'E-Nose'- Design and testing of an electronic device for aroma detection

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ABSTRACT

In the recent past aroma detection has become a significant component in industrial instrumentation and automation field. Electronic noses are developed using a gas sensor array to detect the aroma compounds. These devices are working with the help of pattern recognition software and algorithms. This study describes the design and development of the portable electronic nose device for the detection of the aroma compounds, experimental testing and a mathematical model for the identification of the chemical compounds. The chemical compounds tested are ethanol, acetone and water. The response of sensors raw values were recorded, baseline corrected and averaged. The principal component analysis for these sensor responses are 99.95% of information given with two principal components in the dimensionality reduction. Furthermore, this E-Nose can detect and discriminate among the given substances with 100% accuracy using the 3Nearest Neighbors classification technique.

Key words— aroma detection system; electronic nose; e-nose; gas sensors; MOS sensors.

INTRODUCTION

Electronic Nose (E-Nose) is an artificial olfaction system which can detect different aroma compounds. Electronic noses are used in different types of application such as agriculture and food quality control (Ghasemi-Varnamkhasti, Mohtasebi, Siadat, & Balasubramanian, 2009;Wilson, 2013; Zhou & Wang, 2011;Bhattacharyya *et al.*, 2008; Tozlu & Okumuş, 2018), biomedical applications (Wilson & Baietto, 2011), industrial security purpose (López, Triviño, Calderón, Arcentales, & Guamán, 2017) and environment quality (Bourgeois, Burgess, & Stuetz, 2001; Bourgeois, Romain, Nicolas, & Stuetz, 2003; Capelli, Sironi, & Del Rosso, 2014). E-nose systems consist of sensors which response to different classes of chemical compounds present in a given aroma sample. Accordingly there are sensors which can detect levels of alcohol, hydrocarbons, carbon monoxide, ammonia, hydrogen sulfide, natural gas, etc. (hek, (n.d)). These gas sensors could be either optical (absorption, fluorescence), thermal (pellistor), electrochemical (chemiresistive, potentiometric, amperometric) or gravimetric (James, Scott, Ali, & O'Hare, 2005). The selection of gas sensors for a particular application depends on the aroma profile (Ghasemi-Varnamkhasti et al., 2009; Schaller, Bosset, & Escher, 1999; Wilson & Baietto, 2011). When developing e-nose systems the design of sensors chamber, flow rates, sensor response are important (Schaller et al., 1999). The sensor chamber often consists of a series of gas sensors and the response is recorded as varation of resistance or conductance in aroma sample (Haddi *et al.*, 2011; Sharma, Ghosh, & Bhattacharya, 2013). The system parameters show variations in terms of

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sensor warm up time, purging time and flow rate, sampling time number data recording cycles (sniffing cyles) *(Haddi et al*., 2011; He *et al.*, 2012; Sharma *et al*., 2013; Tian, Cai, & Zhang, 2012). The commonly used statistical methods for e-nose data analysis are principal component analysis (PCA), variance analysis (ANOVA) and clustering methods (Scott, James, & Ali, 2006). In addition artificial intelligence methods are also used for the data analysis (Scott *et al.*, 2006). The e-nose systems currently in market are custom designed (Electronic Nose, (n.d.); Portable elctronic nose, (n.d.)), often preprogrammed to detect a limited number of volatile organic compounds, and offer no flexibility to upgrade through custom programming.

The main objective of this study is to develop a low cost "e-Nose" system and test it in a controlled environment. The unique design of the e-nose system utilizes four metal oxide sensors (MOS) in the sensor chamber and records aroma level as the sensor raw values. In this project alcohol, acetone, and water have been used in order to validate and evaluate the discrimination capacity of the sensor arrays. This device is developed to be used in measuring aroma levels in food related industries where aroma levels can be recorded and compared as a quality controlling device.

METHODS AND MATERIALS

E-Nose Design

The E-Nose system developed here contains three main parts, (i) Data acquisition system hardware, (ii) Gas sensor chamber, and (iii)Vacuum pumps. A schematic diagram of the developed E-Nose system is shown in Figure 1 and the e-nose system constructed is given in Figure 2. Data acquisition system was developed with ARDUINO Mega. Arduino and related hardware are used to design the data acquisition system to record the sensor data when testing a sample. Acquired data from sensors were saved in an SD card. Inlet 1 and Inlet 2 are used to insert the reference air and aroma of sample to the sensor chamber alternatively. The sensor chamber contained four MOS sensor array placed in a closed air tight box. Vacuum pump (12V) was used to draw the reference air and sample air to be analyzed at the inlet and another pump (12V) at the outlet for sensor chamber cleaning. Environment air was used as the reference air in this study and to clean the sensor chamber between two sample measurements.

