Chemosphere 152 (2016) 107–116

Contents lists available at ScienceDirect

Chemosphere

journal homepage: www.elsevier.com/locate/chemosphere

On-line classification of pollutants in water using wireless portable electronic noses

José Luis Herrero [a], Jesús Lozano [b,*], José Pedro Santos [c], José Ignacio Suárez [b]

[a] Department of Computer and Telematics Systems Engineering, University of Extremadura, Avda. de Elvas s/n, 06006, Badajoz, Spain
[b] Department of Electric Technology, Electronics and Automation, University of Extremadura, Avda. de Elvas s/n, 06006, Badajoz, Spain
[c] Institute of Physics Technology and Information, Spanish Council for Scientific Research (ITEFI-CSIC), Serrano 144, Madrid, Spain

HIGHLIGHTS

- A portable electronic nose with wireless communication has been designed.
- 12 water samples with different pollutants have been detected and identified.
- A web-based application is proposed for classifying pollutants in water.
- The use of a server allows external users to perform data classification.
- The remote classification increases the capacity of memory and the computing power of the classifier.

ARTICLE INFO

Article history:
Received 4 January 2016
Received in revised form
22 February 2016
Accepted 25 February 2016
Available online xxx

Handling Editor: I. Cousins

Keywords:
Electronic nose
Neural networks
Web applications
Components
Web services

ABSTRACT

A portable electronic nose with database connection for on-line classification of pollutants in water is presented in this paper. It is a hand-held, lightweight and powered instrument with wireless communications capable of standalone operation. A network of similar devices can be configured for distributed measurements. It uses four resistive microsensors and headspace as sampling method for extracting the volatile compounds from glass vials. The measurement and control program has been developed in LabVIEW using the database connection toolkit to send the sensors data to a server for training and classification with Artificial Neural Networks (ANNs). The use of a server instead of the microprocessor of the e-nose increases the capacity of memory and the computing power of the classifier and allows external users to perform data classification. To address this challenge, this paper also proposes a web-based framework (based on RESTFul web services, Asynchronous JavaScript and XML and JavaScript Object Notation) that allows remote users to train ANNs and request classification values regardless user's location and the type of device used. Results show that the proposed prototype can discriminate the samples measured (Blank water, acetone, toluene, ammonia, formaldehyde, hydrogen peroxide, ethanol, benzene, dichloromethane, acetic acid, xylene and dimethylacetamide) with a 94% classification success rate.

1. Introduction

In 1982, the concept of an "artificial nose" appeared for the first time in (Persaud and Dodd, 1982) to define a system capable of analyzing a pattern of responses from a sensor array to differentiate some volatiles. Later in (Gardner and Bartlett, 1993) the "electronic nose" (or "e-nose") concept was defined as "an instrument, which comprises an array of electronic chemical sensors with partial specificity and an appropriate pattern-recognition system, capable of recognising simple or complex odours". Today, those arrays of sensors are manufactured by using Micro-Electro-Mechanical-Systems (MEMS) technology (Choi et al., 2005; Blaschke et al., 2006). Modern e-noses are presented with different formats, but all of them include the same elements: an array of sensors, signal conditioning circuits, pumps, an air conditioner, an electronic control unit (ECU) and software for data pre-processing, analysis and pattern recognition. The application fields of e-noses are varied, for example, for measuring and controlling food quality

* Corresponding author.
E-mail addresses: jherrero@unex.es (J.L. Herrero), jesuslozano@unex.es (J. Lozano), jp.santos@csic.es (J.P. Santos), jmarcelo@unex.es (J.I. Suárez).

http://dx.doi.org/10.1016/j.chemosphere.2016.02.106
0045-6535/

(Ampuero and Bosset, 2003; Peris and Escuder-Gilabert, 2009), for monitoring air quality (Offermans and Vitushinsky, 2013), in health applications (Fonollosa et al., 2014) and so on.

It is a common practice that MEMS sensors are included in smart nodes based on digital computers (mainly microcontrollers) with wireless communication capabilities constituting Wireless Sensor Networks (WSN) (Yick et al., 2008). Those smart sensors, which can be deployed anywhere, are low power systems because they usually take the energy from a battery. For this reason they also have a small amount of resources (memory, processing and storage capacity, etc.) and communications are low power and low bandwidth systems. The applications of WSN are varied, ranging from natural disaster relief (Castillo-Effen et al., 2014), cultural assets monitoring (Ceriotti et al., 2009; Rodriguez-Sanchez et al., 2011), medical systems (Hsu et al., 2010), military targets tracking and surveillance (Simon et al., 2004; Tuna et al., 2014), to mobile robots (Yick et al., 2005), etc.

