Fast Transient Classification With a Parallelized Temperature Modulated e-nose In Natural Uncontrolled Environments

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Abstract
In this article we introduce a novel operating principle for a temperature modulated electronic nose. The aim is to perform gas discrimination with metal oxide gas sensors in natural, uncontrolled environments where the sensor is exposed to patches of gas only for short periods of time. The proposed Parallelized Temperature Modulated e-nose (PTM e-nose) allows to speed-up discrimination of gases by measuring in parallel the response of N gas sensors of the same type but with a phase-shifted temperature modulation cycle. The basic idea is to replicate the base sensor N times with each sensor instance measuring one different Nth of the modulation cycle. In this way the response to the full modulation cycle for one sensor can be recovered from N different sensors in one Nth of the time while the chemical response of the individual sensors is not compromised by a too fast temperature change. We demonstrate the proposed operating principle with a PTM e-nose that consists of four commercially available tin oxide gas sensors, which are temperature-modulated with sinusoids of the same amplitude but phase-shifted by 90 degrees. We particularly address gas discrimination in the early stages of the transient response and demonstrate that the information contained in one entire modulation cycle can be sufficiently recovered from the responses of the individual sensors.

Keywords: Electronic nose; Odour classification; Natural environments; Temperature modulation; Gas sensor array.

1. Introduction

Gardner et al. defined in 1994 the electronic nose (e-nose) as an instrument that comprises an array of partially selective chemical sensors with an appropriate pattern recognition algorithm capable of recognizing simple or complex odours [1]. Over the past two decades, e-nose systems have been used in a wide range of applications under laboratory conditions (i.e. controlled environments), from wine brand discrimination [2] and food quality control [3] to medical applications for bacteria detection [4]. In a typical laboratory setting, measurements are performed inside chambers where temperature, humidity and gas concentrations are controlled and the sampling process comprises of three phases. The sensors are first exposed to a reference gas, then to the gas analytes were the sensors reach the steady state (dynamic equilibrium for temperature modulated e-noses) response in which the analysis is performed. Finally, the gas analytes are flushed away and the sensors recover.

It is desirable to be able to use e-noses; especially based on inexpensive sensor technology, also outside the laboratory. There are several potential applications in outdoor areas that can be implemented with the use of an e-nose combined with a mobile robotic platform. Examples of such applications are environmental exploration [5], gas distribution modeling [6], buried land mine detection [7] or pollution monitoring [8].

Three phase sampling techniques cannot be applied straight forward when the e-nose is mounted on a mobile robotic platform due to constraints related to weight, space and power consumption [9]. Furthermore; for metal oxide gas sensor, the dynamic equilibrium is hardly reached due to the intermittent nature of turbulent airflow [10] along with the movement of the robot. Consequently, data analysis (i.e. classification) has to be performed in the transient response of the sensory array.

Transient response classification has been proved feasible in previous works. Muezzinoglu et al [11] proposed a method to extract features that are available in early stages of the sensor response and that are correlated with those present in the steady state. The authors performed their experiments in a 3-class gas discrimination problem where the concentrations were kept constant and it was demonstrated that odour processing can be accelerated by means of the transient response features. Trincavelli et al. [12] compared different feature extraction methods and classification algorithms to successfully discriminate between three odour sources using the transient response of the sensors. The data set was collected with an e-nose composed by five tin oxide sensors mounted on a mobile robotic platform.

The operating temperature dependence of the metal oxide sensors has been widely investigated [13-15] and it is shown in several publications, that the information content of the response can be improved by modulating their operational temperature. According to [16], temperature modulation can be grouped into two broad categories: thermal transients and temperature cycling. In the thermal transient approach, the heater voltage of the sensors consists of a step function or a pulse and the discrimination is performed in the transient response induced by the fast change in the temperature. The temperature cycling technique involves of connecting the heating element of the gas sensor to a waveform generator that periodically changes the working temperature of the device. When the sensor operating temperature is modulated, the kinetics of adsorption and reaction that occur at the sensor surface are altered [17]. Therefore, a cycle of the modulation signal (of period T) generates a characteristic pattern (i.e. an ``odour signature'') of a target analyte present in the environment [18].

In this paper we introduce a novel operating principle for a temperature modulated e-nose. The proposed system uses cycling temperature modulation to increase the selectivity of the sensors and the transient response is used to discriminate between three organic solvents (namely Acetone, Ethanol and 2-Propanol). The particular characteristics of our approach is that a single sensor is instantiated n times, each of them measuring one different *nth* of the modulation cycle. By considering the transient response and the parallel operation of the replicated sensors, the required exposure time can be reduced. To the authors best knowledge, parallelized operation of gas sensors of the same type in an e-nose has not been proposed in previous works.