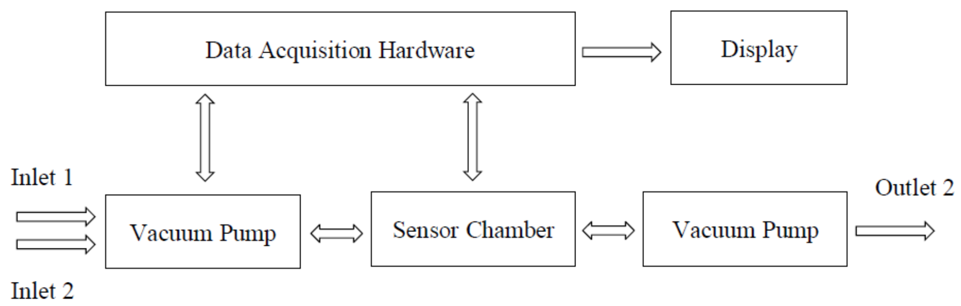

Figure 1: Schematic Diagram of Electronic Nose System

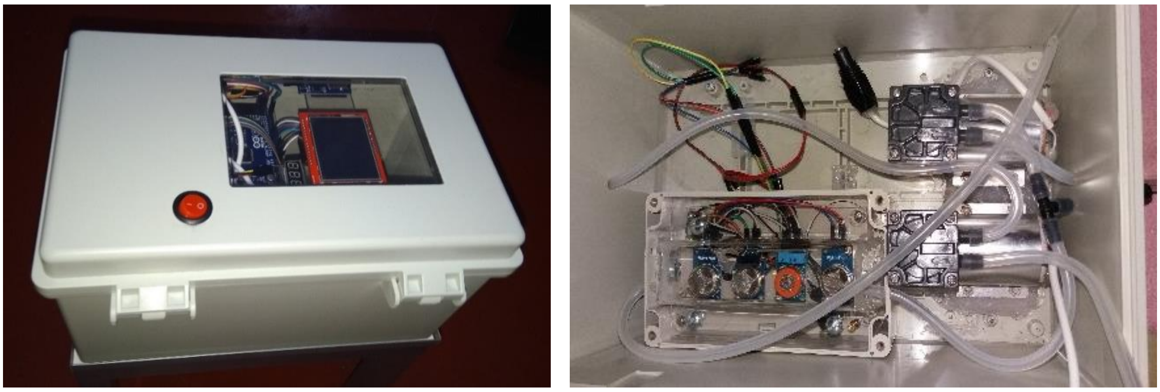

Figure 2. (a) E-nose system developed in this study (b) the sensor chamber

One sniffing cycle of sample contains the following events: sensor cleaning, sniffing process, odor lock, and sensor cleaning. A sample sniffing cycle of E-Nose system is shown in **Figure 3**. At the end of each sniffing cycle, one minute cleaning time is given for the clearing of any residual chemical in the sensor chamber. The next cycle begins soon after the cleaning and the instrument continue to collect data until the process is terminated by the user.

