Australian Journal of Basic and Applied Sciences, 9(5) March 2015, Pages: 360-367

ISSN:1991-8178

Australian Journal of Basic and Applied Sciences

Journal home page: www.ajbasweb.com

Selection of feature analysis electronic nose signals based on the correlation between gas sensor and herbal phytochemical.

[1]U.K. Mohamad Yusof, [1]A. Che Soh, [1]N.F. M. Radzi, [1]A.J. Ishak, [1]M.K. Hassan, [1]S.A. Ahmad, [2]S. Khamis

[1]University of Putra Malaysia, Department of Electrical and Electronic Engineering, 43400 Serdang, Selangor, Malaysia.
[2]University of Putra Malaysia, Institute of Bioscience, 43400 Serdang, Selangor, Malaysia.

ARTICLE INFO

Article history:
Received 12 October 2014
Received in revised form 26 December 2014
Accepted 1 January 2015
Available online 27 February 2015

Keywords:
Gas sensor, electronic nose, gas chromatography-mass spectrometry, herbs classification.

ABSTRACT

Background: Electronic nose consists of commercial gas sensor which detects gas through an increase in electrical conductivity when reducing gases are adsorbed on the sensor's surface. The election of the best gas sensor that suits to the target gas detection is very crucial in order to capture the desired signal to be used in further process to design e-nose for odor detection with high rate of classification. In this study, five herbs were chosen as sample for electronic nose development. The volatile chemical compound in herbs as the source of the odor will be characterized by using gas chromatography–mass spectrometry test. The result of the test is useful to determine the potential gas sensor for e-nose. The process is followed by one to five feature analysis of the e-nose signal to find the best gas sensor array. **Objective:** The selection of gas sensors is investigated in order to design e-nose for odor detection. **Results** Feature analysis shows that five feature analyses by using five types of gas sensor for e-nose give the best result as the 90% accuracy of classification. **Conclusion:** Five types of gas sensors have been determined from the phytochemical's results of GCMS test. Hence, it will be used as sensor array in e-nose application for herbs classification.

To Cite This Article: U. K. Mohamad Yusof , A. Che Soh, N.F. M. Radzi, Selection of feature analysis electronic nose signals based on the correlation between gas sensor and herbal phytochemical. ***Aust. J. Basic & Appl. Sci.,*** *9(5): 360-367, 2015*

INTRODUCTION

The commencement of sensor technology in artificial olfaction begins in 1982 with the invention of the first gas multisensor array (Persaud and Dodd, 1982). These devices, known as electronic noses, were engineered to mimic the mammalian olfactory system within an instrument designed to obtain repeatable measurements, allowing identifications and classifications of aroma. The basic concept of an electronic nose, or machine olfaction, is a measurement unit that generates data for each measurement combined with a pattern recognition technique that interprets data and relates it to a target value or class (Alphus and Baietto, 2009).

The interest in extracting pure component spectra from complex chromatograms started when the instrumental technique of gas chromatography and mass spectrometry (GCMS) is introduced. Biller and Biemann proposed an extracted spectrum method uses maxima in ion chromatograms to detect chromatographic components (Biller and Biemann, 1974). The resolution of this method is improved by Colby where more precise ion maximization times are computes (Colby, 1992). The use of a mass spectrometer as the detector in gas chromatography was developed during the 1950s by Roland and Fred (Roland and Fred, 1993).

The used for GCMS are numerous in the medical, pharmacological, environmental and law enforcement fields. It is actually two techniques of gas chromatography and mass spectroscopy that are combined to form a single method of analyzing mixtures of chemicals. GC separates the components of a mixture, while MS characterizes each of the components individually. However, GCMS are an effective combination for the identifying of volatile chemical compounds in complex mixtures. GCMS is especially useful for air samples but can be used to detect, quantify, and identify chemicals in air, water, soil, plant and animal tissue, and many other substances.

In electronic nose, selection of feature analysis electronic nose signals based on the correlation between gas sensor and herbal phytochemical from GCMS analysis is conferred for the purpose of developing high classification and recognition rates.

This paper is formed as in section 2, the fundamental operation of artificial olfactory system, architecture of sensor array in e-nose and gas chromatographic mass spectrometer used in aroma research. Section 3 is about experimental setup and

Corresponding Author: Azura Che Soh, PhD. University of Putra Malaysia, Department of Electrical and Electronic Engineering, 43400 Serdang, Selangor, Malaysia.
Phone numbers: +603-89466499; E-mail: azuracs@upm.edu.my

measurement process. In section 4, result and discussion will be focusing on GCMS test and the feature analysis of E-nose signal and the conclusion of this paper is summarized in the last session.

