MOS Based Sensor Array System for the Detection of Human Breath Volatile Organic Compounds

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ABSTRACT

This paper discusses the fabrication and testing of an electronic nose (e-nose) system to detect the breath volatile organic compounds (VOC) present in the exhaled breath of humans. The exhaled breath consists of several VOCs in addition to the main components like nitrogen, oxygen, and carbon dioxide. Some of these VOCs are biomarkers for certain lung diseases, and can even identify smokers and drinkers by the variations of VOCs. This involves the use of sensor arrays, consisting of five metal oxide (MOS) gas sensors to detect the VOC profile of interest. This paper describes the gas sensor selection process and sensor array fabrication method, to develop the e-nose system. It uses five MOS sensors, an Arduino, and an analysis of processed sensor data to identify and label the various lung conditions. The e-nose system was tested in a small pilot study involving 10 subjects, to verify the operation of the e-Nose, and the results of the study are also included, along with the conclusions drawn from the work.

Keywords

Breath analysis; e-nose; sensor array; volatile organic compounds

1. Introduction

The exhaled human breath consists of various volatile organic compounds (VOCs) in very low concentrations of the order of parts per million (ppm) or parts per billion (ppb). The major components of the exhaled breath are shown in the figure 1, and the composition is 75% nitrogen, 13% oxygen, 6% water vapor, 5% carbon-di-oxide, and 1% volatile organic compounds. The 1% of VOCs in the exhaled breath consists of more than 1500 gases and produced either by the endogenous or exogenous method [1]. The lung conditions of humans can be identified by the analysis of these breath VOCs and even pulmonary disease classifications can be done. The production of certain VOCs in the human breath is by oxidative stress which is by the degradation of polyunsaturated fatty acids. The exhaled breath VOC components such as isoprene, ethane, acetone, carbon monoxide, pentane, isobutane, propane, etc can give intuitions into several biochemical processes in people affected with various lung diseases and healthy controls [2]. These VOCs are used as disease biomarkers for different pulmonary illnesses like cystic fibrosis, chronic bronchitis, asthma, lung cancer, chronic obstructive pulmonary diseases are shown in table 1.

Breath analysis is an easy, painless, sensitive, and economical method and hence it is becoming more popular in the disease diagnosis of various diseases. [11] Different techniques for the breath gas analysis are Gas chromatography–mass spectrometry (GC-MS) [12,13], Electronic noses (eNoses)[12,13,14], Ion mobility spectrometry (IMS) [12,15], Gas Chromatography-Flame Ionized Detection (GC-FID) [16], Proton Transfer Reaction-Mass Spectrometry (PTR-MS) [17], Laser Photoacoustic Spectroscopy [18], and Differential Mobility Spectrometer (DMS) [12].

Electronic noses are an array of different types of sensors that responds to a mixture of breath VOC gases. E-nose technology is nowadays used in various fields such as food and beverages, chemical analysis, and military [19]. An increasing number of researches being carried out in the VOC analysis of breath using e-nose for disease diagnosis. Electronic noses are almost similar to the human olfactory system which measures the whole VOC spectrum without identifying separate VOC components [14]. The output of e-Nose is a 'breath signature' or 'breath print' which is a breath pattern corresponding to the VOCs come in contact with the sensor array. The breath signature can be analyzed using machine learning and deep learning algorithms for disease diagnosis without recognizing the separate VOCs in the exhaled breath.



Figure 1. Components of exhaled human breath

Table 1. L	ung disease	VOC bio	markers

Disease	VOC Biomarkers	Reference
Asthma	Ethane, Pentane, Isoprene	5
Chronic obstructive	Ethane, Pentane, Undecane,	6
pulmonary disease	Hexadecane, Octadecane	
Cystic fibrosis	Pentane, Carbonyl sulphide,	7
	Ethane, Methyl thiocyanate	
Lung Cancer	Isoprene, propanol, acetone,	8
	hexanal, and toluene	
Pneumonia	Acetone, nonanal, ethanol,	9
	and heptane	
Acute Respiratory Distress	Acetone, Isoprene, n-	10
Syndrome	Pentane	

The gas sensors used for the volatile organic compound analysis should give high responses, high selectivity, and high stability. The various gas sensors used in the sensor array for e-nose fabrication are solid-state electrochemical sensor, colorimetric sensor, metal oxide semiconductor

sensor, surface acoustic wave sensor, conducting polymer sensor, optical sensors, and quartz crystal microbalance sensor [20]. Metal oxide semiconductor (MOS) is one of the most common technologies used in the e-nose system sensor array. Based on the majority carrier type, the MOS sensors are either p-type (majority carriers are holes) or n-type (majority carriers are electrons). The working is based on the equilibrium shift of the surface reactions corresponding to the target analytes [21]. The reducing gases such as carbon monoxide, ammonia, hydrogen, etc cause a rise in conductivity for n-type semiconductors and a fall for p-type semiconductors. Similarly, oxidizing gases such as nitrogen dioxide, chlorine, ozone, etc cause a rise in conductivity for p-type semiconductors and a fall for n-type semiconductors. N-type MOS gas sensors are widely used in the field of breath research due to its high response rate.