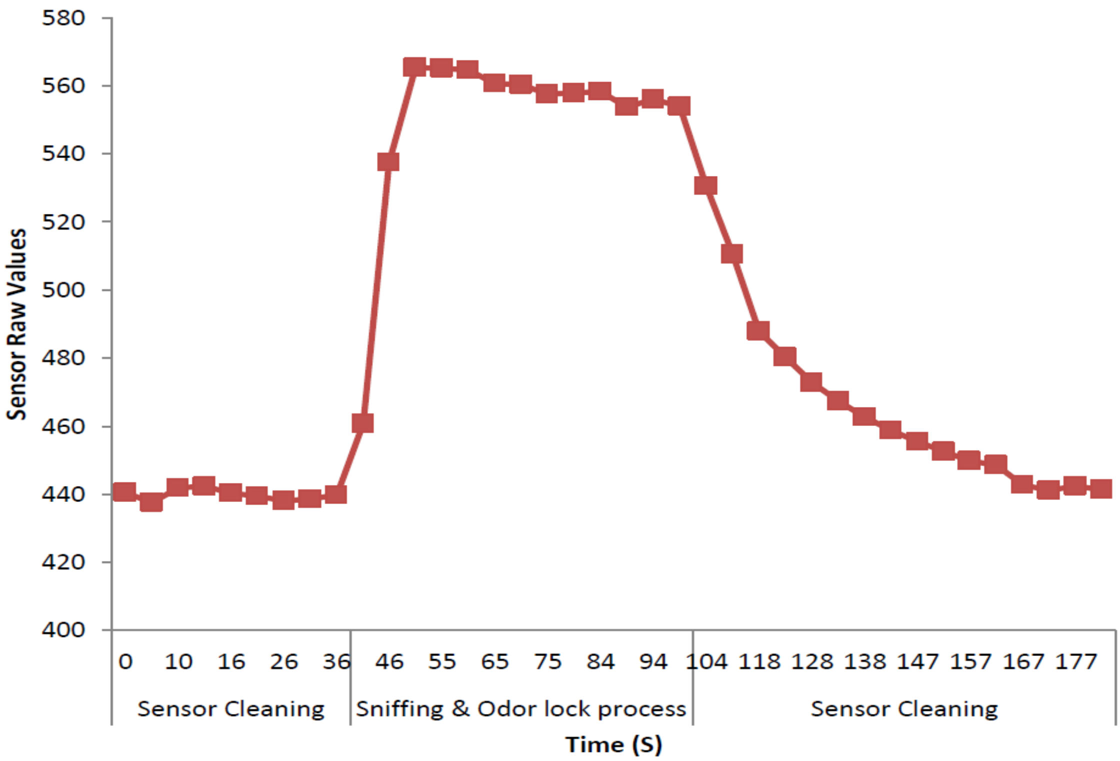

Figure 3. Samplesingle sniffing cycle of E-nose system

The sensor chamber was built using a sensor array encapsulated in an air tight water proof case with dimensions 3.5 cm x 14 cm x 3 cm. MOS gas sensors (MQx (x=2, 3, 4, 5)) were arranged in a linear direction to develop the sensor array in this study.The sensitivity of MOS gas sensors is given in the **Table 1** (HANWEI ELETRONICS CO., 2015; "MQ-2 Semiconductor Sensor for Combustible Gas," 2016; "Mq-4," n.d.; "MQ-5 Gas Sensor Technical Data," n.d.). The sensor chamber and vacuum pumps were connected using transparent tubes.

Table 1: Sensors used in sensor chamber

Sensors	Sensitivity to chemicals
MQ 2	Hydrogen, LPG, Methane, CO, Alcohol, Propane
MQ 3	Alcohol, Benzene, Hexane, LPG, CO, Methane
MQ 4	LPG, CH4, Hydrogen, CO, Alcohol, Smoke
MQ 5	LPG, Hydrogen, Methane, Alcohol, CO

Experimental Set-up

Alcohol, Acetone and Water were used to validate the E-Nose system in this study as pure substances. Small glass bottles (40 mL) were used for the alcohol (9 mL, reagent grade), acetone (9 mL, reagent grade) and water at room temperature. The sensor responses were recorded for three samples of each substance. The time of one sniffing cycle was limited to 3 minutes (1 minute for cleaning, 1 minute for sniffing and odor lock process and I minute for cleaning). The data collection was done for each sample for period of three successive sniffing cycles. Environment air was used to clean the sensor chamber and sample air inlet was closed while sensor chamber was cleaning. A continuous gas flow was maintained in the sensor chamber except during odor lock process. Then same experimental procedure was done for the mixture of those chemicals to evaluate the sensor array. Data obtained from the sensor array were stored in the micro Secure Digital (SD) card to conduct the data analysis.

Discrimination Model

Data obtained from the experiment were preprocessed initially in order to produce the optimal data model. Baseline of sensor response signal and peak alignment correction were done during the preprocessing step (López et al., 2017). In the baseline correction process, sensor response of environment air condition was subtracted from the sensor response of sample. An assumption was made as all experiments started at same time when correcting the peak alignment. In order to avoid the misalignment, all the sensor response of each test was linked together (4 sensors x 50 time points = 200 experimental data points). Finally, 33 experiments were used to build the discrimination model.

After the data preprocessing step, Principal Component Analysis (PCA) (Bartholomew, 2010; Lazaro, Ballado, Bautista, So, & Villegas, 2018; Liu et al., n.d.) was done to build the model to discriminate among the different classes. In the first step, preprocessed data were high (33 experiments X 200 data points). Then these preprocessed data were reduced to 33 experiments X number of principal components. After the dimensionality reduction process, the 3Nearest Neighbors (k-NN, k=3) (Cunningham & Delany, 2007; Moise et al., n.d.) algorithm was used for the classification process. The cross validation technique (Iii, 2009; Jung & Hu, 2015) was used to obtain the classification rate of the model.

