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An active, inverse temperature modulation strategy for single sensor odorant classification

Fernando Herrero-Carrón[a], David J. Yáñez[b], Francisco de Borja Rodríguez[a], Pablo Varona[a,*]

[a] Grupo de Neurocomputación Biológica (GNB), Dpto. de Ingeniería Informática, Escuela Politécnica Superior, Universidad Autónoma de Madrid, Calle Francisco Tomás y Valiente, 11, 28049 Madrid, Spain
[b] Deutecno N&S S.L., C/Pont de Molins 21, 30D, 28038 Madrid, Spain

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ABSTRACT

Metal oxide semiconductors are used as gas sensors and detectors. To improve their odorant discrimination capabilities their temperature can be modulated, exploring different working regimes to which gases will react differently. In this paper we present a temperature modulation algorithm that we call active and inverse. It is active because modulation depends on the online response of the sensor, and inverse because, in contrast to previous work, we first set a target value and then calculate the necessary modulation to drive the sensor to that value. Results show that this algorithm is robust and produces reliable data for odorant classification. Moreover, we successfully classify odorants in a sequence irrespective of the preceding odorant and without any clean-up procedure between them.

1. Introduction

Metal oxide semiconductors are used as gas sensors and detectors. When energized, semiconductor electrons jump to the conduction band and allow electric currents to flow through. Some gases cause a redox reaction on the surface of the sensor, changing the density of free electrons in the semiconductor [1], and therefore causing a change in its conductivity that can be measured. In fact, a naive approach to chemical sensing would be to simply take measurements from the sensor conductivity in the presence of different odorants.[1]

Several studies have acknowledged the fact that semiconductor sensors are not time-invariant (e.g. see [2]): they exhibit hysteresis and aging effects, which means that conductivity values depend not only on present conditions, but also on their past activity. That is, a given odorant induces different conductivities depending on previous odorants and previous conditions of the sensor. Classification with a naive technique is therefore not straightforward.

Different procedures have been developed to overcome this problem. Some researchers include a clean-up phase in their protocols prior to odorant exposure [3]. They try to reset the effects of past history by cleaning the sensor with some inert gas like clean air or argon for a fixed period of time, and thereby restore the sensor to a hopefully known state.

In their commercial form, these sensors have a heating resistor to control the temperature of the sensing surface. Both the energy level of the semiconductor electrons and the reactions that take place there are affected by changes in temperature (see [4] for an extensive review of the chemical processes).

A second procedure includes the modulation of the temperature of the sensor through the heating resistor [3,5]. Researchers have developed different temperature modulation profiles (e.g. see [6–12]). In these approaches, an odorant is not characterized by a single conductivity value but by many, each of them at different heating temperatures. Besides, those profiles are designed to change the internal state of the sensor by repeated heating and cooling, overcoming some of the hysteresis effects.

One further problem is that sensor properties are affected by climatic conditions and that they degrade over time because of accumulation of dirt, chemical aggression, etc. Therefore, directly using sensor measurements to characterize odorants will surely

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* Corresponding author. Tel.: +34 91 497 2263; fax: +34 91 497 2235.
E-mail addresses: fernando.herrero@uam.es (F. Herrero-Carrón), david@deutecno.com (D.J. Yáñez), f.rodriguez@uam.es (F.d.B. Rodríguez), pablo.varona@uam.es (P. Varona).

[1] For the sake of readability, we may use the terms “gas” and “odorant” interchangeably in this paper.

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prove little robust to time. Modulating the heating temperature is a means to improve the discrimination ability of these sensors by exploiting different physicochemical properties at different temperatures. Taking measurements of sensor conductivity at different prefixed temperatures and fixed intervals is a common strategy that yields a many-dimensional representation of odorants using a single sensor.

Osuna and Hierlemann [13] make an extensive review of different modulation methods. The most common strategy is to design a fixed temperature profile to control the sensor heating. Machine learning and artificial intelligence algorithms help then to compensate possible drifts in sensor behavior (for a review and recent approaches see [14–17]). In our opinion these strategies are not adaptive in the sense that temperature profiles remain fixed independent of the actual odorant that the sensor is exposed to.

So called *active sensing* is an approach whereby the conditions of the sensing operation are modulated using online information about the olfactory process itself [18]. In principle, different temperature profiles could then be calculated depending on data provided by the sensor, each of which would be tailored to a specific odorant and/or concentration. This way, the process of modulation provides information in addition to pure sensor data that can be used in solving classification or regression problems.

