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Qualitative Assessment of Volatile Organic Compounds (VOCs) using Electronic Nose (E-Nose)

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ABSTRACT: *Electronic Nose, i.e. E-Nose is an alternate system to assess the quality of food using their odours. The odours have the information about the ripeness of the food and also contain the qualitative as well as quantitative information. To assess this information with the proper sensing system, the quality of the food is to be predicted. In this research work, eight volatile organic compounds (VOCs) are analysed and tested for identification of the different VOCs using the developed e-nose system. The aroma data is recorded using "Vapour Detection UNIT" application program developed in the Laboratory Virtual Instrument Electronic Workbench (Lab VIEW) software environment in the personal computer (PC) for analysis. Peripheral Interface Controller (PIC) microcontroller has all the necessary features to develop an E-Nose system. PIC is used for reading the sensors signal. Analog input channel of microcontroller is used to capture the E-Nose responses. Total eight metal oxide nonspecific gas sensors are used in this research work. The achieved results have very clear discrimination between the different VOC samples. Therefore, using these results, one can have used this research work for the development of their own gas sensing / electronic nose system for different applications.*

KEYWORDS: Volatile Organic Compounds(VOCs), E-Nose Setup, Pattern Recognition, Qualitative Discrimination.

1. Introduction: An electronic nose is setup using different gas sensors/gas sensor array. These are TGS gas sensors which is nonspecific MOS gas sensors. The odor/aroma of VOC is sensed by these gas sensors and gives the changed signal according to their VOC information in voltages. When odor is in contact with volatile compounds, the sensors react and a change occurs in its electrical properties [1]. These signals (data) are recorded by PIC microcontroller via ADC channels after signal conditioning. These signals are used by different preprocessing techniques, data reduction techniques and pattern recognition for the qualitative discrimination between different samples and are used for odor sample identification. The block diagram of developed electronic nose is given in figure 1. This E-nose system is used for the classification of eight volatile organic compounds (VOCs). These VOCs are very harmful for human and can be identified the diseases, like cances, using VOCc studies and are present at common places such as museum [2-10].