In this work, we have developed an e-nose system using MOS gas sensors to detect the presence of volatile organic compounds present in the expelled breath of humans. The VOC profile of humans is a signature pattern and varies for individuals. The lung conditions of humans can be analyzed with the developed system. It is an economical system with five MOS gas sensors, an Arduino Uno Rev3 developer board, and an analysis of the processed data. The breath samples of ten study subjects were analyzed using e-nose to understand their lung conditions. This system can be further used for the detection of various pulmonary diseases like lung cancer, bronchitis, chronic obstructive pulmonary disease, etc.

2. Materials and Methods

2.1.Gas Sensors

The gas sensors used in this work are common semiconductor metal oxide gas sensors developed by Figaro USA. They are TGS 2600, TGS 2610, TGS 2620, TGS 822, and TGS 826. The details and specifications of the sensors are shown in table 2 [22]. When the detectable gases are present, the sensor's electrical resistance decreases depending on the gas concentration in the air. This can be converted into an output signal with the help of a simple electrical circuit.

The features such as highly sensitive to air contaminants, consumes low power, durability, reduced cost, and tiny size made this sensor of our choice. All these sensors are cross response sensors and not gas specific sensors. The circuit voltage and heater voltage of TGS sensors are 5 V, but for circuit voltage 5V DC is compulsory whereas for heater either DC or AC is acceptable. For all the sensor circuits, the minimum value of load resistor required is 0.45 K.

The TGS 2600 sensor gives high sensitivity to air contaminants such as methane, isobutane, ethanol, and carbon monoxide. TGS 2610 is used for the detection of petroleum gas. They give high sensitivity to ethanol, hydrogen, methane, isobutene, and propane. TGS 2620 is used for the detection of solvent vapors and gives high sensitivity to ethanol, hydrogen, methane, carbon monoxide, and isobutane. TGS 822 are commonly used in alcohol detectors and this sensor is highly sensitive to benzene, acetone, ethanol, and methane. TGS 826 gives high sensitivity to ammonia, ethanol, hydrogen, and iso-butane.

Sensor	TGS 2600	TGS 2610	TGS 2620	TGS 822	TGS 826
Model					
Detected	Methane,	Ethanol,	Carbon	Acetone,	Ammonia,
Compounds	Isobutane,	Methane,	Monoxide,	Ethanol,	Ethanol,
	Ethanol,	Propane, and	Ethanol,	Benzene, and	Hydrogen, and
	and	Isobutane	Isobutane,	Methane	Isobutane
	Carbon		and Methane		
	Monoxide				
Detection	1-100	300-10000	50-5000	50-5000	30-300
Range (ppm)					
Picture	60 13 T 4		2620 292TD		
Heater	5.0±0.2V	5.0±0.2V	5.0±0.2V	5.0±0.2V	5.0±0.2V
Voltage(VH)	AC/DC	AC/DC	AC/DC	AC/DC	AC/DC
Circuit	5.0±0.2V	5.0±0.2V	5.0±0.2V DC	5.0±0.2V DC	5.0±0.2V DC
voltage (VC)	DC	DC			
Load	Min 450 Ω	Min 450 Ω	Min 450 Ω	Min 450 Ω	Min 450 Ω
resistance					
(RL)					
Heater	83 Ω	59 Ω	83 Ω	38±3 Ω	30±3 Ω
Resistance					
Heater	42±4mA	56±5mA	42±4mA	42±4mA	167mA
current					
Heater power	210mW	280mW	210mW	660mW	833mW
consumption					
Sensor	10kΩ -	1kΩ -10kΩ	$1k\Omega - 5k\Omega$	1kΩ -10kΩ	20kΩ -100kΩ
resistance	90kΩ				
Sensor	0.3-0.6	0.45-0.62	0.3-0.5	0.3-0.5	0.4-0.7
resistance					
ratio					

Table 2. Details and sp	ecifications	of TGS	sensors
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2.2. Arduino Uno Rev3 developer board

Arduino Uno Rev 3 is an ATmega328P based microcontroller board that has numerous applications. A picture of the developer board is shown in figure 2. The Uno has fourteen digital I/O (input-output) pins, in which six can be used as pulse width modulation (PWM) outputs, six analog inputs, and a 16 MHz ceramic resonator, In-Circuit Serial Programming header, a universal serial bus connection, a power jack, and a reset button. The developer board has everything required to support the controller, easily connect the board to a PC/laptop with a USB cable or else power it using a DC adapter/battery. The Arduino Uno Rev 3 has an 8-bit AVR

Microcontroller with 32K Bytes in-system programmable flash, ATmega 328P. The board can be powered either with an external power supply or with a USB connection. An external input voltage of 6 V to 20 V can be applied to the board, but the recommended voltage level is 7 V to 12 V [23].