RESULTS AND DISCUSSION

Figure 4, Figure 5 and Figure 6 show that the raw signal response values of the sensor array when the E-Nose was exposed to ethanol, acetone, and water, respectively. According to these figures, during the first 36 seconds, the sensor chamber was exposed to the environment air. Then the sensor response was changed when sample air was sniffed to the sensor chamber. This sniffing and odor lock process was done for 50 seconds. An elevated sensor raw value is obtained for each sensor MQx during odor lock period, which ultimately decreased during 70 seconds of cleaning process

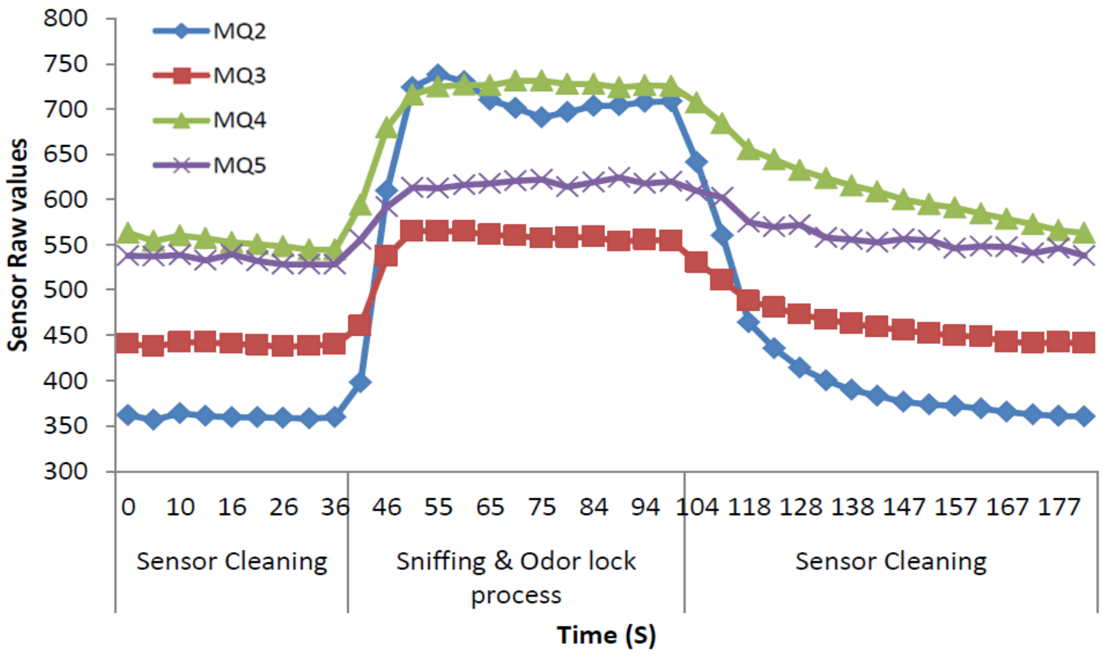