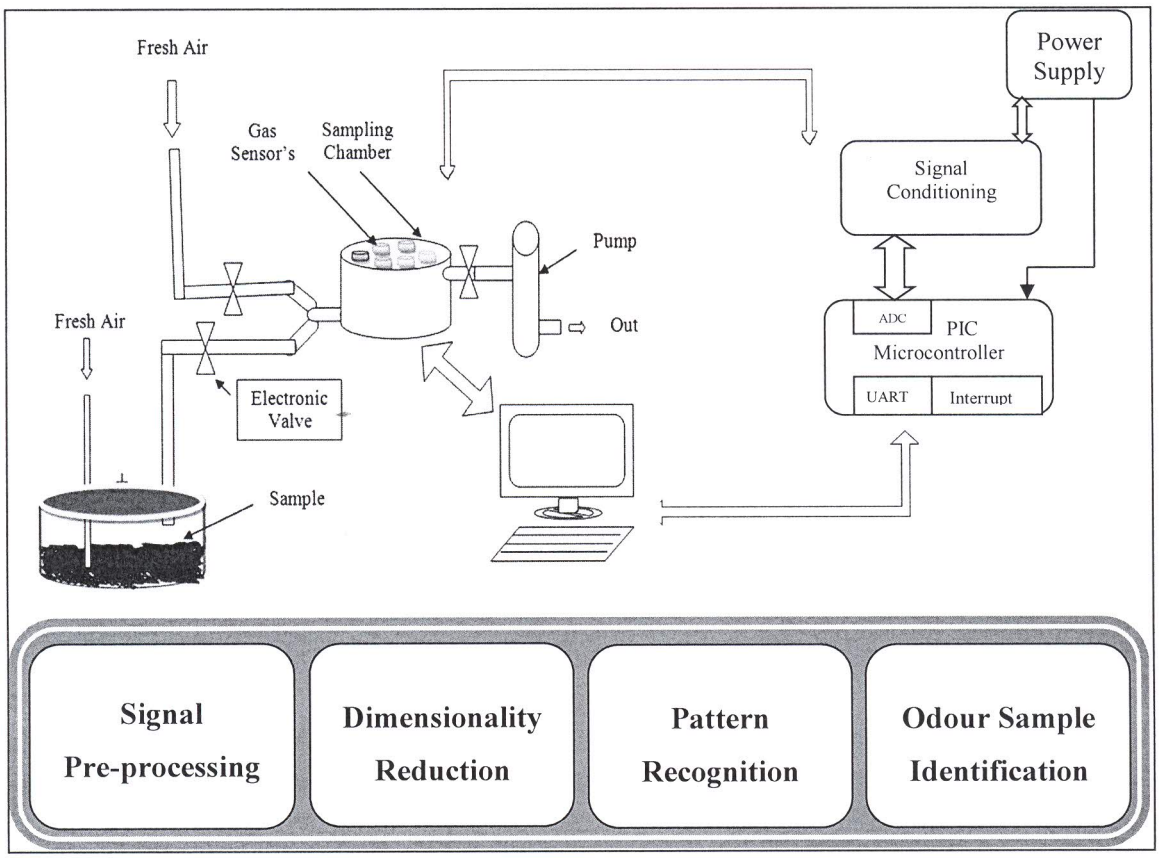

Figure 1: Block Diagram of E-Nose System

2. VOLATILE ODOUR IDENTIFICATION BY E-NOSE: Electronic nose can be used to discriminate complex vapor mixtures containing many different types of volatile organic compounds (VOCs) [11]. VOCs are also analyzed using solid phase microextraction (SPME) fibres and a newly developed method of analysis; collection of VOCs onto a polydimethylsiloxane (PDMS) elastomer strip [12]. The different organic compound is assessed with the developed e-nose sensor system. The odors of eight volatile organic chemical compounds are recorded and analyzed with different techniques. The Liquid organic chemical compound of 0.05 ml is used to make the VOC samples for E-Nose data analysis from each sample. All the analysis is done with 'The Unscrambler' and Matlab software. The samples are taken using BD U-40 Insulin syringe of 1.00 ml capacity. The analyzed volatile chemical compound is –

1. Methanol
2. Ethanol
3. Acetone
4. Isopropyl Alcohol
5. Benzene
6. Di-Ethyl Ether
7. N-Butyl Acetate and
8. Toluene

3. **PLATFORM USED:** The program is written in the C language in 'mikroC PRO for PIC', which is an open source software. The developed program can be easily dumped into the microcontroller by using the different available flash software for PIC microcontroller as mikroProg Suit, MPLAB IPE v2.30 etc. The PICkit 3 hardware is used for programming the microcontroller. The development of E-Nose is given here for the structure and functional working of electronic nose.

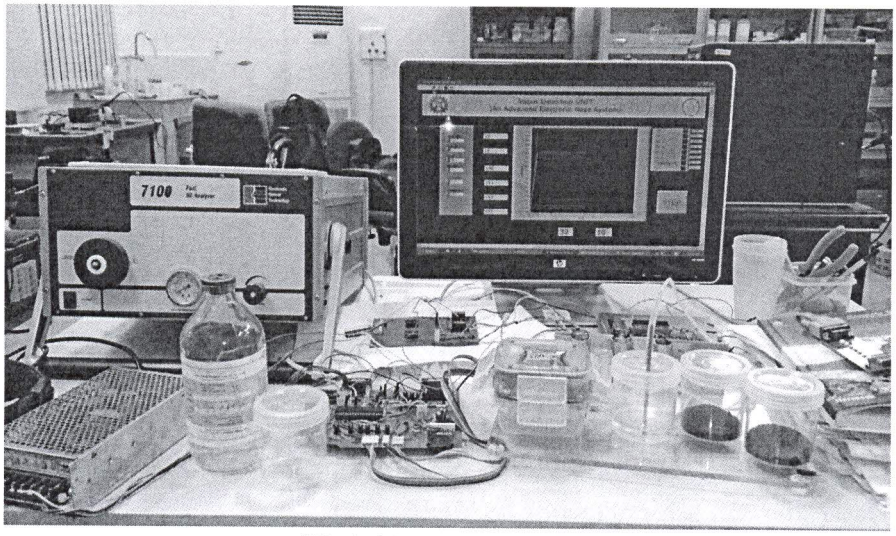

Fig2 (a)- E-Nose Setup

Fig(b)