2. Bio-Inspired System of Electronic Nose:

Nature has developed through thousands of years of evolution, sensing organs and strategies that stand out in versatility, performance, sensitivity or tolerance to saturation (Valle, 2011). As well as for the mammalian olfactory system for detection and capabilities to discriminate various odorants with high precision. Despite the importance of olfactory systems of odor and flavor, more analytical approach has been developed in response to overcome dispute in comparing different person experience of smell and quantifying of odor. Research into alternative olfactorial sensing methods within an electronic nose as quantitative measurement intended to fill up this desire.

2.1 The Mammalian Olfactory Architecture:

The olfactory system is stimulated by information contained with odorants that are released from an object. An odor in the inhaled air that upon coming in contact with the human sensory system is able to encourage an anatomical response (Magda Brattoli *et al*., 2011). From Figure 1, odor molecules are trapped and dissolved into olfactory epithelium as in which is the area where the olfactory receptor cells exist.

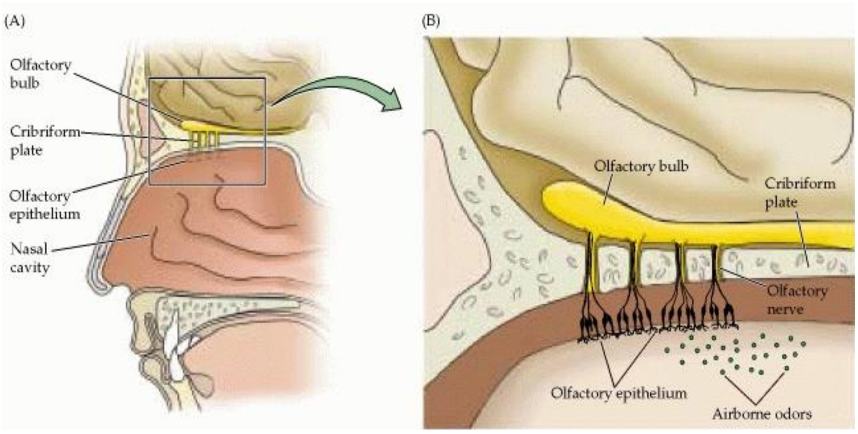

Fig. 1: Human olfactory system

In small region of both nasal cavities, odorants excite an electrical response and transmitted to the olfactory bulb. Process of enhances sensitivity, improves immunity to noise, increase selectivity and allows for the constant regeneration of the olfactory cells occur in this stage. The olfactory signal is thus send to the pyriform and entorhinal cortex. The final perceived odor results from a series of neural computations in brain. Due to its nature, mimic a human olfaction becoming a straightforward importance tool in electronic nose to accommodate a sensor and some form of pattern recognition algorithm.

2.2 The Principle Operation of Electronic Nose:

Electronic sensing technology is developing field of study that has greatly advanced over the decade. Nowadays, electronic nose has been developed in many industries such as to measure the quality of food, drinks, perfumes, cosmetic, in environment issues, as well in chemical products (Magda Brattoli *et al*., 2011; Craven, 1997; Chew *et al*., 2003; Nollet, 2007; Li *et al*., 2010; Baietto, 2009; Ammar *et al*., 2010; Wahyu *et al*., 2010; Elizabeth *et al*., 2011; Hasin, 2013). The basic concept of an electronic nose or machine olfaction is a measurement unit that generates complex multi-dimensional data for each measurement combined with a pattern recognition technique that interprets the complex data and relates it to a target value or class (Hasin, 2013).

Over the last decades, chemical senses captured the attention of scientists who started to investigate the different stages of olfactory pathways. This growing knowledge took over in replication of mammalian olfactory system to develop E-nose system. As a consequence, some of the functions for both systems were resemblance as shown in Table 1.

