CHARACTERIZATION OF SELECTED VOLATILE ORGANIC COMPOUND IN HOUSE HOLD PRODUCT USING GAS SENSORS AND LABVIEW – PILOT STUDY

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Abstract— Certain organic compounds are present in alcoholic beverages, and house hold products which may cause a serious health effects. Since it consists of a wide range of compounds, comprising of acids, alcohols, esters, aldehydes, and other trace level aroma compounds. These compounds play an important role as they provide relative information on the product quality and enhance product acceptability and also can be used to assess the person's health. A pilot study has been done to observe the gas sensor reaction towards the toxic gases using LabVIEW software

Keywords- VOC's identification; gas sensor; LabVIEW

I. INTRODUCTION

Volatile Organic Compounds (VOCs) are a large group of carbon-based chemicals that easily evaporate at room temperature which means that these chemicals are carbon based and can easily evaporate into the air from products. These kind of chemicals can enter the body through breathing, touching or swallowing. It have application in industry and science as reagents or solvents. It can be used as a solvent in medical drugs, vegetable essences such as vanilla, alcoholic beverages, and personal care product such as nail polish remover, perfumes, hair spray, and mouthwash. The possible volatile organic compounds (VOCs) used in house hold products arebenzene, toluene, ethylbenzene, xylene, hexane, cyclohexane, 1,2,4-trimethylbenzene, Acetone, ethyl alcohol, isopropyl alcohol, methacrylates (methyl or ethyl), ethyl acetate, tetrachloroethene, (perchloroethene (PERC), trichloroethene (TCE)), d-limonene (citrus odor), a-pinene (pine odor), isoprene, tetrahydrofuran, cyclohexane, methyl ethyl ketone (MEK), Methylene chloride, 1,4-dichlorobenzene, naphthalene, Formaldehyde.

Hair spray is the most widely used dangerous beauty product consists of toxic VOCs that can harm ozone. The compounds such as methane are famously known as CFC's or chlorine, fluorine and carbon have been directly related to global warming; common chemicals found in hairspray are aerosol propellants, alcohol, carcinogenic polyvinylpyrrolidone plastic, formaldehyde and artificial fragrance, which can cause low blood pressure, breathing difficulty, as well as irritation of the skin, eyes and lungs . These chemicals also increase the risk of developing the lung disease thesaurosis over a period of time. The high content of formaldehyde in mouth wash can cause oral cancer, in alcoholic beverages cause blindness or death and in nail polish remover can cause irritation to skin and eyes. The mixes of alcohol in drugs cause a problem such as liver damage, heart problems, internal bleeding and impaired breathing. As the alcohol contains many toxic VOCs such as ethyl alcohol, methyl alcohol, propylene glycol, etc., it may severely affect the human system while consuming it.

Monitoring of the numerous VOCs is a promising field and expanding field. In conventional real-time, gas sensing measurement has been based on two different kinds of gas sensing method, they are method based on electrical variations with different materials such as polymer, metal oxide semiconductor, electrochemical and carbon nanotubes. Another method based on other variations including optical methods, acoustic methods, gas chromatograph and calorimetric methods. While selecting the gas sensing methods certain parameters should be considered such as sensitivity, selectivity, response time, operating temperature, fabrication cost and size.

Sensitivity is nothing but the gas sensor could be able to detect the target gases, even though the volume concentration of the target gas is minimum. Selectivity is the ability of the gas sensors to identify a specific gas among the gas mixture. Response time is the period when the gas concentration reaches the peak value from that time to that when sensor generates a warning signal. Under the parameters as mentioned above metal oxide semiconductor (MOS) gas sensor is provided with high sensitivity, rapid response time, ability to operate in high temperature and pressure and low cost compared to other gas sensors.