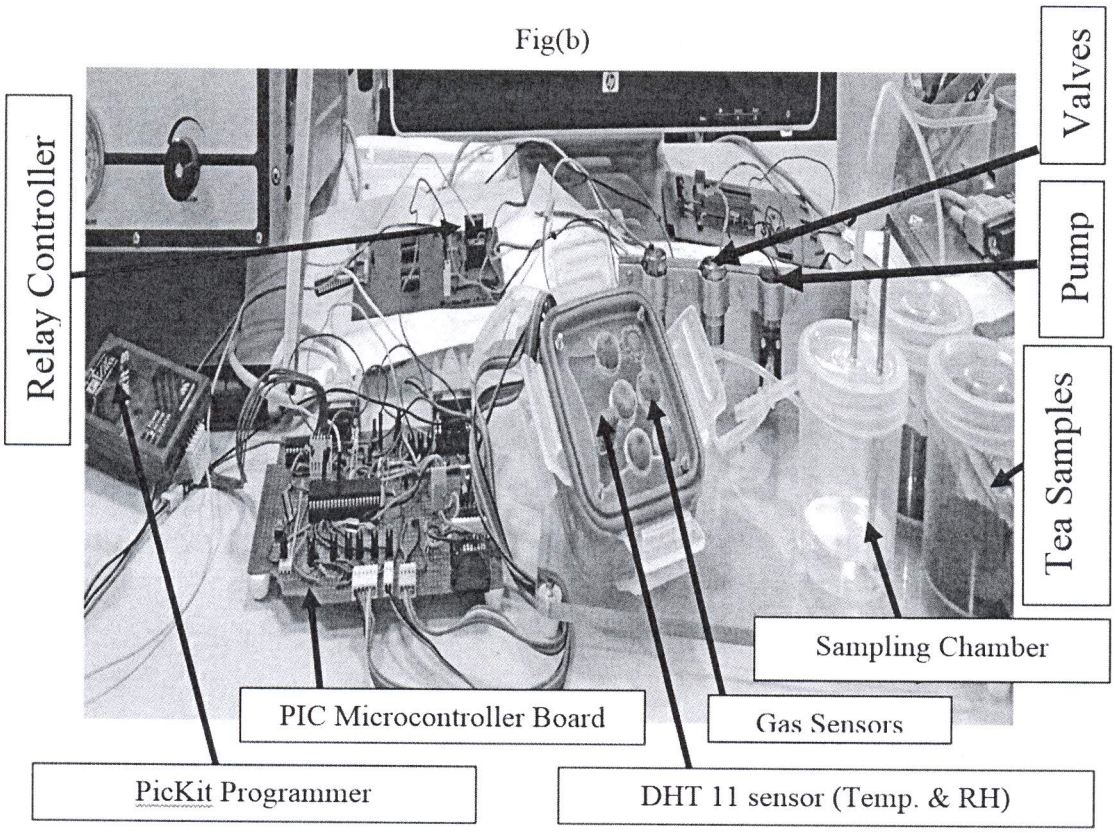

Figure 2. (a)- E-Nose Setup, (b)- Hardware

4. E-NOSE EXPERIMENTAL SETUP:

The E-nose (gas sensor array) is interfaced with the PIC 16F877A microcontroller. The microcontroller is interfaced with GAS sensors, Valves (for purging and sensing), pump (for odor sucking) and serial port (for microcontroller data to PC). LabVIEW application software is developed in PC for receiving the data from PC serial port and saves the data for further data analysis. The E-Nose system and their hardware setup is given in Figure 2(a) and 2(b).

