



Acceleration of chemo-sensory information processing using transient features[☆]

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ABSTRACT

A snapshot from the steady-state response of chemical sensors conveys, on average, more mature and relevant information regarding the analyte than a snapshot from the transient can provide. Nevertheless, time constraints in many applications make it infeasible to wait for and extract steady-state features. Substituting them by transient ones is the only viable solution to accelerate odor processing. Based on measurements recorded from metal-oxide sensors, we point to a correlation between a transient feature and the steady-state resistance that are observed in response to fixed analyte concentration. We utilize this correlation to expedite standard quantification and classification substantially while ensuring the performance that the steady-state feature can provide.

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1. Introduction

Shortcomings of metal-oxide based gas sensors in providing a highly sensitive, selective, long-term stable, and fast response [8,13,5,16] constitute the major limitations on their practical value [18,20]. Signal processing is the most sensible approach to overcome these barriers, yet with limited success [10].

Feature selection is a decisive step in sensory signal processing. Nevertheless, a systematic selection rule that fits all applications does not exist. A practical approach is to produce a set of candidate features and then eliminate the redundant ones in training the recognition system.

Since each additional feature selected for further processing adds to the dimensionality of the problem, redundant (or non-informative) features may induce severe computational costs in subsequent stages. It is therefore necessary in many applications to perform a redundancy check on the feature set and filter out the ones that do not contribute to the recognition. Given a set of candidate features, finding the minimal set that covers all of information regarding the problem is a combinatorial problem, which can be tackled in a principled manner by quantifying the correlation or mutual information [4].

In addition to the amount of complexity added to the recognition problem, there may be other application-specific criteria that can make certain features less preferable than others, or maybe even totally infeasible. This study observes such a constraint, namely the overall processing time as determined by the time the latest feature occurs in a temporal pattern. In particular, we deal with the time profile of metal-oxide sensor resistance in response to a chemical vapor at a constant concentration.

Fulfilling time constraints in chemo-sensor driven processes is usually difficult since the characteristic time of sensor response is traditionally slow. Considering that the transient period in a typical metal-oxide sensor response is in the order of a minute, it is imperative in many critical applications to focus the attention exclusively on the transient features, which would be available much earlier.

There are multiple ways to induce a transient sensory response. Two common ones are a controlled change in analyte concentration [23,14,9,17,19,24,21] or in operating temperature [24,15,2,12,22]. We focus on the former method in this paper.

A number of transient features for odor sensors and their evaluation with respect to the classification/quantification performance have been reported in the literature [23,14,9,17,1]. The common approach in utilizing transient features in recognition has been to use them together with some steady-state features. The underlying idea is that the transient phase may be conveying additional information regarding the analyte that steady-state does not tell. Hence, when used as an aid to steady-state ones, transient features can boost the performance. While such reasoning is absolutely valid, it

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might not be of much help when it is not feasible to wait until the steady-state.

In contrast, our treatment of transient features aims at making them successful *substitutes* for the steady-state ones. Note that such a substitution is the only feasible option, when reduction in processing time is necessary.

For this purpose, we investigate the peak value of the exponential moving average (denoted by E_α) of sensor resistance. The suggested feature is available at a particular time instant in early transient, long before the sensor response reaches its steady-state. Due to the (single) parameter involved in its calculation, the exact time E_α occurs in the transient can be adjusted. This flexibility enables using an bank of feature extractors on the same signal, where the recognition process is fed with new information from the transient on-the-fly as each feature becomes available.

We show on recordings from a metal-oxide sensor array that, within a fairly wide concentration interval, E_α correlates with the most preferred steady-state feature ΔR of sensor response in a one-to-one fashion. We take advantage of this relation in predicting the analyte concentration shortly after the gas injection and minutes earlier than the conventional scheme. We also investigate the classification performance of the proposed feature using three analytes. We conclude that E_α is a successful substitute to ΔR , provided that the recognition system has access to the transient of the transduction process.