The organization of this paper is as follows: section 2 describes the proposed operational principle, the sensory array, the experimental setup along with the pattern recognition methods used for classification. In section 3, the obtained results are presented and discussed. We conclude with discussions and description of future works.

2. PTM E-Nose Concept

The exposure time needed to record an "odour signature" is a function of the period (T) of the modulation signal. Fig. 1.A shows the responses in dynamic equilibrium of a single TGS 2620 gas sensor exposed to Acetone, Ethanol and 2-Propanol. In this example the odour signatures are collected in a period (T). An approach to reduce the exposure time is to increase the frequency of the modulation signal. However, due to the physical limitations a of a gas sensor (i.e. the thermal time constant), fast changes in the modulating temperature might not significantly alter the sensor's conductance profile [19].

The proposed PTM e-nose aims to reduce the exposure time without increasing the modulation frequency. It consists of an array of n gas sensors of the same type, individually modulated with sinusoids of the same amplitude and DC level but shifted in phase. This configuration aims to replicate the sensor n times, where each one of the sensor instances is measuring one different *nth* of the modulation cycle. Thus, a full odour signature can be recovered from the replicated sensors in an *nth* of the modulation cycle.

3. Experimental Setup

3.1. PTM e-nose configuration

In Fig. 1.B, The PTM e-nose configuration used in this work is shown. It consists on four gas sensors independently modulated with sinusoids of DC level equal to V_{ai} (i=1,...,4), amplitude equal to V_{bi} and frequency f. The working parameters (V_a, V_b and f) are kept at same values for the whole sensory array and the sinusoidal signals are shifted in phase by 90 degrees, effectively instantiating the base sensor four times. The four sensors in the array are able to collect data in parallel from $t=0$ to $t=T/4$, each one of them covering one quarter of the modulation period (Fig. 1.C). By appending the readings from the four sensors (x_1 to x_4) and eliminating discontinuities with a 4^{th} order Fourier approximation, a full odour signature can be approximated in a quarter of the modulation cycle as shown in Figure 1.D.

The sensory array consists of four TGS2620 gas sensors that, according to the manufacturer, are highly sensitive to the vapor of organic solvents and also to a variety of combustible gases such as carbon monoxide, making it a good general purpose sensor [20]. They are enclosed in an Aluminum tube of 0.05m diameter and 0.05m length and mounted close to each other in order to have a gas exposure that is as similar as possible across the sensor array. A fan is placed at the opening of the tube in order to create a constant airflow towards the sensors.