- PicKit device programmer is used to program the hex file into PIC microcontroller.
- LabVIEW software is used for developing the application in PC for receiving the data from PC COM port, and visualizing the data in Graphical form and data storing into text file.
- MicroC software is used here to read the gas sensor's signal through the analog input port and to control the valves and pumps accordingly and sends the data to COM port.
- E-Nose has gas sensor array with following metal oxide sensors-

TGS – 813	(for detection of Combustible Gases)
TGS – 816	(for detection of Combustible Gases)
TGS – 821	(for detection of Hydrogen Gas)
TGS – 822	(for detection of Organic Solvent Vapors)
TGS – 823	(for detection of Organic Solvent Vapors)
TGS – 825	(for detection of Hydrogen Sulfide)
TGS – 2611 and	(for detection of Methane)
TGS – 2620	(for detection of Solvent Vapors)

- The sensing element of Figaro gas sensor, which consists of a Tin Oxide (SnO2) semiconductor has low conductivity of clean air. In the presence of a VOCs/detectable gas, the sensor's conductivity increases depending on the aroma/VOCs concentration in the air. A simple electronic circuit is used to converts the change in conductivity as an output signal, which corresponds to the VOCs concentration [13].

5. LAB VIEW PROGRAM FOR E NOSE SYSTEM

Data Recording is done using developed LabVIEW Application program. The application window is given the name as Vapour Detection UNIT. The PC serial port is configured to read data from PIC microcontroller serial port. The sensors data are coming from PIC microcontroller and these sensors data are stored in the PC for further data analysis.
The setting for the PC Serial Communication is –

Baud rate = 9600 (same as PIC baud rate)
Data bit = 8
Parity = none
Stop bit = 1
Flow control = none
Time out = 10000 ms