The paper is organized as follows: In the next section, we introduce the suggested feature E_α and its properties. We also show on actual measurements that it is correlated with the standard steady-state measure. In Section 3, we demonstrate its quantification and classification performance. Concluding remarks are given in Section 4. The details of the measurement setup used in the experiments are given in [Appendix A](#). The measurement data used in this paper are available in the [supplementary material](#).

2. The proposed feature E_α

2.1. Definition

We consider the response (resistance) of a metal-oxide sensor, which is subjected to a specific analyte in a constant flow. We assume that the analyte is applied in constant concentration beginning $t = t_0$ until the end of processing. The sensor resistance $r(t)$ is sampled and recorded at a constant rate σ .

For the recorded $r[k]$, $k \geq \sigma \cdot t_0$, we propose the real-valued feature:

$$E_\alpha\{r[\cdot]\} = \max_k \text{ema}_\alpha(r[k]).$$

Here, $\alpha \in [0, 1]$ being a smoothing parameter, the exponential moving average operator ema_α transforms a given discrete-time signal $x[k]$ into

$$y[k] = (1 - \alpha)y[k - 1] + \alpha(x[k] - x[k - 1]) \quad (1)$$

with the initial condition $y[0] = 0$. Note that ema_α implements a linear filter from x to y . [Fig. 1](#) shows $\text{ema}_\alpha(r[k])$ for three different α values.

Exponential moving average is a popular smoothing technique in time-series analysis. When applied on the (time-derivative of the) saturated exponential signal:

$$s(t) = S \cdot \left(1 - \exp\left(-\frac{t}{\tau}\right)\right), \quad (2)$$

which can be considered as an over-simplified model of metal-oxide sensor response to an analyte under the assumptions given above, the transform ema_α gives a time-series with a single peak within its transient. The exact location of the peak in time depends

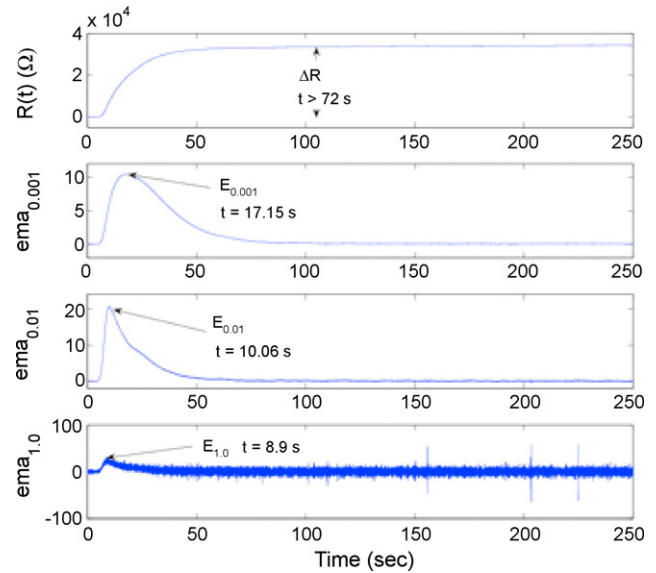


Fig. 1. A raw metal-oxide sensor response (with offset removed) to 250 ppm ethylene (top row) and its ema_α transforms for $\alpha = 0.001, 0.01, 1.0$ (following three rows).

on the smoothing parameter α , which also determines the bandwidth of the filter implemented. For a constant α and τ , the magnitude of this peak is linearly correlated with the steady-state value S of the signal, due to the linearity of the transform.