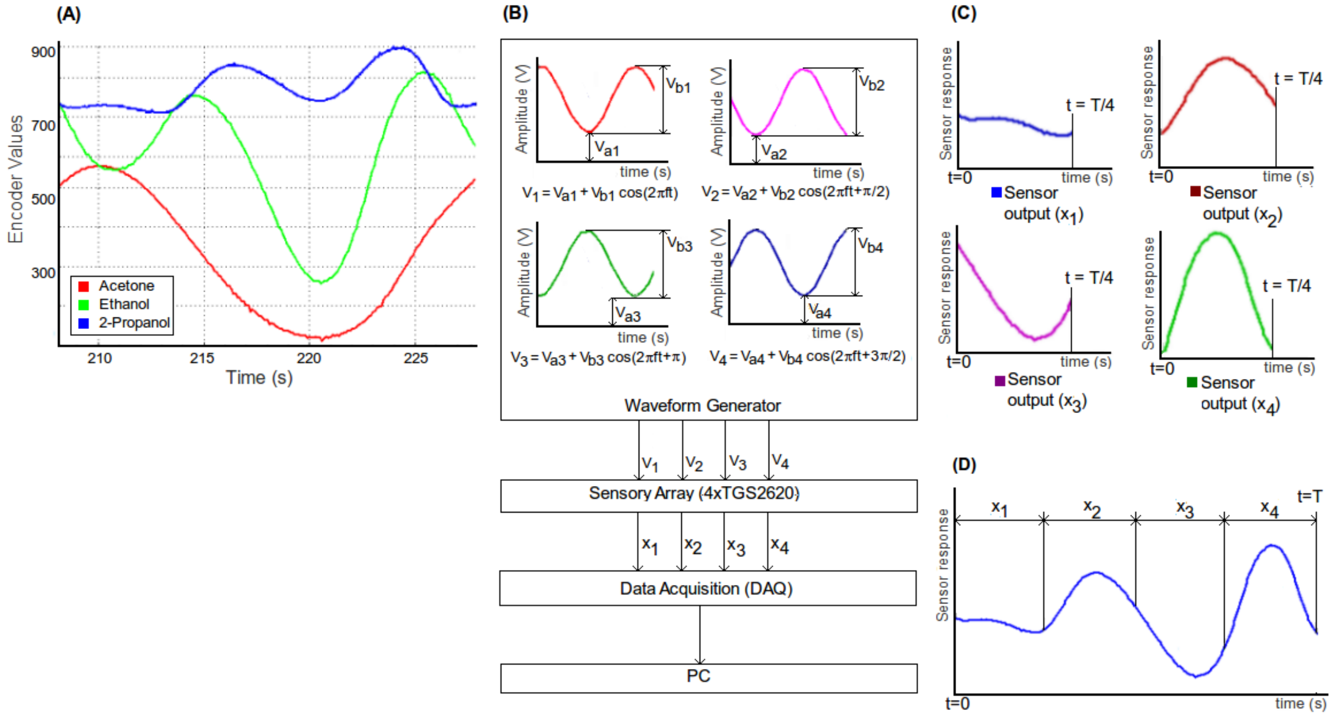

Fig.1 A) Responses in dynamic equilibrium to different analytes recorded with a single TGS2620 sensor modulated by a sinusoidal signal of 1.7V DC Level, 3.3V amplitude voltage and a modulation frequency of 0.05hz. B) Block Diagram of a PTM e-nose composed by four TGS2620 sensors. C) Portion of the response of the gas sensors array in dynamic equilibrium when exposed to a sample of 2-Propanol with working parameters equal to V_a=1.7V DC Level, V_b=3.3V and f=0.05hz D) 4th order Fourier approximation of the 2-Propanol odour signature using the four sensors readings

3.2. Gas sources

Ethanol (C_2H_5OH), 2-Propanol (C_3H_8O) and Acetone (C_3H_6O) have been chosen for the experiments. Ethanol and 2-Propanol have comparable vapor pressure at room temperature while the vapor pressure of Acetone largely differs from Ethanol and 2-Propanol. In order to perform discrimination with gases at comparable vapor pressure levels, some experiments were carried out with samples of Acetone cooled down to -10¶C. These analytes are invisible in the air and, in small quantities, harmless for humans.

3.3. Sampling in controlled environments

The experiments in controlled environments are carried out using a three phase sampling process [21] as follows: the PTM e-nose is placed inside a 7.9l Plexiglas chamber to be exposed first to a reference gas (i.e. fresh air) for 2 minutes to sample the baseline response. Then, a cup filled with one of the three target analytes is placed inside the chamber and the top is closed. The PTM e-nose is exposed to the target analyte long enough to sample the response of the sensors in dynamic equilibrium. The last step consists of opening the chamber and removing the analyte in order to let the sensors to recover the baseline level.

3.4. Sampling in natural uncontrolled environments

The setup for natural uncontrolled environments is shown in Fig. 2. A bottle with a few deciliters of one of the target analytes is connected to a pump by a plastic tube. The analyte inside the bottle evaporates and mixes with the overhead air. In addition, incoming fresh air is led with another tube to the bottom of the bottle. The electronic nose is placed at a distance of 0.2m from the outlet of the pump and the whole system is placed in an outdoor area.

The experimental process starts with exposing the PTM e-nose to the reference gas for 2 minutes. Then the pump is activated to allow the mixture of air and the target analyte to reach the electronic nose and the transient response of the sensor array is recorded for further processing. The pump is then deactivated and the sensor array is exposed to the reference gas to recover to the baseline level.