In this paper we present a modulation technique that contributes to discriminate odorants using a single sensor in uncontrolled and unexpected conditions. Our goal is to go beyond the common method of applying fixed temperature profiles and develop a temperature modulating strategy that adapts to the online activity of the sensor. On one hand, our strategy will explore relationships among values of the sensor, like minimum/maximum conductivity when exposed to a given odorant, rather than relying on absolute sensor measurements, which are ambiguous and unstable with respect to time. On the other hand, we expect that the active temperature modulation process will itself provide us with additional relevant data about each odorant to be classified.

2. Materials and methods

We present a new active sensing algorithm for a single sensor that yields data that are highly separable for single odorant classification problems across a variety of conditions.

2.1. Inverse temperature modulation

The usual modulation scheme aims to explore how the sensor behaves for different values of the modulation parameter, in this case heating temperature. In most cases a fixed temperature profile is followed that drives the heating up and down to different operating regimes (see [3], for instance), and sensor conductivity is recorded at each modulation step. This is made in the hope that the same sensor values will be obtained in future experiments for the same temperature values.

Recently Martinelli et al. [19] have proposed a self-adapted temperature modulation method based on the fact that the gas sensitivity of the sensor resistance depends on the operating temperature, and, conversely, the sensitivity to the temperature depends on the gas. In this method a closed-loop is built by connecting the sensitive terminals to a circuit interface, and by using the circuit output as the input signal of the sensor heater. Thus, the resulting temperature frequency modulation depends on the resistance of the sensor changing according to the interaction with the gas, which can be used for gas identification.

Similarly, our goal is to explore different dynamical operating regimes by adjusting the temperature profile both to the odorant being sensed and to the sensor's response. In this approach, the process of modulation of the sensor itself yields additional information about the odorant. The proposed modulation process discovers the minimum and maximum conductivity values of the sensor under the presence of a given odorant. These two values are highly reproducible and characteristic of each individual odorant.

Table 1
PID controller constant values.

Constant	Value
K_p	0.6·0.3 = 0.18
K_d	50/8 = 6.25
K_i	50/2 = 25

While traditional modulation techniques first set a fixed heating voltage or temperature and then read sensor conductance, our method sets a target sensor value and calculates the temperature needed to drive the sensor to that value. That is why we call our approach the *inverse* modulation strategy. The key point is that there is a process that continuously updates the target or reference sensor value depending on the recent history of the sensor. In the following sections we will describe the modulation procedure. See Fig. 1a for a conceptual diagram of the algorithm explaining both how the temperature is modulated and how the reference point is updated.

2.1.1. Oscillatory exploration

In order to explore how the sensor behaves at different operating regimes, we want to drive it in an oscillatory manner. Unlike previous work like [2], in which temperature is directly modulated with a sinusoidal, we set instead a sinusoidal target value and then calculate the necessary temperature profile for the sensor to follow it.

Considering real sensor response dynamics we decided to set the period of the reference sine wave to 40 s. If the frequency of the wave were too low, it would take too long to obtain the desired measurements. If it were too high, the sensor may not be able to respond fast enough and we might end up losing valuable information. This is a heuristic approach rather than an optimum, but we have achieved positive results, so it remains for a future work to explore the optimum frequency of the reference wave (see [8] for a study of optimum modulation frequencies in direct, passive modulation).

The top panel in Fig. 1b shows the reference sinusoidal signal, the online calculated temperature profile and the actual sensor values read when that temperature profile is applied to the sensor heater. The temperature profile is calculated by a PID controller whose input is the error between the target and the actual sensor values. It has been hand-tuned following the widely known Ziegler-Nichols heuristic rule. Its parameters remain fixed during and across experiments. Eqs. (1)–(4) show the implementation of our PID controller, and Table 1 shows the values of the constants used.

$$e_p = \text{reference\_value} - \text{sensor\_value} \tag{1}$$

$$e_d = \Delta e_p \tag{2}$$

$$\Delta e_i = e_p \tag{3}$$

$$\Delta u = K_p \left(e_p + K_d \cdot e_d + \frac{1}{K_i} \cdot e_i \right) \tag{4}$$

where e_p is the proportional error, e_d is the derivative of the error, e_i is the integral of the error, K_p, K_d and K_i are the PID controller proportional, derivative and integrative constants respectively and Δu is the update of the control parameter, or sensor heating in our case.