identify quantitatively the therapy effects of variety natural oils.

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The present paper describes a preliminary study of a diffusion/detection system designed to control the odor intensity. Two essential oils (pin and lavender) at several concentrations are studied and the performance of commercial gas sensors is tested to identify accurately low concentrations of evaporated oil components.

2. Method and Materials

The studied equipment is mainly composed of two units: an electronic nose (Strobel et al., 2004) for the concentration detection of the evaporated essential oil and an oil diffuser unit. For the detection, eight metal oxide gas sensors (SP-AQ1, SP-MW0 from FIS and TGS 882, 2600, 2602, 800, from Figaro) have been tested taking into account their sensitivities to solvent vapours, odorous gases or VOCs. The oil diffusion unit is based on a constant inflow of synthetic air bubbling into a bottle containing liquid oil. In this work, the outlet flow (containing evaporated EO substances) is combined with a flow of synthetic air to generate different oil concentrations at a constant flow rate (100ml/min). This created atmosphere is directly introduced into the sensor cell of the electronic nose to evaluate the sensor's performances in the detection of low oil concentration variations. So, the oil concentrations are reported as the percentage of the air flow rate coming from the oil bottle over the total flow rate (Fig.1). By varying this inflow rate different concentrations of evaporated EO are created.

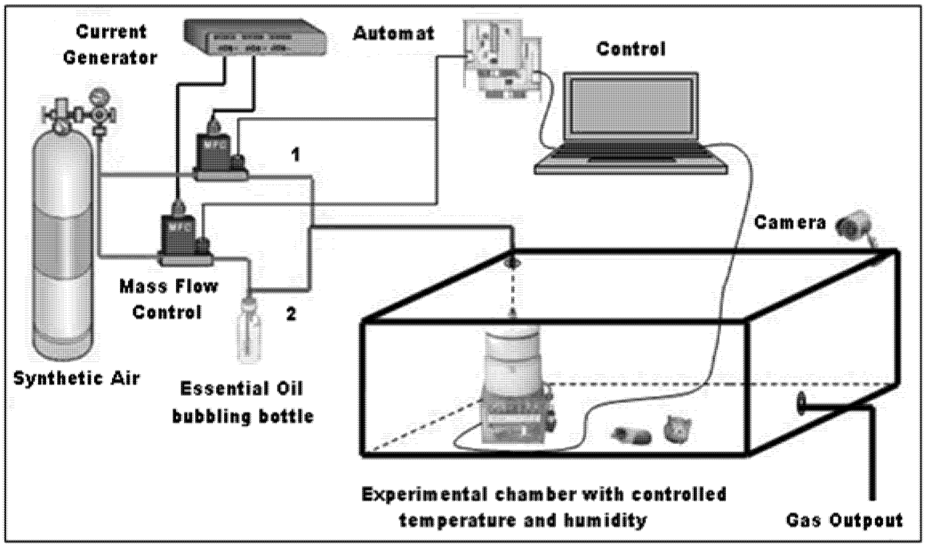


Figure 1: Schematic diagram of the experiment set-up with the electronic nose inside of a closed chamber

2.1 Measurement procedure

Measurements were performed under atmospheres composed of a selected essential oil (pin or lavender) at low concentrations in synthetic air. The concentration range of each studied EO was defined by a human olfaction panel.

Table 1- Pleasant smelling appreciation for different concentrations of pin oil given by a jury of 4 persons

	1%	2%	3%	4%	5%	6%	7%
Person1	yes	yes	yes	no	no	no	no
Person2	yes	yes	yes	yes	yes	yes	yes
Person3	yes	yes	yes	yes	yes	yes	yes
Person4	yes	yes	yes	yes	yes	no	no

These ranges (Tab. 1) are 1% - 7% (step 1%) for pin oil and 5% - 15% (step 2 or 3%) for lavender oil. Conductance variations of the sensor are digitalized and recorded in terms of sensor's voltage (Volts).

Our first approach was to overcome the sensor drift and low response-time which constitute a limitation of their utilization in the gas detection system. In this idea, we have tested several measurement protocols [Sambemana et al., 2009] and examined the sensor's responses to minimize the drift magnitude after each gas exposure. Regarding the lowest and the highest concentrations, and the drift minimizing, the best cycle is composed of 10 minutes of gas exposure followed by a recovery time of 20 minutes (Fig. 2).The interest of this exposure time is to allow us to reach the dynamic response as well as the permanent responses of the sensors. Then our objective was to select and to compare several characteristic features to obtain the best accurate quantification.