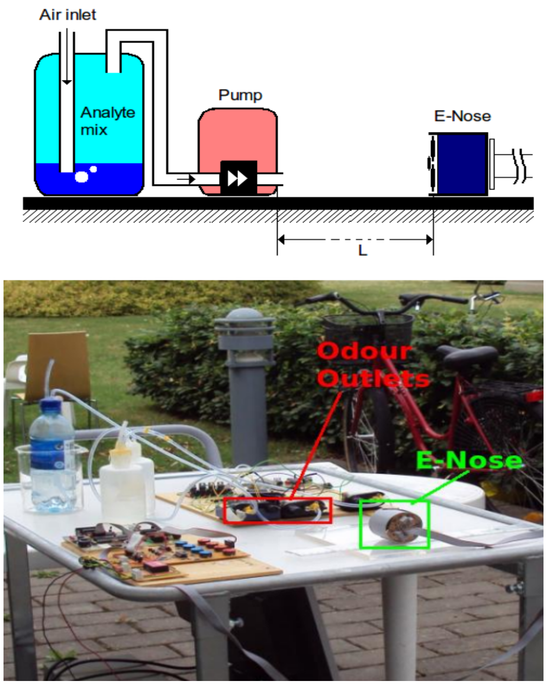

Fig. 2. Setup used for natural uncontrolled environment experiments

3.5. Data analysis

In the controlled environment setup, the analysis was performed in both, transient and dynamic equilibrium segments of the sensor response while for the uncontrolled setup, in which the sensors do not reach the dynamic equilibrium state, only the transient response could be processed. In both cases, the data analysis comprised four stages namely signal segmentation, feature extraction, dimensionality reduction and classification.

In the segmentation stage, the full sensors response was segmented in rising, equilibrium and decay edges using the gradient of the sensor response as suggested in [22].

As previously shown in Fig. 1.A, the sensor responses in dynamic equilibrium are given by a stationary signal. Hence, a suitable tool for feature extraction is the Discrete Fourier Transform (DFT). The DFT was computed over the equilibrium response of the sensors and the phase and magnitude values of the first three harmonics of the modulation signal were taken as features.

In the case of the transient response analysis, the readings are given by non stationary signals that evolves over time. One of the drawbacks of the DFT is that when a signal is transformed to the frequency domain its time domain information is lost [14], thus the Discrete Wavelet Transform (DWT) is used instead. The DWT provides both frequency and temporal information, and is defined as a multilevel decomposition technique that returns a series of descriptors (named approximation and detail coefficients) that are calculated for different scales of a generating function known as the mother wavelet.

The analysis for the transient response was performed by applying the DWT over the rising edge of the sensors readings in order to extract those coefficients located in the frequency band of the modulation signal (in this case, the 5^{th} level detailed coefficients).

The Linear Discriminant Analysis (LDA) technique was used for the dynamic equilibrium and for the transient response analysis for dimensionality reduction purposes. LDA is a transformation that projects the data into a *C-1* dimensional space (*C* is the number of classes in the discrimination problem) where the within-class distance is minimized and the distances between classes are maximized [23].

Classification was performed by using a Support Vector Machine (SVM) with a linear kernel. SVM is a maximum margin classifier [24]. One of its most important properties is that the estimation of the model parameters is a convex optimization problem, and therefore any local solution is a global maximum. Since SVM is by definition a binary classifier, an extension of the original algorithm named “one-versus-rest” was used. In this approach, an individual SVM is trained for each class C_k in the discrimination problem where all the elements that belong to the C_k are considered as the positive class while the rest of the elements in the training set corresponds to the negative class.

4. Results and Discussion

4.1. Performance in controlled environment

For each analyte, 16 experiments were made in a random sequence for a total of 48 measurements. The working parameters of the PTM e-nose were set as follows: Va=1.3V, Vb=3.7V and f=0.5Hz and classification was evaluated in both, the transient response and the dynamic equilibrium states.

Fig. 3.A and Fig. 3.B show a comparison between the LDA plot obtained with data collected by a single sensor during a full modulation cycle and the LDA plot from data collected with the PTM e-nose in one fourth of the modulation cycle, both in dynamic equilibrium. As shown in the figures, in both cases well defined and separable clusters were obtained. With the linear SVM classifier and an 8-fold cross validation, the success rate obtained with both methods was 100%. However, the exposure time with the PTM e-nose was reduced to 0.5s compared to 2s with the standard e-nose approach.