Figure 4. Response values of sensor array when exposed to ethanol

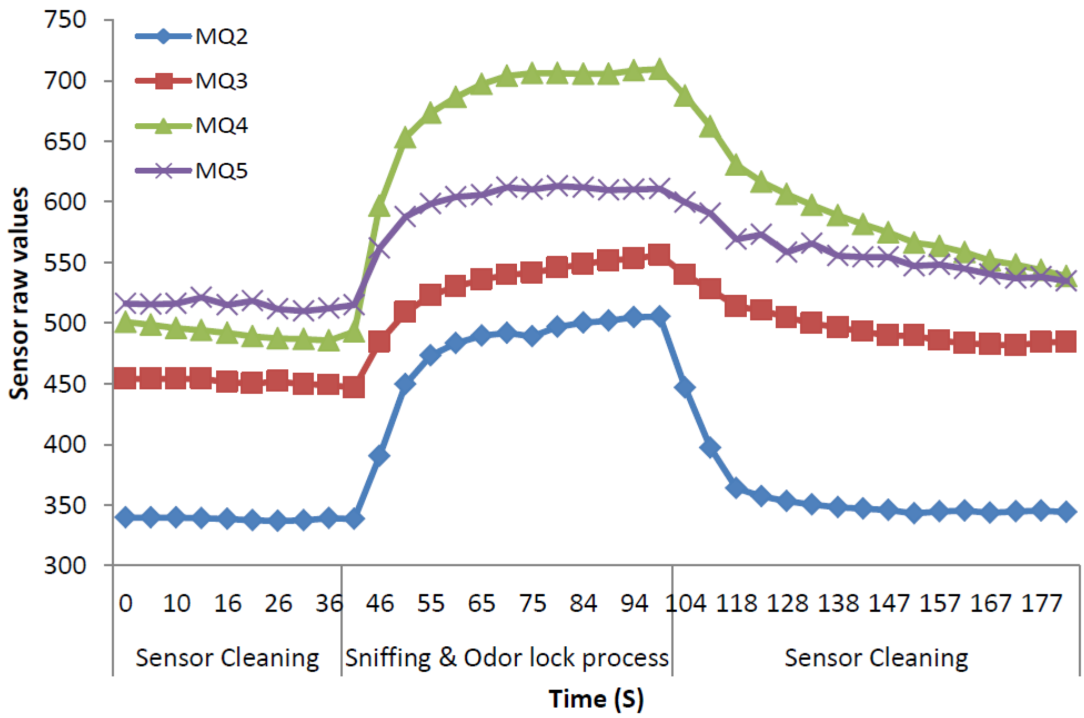

Figure 5: Response values of sensor array when exposed to acetone

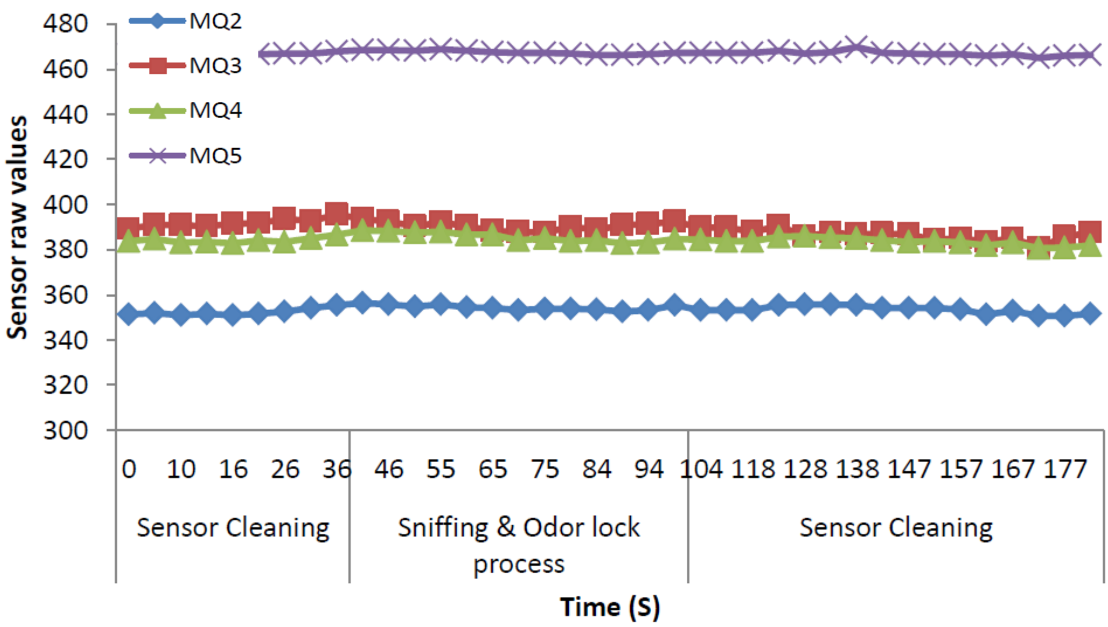

Figure 6. Response values of sensor array when exposed to water

However, the sensor raw values for baseline corresponding to the time period prior to the odor lock and after the odor lock are different for each sensor. Therefore, baseline correction is necessary to compare sensor raw values obtained for each MQx sensor. Figure 7 and Figure 8 show that the baseline corrected sensor raw signal response values when exposed to ethanol and acetone.

