Available online at www.sciencedirect.com

ScienceDirect

Procedia Engineering 87 (2014) 556 – 559

Procedia Engineering

www.elsevier.com/locate/procedia

EUROSENSORS 2014, the XXVIII edition of the conference series

Detection of pollutants in water samples with a wireless hand-held e-nose

J. Lozano[a*], J.P. Santos[b], J.I. Suárez[a], P. Arroyo[a], J.L. Herrero, A. Martín[a]

[a] *Department of Electric and Electronic Engineering and Automation, University of Extremadura, Badajoz, Spain*
[b] *GRIDSEN, Spanish Council on Scientific Research, Madrid, Spain*

Abstract

We present in this communication a home-made and home-developed portable electronic nose. It is capable of working with several types of resistive microsensors, it has an electronic pump and an electrovalve to control the way of the sampling gas, embedded control and instrumentation electronics, rechargeable batteries, touch screen and IEEE 802.11 transceiver for wireless communication. Several measurements are made in order to check the discrimination capability of the prototype in the detection of pollutants in water samples. Principal Component Analysis (PCA) and classification with Artificial Neural Networks are made as data processing methods. A web service infrastructure is also integrated with the aim of providing services such as retrieving the acquired data and requesting a classification value from an unknown sample measurement.

Peer-review under responsibility of the scientific committee of Eurosensors 2014

Keywords: Electronic nose, gas sensors, water pollution, pattern recognition

1. Introduction

In last years, the development of innovative instrumentation systems such as electronic nose (e-nose) has been investigated and implemented. The e-nose, can mimic the human sense of olfaction and can be used for detection, recognition and classification of volatile compounds and odours [1]. These devices have been applied widely in food industry [2] as well as for air quality monitoring [3].

The commercial available electronic noses, generally, do not address the current market needs. This is because the market demands a simple, low cost, portable and multifunctional product. E-Nose miniaturization is not an easy task, one of the reasons for the difficulty in reducing the size of these systems is the need to perform odor signal manipulation and classification, which demand high powered

Peer-review under responsibility of the scientific committee of Eurosensors 2014
doi:10.1016/j.proeng.2014.11.548

central processing units (CPUs), due to the complexity of the algorithms involved. A hand-held electronic nose is one of the solutions to the market demand. The proposed e-nose is a truly portable product. It can be used in field for sample recognition and classification without using a personal computer to process input data.

UEX and CSIC have been carried out for years the design of several prototypes of electronic noses for different applications [2-4]. The main novelty of this device is the size, the autonomy, the possibility of forming a network of electronic noses in order to realize distributed measurements and the connection to a web service infrastructure in order to perform on-line data storing, monitoring and data classification. In this sense, the data and results of classification can be available from different devices (PCs, tablets and smartphones). Moreover the composition and operation of the sensors are optimized to obtain the best classification rate. Although this device has been developed for indoor applications it is versatile enough to be used as a general purpose low cost electronic nose.

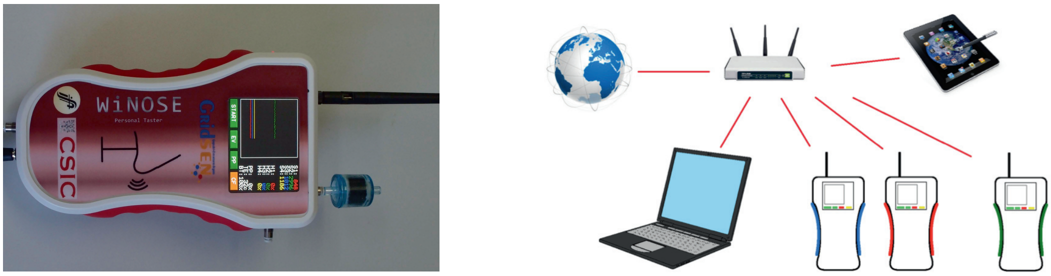

Fig. 1. (a) Portable electronic nose; (b) Configuration of the e-nose in the network.

2. Material and methods

We present in this communication an electronic nose (Fig.1a) with wireless communications capable of forming a network of e-noses for distributed measurements (Fig.1b). It has been designed to work with several types of resistive microsensors, it has an electronic pump and an electrovalve to control the way of the sampling gas, embedded control and instrumentation electronics, rechargeable batteries, touch screen and IEEE 802.11 transceiver for wireless communication (Fig.2).