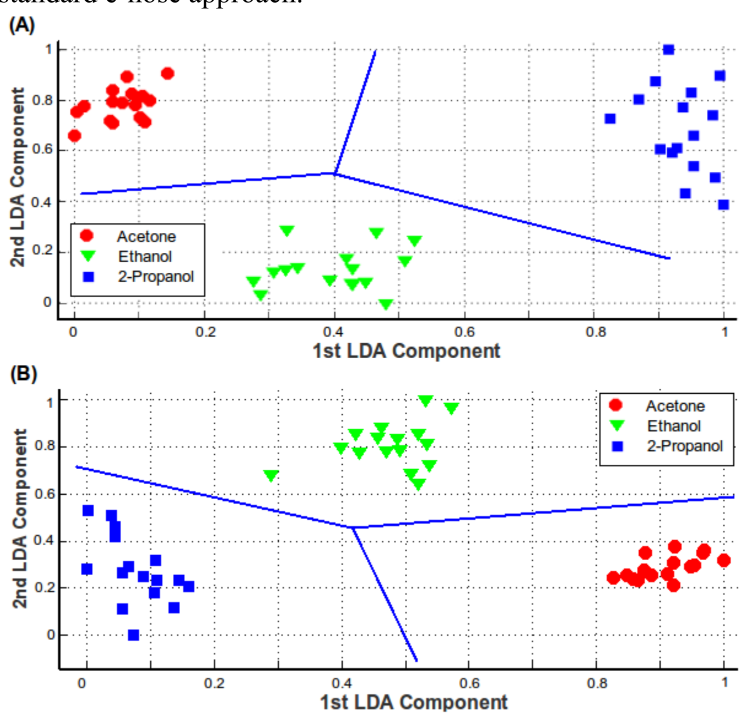

Fig. 3. LDA plots obtained in dynamic equilibrium (f=0.5Hz, Va=1.7V, Vb=3.3V): A) Classical method, one sensor collecting data during *T*. B) Proposed PTM e-nose operating under the same working parameters collecting data during *T*/4.

With the same dataset, classification success rates were investigated using three different segments of the transient response. First, as soon as the rising edge of the sensor response is detected (number 0 in Fig. 4.A), data were collected during the first 0.5s of the transient (one fourth of the modulation cycle, number 1 in Fig. 4.A).

In the second portion of the transient considered, the sensors were exposed to the target analytes for an entire modulation cycle (*T*=2s) after the rising edge, plus one fourth of the second (*T/4=0.5s*) for a total exposure time to the odours of *t=2.5s* (from point 0 to 2 in Fig. 4.A). Similarly, in the third portion considered, the sensors were exposed to the analyte for two entire modulation cycles plus one fourth of the third for a total of *t*=4.5s (from point 0 to 3 in Fig. 4.3). In the last *T*/4 portion of the transient considered, the PTM e-nose collects the information needed to approximate the response of one modulating cycle (*T*) as described in Section 3.

The success rates of the linear classifier obtained by using an 8-fold cross validation were 54.0%• 18.0% for t=0.5s, 93.0%• 7.0% for t=2.5s and 100.0% for t=4.5s. The LDA plots for the three transient segments are shown in Fig. 4.B to Fig 4.D. It can be seen from the results obtained that the classification performance improves as the transient response progresses, having good classification performance at 2.5s and 4.5s.