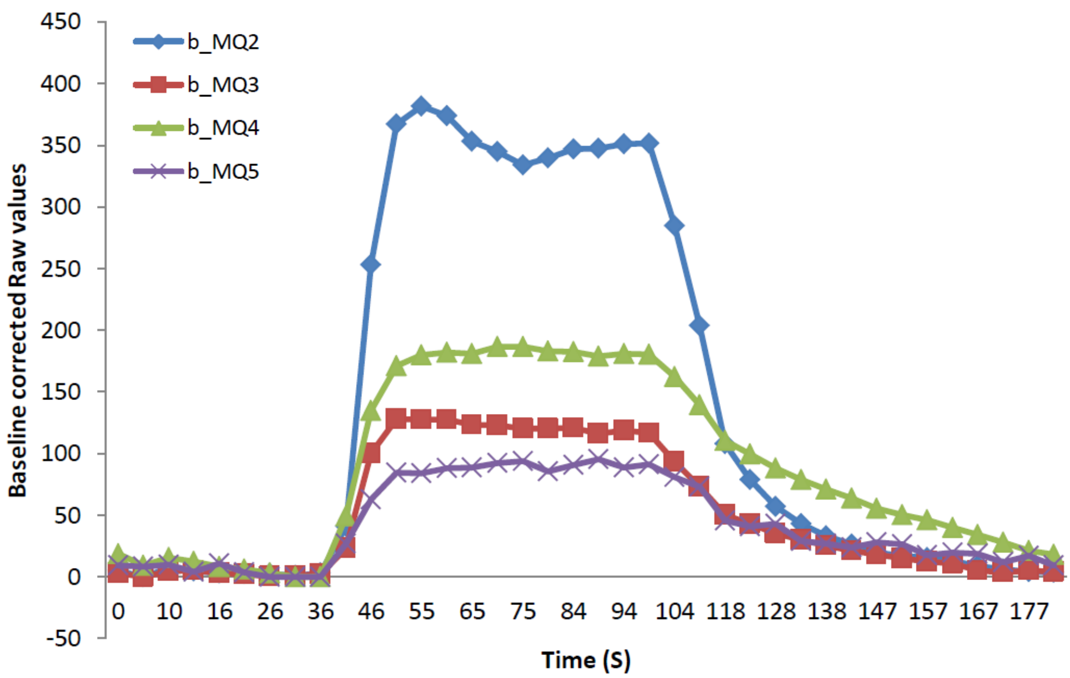

Figure 7. Base line correctedsensor response values when exposed to ethanol

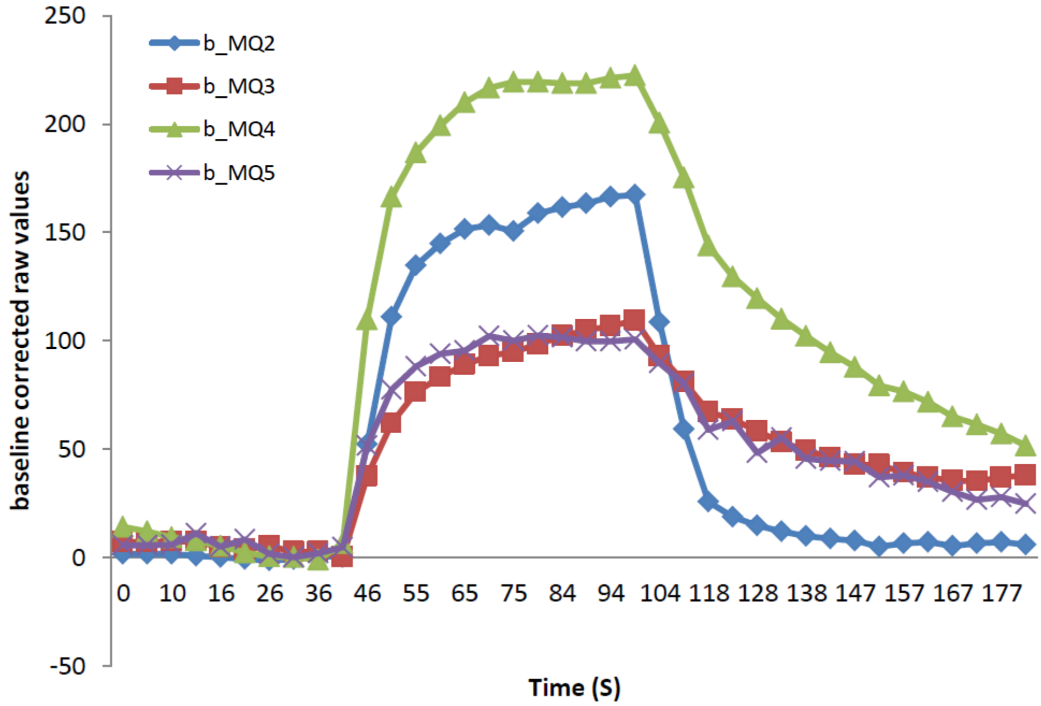

Figure 8. Base line correctedsensor response values when exposed to Acetone

According to the Figure 7, MQ2 sensor is most sensitive to the ethanol and MQ5 is least sensitive to the ethanol. It can be seen in Figure 8 that MQ4 and MQ2 are more sensitive to the acetone than others. Then peak alignment was done to the base line corrected odor locked sensor response signal values.