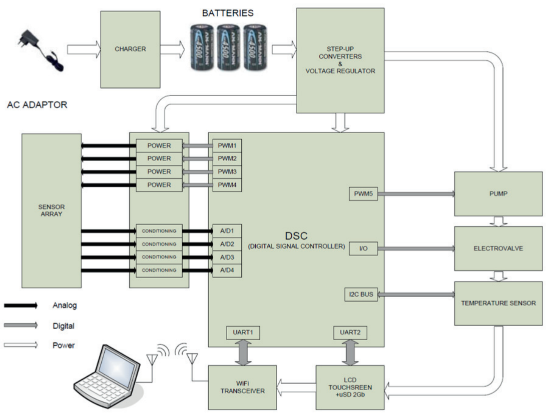

Fig. 2. Block diagram of the main components of the developed portable e-nose.

A network is formed with several identical devices using a router to connect them with the host computer in order to control the electronic nose externally and store the data for further analysis. Solutions of several compounds (1- Blank water, 2-acetone, 3-toluene, 4-ammonia, 5-formaldehyde, 6-hydrogen peroxide, 7-ethanol, 8-benzene, 9-dichloromethane, 10-acetic acid, 11-xylene and 12-dimethylacetamide) are prepared and measured with this device, a total of 20 measurements are made with each compound. Linear pattern recognition techniques such as principal component analysis (PCA) and nonlinear ones such as Artificial Neural Networks have been programmed in Matlab for identification and classification purposes. Comparison between these methods is accomplished.

Data accessibility is an important issue that must be taken into consideration when developing software applications, since we believe that providing full access to data and services is an important challenge for the applicability of a pollutant water detection project. In this regard, offering an easy to use application with low requirements and available from different devices (PCs, tablets and smartphones), is one of the major challenges to be achieved in this field.

3. Results

This work shows the viability of a hand-held e-nose to detect several pollutants in water and a comparison of the discrimination capability of the system increasing the number of pollutants is performed. The prototype uses headspace sampling system: the headspace of samples stored in 15 ml vials is carried to the sensors cell by using an integrated pump. The measurement setup includes cycles of 60s of adsorption and 540s of desorption. It also uses an integrated micromachined gas sensor in silicon composed by four tin oxide gas sensors with different geometries and operating at different temperatures between 400 and 500ºC.

Once the measurement of the samples was performed, the data was preprocessed, and after feature extraction (relative response baseline manipulation and sensor normalization), PCA was performed on the data to reduce data dimension and show it in a plot. Figure 3 shows the plot for the two first principal components of adulterated water with 7 and 11 pollutants respectively. It can be noticed that the clusters of the different pollutants are clearly separated in figure 4 and when a great number of pollutants are required for discrimination, some partial overlapping between the clusters appears.

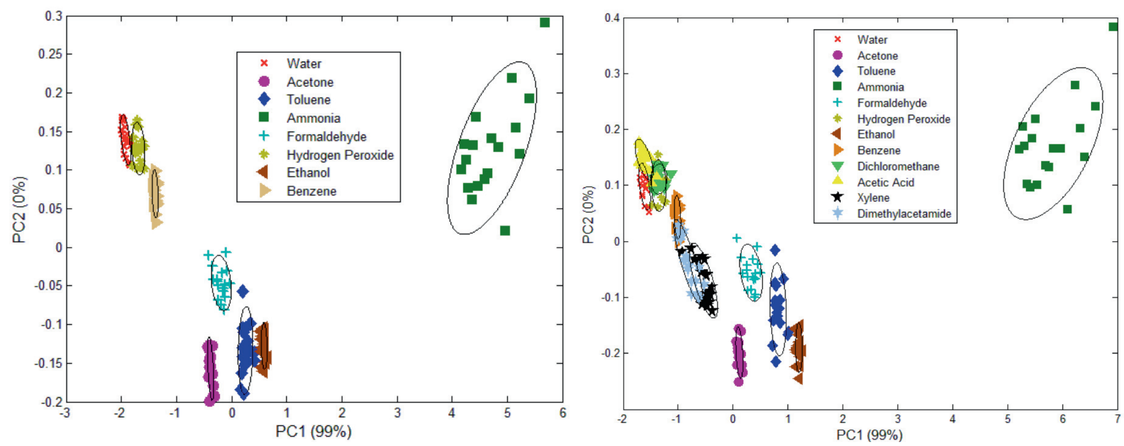

Fig. 3. PCA Score plot of measurements of water samples and 7 (left) and 11 (right) pollutants.