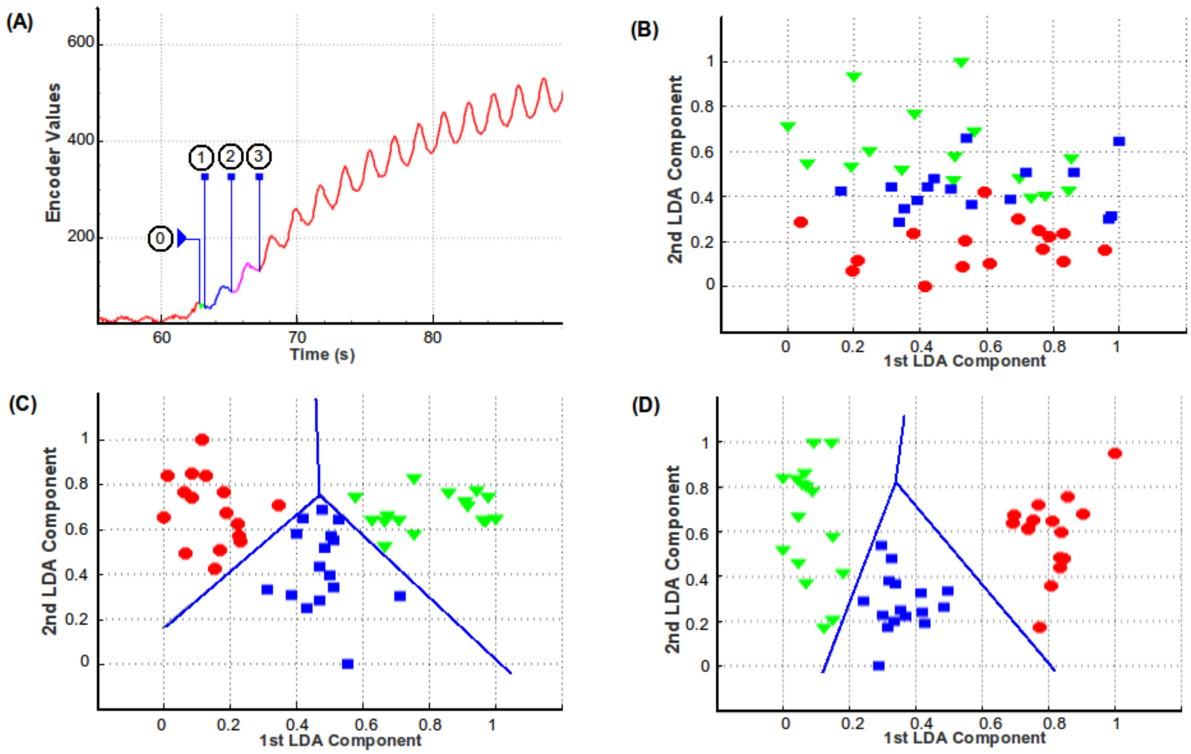

Fig. 4. A) Sensors transient response. Highlighted are the different transient segments used for classification. B) C) D) LDA plots for classification in transient response (controlled environments) for t=0.5s, t=2.5s and t=4.5s respectively.

4.2. Performance in natural uncontrolled environments

In natural uncontrolled environments, 63 experiments were recorded (21 for each of the target analytes) during two consecutive days where the ambient temperature fluctuated between 20¶C to 25¶C. As shown in Fig. 5.A, the equilibrium state in the sensor readings was never reached, therefore the classification was performed only in the early stage of the transient response, where the PTM e-nose is supposed to be in the plume of the analytes.

Similarly to the case of controlled environments, classification was performed and compared in two different stages of the transient response (t=2.5s and t=4.5). The transient segments obtained at 2.5s and 4.5s are shown in Fig. 5.B. Fig. 5.C and Fig. 5.D show the LDA plot and the decision boundaries for the two transient segments investigated, t=2.5s and t=4.5s respectively. An 8-fold cross validation was applied on the obtained data set to evaluate the performance of the proposed system. The classifier accuracies were 86.3%• 13.0% for t=2.5s and 92.3%• 7.0% for t=4.5s. The performance is lower compared with the transient classification in closed environments. This result can be expected due to, in natural environments the interaction with the airflows present, produces irregular concentration patterns (Fig. 5.A) while the volatiles travel from the pump outlet to the PTM e-nose.