Moreover MOS gas sensors have a greater sensitivity over a broad range of volatiles and have higher

attraction towards alcohols, aldehydes and ketones and less responsive to molecules like terpenes, aromatic compounds or organic acids. MOS gas sensors have a limitation in terms of selectivity. Several research work has been done to overcome the selectivity problem .The lack of selectivity problem can be overcome by doping the sensing film surface with a suitable catalyst material, by varying the working temperature the desired selectivity range can be occurred, as mentioned above, the charge of oxygen species adsorbed at the oxide's surface depends on temperature. The most commonly used method to enhance the selectivity is by utilizing the sensor array with different sensing materials

Hence all adsorption, desorption, and diffusion processes are temperature- dependent, so the temperature modulation in sensitive layer can help to increase the selectivity. The rest of the paper deals about the metal oxide semiconductor gas sensor working principle, chapter II reviews the experimental techniques such as design of sensor chamber, calculation for finding the desired concentration of analyte which is to be injected inside the chamber. Chapter III describes the experimental results obtained using the array of gas sensors. Chapter IV deals with the conclusion and future works.

Metal oxide semiconductor gas sensor

Metal oxide semiconductor is being the most commonly used sensing materials. It provides a sensor with high sensitivity and low cost compared to all other gas sensors. Metal oxide such as SnO2, CuO, Cr2O3, V2O5, WO3 and TiO2 can be mainly exploited to detect combustible gases, chlorinated solvents and toxic gases. Tin dioxide (SnO2) is the commonly used gas sensing material. The detection principle of metal oxide semiconductor based gas sensors is based on chemical adsorption and desorption of gases on the sensor's surface: in air, at temperatures between 150 and 400°C, oxygen is adsorbed at the surface of the metal oxides by trapping electrons from the bulk with the overall effect of increasing the resistance of the sensor, for n-type materials, or decreasing it, for p-type materials. The occurrence of a target gas in the atmosphere, which reacts with the pre- adsorbed oxygen or directly with the oxide, determines a change of the sensor resistance, which is recorded as a sensor signal and the magnitude of which is correlated to the concentration of the target gas.

Literature review

Miguel Macìas Macìas et al. developed a system consisting of commercially available MOS sensor to measure an ethanol content of synthetic wine. Four metal oxide gas sensors from Figaro Gas Sensors – TGS2602, TGS2611, TGS2600, TGS2620, two auxiliary sensor as temperature and humidity sensor have been installed in their system. Each gas sensor shows a certain response towards a specific gas but are sensitive towards a wide range of gas types with overlapping sensitivities. They have designed a stainless steel sensor chamber where the sensors have been mounted, in order to avoid the exposure of unspecific gas. The result of the experiment shows a fast response time, high sensitivity and selectivity towards specified analyte.

Mazlina Mamat et al., designed a system to sense alcoholic beverages VOCs. The gas sensors used in this system were TGS 8XX, TGS 26XX, the sensor chamber they have designed was very compact and the material used for to design the chamber was remarkable. The result of this experiment shows better sensitivity and selectivity. Kea-Tiong Tang et al., Faycal Benrekia et al, DongminGuo et al, Jun Wang et al. designed a system especially for food analysis, sensors that were used in their experiment was FIGARO gas sensor, since it has many advantages as they give the fast response to the target analyte, to attain better selectivity an array of gas sensors were used for to sense the specific gas among the gas mixture.

II. MATERIALS AND METHODS

A. Experimental characterization

To design this proposed system three parts has played a vital role they are: (1) designing gas sensor chamber and to select a suitable gas sensors (2) data acquisition (3) signal pre-processing. An automated experimental setup was built in order to perform electrical and gas sensing characterization. LabVIEW program was developed to acquire sensor signal and to control the fan which is being placed inside the sensor chamber. The block diagram for the proposed system is shown in the figure 1.

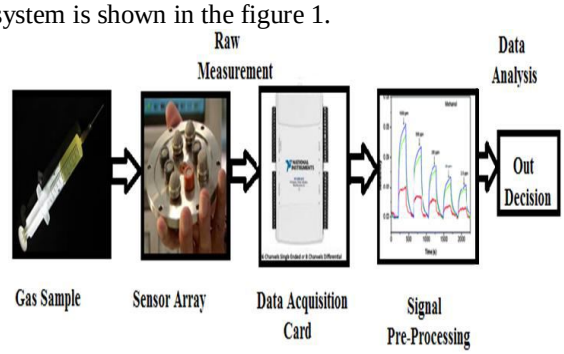


Figure 1. Block diagram of proposed method

In our experiment, we have taken the most toxic VOCs in house hold product. A microliter syringe was used to inject the sample into the gas sensor array chamber. NIDAQ card was used to acquire the sensor signal for further analysis and classification.

