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Extracting discriminative information from the Padé-Z-transformed responses of a temperature-modulated chemoresistive sensor for gas recognition

F. Hossein-Babaei*, S.M. Hosseini-Golgoo, Amir Amini

Electronic Materials Laboratory, Electrical Engineering Department, K.N. Toosi University of Technology, Tehran 1635-1355, Iran

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ABSTRACT

The response patterns of a temperature-modulated chemoresistive gas sensor were transformed to multi-exponential functions which facilitated the extraction of their discriminative features for gas diagnosis. The patterns were generated for air contaminated with different concentrations of various volatile organic compounds by applying a staircase heating voltage waveform to the microheater of a tin oxide-based sensor that modulated its operating temperature in the 50–400 °C range. Padé-Z transform was utilized for the transformation, and a novel heuristic procedure facilitated the extraction of the components of the feature vectors from the transformed data. These vectors were classified by the available techniques. The method differentiated the patterns generated for methanol, ethanol, 1-propanol, 1-butanol, and acetone contaminations in the wide concentration range examined. The method was also used to separately estimate the amount of the discriminative information in various steady state and transient response features; the results are anticipated to help design more elaborate temperature-modulated sensors for gas diagnosis.

1. Introduction

Their attractive combination of quality factors has rendered chemoresistive gas sensors [1–9] suitable for applications ranging from the simplest household CO and fire detectors [8] to sensor arrays utilized in artificial olfaction systems [10–13]. In these devices, the electrical resistance of a polycrystalline oxide semiconductor pallet varies with the composition of the surrounding atmosphere, and the magnitude of this variation defines the response to any polluting, combustible, or poisonous contaminant [1–5]. The sensitivity as well as the response level vary from one target gas to the next, but, in practice, no selective detection is expected from a single sensor as its response to gas A at concentration C_A can be similar to that to gas B at a different concentration C_B. Different techniques have been used to overcome the lack of selectivity in these sensors [4,14–18], among which the modulation of their operating temperature is well known [18–29].

Chemoresistive gas sensors operate at elevated temperatures, and their responses are strongly temperature dependent [7]. A pre-programmed variation of the operating temperature results in a complex temporal response pattern that contains information on the nature and concentration of the contaminant present [19]. It has been shown that the extraction and classification of this information can facilitate contaminant diagnosis [22–29]. The temporal modulation of the operating temperature is achieved by applying the power waveforms of different shapes to the heating element of the sensor [21–24]; an example is the staircase voltage waveform applied to the sensor heater [24,25]. Each step of the staircase brings the sensor to its corresponding temperature plateau and allows enough time for the sensor response to approach its steady state level at that temperature. The created complex temporal pattern contains a number of rises, plateaus, and falls, the details of which are related to the composition of the surrounding atmosphere of the sensor [25].

The response patterns of the temperature-modulated sensors have been processed both in time [24] and frequency domains [26] for the extraction of the diagnostic information. The temporal response pattern obtained for a specific target gas amounts to a large pile of numerical data; the complications of the high dimensional calculations involved are avoided by the application of proper mathematical transformations on the generated patterns, which map them into a low-dimensional space where they can readily be classified by using appropriate classification techniques. Utilization of the fast Fourier transform for this dimensional reduction has resulted in a successful classification of the responses of a temperature-modulated sensor to the binary mixtures of CO and NO_2 in a wide concentration range in air [21]. Wlodek et al. attempted feature extraction by fitting a family of

* Corresponding author. Tel.: +98 21 8873 4172; fax: +98 21 8876 8289.
E-mail addresses: fhbabaei@kntu.ac.ir, fhbabaei@yahoo.com (F. Hossein-Babaei), smhosseini@ee.kntu.ac.ir (S.M. Hosseini-Golgoo), amir.amini@ee.kntu.ac.ir (A. Amini).

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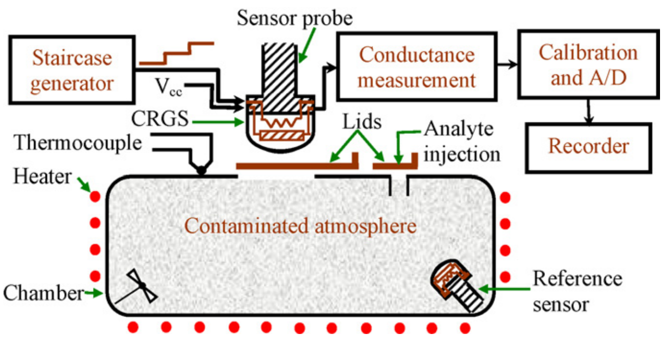

Fig. 1. The schematics of the experimental setup (colored online).