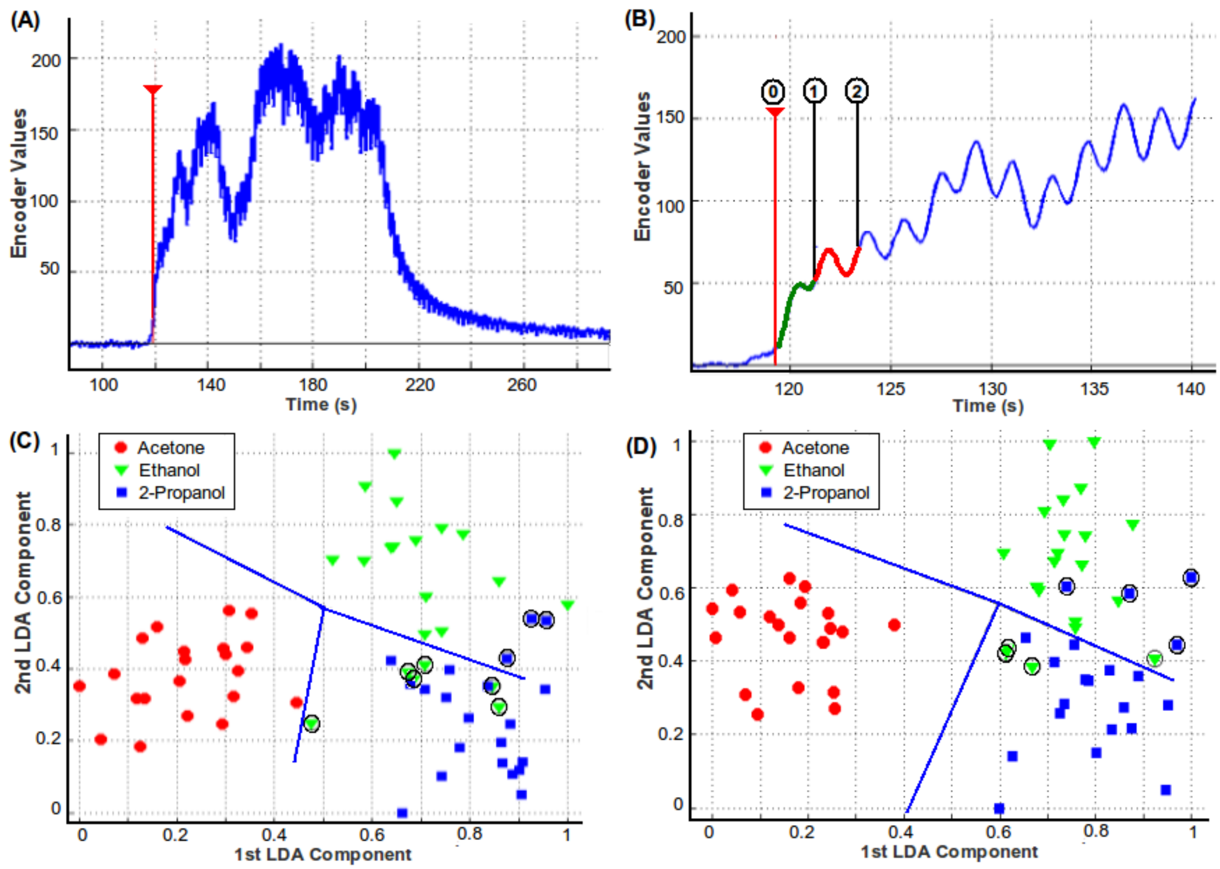

Fig. 5. A) Sensor response when exposed to an Ethanol patch of gas in natural environments. B) Highlighted are the different transient segments used for classification. C) D) LDA plots for classification in transient response (natural environments) for t=2.5s and t=4.5s respectively.

5. Conclusions

A fast sensitive low cost device is a key component for gas sensing applications in natural uncontrolled environments. In this work we introduced the PTM e-nose concept which is an intuitive but effective means to reduce the exposure time to a target analyte by replicating a base sensor *n* times and using phase shifted modulation sinusoid signals.

The proposed system was tested in both, laboratory and outdoor conditions to perform discrimination of organic solvents (namely Ethanol, Acetone and 2-Propanol). The results obtained showed that in laboratory conditions and when discrimination is carried on in the equilibrium state of the sensors response, the performance is similar to the results obtained with a single gas sensor but with a considerable reduced exposure time. Also in transient response under the same conditions, a high classification success rate can be obtained at 2.5s after the rising edge of the signal was detected.

In the case of natural uncontrolled environments, it was demonstrated that successful classification can be obtained at 2.5s, however, the performance is diminished due to external disturbances and irregular gas concentrations. It was also observed that at 4.5s a success rate similar to laboratory conditions (at 2.5s) can be obtained.

Future work will explore the feasibility of adding more than four sensors to a PTM e-nose array. Another future application would be the use of a PTM e-nose mounted in a mobile robotic platform for gas discrimination experiments and gas distribution mapping.

References

[1] J. W. Gardner and P. N. Bartlett, “A brief history of electronic noses”, Sens. Actuators B, vol. 18, no. 1-3, pp. 210-211, 1994.

[2] M. García, M. Aleixandre, J. Gutiérrez and M.C. Horrillo, *"Electronic nose for wine discrimination"*, Sens. Actuators B: Chemical, vol. 113, no 2, pp. 911-916, 2006

[3] S. Ampuero and J. O. Bosset, "The electronic nose applied to dairy products: a review", Sens. Actuators B, vol. 94, no. 1, pp. 1-12, 2003.

[4] M. Trincavelli, S. Coradeschi, A. Loutfi, B. Soederquist and P. Thunberg, *"Direct Identification of Bacteria in Blood Culture Samples using an Electronic Nose"*, Biomedical Engineering, IEEE Transactions on (to appear), 2010.

[5] M. Trincavelli, S. Coradeschi and A. Loutfi, *"Online Classification of Gases for Environmental Exploration",* Intelligent Robots and Systems, 2009. IROS 2009. IEEE/RSJ International Conference, pp. 3311 - 3316, 2009.