It is known that the transient phase of the transduction by tin oxide sensors are governed by multiple chemical reactions at different time-scales [7]. Therefore, the transient response of such sensors are actually more complicated than pure exponential behavior. This fact is the motivation for more detailed response models, such as the summation of exponentials, also known as the Gardner transform [9]. Nevertheless, when the sensor is subjected to a constant concentration of the analyte, the response follows a monotonically increasing and saturated profile, unless the measurement is contaminated by an irregularity in the flow or by another analyte (two possibilities that were disregarded due to our assumption above). Despite its deviation from a pure exponential, this time profile still ensures a distinct peak value in the transient after the EMA transform (see [Fig. 1](#)).¹ Next, we show experimentally that this peak value is still correlated with the (projected) steady-state value:

$$\Delta R_{\text{MAX}} = \lim_{t \rightarrow \infty} (r(t) - r(t_0)), \quad (3)$$

yet in a nonlinear way. This nonlinearity should be attributed to the multiple chemical processes during transient that causes the actual r deviate from the pure exponential $s(t)$.

2.2. Correlation with ΔR

ΔR_{MAX} is the most popular feature used in chemo-sensory data processing. According to different rankings [1,19] based on various criteria and datasets, this steady-state feature stands among the most informative ones that can be extracted from sensory response in a memoryless way. There are two practical issues in capturing ΔR_{MAX} : first, it becomes available late in the response, and second, it is susceptible to drift.

¹ The optimal number of components in the Gardner expansion are found to be no more than a few in practice.

Table 1
Concentrations of the three pure analytes sampled in the database

Analyte	Concentrations (ppm)
Ethanol	10, 20, 30, 40, 50, 75, 100, 125, 150, 175, 200, 225, 250, 275
Ethylene	10, 20, 30, 40, 50, 75, 100, 125, 150, 175, 200, 225, 250, 275
Acetone	25, 50, 75, 100, 125, 150, 175, 200, 250, 300, 350, 400, 450, 500

Each dataset contains five replicates from each concentration.

We have observed the correlation between ΔR_{MAX} and E_α on three datasets, each containing pre-recorded responses of a metal-oxide sensor array to a certain analyte at various concentrations. The analytes and their concentrations contained in the database are listed in Table 1. See the Appendix A for details on the measurement setup. The database is available in the supplementary material.

Fig. 2 shows the two features mapped against each other for each ethanol measurement in the dataset. The measurements are in the increasing order along the fit (from the origin to the northeast direction) with respect to the concentration. As α is reduced, the clear improvement in the correlation can be observed between the two features (see the mean square error in the quadratic fits for each α in the figure).

There are two different reasons for this outcome: First, with a small α , ema_α has a better noise-rejection capability so that the peak becomes more clear after the transform. Second, it delays the occurrence of E_α such that it captures a longer history of the measurement, thus gives a more mature and informative indicator.

The price paid for a higher-quality E_α is the extended period until it becomes available in the signal. We define the occurrence time of a feature as the time elapsed from the gas injection until the latest peak observed in the 16 sensor responses. The average of this time with respect to concentration in the ethanol dataset is given in Fig. 3 for different α values and for ΔR_{MAX} for comparison. For practical purposes, instead of the actual time of ΔR_{MAX} as defined in (3), we record its availability at the time that the response enters the $\pm 2\%$ band of ΔR_{MAX} . Clearly, for each α , E_α becomes available in the measurement substantially earlier than ΔR_{MAX} . Also note that the ΔR_{MAX} time is highly sensitive to measurement noise, which poses a challenge in deciding when to extract it.