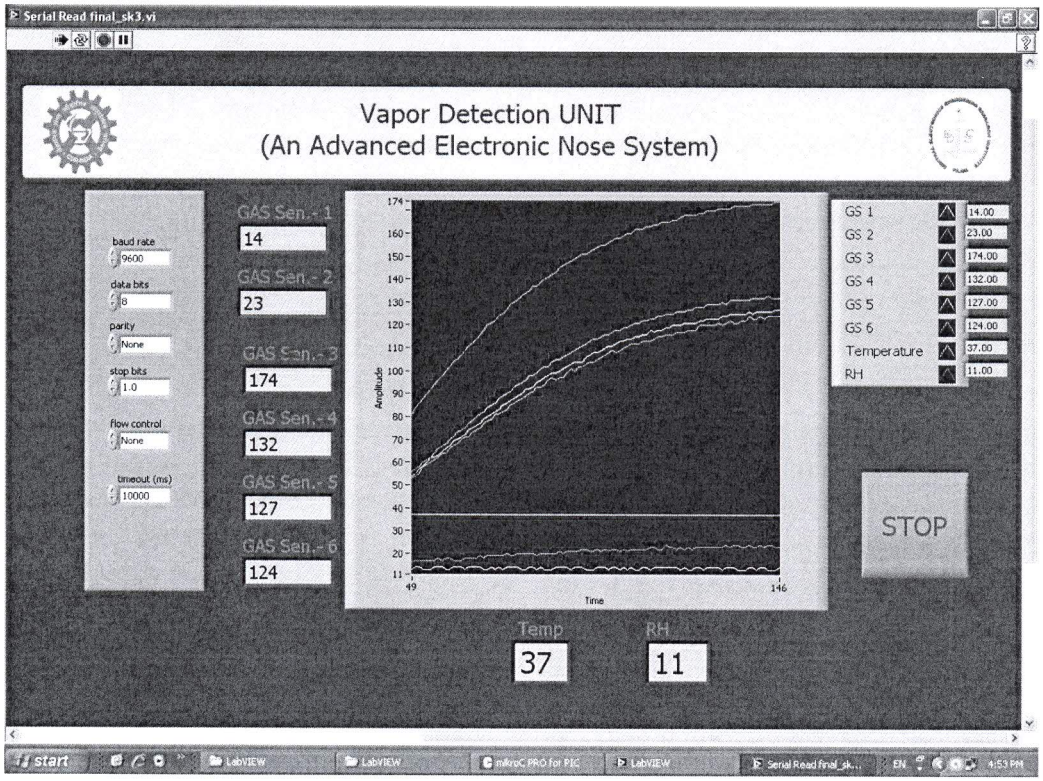

Fig 3: E-Nose Front Panel Software in Labview

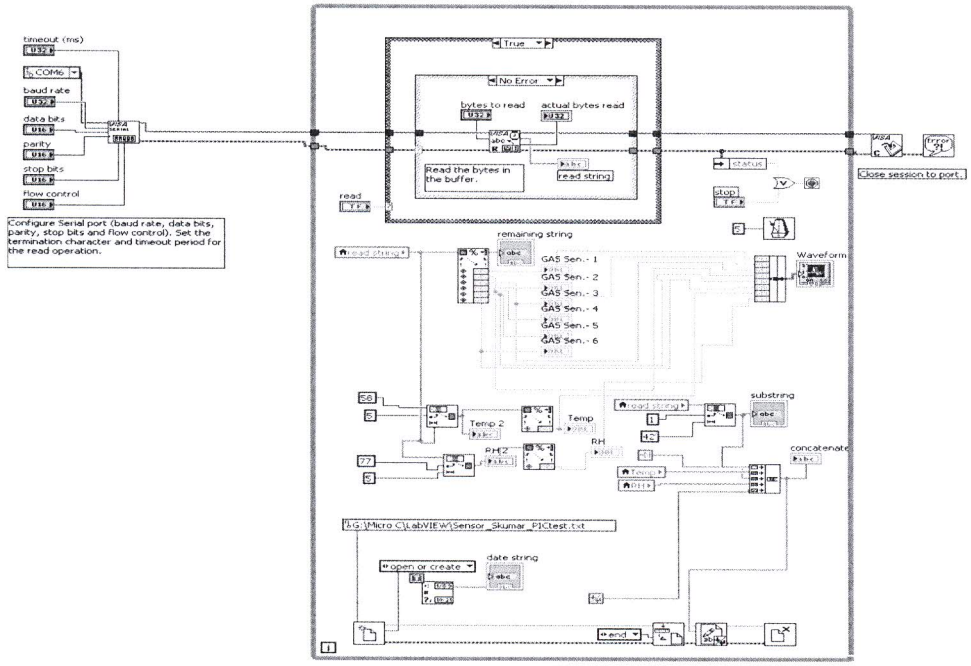

Figure 4: E-Nose System Diagram (Application Program in Labview)

Using the Pic Programming and LabVIEW application program (Figure 3,4), we have achieved excellent results and any one can develop their own application in C program or in any language to develop the electronic node setup and utilise these research for different aroma/ odor

discrimination qualitatively as well quantitatively. For Quantitative means of analysis, one need to develop very precise system using hardware and software. Any odour can be analysed with proper airtight E-Nose sampling system.

6. RESULTS AND CONCLUSION:

The above volatile organic compounds are analyzed with 'The Unscrambler', a standard statistical software package. The data is first normalized using maximum normalization method. This normalized data is used for PCA analysis, the normalized data plot is given in figure 5. Scores achieved by PCA analysis are used to develop the linear Discriminant analysis model. The LDA model gives 98.75 % classification accuracy with 2 principal components (PC) and 100% accuracy with 3 PCs. All these 8-VOCs are successfully identified in their respective group of clusters as shown in figure 6.