[6] A. J. Lilienthal, M. Reggente, M. Trincavelli, J. Blanco Claraco and J. Gonzalez Jimenez, *"A Statistical Approach to Gas Distribution Modeling with Mobile Robots – The Kernel DM+V Algorithm"*, Intelligent Robots and Systems, 2009. IROS 2009. IEEE/RSJ International Conference on, pages 570 - 576, 2009 .

[7] M.Y. Rachkov, L. Marques and A. de Almeida *"Multisensor demining robot"*, Autonomous Robots, vol. 18, no. 3, pp. 275-291, 2005.

[8] G. Ferri, A. Mondini, A. Manzi, B. Mazzolai, C. Laschi, V. Mattoli, M. Reggente, T. Stoyanov, A. J. Lilienthal, M. Lettere and P. Dario, *"DustCart, a Mobile Robot for Urban Environments: Experiments of Pollution Monitoring and Mapping during Autonomous Navigation in Urban Scenarios"*, ICRA Workshop on Networked and Mobile Robot Olfaction in Natural, Dynamic Environments, 2010.

[9] A. J. Lilienthal, A. Zell, M. Wandel and U. Weimar, *"Experiences Using Gas Sensors on an Autonomous Mobile robot”*, Proceedings of EUROBOT, 2001, pp. 4005-4010

[10] B. Shraiman and E. Siggia, *"Scalar Turbulence"*, Nature, vol. 405, pp. 639– 646, 2000

[11] M. Muezzinoglu, A. Vergara, R. Huerta, N. Rulkov, M. Rabinovich, A. Selverston, H. Abarbanel, *"Acceleration of chemo-sensory information processing using transient features"*, Sens. Actuators B, vol. 137, no. 2, pp 507-512, 2009

[12] M. Trincavelli, S. Coradeschi and A. Loutfi, *"Odour classification system for continuous monitoring applications"*, Sens. Actuators B, vol. 139, no. 2, pp. 265 - 273, 2009.

[13] W. M. Sears, K. Colbow, R. Slamka, and F. Consadori, “Selective thermally cycled gas sensing using fast fourier transform techniques,” Sens. actuators B, vol. 2, pp. 283–289, 1990.

[14] R. Ionescu and E. Llobet, *“Wavelet transform based fast feature extraction from temperature modulated semiconductor gas sensors,*” Sens. actuators B, vol. 81, pp. 289–295, 2002.

[15] A. Vergara, E. Llobet, E. Martinelli, C. D. Natale, A. D’Amico, and X. Correig, *“Feature extraction of metal oxide gas sensors using dynamic moments,”* Sensors and actuators B, vol. 122, pp. 219–226, 2007.

[16] R. Gutierrez-Osuna, A. Gutierrez-Galvez, N. Powar. *"Transient response analysis for temperature-modulated chemoresistors"*, Sens. Actuators B, vol. 93, no. 1-3, pp. 57- 66, 2003.

[17] R. Ionescu, E. Llobet, S. Al-Khalifa, J. G. b, X. Vilanova, J. Brezmes, and X. Correig, *“Response model for thermally modulated tin oxide-based microhotplate gas sensors,”* Sens. actuators B, vol. 95, pp. 203–211, 2003.

[18] A.P. Lee and B.J. Reedy, *”Temperature modulation in semiconductor gas sensing”,* Sens. Actuators B, vol. 60, (1999) 35–42.

[19] A. Far, B. Guo, F. Flitti, and A. Bermak, *“Temperature modulation for tin oxide gas sensors,”* in 4th IEEE International Symposium on Electronic Design, Test and Applications. Delta(2008), pp. delta, pp.378–381, IEEE, 2008.

[20] TGS 2620 - for the detection of Solvent Vapors. Figaro Gas Sensor Company.

[21] T. Pearce, S. Schiffman, H. Nagle, and J. Gardner, *"Handbook of machine olfaction"*, Wiley, Germany, 2003, ISBN 2527303588.

[22] M. Trincavelli and A. Loutfi, *"Feature Selection for Gas Identification with a Mobile Robot"*, Robotics and Automation, 2010. ICRA '10. IEEE International Conference on, pages 2852 - 2857, 2010.

[23] C. M. Bishop, *"Pattern recognition and machine learning (information science and statistics)"*, Springer, 2006, ISBN 0387310738.

[24] C. J. C. Burges, *"A tutorial on support vector machines for pattern recognition"*, Data Mining and Knowledge Discovery, vol. 2, no. 2, pp. 121-167, 1998.