



Signal model of electronic noses with metal oxide semiconductor



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ABSTRACT

Electronic noses have found wide applications as a promising tool in many fields. However, a model for their signals has not been clearly elucidated thus far. Here, we have developed a signal model for electronic noses based on the relationship between the signal intensity and the amount of odorant molecules absorbed onto the surface of a sensor. We applied an alternative least square algorithm to solve the model. We successfully applied this model to the analysis of benzene and six perfumes using data from a commercial system.

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1. Introduction

Electronic noses [1,2] mimic the mammalian olfactory system, and they are usually composed of two important components: the chemical-sensing system and the pattern-recognition system. However, the discrimination ability of man-made electronic noses is presently highly limited compared with that of mammalian noses [3,4]. Nevertheless, because electronic noses are sensitive, fast and easy to operate, researchers have attempted to apply them to many fields, such as disease diagnosis [5–7], the detection of explosives [8], and food safety control [9,10]. Electronic noses are expected to be a widely used tool in an increasing number of fields in the near future because their sensing system is essentially based on sensor array technologies, which have been widely studied in recent years [11–13]. Contrary to the substantial interest in developing various sensors, considerably less attention has been focused on a signal model for electronic noses. In the published literature, the signals generated from electronic noses are naturally arranged as two-dimensional data arrays, and pattern-recognition methods based on principal component analysis are commonly applied to the data arrays [14]. The present situation is very similar to that described by Brereton [15] that users prefer commercial package to understanding the details. Fortunately, most of the applications seem promising because they focus on the descriptive analysis of a system [16]. However, identification of “true underlying” influences on a system [16] requires the development of a real signal

model for electronic noses. Otherwise, improper signal models will result in important information being missed or will provide a suboptimal final interpretation of a system [17].

In this work, we provide a new signal model for electronic noses made from metal oxide semiconductors (MOS). It must note that the MOS is a widely used as sensor in commercial instruments of electronic noses. More than one thousand research papers based on commercial instruments have been published in the last decade. Unlike previous models based on gaseous odorant concentration, our model was established from the amount of odorant absorbed onto sensors. We show that the signals are essentially related to the amount of odorant absorbed onto the surface of the sensors rather than to the gaseous odorant concentration [18]. Notably, we will not provide experimental proof of the validity of our model because the direct measurement of the amount of odorant absorbed onto the sensor surfaces is beyond the scope of this work. Instead, we develop this model from the theoretical results of Yamazoe et al. [18] The model was applied to real odor samples, and interesting results were obtained.

2. Signal model

Yamazoe et al. [18] noted that the signal intensity and the absorbed concentration at a given depth from the top surface of a porous sensing layer of a sensor exhibit a linear relationship. As the total absorbed amount is an integration of the concentration in the porous sensing layer, the total signal intensity is still linearly related to the total amount of odorant absorbed. Therefore, a linear equation for signal intensity is as follows:

$$r^{(A)} = \gamma^{(A)} m^{(A)} \quad (1)$$

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where superscript A represents odorant molecule A, r is the total signal intensity, m is the total absorbed amount, and γ is the response of unit amount of odorant molecule absorbed on the sensor. Parameter γ can be interpreted as an odorant constant for odorant molecule A. When Eq. (1) is applied to a sensor array that includes k different sensors, we obtain the following equation:

$$r_i^{(A)} = \gamma_i^{(A)} m_i^{(A)}, \quad i = 1, 2, \dots, k \quad (2)$$

where r_i is the response of the i th sensor, γ_i is the response of unit amount of odorant molecule absorbed on the i th sensor, and m_i is the total amount of molecule A absorbed onto the i th sensor. If t measurements are made using the sensor array, we get a response matrix $\mathbf{R}_{t \times k}$ as follows:

$$\mathbf{R}_{t \times k} = \begin{bmatrix} r_{11}^{(A)} & r_{12}^{(A)} & \dots & r_{1k}^{(A)} \\ r_{21}^{(A)} & r_{22}^{(A)} & \dots & r_{2k}^{(A)} \\ \vdots & \vdots & \ddots & \vdots \\ r_{t1}^{(A)} & r_{t2}^{(A)} & \dots & r_{tk}^{(A)} \end{bmatrix}_{t \times k} = \begin{bmatrix} m_{11}^{(A)} & m_{12}^{(A)} & \dots & m_{1k}^{(A)} \\ m_{21}^{(A)} & m_{22}^{(A)} & \dots & m_{2k}^{(A)} \\ \vdots & \vdots & \ddots & \vdots \\ m_{t1}^{(A)} & m_{t2}^{(A)} & \dots & m_{tk}^{(A)} \end{bmatrix}_{t \times k} \begin{bmatrix} \gamma_1^{(A)} & 0 & \dots & 0 \\ 0 & \gamma_2^{(A)} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \gamma_k^{(A)} \end{bmatrix}_{k \times k} \quad (3)$$

In Eq. (3), the diagonal elements of γ_i construct a response vector of unit amount of odorant molecule absorbed on the sensor array. It can be viewed as the odorant spectrum of molecule A on the sensor array, which is similar to the UV–Vis spectrum. In Eq. (3), the present form of the absorbed quantity matrix $\mathbf{M}_{t \times k}$ (the left matrix on the right side of the equation) does not properly represent the physical–chemical reality in the system and further factor analysis is required to find the true underlying factors. As a general factorization strategy for a system containing only one molecule A, matrix $\mathbf{M}_{t \times k}$ can be factorized as the outer product of an absorbed amount profile vector c (unit length) and an absorbed amount ratio vector n . Thus, Eq. (3) is changed to

$$\mathbf{R}_{t \times k} = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_t \end{bmatrix}_{t \times 1} [n_1 \quad n_2 \quad \dots \quad n_k]_{1 \times k} \begin{bmatrix} \gamma_1^{(A)} & 0 & \dots & 0 \\ 0 & \gamma_2^{(A)} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \gamma_k^{(A)} \end{bmatrix}_{k \times k} \quad (4)$$

In Eq. (4), the elements of vector n are the scaling factors of vector c on the sensors. From a purely mathematical point of view, vector n and the Gamma matrix (right-hand matrix in Eq. (4)) can be combined into a row vector and Eq. (4) can be transformed into a conventional bilinear model. However, the combination will completely destroy the inner specialty of the Gamma matrix and the profile of the diagonal vector. So, it is reasonable to keep the original form of the Gamma matrix shown in Eq. (4). The more interesting thing is that we found that matrix $\mathbf{M}_{t \times k}$ cannot be described by one factor even if there is only one odorant molecule A when we checked the responses of benzene (Fig. 1A). Thus, matrix $\mathbf{M}_{t \times k}$ should be factorized into two matrices $\mathbf{C}_{t \times p}$ and $\mathbf{N}_{p \times k}$. Therefore, Eq. (4) has the form

$$\mathbf{R}_{t \times k} = \mathbf{M}_{t \times k} \Gamma_{k \times k} = \mathbf{C}_{t \times p} \mathbf{N}_{p \times k} \Gamma_{k \times k} \quad (5)$$

where p is the factor number, $\mathbf{C}_{t \times p}$ is a matrix of absorbed amount profiles whose each column is unit length, $\mathbf{N}_{p \times k}$ is a scaling matrix of absorbed amount ratios, and $\Gamma_{k \times k}$ is a matrix of odorant profiles. Eq. (5) shows that the signal model for a single molecule needs more than one factor to describe.