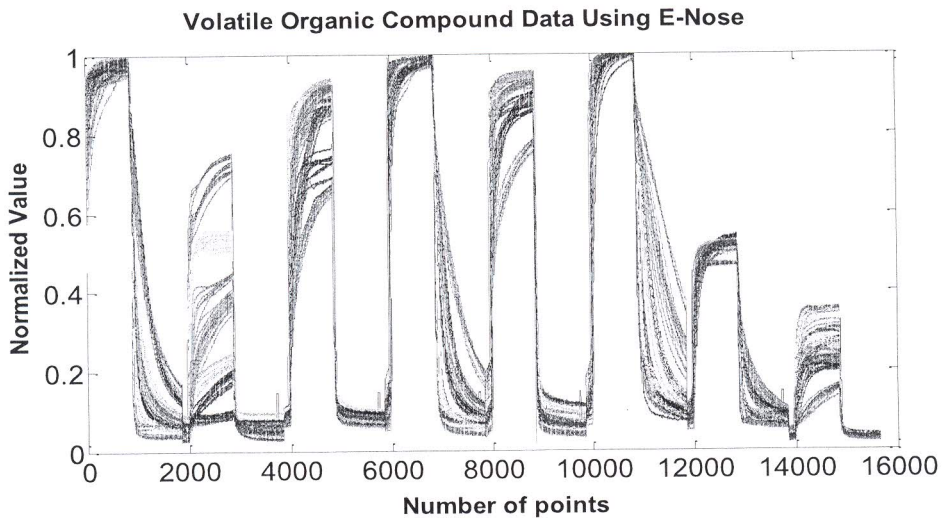

Figure 5: E-Nose Sensor Response of VOCs

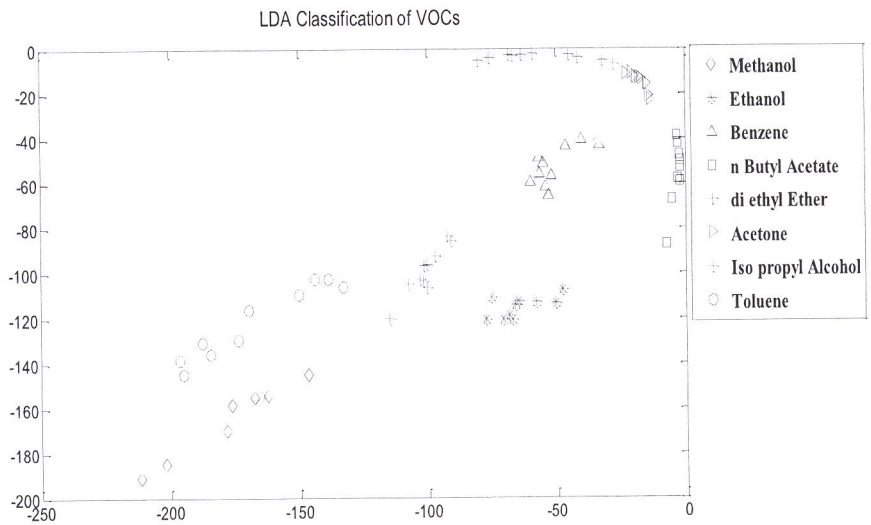

Figure 6: LDA Classification of VOCs

Therefore, the response achieved by e-nose system is very encouraging for analyzing the different VOCs samples. The interaction of the volatile compounds and the conducting polymer surface produced a change in electrical resistance and then produced a signal which can be measured and analyzed by data processing system [14]. Now in the future, we have to take the food samples for their quality assessment using this nondestructive aroma analysis. E-nose gives sufficient information, so that the aroma is used to identify the samples variety using these techniques over E-nose aroma data. we have to acquire some knowledge about data preprocessing techniques and pattern recognition analysis. The MATLAB gives sufficient information with various examples. The electronic nose can be used in the food applications and it is also very useful system to identify the different disease [15]. The advanced electronic system i.e; gas chromatography-mass spectrometry (GC-MS) method are also used to get the compositions of VOCs [16]. The electronic nose setup is the futuristic requirement for the detecting of atmospheric volatile organic compound because of its increasing level in different time periods of the day and seasons and accordingly the need of alarming system for different VOCs [17]. The application can be utilized in different methods like , bar chart, profile, polar and offset polar plots, Multivariate data analyses (MDA), principal component analysis (PCA), canonical discriminate analysis (CDA), featured within (FW) and cluster analysis (CA), Network analyses: artificial neural network (ANN) and radial basis function (RBF) [18]. Therefore, this research work can be utilized by the young researchers as well as the researchers have some interest in this field can take the benefits from MATLAB and utilize the given research.

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