B. Sensor chamber

The sensor chamber has been designed with the inner dimension of 26 cm x 14.5 cm x 12 cm (see figure 2).

The system encompasses three gas sensors, and one auxiliary sensor as temperature sensor (60°c). The gas sensors require a simple heating circuit to work. The gas sensors were selected with the inbuilt heater circuit, which is to be heated to certain temperature by providing a constant dc voltage. At an elevated temperature, the sensor is expected to be sensitive to a particular gas present in the air. In the presence of a detectable gas, the sensor conductivity increases and the measuring circuit converts the change in conductivity to a voltage signal. The chamber also contains a fan to clean the entire system to avoid the interference with the next measurement and also for circulating the analyte during the test.

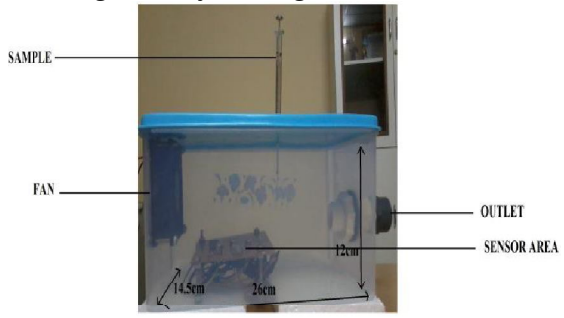


Figure 2. Gas sensor chamber

Table.1 shows the list of gas sensor that was used in the sensor array circuit. To test the system thinner gas was given as the target analyte. The possible VOCs of LPG gases are methane, propane, butane and for thinner gases propane, butane. A simple electronic circuit was designed for the gas sensors to get active toward the exposure of analyte.

TABLE 1.List of sensors to form the sensor array

No.	Sensors	Target Gases
1	MQ6	Combustible Gases(methane, propane, butane)
2	MQ5	LPG (propane, butane)
3	TGS2600	Air Contaminants (hydrogen, carbon monoxide)
4	LM35	Temperature

To get the toxic VOCs into the sensor array such as methanol and ethanol with the desired concentration calculation should be done to know the concentration of the analyte. The forth coming section gives the calculated value for methanol and ethanol desired concentration.

C. Calculation for methanol and ethanol concentration

In our experiment the desired concentration of different types of VOCs such as ethanol, and methanolhas been calculated (see table 3). Since the volume of the box or chamber is known 4500 cm3 it is easy to calculate the concentration of the analyte with respect to the volume.Table 2 shows the analyte concentration vs. analyte volume

TABLE 2. Analyte concentration Vs. Analyte volume

Analyte concentration (ppm)	Volume of analyte (cm^3)
50	0.225
100	0.45
200	0.9
400	1.8
500	2.25
800	3.6
1000	4.5
2000	9

The amount of volatile compounds needed to create the desired concentration in the sensor chamber was introduced in the liquid phase using high precision liquid chromatography syringe. The desired concentration of the different volatile species injected into the chamber could be calculated using the ideal gas theory. Taking ethanol as an example for calculating the ppm, the molecular weight and density should be known. Ethanol has a molecular weight (MW) = 46.0644 g/mol, density(ρ) = 0.789 g/cm3. To get 100 ppm of ethanol into the chamber, from table 2, 0.45 cm3 = ~ 0.45 ml have used to calculate the concentration.

The density of gas of methanol is:

$\partial = P * M \; WR * T$ (1)

where

∂ = the density of the gas of methanol in g/l

P = the standard Atmospheric pressure (in atm) is used as a reference for gas densities and volume (equal 1 atm)

MW = molecular weight in g/mol

R = universal gas constant in atm/ mol.K (equal 0.0821 atm/mol.K

T = temperature in kelvin (Tk = Tc +273.15);

Tc =200C

$\partial = 101.325k \; pa * 32.04 \; g/mol 0.0821 \; atm/mol.k * 293.15$

∂ = 1.34g/l

1.93 g/l is the density of the gas of ethanol, calculated using ideal gas theory equation as derived

To find the volume of the ethanol in liquid phase, is calculated using the formula given below:

Mass = Vgas* ∂ = Vliq * ρ (2)

where

Vgas = the volume of the gas of ethanol

∂ = the density of the gas of ethanol

Vliq = the volume of the liquid of ethanol

ρ = density of the liquid of ethanol

By substituting the corresponding value in equation (2) the volume of methanol for 100 ppm which is to be injected inside the chamber is 0.76*10-6lwas calculated. The calculated value of various concentration for different analyte is shown in table 3.