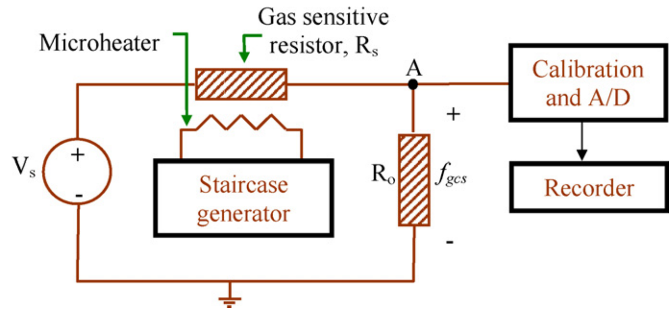

Fig. 2. The schematic diagram of the measurement circuit (colored online).

the Gaussian functions to such temporal responses [22] to discriminate between hydrogen, propane, isopropanol and carbon monoxide. Kunt et al. used the wavelet network method to model the response patterns of a microhotplate-equipped chemoresistive gas sensor, and used the effectiveness of the recovered diagnostic information as the guideline for the determination of the optimum temperature-profile [23]. Gutierrez et al. [24] analyzed the transient responses of a temperature-modulated sensor array using five different transient analysis techniques, including Padé-Z transform, and concluded that both the effective sensitivity and the selectivity of the sensory system are enhanced when the temperature transition modes are utilized instead of the stationary thermal conditions for the operation of the sensors. Finally, two of the present authors employed the method of linear system analysis for the approximate description of the response patterns of a temperature-modulated sensor, and showed that the extracted discriminative information was sufficient for distinguishing between four target gases of considerable chemical similarities [25].

Here, the results of analyzing the temporal response patterns of a single temperature-modulated sensor by their mapping to a time constant domain for gas diagnosis and the separate estimation of the amount of the selective information in the different response features are reported. Padé-Z transform is utilized for this transformation, and the analyte discriminating features of the transformed information are extracted by a novel heuristic method. The effectiveness of the method has been demonstrated by the application of the linear discriminant analysis (LDA) technique [30] to classify the discriminative information obtained on five different volatile organic compounds of certain chemical similarities.

2. Experimental

Experiments were carried out to establish a database of the transient responses of a temperature-modulated chemoresistive gas sensor to the air contaminated with certain volatile organic compounds at different concentration levels. The schematics of the system utilized for the generation and recording of the response patterns is shown in Fig. 1. A 5-l borosilicate glass container was used as the chamber of the controlled atmosphere. The contaminants were methanol, ethanol, 1-propanol, 1-butanol and acetone vapors. Predetermined volumes of the liquid chemicals evaporated upon injection into the chamber and created contamination levels in 100–2000 ppm range in the closed chamber. The contamination levels were continuously monitored during the measurements using a calibrated reference gas sensor installed inside the chamber. To prevent local condensation of the contaminant, the chamber walls were heated to 50 °C by a controlled electric heater distributed over the outer surface of the chamber. The chamber atmosphere was mildly agitated for homogenization by a small electric fan placed inside the chamber.

The electric circuit used to record the variations of the sensor's resistance is depicted in Fig. 2. It comprises a series resistance to convert the variation of the gas sensitive resistor to a measurable voltage signal. The output signal is sent to the recorder through an A/D converter. The sensor employed was a tin oxide-based commercially available general gas detector (SP3-AQ2, FIS Co., Japan) which is equipped with an alloy wire microheater to provide the elevated temperatures required for its operation. The operating temperature changes with the voltage applied to the microheater. A constant voltage level corresponds to a constant temperature at the sensitive surface of the sensor's pallet; while a varying voltage waveform results in a time-varying operating temperature. The sensor's resistance depends on both the temperature maintained at the sensitive surface of the device and the composition of the surrounding atmosphere. The conductance–temperature relationship was experimentally recorded for the sensor used by the measurement of the device resistance at different temperatures in clean air. The temperature of the sensor at any applied heating voltage was measured by placing a fine (diameter of 0.04 mm) platinum-based thermocouple junction in physical contact with the surface of the tin oxide pallet. The relationships between the applied heater voltage, tin oxide pallet surface temperature, and the measured conductance of the device in clean air are presented in Fig. 3. The sharp fall in conductance, observed in Fig. 3b at around $t = 0$, is due to the prior state of the sensor heater set at 5 V (see below); the rest of the conductance variations observed in Fig. 3b are typical of the SnO_2-based gas sensors and are caused by the combined influences of many different temperature dependent parameters such

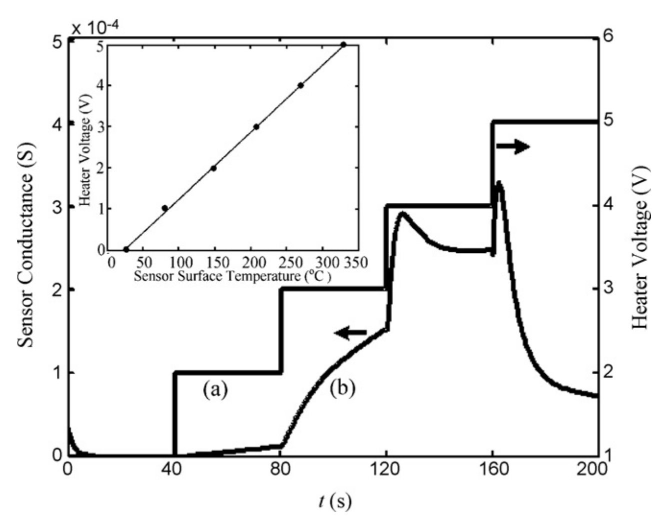

Fig. 3. The staircase voltage applied to the microheater of the sensor (a) and the resulted temporal variation of its electrical conductance (b) in clean air. The insert presents the experimental relationship obtained between the surface temperature of the sensor and the voltage applied to the microheater.