The IEEE 802.11.4 (ZigBee) protocol is widely used for WSN in different fields (Braidot et al., 2013; Tung et al., 2014), because it is specifically oriented to low power and low data rate systems. Recently, the use of the IEEE 802.11 (WiFi) protocol has been proposed for different applications. In spite of its larger power consumption, IEEE 802.11 protocol is adopted in order to cover larger areas with better bandwidths (Lloret et al., 2011; Campbell et al., 2011). The Bluetooth protocol is used in some applications with e-noses (Moon et al., 2013; Tiwari et al., 2014), however it has some drawbacks when compared with WiFi, such as its lower data rate and range. Moreover it is usually used in two-nodes instead of multiple-nodes networks.

E-noses are starting to be used in WSN, especially in air quality monitoring applications and with low cost ZigBee adapters. In reference (Leilei and Yang, 2009), odours around a livestock farm are remotely monitored with an e-nose wireless network. Each e-nose makes use of a ZigBee radio transceiver to communicate to a central control station. All the data collected from the sensor nodes are processed and analyzed by a sensor fusion algorithm in the central station. The odour plume dispersion is calculated, displayed dynamically and predicted in real-time. Reference (Young-Wung et al., 2009) describes a wireless e-nose network, based on ZigBee protocol, proposed for monitoring gas mixtures (NH_3 and H_2S) in real-time. Each node has a powerful 16-bit microcontroller to classify and estimate the concentration of the gas mixture. That information is transmitted to a central station in order to monitor the evolution of gas mixtures in each location. A web service is implemented to enable monitoring and control from any place that has access to the internet.

Despite the massive use of the IEEE 802.11.4 (ZigBee) protocol, IEEE 802.11 (WiFi) protocol presents some advantages that may be taken into consideration in e-nose systems. Other than the previously aforementioned (longer transmitting range and higher data throughput), WiFi devices can be accessed from any modern equipment (pcs, smartphones, tablets, etc.) without any protocol adapter. That is one of the strengths of the e-nose presented in (Wongchoosuk et al., 2012), which is used for monitoring indoor air contaminants that communicate via a laptop. Regardless of its advantages, WiFi is still underused for e-nose systems and in that respect references are difficult to find.

As stated by Marco (Marco and Gutierrez-Galvez, 2012), every particular implementation of an electronic nose includes a data analysis and interpretation module to obtain the final prediction based on the sensor responses. Data processing can be carried out integrating directly into the instrument for on-line evaluation (Perera et al., 2002), or using a desktop computer with dedicated software. The first alternative requires the integration of complex software to support pattern recognition for machine olfaction into e-nose devices, which increases development costs. Another drawback that can be highlighted is that the information required to classify odours is incorporated into the pattern software, making e-nose software updates and information sharing very difficult tasks. Finally it is noteworthy that this integration provides a limited memory capacity and computing power.

To deal with these problems, this paper proposes an e-nose system that provides odour detection software through the web. According to this approach, e-nose devices do not require to integrate complex software, reducing system cost, while odour information is stored and processed in a web-based server, which simplifies software updates, offers a central location to share odour information, exposes web-based services to response user's requests, increase computing power and offers greater memory capacity. In e-nose systems connected to remote stations, where data processing is carried out, it is a common practice to store information in a database system in order to be used for pattern-recognition algorithms. The technology employed in e-nose systems for storing sensor signals and odour information relies both on well-known commercial (proprietary) packages, such as Microsoft SQL Server, and open source systems, for example MySQL (Pogfay et al., 2012). However, this approach requires specialized software algorithms to extract information from databases, connect to ANNS and request classification values. Furthermore, in our proposal we believe that giving open and on-line access to operations for requesting pollutants in water should be an important benefit to be achieved.

On the basic of such reasoning, the system proposed in this paper approaches these challenges and supports data acquisition from electronic noses through Wi-Fi connection, classifies pollutants in water using a neural network specifically developed for this purpose, provides a persistent repository where data is stored, and finally offers a web-based framework that provides on-line services to deliver classification results in response to online requests.

The rest of the paper is organized as follows. Section 2, describes the e-nose, methods, control programs and the framework used for data acquisition, processing and requesting. Section 3 presents the results obtained from the evaluation of the system and the web-based application developed for online classifications. Finally, Section 4 draws some conclusions and future works.

2. Material and methods

2.1. Samples

In order to check the discrimination capability of the system, several measurements are taken from water solutions (Blank water, acetone, toluene, ammonia, formaldehyde, hydrogen peroxide, ethanol, benzene, dichloromethane, acetic acid, xylene and dimethylacetamide). Chemical compounds were supplied by Sigma–Aldrich, and Milli-Q water was used for solutions. One mL of each compound was placed in a 20 mL vial and kept at 16 ± 1 °C by a Peltier system.

2.2. Wireless electronic nose

The core of the electronic nose is the sensor array. The WiNOSE 3.0 has been home-designed to support several types of microsensors. Fig. 1 shows some designed cells with their respective microsensors.

For this work we used a 4 sensor array made by four commercial individual tin oxide sensors (e2V 2xMICS-5524, MICS-5526 and MICS-5914), with integrated heaters, SMT encapsulated, capable of reaching 500 °C with tenths of mW power consumption. The fluidics inside the e-nose is formed by two gas inlets that are switched