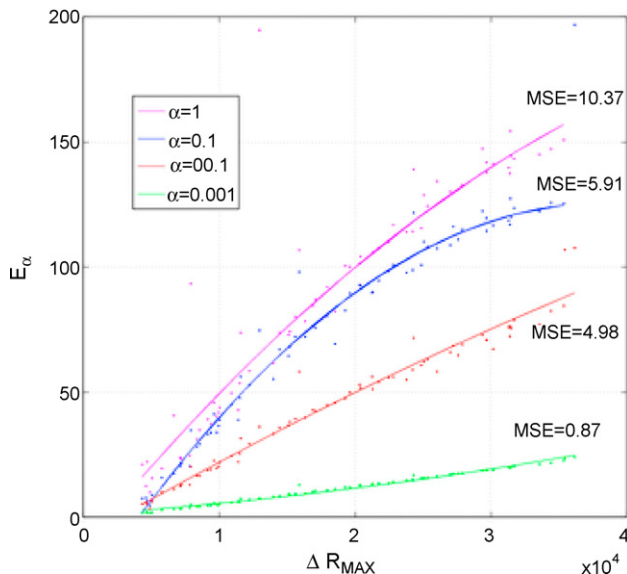


Fig. 2. All 70 ethanol measurements mapped on the 2D feature space ΔR_{MAX} vs. E_α for each $\alpha \in \{0.001, 0.01, 0.1, 1.0\}$ (each color-coded). The dots are the actual data extracted and the curves are quadratic fits with their mean-square-errors indicated.

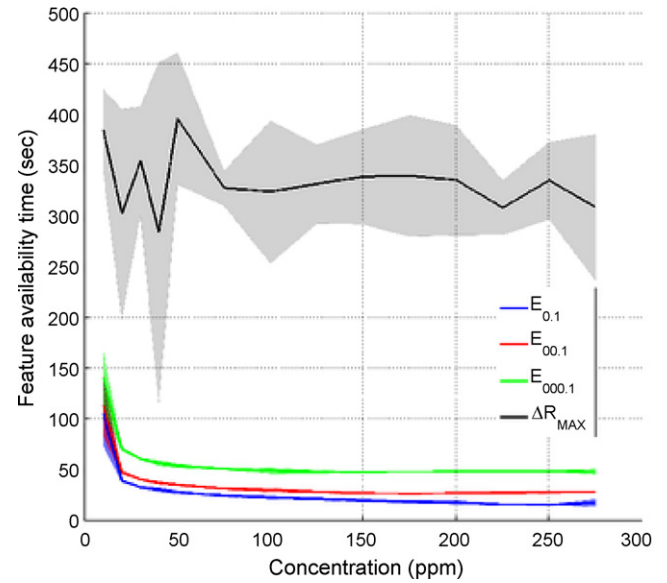


Fig. 3. The times when E_α and ΔR_{MAX} become available in ethanol measurements versus the concentration range swept. The curves show the mean times calculated over the five replicates and the shaded bands around them indicate the standard deviation.

We have verified this trade-off in other datasets on the same feature space.

One can take advantage of the illustrated correlation and the time difference in expediting quantification and identification of analytes. We demonstrate this idea on two problems in the next section. Before that, we would like to point out a generic processing scheme that can be useful in balancing the demands on the processing time and the performance when the proposed feature is used.

2.3. Bank of E_α features

Despite being a better indicator of ΔR_{MAX} as α goes to zero, the quantity E_α with a small α does not necessarily supersede the transient features with larger α values. In other words, E_α with a large α could still have something novel to convey about the measured analyte. Therefore, using multiple features in parallel on the same sensor response can be useful.

We propose the scheme shown in Fig. 4. Here, the features become available at different times since they have different α values. As soon as a feature becomes available, it is passed on to the decision unit. In this way, the decision unit would have access to a rich variety of information sources regarding the same process. This variety comes at the expense of increasing the dimensionality of problem.

Would employing multiple features in such an incremental arrangement require an update on the decision rule during the process? The answer is no, since the information base would be nested with respect to time, i.e., the content $\{E_{\alpha 1}, E_{\alpha 2}, \dots, E_{\alpha i}\}$ available to the decision unit at a given time T is necessarily contained in the base at any $t > T$. Assuming that the unavailable features in the system are substituted by a constant, say 0, the pattern space for the decision unit grows in dimension by time, with the previous content retained in the subspaces. In this particular case, an optimum unbiased classifier/regressor, such as a Support Vector Machine (SVM), designed for the full n -dimensional space, would still be optimal in each subspace, i.e., before all n features are available. Therefore, the same decision unit (without