After the preprocessing step, three experiments of each substance are shown in Figure 9.Intensity of water is nearly zero while acetone and ethanol give high response to the sensor array. The intensity of ethanol is higher than acetone and water. MQ2 and MQ5 have nearly same response to the ethanol and acetone. MQ3 has some sensitivity compared to other sensors when the sensor array is exposed to water. Sensitivity of sensors MQ3 for ethanol is higher than acetone and water as expected according to Table 1 above.

After the preprocessing step, dimensionality reduction was done using principal component analysis. There may be variance loss, when converting the dimensional space to two dimensional space during PCA process. Therefore, variance ratio explained should be identified to find how much variance can be attributed to each of the principal components when performing dimensionality reduction. In this PCA model, first principal component contains 93.67% of the variance and the second principal component contains 6.28% of the variance. Together two components contain 99.95% of the information. Therefore, the raw matrix is reduced to 2 principal components.Eleven samples of each class are projected in the PCA model. Dimensionality reduced PCA model results are shown in Figure 10. It can be seen that acetone, water, and ethanol are completely separated when projecting the PCA model (blue- acetone, red- ethanol, yellow- water) in Figure 10. It is because of the variation in the sensor responses in the presence of different organic compounds. It can be stated that E-Nose system can discriminate among the different substances. Therefore the preprocessing step is important for the model evaluation.