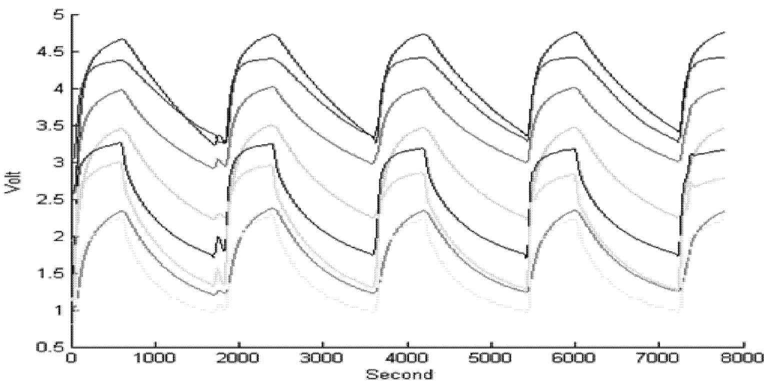
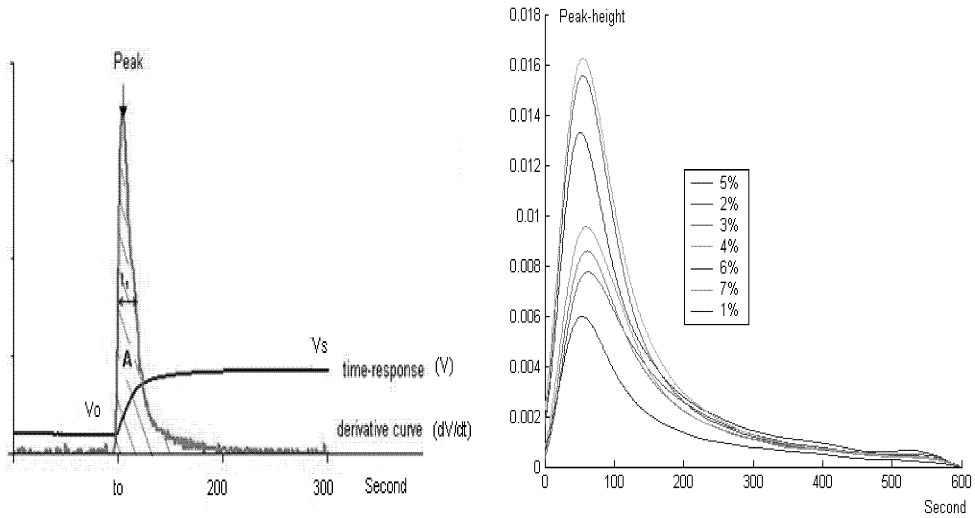


Figure 2: Gas sensor responses obtained by repeating gas exposure (5% pin oil) and regeneration phases. Good recovery is observed for the eight sensors

2.2 Feature selection

The analysis of the sensor response and the selection of the features constitute an essential part of such developments. Plotting sensor responses over time, dynamic and quantitative differences are observed along with the EO concentrations. So, the transient phase of the sensor responses has been studied in terms of their time derivative curve. To obtain accurate features on the derivative curves, we first applied digital filters on the sensor responses. Chebyshev filters were used and filter coefficients were different for each sensor type taking into account their response-time. To characterize the permanent response we have chosen the initial V_0 and the final Vs response values of the eight sensors (Fig. 3-a).