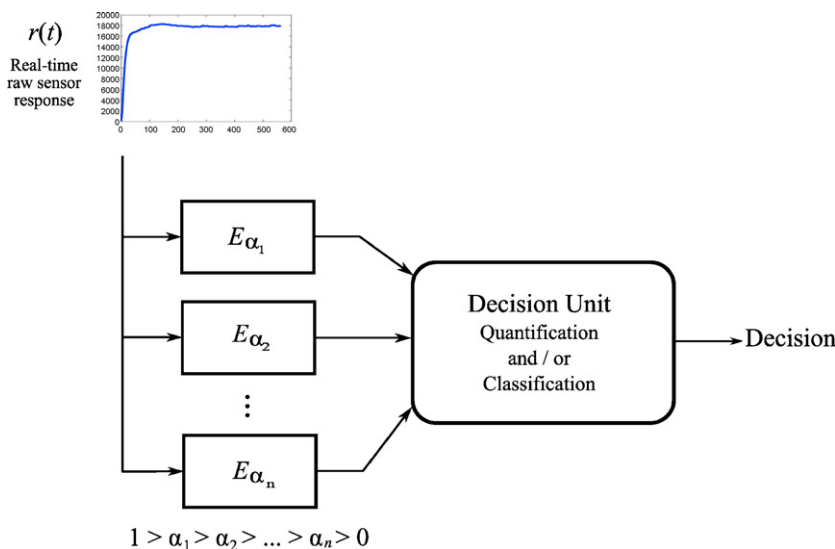


Fig. 4. A bank of features with different smoothing parameters can be evaluated in parallel and in real time.

any change in its parameters) can be used throughout the process.

3. Simulation results

In this section, we make use of the proposed transient feature as a substitute of ΔR_{MAX} in two standard applications, namely quantification (i.e., concentration prediction) and classification (i.e., analyte type identification). We finally demonstrate the idea of E_{α} feature bank in the combined problem.

3.1. Quantification

We consider first the problem of predicting the analyte concentration given a sensor array response, assuming that the analyte identity is known.

The concentration is a continuous variable, hence the prediction should be made by a regressor which takes 16 features from the sensors and output a real number. Nevertheless, the problem can also be cast as a classification one when the considered concentration interval is discretized and each interval is assigned as a class. Our dataset is especially suitable for the latter approach since the concentration levels are already quantized (see Table 1).

Considering the three datasets separately, we extracted four features, namely ΔR_{MAX} , $E_{0.001}$, $E_{0.01}$, $E_{0.1}$, from each one of the 70 records. In each case, we constructed a 16-dimensional real vector for each measurement and labeled it with its concentration.

In evaluating each feature, we used a linear SVM classifier with 16 inputs. In particular, we randomly split the dataset into 80% training and 20% test sets. The training part was used in the design of linear SVM design, which we performed using [3]. Then, we tested the performance of the decision unit on the test data and recorded the correct classification rate. We repeated this design-test procedure 100 times with different random splits.

The average prediction rate over these trials are listed in Table 2 for each dataset and for each feature used.

ΔR_{MAX} is known to be strongly correlated with the analyte concentration [8]. Therefore, in quantification, E_{α} with a small α is consistently a better indicator, as it is more tightly correlated with ΔR_{MAX} than an E_{α} with a large α .

3.2. Identification

The high dimensionality of the considered data, high quality of measurements, and the small number of analyte classes makes the identification problem a straightforward one when all 16 sensor responses are used. The classification performance hits 100% on the dataset when any pair of sensors are used with any features considered in this work. Therefore, in the identification test, we used a single sensor response (sensor no. 1) and disregarded others. We used the four features ΔR_{MAX} , $E_{0.001}$, $E_{0.01}$, $E_{0.1}$ of the single channel time-series, which was extracted in the previous test.