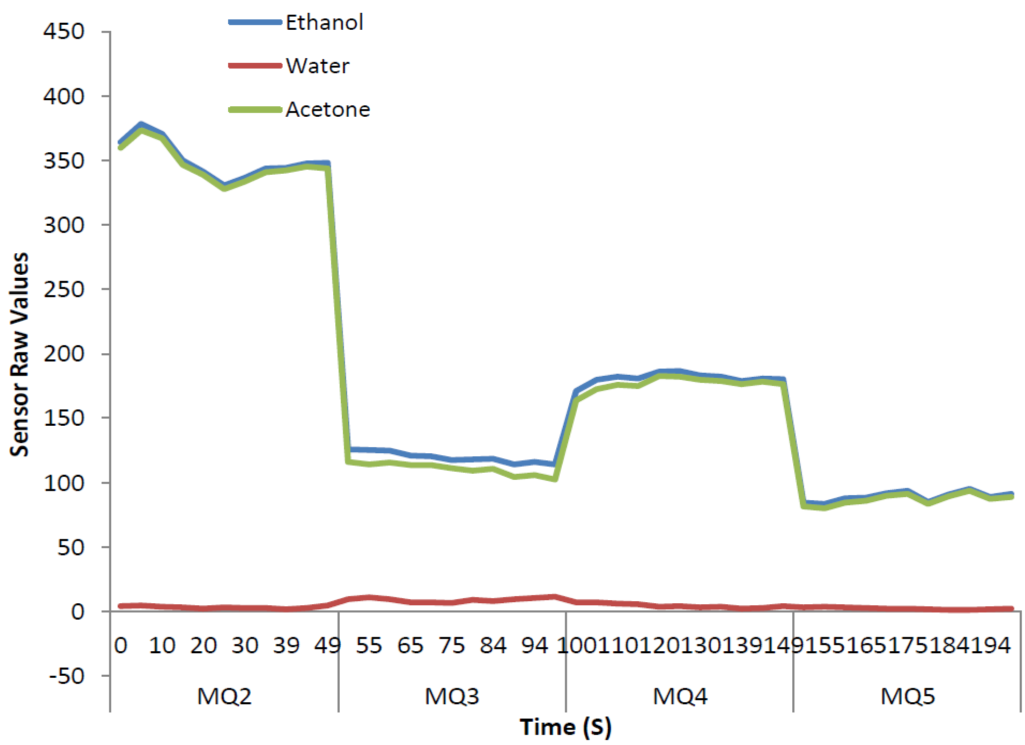

Figure 9. preprocessed sensor array values of ethanol, acetone, and water

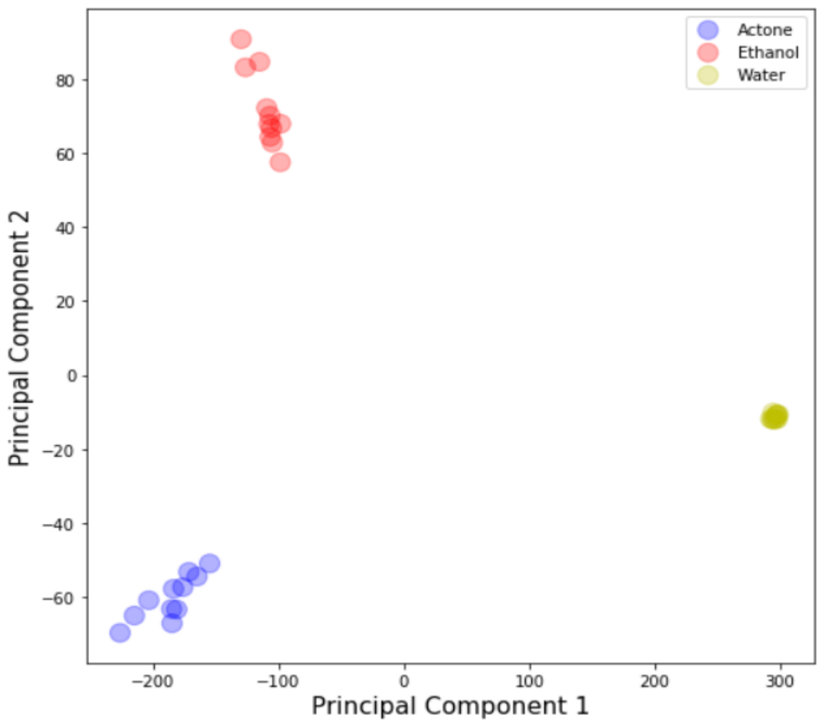

Figure 10. Two dimensional representation of the classification problem

A k-fold cross-validation method was used to assess the performance of classification in a practical way. Classification results were estimated using 10-fold cross validation technique and performed using k-NN (k=3) classification process. Classification rate was obtained as 100% with k=3. Confusion matrix of this classification process is given in Table 2.

Table 2: Confusion matrix obtained from 3-NN classification process

Confusion Matrix		**Predicted class**			**Total**
		Acetone	Ethanol	Water	
Real Class	Acetone	2	0	0	2
	Ethanol	0	4	0	4
	Water	0	0	3	3
Total		2	4	3	9

According to the Table 02, it can be said that samples are predicted 100% correctly as real samples. The sensor array was exposed to mixture of those chemicals. The response of sensor array when exposed to mixture of chemicals is represented in Figure 11.

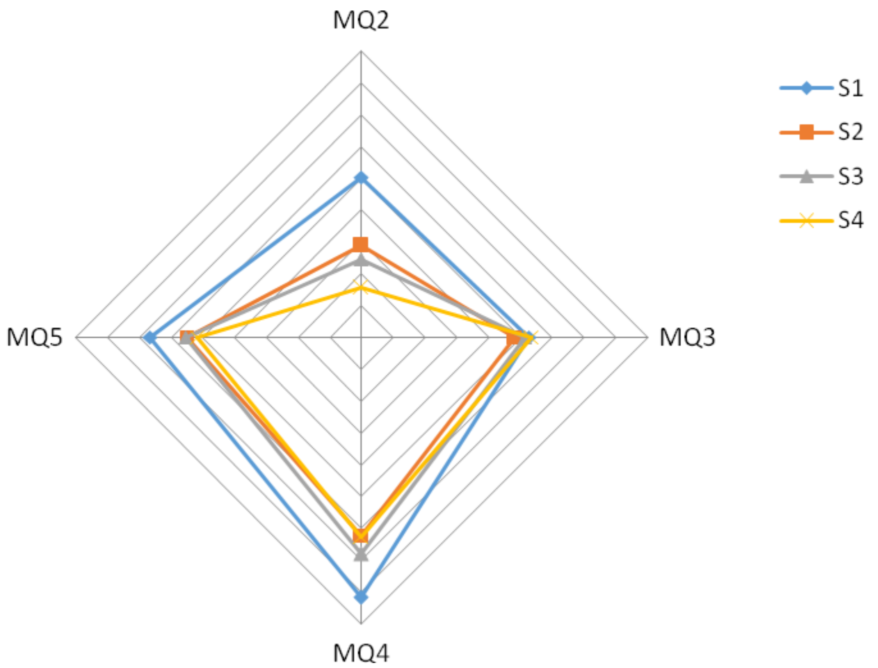

Figure 11. Sensor response when exposed to a mixture of chemicals
(S1: Acetone/water mixture 1:1, S2: Ethanol/water mixture 1:1, S3: Acetone/ethanol mixture 1:1, S4: Acetone/ethanol/water mixture 1:1:1)

When considering the outset of the spider, it can be clearly found out each mixture has a unique response for each of four sensors.

CONCLUSIONS

An effective aroma detection system developed using an array of gas sensors is presented in this paper. Three different organic substances were analyzed using the developed system and 100%

accuracy obtained by a k-nearest neighbor classification process. The 2 component PCA model indicates clear discrimination among three substance with 99.95% information. Validation of the system using more organic solvents and real world products is ongoing at present.

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