Figure 2. Arduino Uno developer board

2.3. The e-Nose system

The final arrangement of the e-nose system is shown in figure 3. The sensor array set up is as shown in the figure and the output of each TGS sensor is driven using a load resistance of 1 K. The input voltage and heater voltage supplied to each sensor is 5 V DC. The working of the system is such that in response to the changes in input gas concentrations a change in analog output voltage occurs which is between 0 V and 5 V. The arduino board converts that signal into a digital signal for further data analysis.



Figure 3. The e-Nose system

2.4. Study participants and data collection

For this study, we enrolled 10 volunteers and collected their breath samples, using the e-nose system. All the study subjects were from the Kottayam municipality of Kerala state in India. The major characteristics of the study subjects are shown in table 3. We have collected written informed consent from all the volunteers under the study. Out of the ten participants, six were male and four were female. To get a clear idea about the changes of breath VOCs for person to

person, we have selected smokers, non-smokers, drinkers, non-drinkers, and subjects with the consumption of daily medicines. We have also considered the age of the participants which varied from 18 to 65. The education and occupation of the study subjects were also different.

Sex	Age	Type of work	Weight (Kg)	Cigarette Smoking	Alcohol Drinking	Remarks
Female	65	Housewife	73	Non- smoker	Non- drinker	Daily medications for hypertension
Male	60	Retired builder	81	Heavy smoker	Heavy drinker	Daily medications for diabetes mellitus, high cholesterol, and hypertension
Male	54	Mason	64	Heavy smoker	Moderate drinker	Daily medications for diabetes mellitus
Male	46	Farmer	74	Moderate smoker	Heavy drinker	Chronic Bronchitis
Male	38	Software tester	108	Light smoker	Moderate drinker	No major diseases and daily medications
Male	33	Teacher	72	Non- smoker	Non- drinker	No major diseases and daily medications
Female	30	Nurse	54	Non- smoker	Non- drinker	No major diseases and daily medications
Female	28	Web developer	53	Non- smoker	Light drinker	Daily medications for migraine
Male	24	Student	66	Light smoker	Light drinker	Had Hyperpyrexia two weeks back
Female	18	Student	48	Non- smoker	Non- drinker	Asthma
Heavy smoker- Smokes more than 25 cigarettes per day						

 Table 3. Details of the study subjects

Heavy smoker- Smokes more than 25 cigarettes per day Moderate smoker- Smokes more than 10 but less than 25 cigarettes per day Light smoker- Smokes 10 or fewer cigarettes per day Heavy drinker- Consumes more than 3 drinks per day Moderate drinker- Consumes 1 to 2 drinks per day Light drinker- Consumes 1 to 3 drinks per week

The sensor array gave a 'breath print' corresponding to all the study subjects' exhaled breath. The breath profiles of each individual were different based on the amount of VOCs present in their breath. The measurement cycle was two minutes and we sampled the exhaled breath from all the participants nine times. The samples were taken at 8 am before breakfast, at 1.30 pm after lunch, and at 7 pm before dinner in three days. The subjects selected for the breath test were restricted

from smoking and drinking alcohol on the breath sampling and a day before the test. The sensor array response was almost similar for all the nine measurements and thereby verifies the good repeatability of the system.

3. Results and Discussions

The sensor array was able to discriminate between smokers and non-smokers, and alcoholic and non-alcoholic (fig 4 to fig 13). The average values of all nine measurements are shown in figure 4 to figure 13. Referring to the figures we can say that the output voltages of all sensors are higher for smokers and alcoholics than non-smokers and non-alcoholic. This is the result of detected VOCs like carbon monoxide, ethanol, and ammonia with the sensors. When a combination of VOCs is exposed to particular TGS sensors, and when the concentration of that gaseous mixture increases the sensor resistance decreases, and thereby the output voltage across the load resistor connected with the sensor increases.



Figure 4. Sensor array response to 65-year-old female



Figure 5. Sensor array response to 60-year-old male



Figure 6. Sensor array response to 54-year-old male



Figure 7. Sensor array response to 46-year-old male

The sensor TGS 2610 which is highly sensitive to ethanol gave a maximum output voltage of 1.37 V for the gas sample from the volunteer who is a heavy alcoholic and heavy smoker aged 60. The daily medicines for diabetes mellitus, high cholesterol, and hypertension also affected the high output response. For a male moderate drinker with an age of 38 and with no major diseases or daily medications, this sensor gave a maximum output voltage of 1.31 V. For another moderate drinker who is a mason aged 54 and using medicines for diabetes, the sensor gave a maximum output of 1.33 V. The light drinkers selected for the study was a master's student and a web developer, and the maximum output voltage produced in response to exhaled breath is 1.23 V and 1.25 V respectively. From the figures, we can say that the output voltages to exhaled breaths of non-alcoholic study subjects reduced significantly.