TABLE 3. Analyte concentration Vs. Analyte quantity

Analyte concentration (ppm) /Analyte	50	100	200	400	500	1000	2000
Ethanol (µl)	0.55	1.1	2.2	4.4	5.5	11.0	22.0
Methanol (µl)	0.38	0.76	1.5	3.0	3.8	7.61	15.2

The sensor chamber has been tested, by giving the VOCs of house hold product (nail polish remover, thinner), the corresponding sensor can able to identify the gas, where MQ5, MQ6 are made to sense the butane and propane gas, the response was achieved from these sensor but not from the TGS 2600 gas sensor. Since TGS 2600 is highly sensitive to hydrogen and carbon monoxide gas, it could able to sense the combustible gas.

D. Sensor Data Acquisition

The signals from the sensor chamber were acquired using NI DAQ card. Each sensor voltage was measured with dedicated channel of the DAQ device to the computer with LabVIEW software. The DAQ card has eight ADC port and five DAC port. The LabVIEW program was developed to acquire the sensor signal as well as to control the fan for every 120 seconds because the experiment has taken 120 seconds for the sensors to give the response time period. After the 120 seconds the sensors data have to go down which means to indicate there is no exposure of gas into the sensor array. As mentioned above the fan was used to drive the gas out of the gas sensor chamber to avoid the contamination for the next measurement. The acquired signal was shown in figure 2.

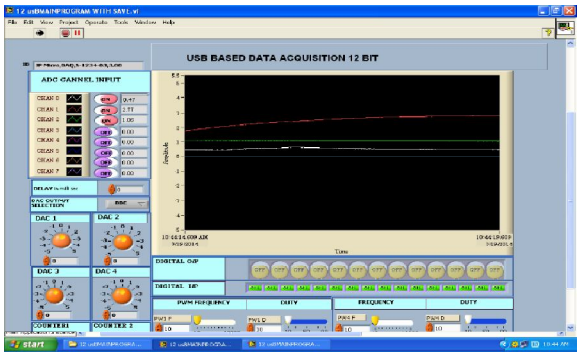


Figure 2. Screen shot of front panel for the acquisition sensor signal data from the sensor chamber

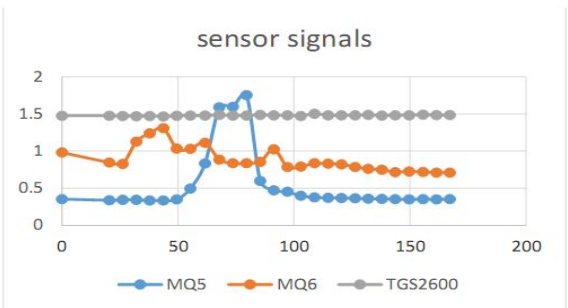


Figure 3.Graph for acquired signal data(Microsoft xl)

For 120 seconds we got 55,000 sensor data, the obtained data was down sampled to get 30 sampling points for the explicit view. Thus the graph shows (see figure 3) that the given analyte was sensitive to the corresponding gas sensors. Whereas TGS2600 is less sensitive to LPG gas no variation was seen in the sensor data. According the target gas the sensor has to be selected to sense the specific gas, for to sense the toxic VOCs of alcohol such as methanol and ethanol different gas sensor has to be used to sense these analyte.

III. CONCLUSIONS AND FUTURE WORK

In this paper, the system has been designed to monitor and measure toxic VOCs in house hold products. The system performance has been tested using house hold product (thinner, nail polish remover) VOCs. The experiment has achieved good sensitivity, and selectivity towards the particular analyte was observed.

From this pilot study the observation obtained was, to get a better sensitivity result the sensor chamber should small as possible and the material used to design the chamber should be non-reactive to the vapors present inside the chamber. The gas sensor should be selected in an appropriated way for the specific gas to be detected. In the future, by using this methodology an alcohol VOCs will be measured and monitor, with different gas sensor with the help of literature review.

The desired concentration for methanol and ethanol analyte was calculated for the future development. The LabVIEW program is being designed for the signal analysis and classification.

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