We grouped the extracted scalar features by the feature type and, within each group, labeled the data by the analyte identity (regardless of the concentration). Note that each group induces a three-class classification problem, which we attacked, once again, with a linear SVM. We employed the same train-test procedure followed in the previous test.

The average correct classification rate was 85.3%, 82.9%, 89.5%, and 93.8% for $E_{0.1}$, $E_{0.01}$, $E_{0.001}$, and ΔR_{MAX} , respectively. Comparable results have been obtained when other sensors were used individually in this experiment.

The steady-state feature stands as the best one again. However, as opposed to the quantification test, an earlier E_{α} feature with a large α does not necessarily yield a worse performance than the later features in identification.

3.3. The combined problem

As shown in the previous tests, two E_{α} features extracted from the same sensor response can convey independent statistics regarding the process, particularly in classification. This supports the idea of using a multi-dimensional feature, containing multiple E_{α} fea-

Table 2

Average correct prediction rates (in %) when linear SVM is applied on the quantification of the indicated analyte using the selected feature.

	$E_{0.1}$	$E_{0.01}$	$E_{0.001}$	ΔR_{MAX}
Ethanol	66.9	69.3	81.0	85.1
Ethylene	76.1	76.6	85.5	86.9
Acetone	71.0	75.3	76.7	75.2

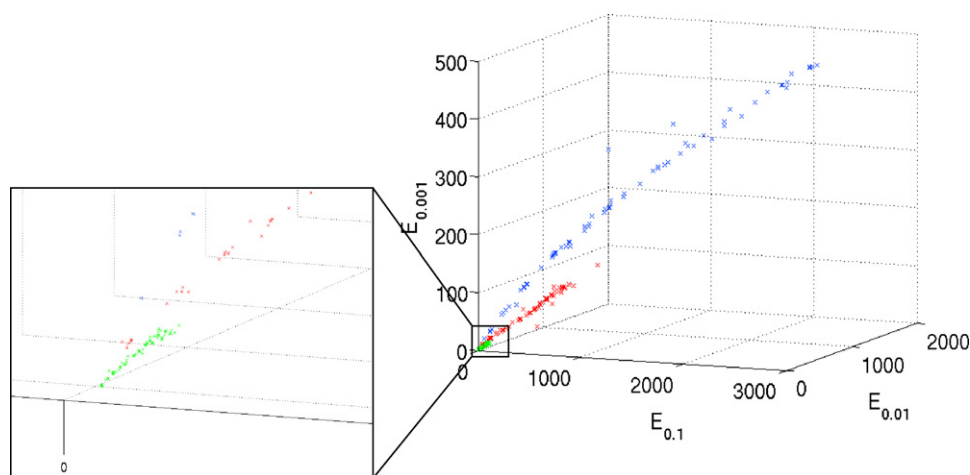


Fig. 5. Map of all responses recorded from a single sensor on a 3D feature space induced by three transient features. The analyte identities are color-coded (ethanol in red, ethylene in blue, and acetone in green).

tures of the same sensor transient, to improve the accuracy of decision.

We demonstrated this idea on the joint problem of quantifying and identifying a given measurement. As in the identification test, we focused on a single sensor response (number 1 in the array). This task was qualitatively more difficult than the individual problems investigated above, because two decisions had to be made simultaneously on-the-fly and based on a single-channel time series.

For this purpose, we considered the triple of features $E_{0.1}$, $E_{0.01}$, and $E_{0.001}$. We mapped each sensor response in the three analyte datasets to these features and labelled them both with the concentration and the analyte identity. Hence, the problem was to classify a given single-channel measurement into 42 categories (each corresponding to a analyte type at a concentration level) using 3 transient features. We used the linear SVM evaluation method as performed in the previous tests.