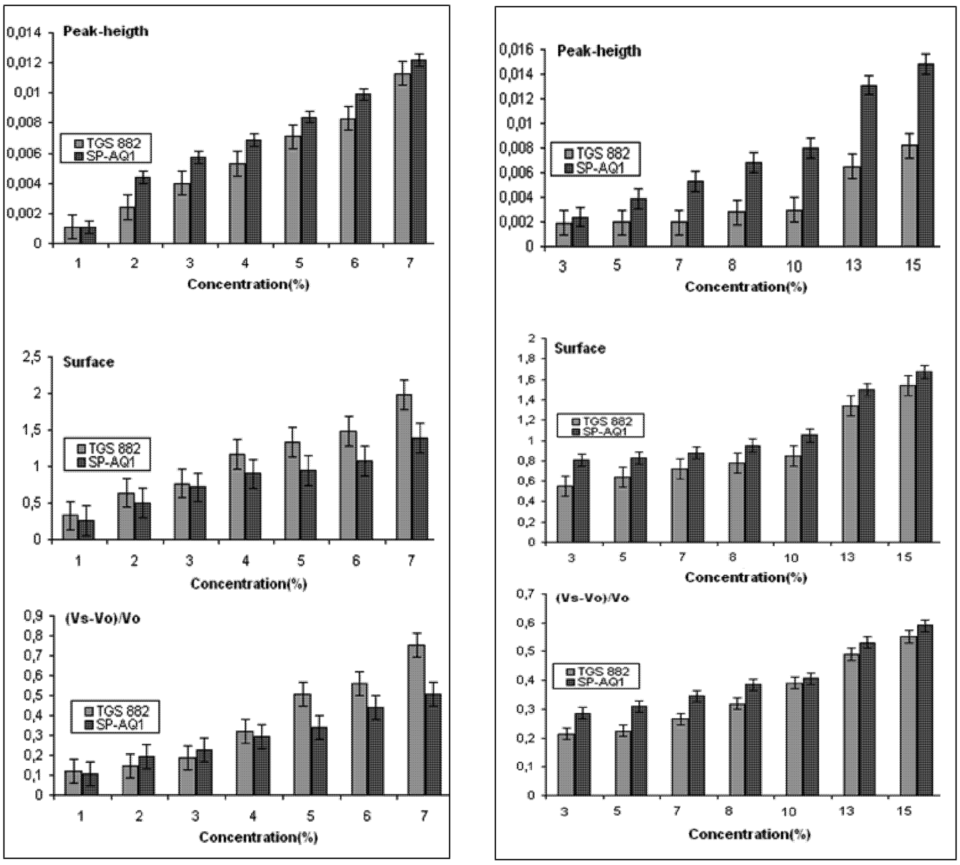
(a) *(b)*

Figure 3: Schematic representation of selected features on the derivative and the time-response curves (a); Derivative curves of TGS-882 gas sensor at different concentrations (b)

All the derivative curves present a characteristic peak (Fig. 3b). So, we have selected the peak height value, the half-height peak width, curve surface under the peak, and the peak occurrence time. These parameters were tested for their capability to differentiate the oil concentrations. The more accurate derivative features have revealed to be the peak height and the surface values which are presented in the following section. For the permanent phase, the initial and the final values have often been used in literature almost in different forms of combinations (Delpha et al., 2004; Nicolas, 2000). We utilize them in this work to compare their concentration discrimination power with the new proposed features (named derivative features).

3. Results

Some conclusions can be made about the gas sensors. We note fast and stable response of the SP-AW0 sensor (FIS). Among the Figaro sensors, the 2602 presents irreversible important drift during the experimentation. Other Figaro sensors (with a preference for the 8xx series) and the FIS SP-AQ1 have more or less the same behavior.
Each studied atmosphere is repeated more than 10 times. Features are calculated and the mean values as well as the standard deviation are studied. In figure 4 we have reported the variations of three representative parameters along with the concentration of pin and lavender oil, for two gas sensors (SP-AQ1 and TGS-882). Considering these parameters over the EO concentration, significant and uniform changes (with acceptable errors) were observed for the two derivative features (peak-height and surface) as well as the well known $(Vs-V_0)/V_0$ coefficient corresponding to the permanent parameter. We can also note that generally gas sensors are more sensitive to pin than to lavender.



a) pin oil *b) lavender oil*

Figure 4: Averaging replicates of the 3 selected features for two gas sensors (TGS-882 and SP-AQ1)

These parameters are used in classification techniques for the concentration identification. The linear Discriminant Factorial Analysis (DFA from SPSS software version 11.0) was applied on data grouping features of all the sensors and all the measurements. Figure 5 shows the DFA classification diagram obtained for pin and lavender oils when using only the two derivative features (peak-height and surface). We note a good differentiation of the concentrations in the two cases of EO. The success rates given by cross validation technique was 100% for pin oil and 86.2% for lavender oil. But, when using these two derivative parameters combined with the $(Vs-V_0)/V_0$ coefficients, the success rates fall to 98.8% (pin) and 79.3% (lavender).

That shows the interest of the two derivative features for the concentration evaluation. In this way, it is not necessary to wait for the response stabilization. This result offers advantageous consequences: a) the possibility to develop rapid detection system (stabilization is not necessary); b) minor drift of the gas sensors after exposure.

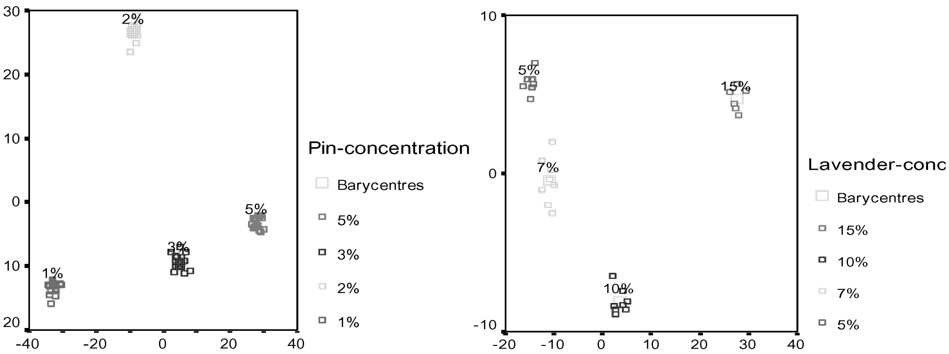


Figure 5: DFA diagram for pin and lavender concentration discrimination

Conclusion

Metal oxide gas sensors were tested to identify essential oil concentration diffused in neutral air. Our work was more devoted to study their dynamic response, in terms of the derivative curve. So, two new "derivative features" revealed to have a good discrimination power for a low range of EO concentrations, tolerable by a human subject, compared to other parameters often cited in the literature.

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