TGS 2600 and TGS 2620 are sensitive to ethanol and carbon monoxide, thereby producing more output voltages for exhaled breaths of smokers and drinkers. It can be noted from the graph that TGS 2600 and TGS 2620 output is almost constant for the whole measurement period for all the study subjects. Both of these sensors gave an output voltage in the mV range. For non-smoker group, the sensor TGS 2600 produced a minimum voltage of 137 mV and a maximum of 235 mV whereas the minimum output voltage of TGS 2620 was 204 mV and a maximum of 450 mV. For

the retired builder aged 60 who is an alcoholic and heavy smoker for the past 35 years, TGS 2600 sensor produced a maximum voltage of 259 mV at a measurement time of 34th second. The TGS 2620 output for the exhaled breath of him was gradually increased from 274 mV to a maximum value of 489 mV and then reduced finally to 338 mV at the final seconds of measurement. Both the sensor responses to the exhaled breath of a male student who is a light drinker and smoker, and a female web developer who is a light drinker and non-smoker were almost the same.







Figure 9. Sensor array response to 33-year-old male

The sensor TGS 826 is highly sensitive to ammonia. Since the cigarette smoke contains ammonia, the exhaled breath of smokers can detect the presence of ammonia. For the exhaled breath of heavy smokers, the TGS 826 produced a higher voltage than that of non-smokers or light smokers. For the retired builder and mason (heavy smokers) this sensor had given a maximum voltage of 853 mV and 813 mV respectively. The maximum value for this sensor noted in non-smokers is in male teacher aged 33 and is 588 mV. For the only moderate smoker of our study who is a farmer aged 46, this sensor output voltage increased from an initial value of

437 mV to 759 mV at the 38^{th} second of the measurement cycle and then continuously reduced to a final value of 640 mV at the end of the second minute.

TGS 822 gas sensor gives high sensitivity to acetone and ethanol, thereby giving increased output voltages to exposed breaths of alcoholic than non-alcoholic. For the non-drinker study subjects a teacher aged 33, a nurse aged 30, a housewife aged 65, and a student aged 18, this sensor produced a maximum output voltage of 656 mV, 625 mV, 696 mV, and 658 mV respectively. For the moderate drinkers, software tester and mason the maximum output voltage produced is 848 mV and 874 mV respectively. To the exhaled breath sample of the retired builder, the sensor output voltage started from an initial value of 659 mV and gradually increased to a maximum value of 889 mV and returned to a reduced value of 718 mV at the 120th second. Similarly for the farmer from a starting value of 572 mV at the first second of the measurement elevated to a value of 805 mV at the 41st second of the measurement phase and then finally at the 120th second the value reduced to 630 mV.



Figure 10. Sensor array response to 30-year-old female



Figure 11. Sensor array response to 28-year-old female



Figure 12. Sensor array response to 24-year-old male



Figure 13. Sensor array response to 18-year-old female

4. Conclusions

The e-nose system was able to detect the presence of volatile organic compounds in the exhaled breath of participants under study. The system could recognize the 'breath signature' based on human breath and can be extended in the study of patients with various respiratory diseases. Here we have presented the possibility and adaptability of the e-nose system in examining the breath VOC components of the subjects with dissimilar sex, age, height, weight, profession, medical conditions and history, drinking and smoking habits. In the developed sensor array system, all the MOS sensor output voltage was directly proportional to the input VOC gases applied to it. For example, the elevated levels of ethanol in the exhaled breath of drinkers produced more output voltage for all the sensors, as all the TGS sensors used in the sensor array was sensitive to ethanol. It is also noticed that the TGS sensors generate an output voltage for a mixture of VOCs from the exhaled breath rather than predicting the value of a particular VOC

From this pilot study conducted in ten volunteers, we have identified that there are significant variations in the VOC profiles of smokers and non-smokers. The amount of exhaled VOCs is also different for alcoholics and non-alcoholics. The effect of medicines, lifestyle, age, and profession may also affect the exhaled VOC values of humans. Briefly, the e-nose system developed was simple and economical. The major advantage of the system is that it produces rapid responses and also the sampling is non-invasive. With the integration of machine learning methods for sensor data processing, the fabricated sensor array system can be effectively used for the discrimination of pulmonary diseases such as asthma, chronic bronchitis, COPD, cystic fibrosis, lung cancer, and healthy controls. Based on the conclusions drawn from this study, our future work is to develop a system to predict lung cancer at its early stage.

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