When $E_{0.1}$, the earliest feature, was used alone, the linear SVM, trained and tested as in previous simulations, was 62.1% accurate in identifying the correct identity and concentration. As was reported above, this single feature is 85% accurate in identifying the correct analyte only. So, the drop in the performance is due to the increased complexity of the problem by the quantification aspect.

When $E_{0.1}$ and $E_{0.01}$ features are used together to solve the problem, the performance of the SVM (now with two inputs) advanced to 89.5% on the combined problem. These two features gave 93.6% accuracy in predicting the correct identity, when the quantification aspect is ignored.

The three transient features gave 92.9% correct classification rate on the combined problem, where they were 100% accurate in identifying the analyte type. The advantage that is gained by using these features together on the problem is illustrated in Fig. 5. As observed from the figure, using multiple features together reduces the confusion (overlap) in class representations, making classification an easier task. Adding more transient features (i.e., new blocks to the feature bank in Fig. 4) can further improve the performance at the expense of an increase in availability time.

The ΔR_{MAX} feature alone is only 63.3% accurate in making the correct classification on the combined problem.

4. Conclusions

We have presented a transient feature, E_{α} , of the metal-oxide sensor response to a constant concentration of analytes. The feature is available much earlier than the standard steady-state feature

ΔR_{MAX} , but gives comparable results both in quantification and identification problems. The feature is parameterized by a single real variable α , which adjusts its availability in time and its qualities. The extraction process is computationally straightforward and suitable for parallel computation. This enables one to use multiple features with different qualities on the same slowly-saturating time series.

A clear transient is necessary to extract the suggested feature. Therefore, an effective flow control, such as sniffing, in the acquisition is required. On the other hand, since it captures only a short period within the transient, E_{α} is not affected by the drift or other long-term hazards.

Various transient regimes that can be observed in the sensor response, such as the one caused by switching the temperature [11], makes transient features feasible options in chemo-sensory signal processing. These features are vital in expediting the decisions.

The derivative-based E_{α} spans just one half of the dynamical feature spectrum regarding the sensor transients. The other half contains integral features, which we are currently investigating.

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Appendix A. Measurement setup and database

An array of 16 commercially available metal-oxide based gas sensors were placed in a 60 ml volume test chamber to measure vapors at different concentrations. This chamber was connected to a computer-controlled continuous flow system that allowed us to obtain, starting from calibrated gas bottles, the desired concentrations of the different gases and gas mixtures in a highly reproducible way. The carrier gas was dry air. The total gas flow was set to 200 ml/min and kept constant. Moisture level was kept at 10% R.H. (measured at $30^{\circ}\text{C} \pm 1^{\circ}\text{C}$) during the entire measurement process. The following (four from each) screen-printed sensors by Figaro Inc. [6] were used in this study: TGS2620, TGS2610, TGS2602, TGS2600.

The response of the micro-gas sensor array was measured when the operating temperature of sensors was fixed at 400°C . The data acquisition board was controlled by a LABVIEW[®] program running on a PC platform.

Fourteen different concentrations of each analyte (ethanol, ethylene, and acetone—see Table 1) were measured using the gas sensor-array. Each measurement was replicated 5 times (performed

in a disordered way), which gave a total of 70 measurements from each analyte. The measurement procedure consisted of the following steps: First, a constant flow of dry air was circulating through the sensing chamber while the gas sensor array were kept at a stable working temperature of 400 °C. This was done to measure the baseline steady-state sensor response. Afterwards, the desired concentration of the gas was injected by the continuous flow system into the sensing chamber. Finally, in the third step (cleaning phase) the vapor was vacuumed away from the sensor array and the chamber was cleaned with dry air before the concentration phase of a new measurement could start. The acquisition of these measurements took about 20 min to complete, i.e., 10 min for the gas injection phase and 10 min for the recovery (cleaning) phase. We discarded the recovery phase and subtracted the baseline from each record. The sampling rate was set to $\sigma = 10$ Hz.

Appendix B. Supplementary data

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.snb.2008.10.065.

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