These results are confirmed with the classification with several types of Artificial Neural Networks (ANNs). Two common ANNs have been used: Probabilistic Neural Network with Radial Basis Functions (RBF) and Feedforward Neural Network with Backpropagation (BP) learning algorithm. Leave One Out crossvalidation [5] is used to performance estimation. The success rate (percentage of cases correctly classified in validation) obtained was 100%, 100% and 92% for 4, 7 and 11 pollutants respectively using RBF network and 100%, 100% and 94% for 4, 7 and 11 pollutants using BP network. The confusion matrix obtained in Leave One Out validation with both networks is shown in Fig.4. A web-based application has been developed where web users can introduce sensor values from portable electronic noses and request a classification value. This tool integrates an Artificial Neural Network to provide the classification service

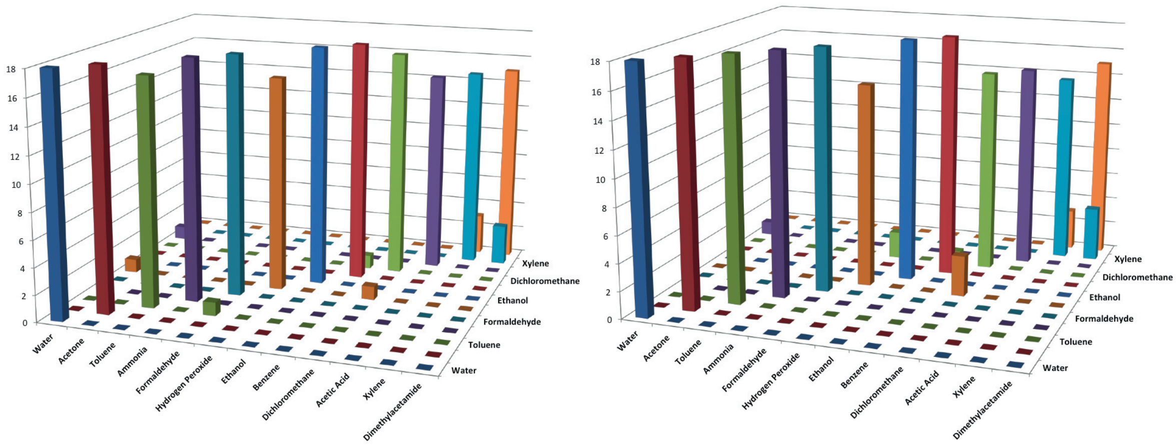

Fig. 4. Matrix confusion of RBF (left) and BP (right) networks obtained in Leave One Out validation.

4. Conclusions

A home-made and home-developed portable electronic nose is used for discrimination of pollution in water samples. Principal Component Analysis and classification with Artificial Neural Networks show good results (more than 94%) in discrimination of samples.

Acknowledgements

Authors want to thank Spanish Ministry of Science and Technology for supporting the projects TEC2010-21357-C05-02 and TEC2013-48147-C6-5 and Regional Government of Extremadura for supporting GR10097.

References

[1] J. Lozano, New Technology in sensing odors: From human to artificial noses in J.A. Teixeira da Silva (ed.): Floriculture, ornamental and plant biotechnology: advances and topical issues (1st ed), Global Science Books, 2006, cap. 13, pp. 152-161.

[2] J.P. Santos, J. Lozano, M. Aleixandre, T. Arroyo, J. M. Cabellos, M. Gil, M. C. Horrillo, "Threshold detection of aromatic compounds in wine with an electronic nose and a human sensory panel" Talanta 80 (2010), pp. 1899-1906.

[3] J.P. Santos, J. Lozano, J.I. Suárez and M. Aleixandre, "Electronic Nose Network For Detection Of TATP Precursors" Proceedings of ISOEN 2013. Daegu (South Korea), July 2nd 2013.

[4] [1] Aleixandre, M.; Lozano, J.; Gutiérrez, J.; Sayago, I.; Fernández, M.J.; Horrillo, M.C. Portable E-Nose to Classify Different Kinds of Wine. Sens. Actuat. B-Chem. 2008, 131, 71-76.