Eq. (5) can be extended to describe a system that contains more than one odorant molecule. Before we make that extension, we assume that the total response of a sensor is the summation of the responses from c absorbed odorant molecules. Our experience with chemistry also tells

us that adjusting the experimental conditions can support the linear summation. For the conciseness, we provide a model extension example of two odorant molecules. We assume that there are two odorants A and B in a system. The response of a sensor is the linear addition of responses from the two odorants on the sensor. So, we have responses of a sample on the k sensors as follows

$$\begin{aligned} r_1 &= \gamma_1^{(A)} m_1^{(A)} + \gamma_1^{(B)} m_1^{(B)} \\ r_2 &= \gamma_2^{(A)} m_2^{(A)} + \gamma_2^{(B)} m_2^{(B)} \\ &\dots \\ r_k &= \gamma_k^{(A)} m_k^{(A)} + \gamma_k^{(B)} m_k^{(B)}. \end{aligned}$$

The response vector \mathbf{r} of the sample can be expressed as follows:

$$\mathbf{r} = [r_1 \quad r_2 \quad \dots \quad r_k] = \left[\left(\gamma_1^{(A)} m_1^{(A)} + \gamma_1^{(B)} m_1^{(B)} \right) \dots \left(\gamma_k^{(A)} m_k^{(A)} + \gamma_k^{(B)} m_k^{(B)} \right) \right].$$

Above equation can be rearranged as follows:

$$\mathbf{r} = \left[\begin{matrix} (m_1^{(A)} & m_1^{(B)}) & \dots & (m_k^{(A)} & m_k^{(B)}) \end{matrix} \right] \begin{bmatrix} \gamma_1^{(A)} & 0 & \dots & 0 \\ \gamma_1^{(B)} & \dots & \dots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \dots & \gamma_k^{(A)} & \dots \\ 0 & \dots & \gamma_k^{(B)} & \dots \end{bmatrix}.$$

So, the response matrix \mathbf{R} of t samples gives

$$\mathbf{R}_{t \times k} = \mathbf{M}_{t \times 2k} \begin{bmatrix} \gamma_1^{(A)} & 0 & \dots & 0 \\ \gamma_1^{(B)} & \dots & \dots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \dots & \gamma_k^{(A)} & \dots \\ 0 & \dots & \gamma_k^{(B)} & \dots \end{bmatrix} = \mathbf{M}_{t \times 2k} \Gamma_{2k \times k}.$$

Matrix $\mathbf{M}_{t \times 2k}$ is expressed as the product of two matrices $\mathbf{C}_{t \times p}$ and $\mathbf{N}_{p \times 2k}$ of p factors. Thus, the response matrix is as follows

$$\mathbf{R}_{t \times k} = \mathbf{C}_{t \times p} \mathbf{N}_{p \times 2k} \Gamma_{2k \times k}.$$

The model for c odorant molecules can be written as

$$\mathbf{R}_{t \times k} = \mathbf{C}_{t \times p} \mathbf{N}_{p \times (c \cdot k)} \Gamma_{(c \cdot k) \times k} \quad (6)$$

where $\Gamma_{(c \cdot k) \times k}$ becomes a band-diagonal matrix.

To solve Eq. (6), we used alternating least squares [19,20]. The main points of our algorithm are (1) matrices \mathbf{C} , \mathbf{N} , and Γ are calculated using alternating least squares from random initial conditions; (2) non-negative constraints are used for matrices \mathbf{C} , \mathbf{N} , and Γ ; (3) unimodal constraints and normalization to unit length are used for the columns of matrix \mathbf{C} ; (4) a band-diagonal constraint is used for matrix Γ ; and (5) the sum of squared residuals (SSR) is used as a convergence criterion. This algorithm was used for the data arrays generated from electronic noses, and the results were interesting.

3. Experiments

3.1. Instrumentation

All the samples were analyzed on an α -Fox-4000 electronic nose manufactured by Alpha Multi Organoleptic System (MOS) (Alpha MOS, Toulouse France). The whole analytical system consists of 18 MOS sensors distributed in three chambers, HS-100 auto-sampler and AG2301 high pure air generator.

3.2. Measurement methods

Benzene, ethyl acetate, and cyclohexanone samples: Blank papers of 1 cm \times 5 cm were dried at 100 °C for 60 min to volatilize substances

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