Table 1: Function of component in mammalian olfaction system and E-nose system

Mammalian olfaction system	E-nose system	Functions
Nostril	Sampler	Serves as gas detection chamber
Primary neuron	Sensor array	Sense odor and collect data
Secondary neuron	Signal conditioning & data pre-processing	Analyze and process data
Brain	Pattern recognition	Classify and identify the smell

2.3 The Fundamental of Gas Chromatography Mass Spectrometer:

Gas Chromatography Mass Spectrometer is an instrumental technique which comprising a gas chromatography coupled to a mass spectrometer purposely for complex mixtures of chemicals may be separated, identified and quantified (Alphus and Baietto, 2009; Biller and Biemann, 1974). Figure 2 and Figure 3 shows the block diagram and schematic illustration of GCMS, respectively. The GCMS instrument is made up of two parts. The GC portion separates the chemical mixture into pulses of pure chemicals and the MS identifies and quantifies the chemicals. GC uses a carrier gas to move analytes through a coated, fused silica capillary. Separation occurs based on differential partition between the gas phase and the coating inside the capillary. Separation occurs based on differential partition between the gas phase and the coating inside the capillary. Meanwhile, effluents from a GC column are passed into a mass selective detector or MS to provide the information on molecular weight, identification and confirmation of compounds through their mass spectra as well as quantitation of compounds (Biller and Biemann, 1974).

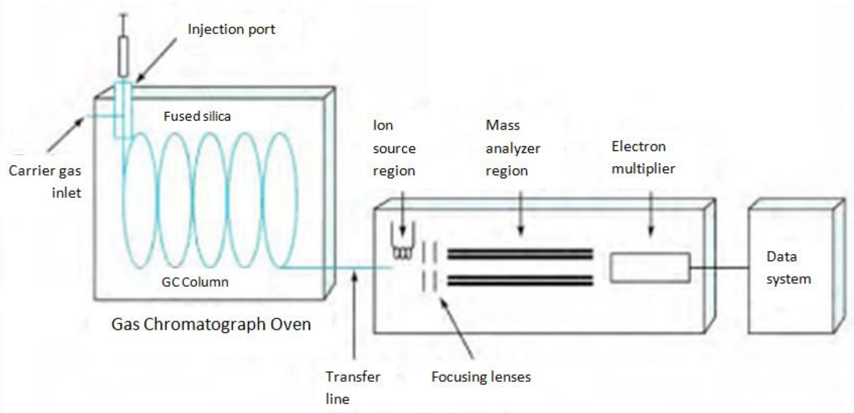

Fig. 2: Block diagram of a GCMS

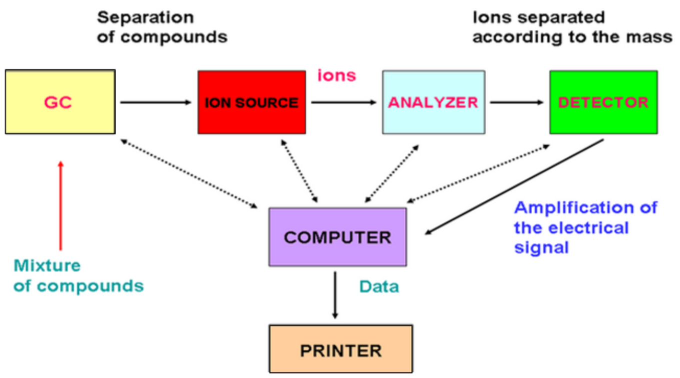

Fig. 3: Schematic illustration of a GCMS

Among its uses is drug testing and environmental contaminant identification. In order for a compound to be analysed, it must be sufficiently volatile and thermally stable. In addition, functionalised compounds may require chemical modification, prior to analysis, to eliminate undesirable adsorption effects that would otherwise affect the quality of the data obtained. Samples are usually analysed as organic solutions consequently materials of interest need to be solvent extracted and the extract subjected to various wet chemical techniques before GCMS analysis is possible.

2.4 Metal Oxide Gas Sensor and Type of Gas Detection:

The Figaro metal oxide gas sensors are chosen to form sensor arrays of proposed e-nose. The principle of operation of the gas sensor is when the tin oxide (SnO_2) in gas sensor is heated, oxygen from the air is adsorbed on the crystal surface. Electron is transferred from the SnO_2 to the adsorbed oxygen, leaving the positive charges at the conduction band near surface. Due to this removal of the electron, an insulating region is produced and increases the contact resistance between powder grains (Craven, 1997).

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Surface density of negatively charged oxygen decreases in the presence of a deoxidizing gas, so barrier height in the grain boundary is reduced. The reduced barrier height decreases sensor resistance, thus, an output signal will be formed. Sensor type being used and type of gas detection is shown in Table 2. According to the table, it can be concluded that each sensor being selected is sensitive to ethanol chemical compound which is originated from alcohol family.

Table 2: Sensor type and type of gas detection

Sensor Type	Type of gas detection
TGS 2610	Liquefied Petroleum (LP), Ethanol, Hydrogen
TGS 2611	Methane, Ethanol, Iso-butane
TGS 2620	Carbon Monoxide, Ethanol, Hydrogen
TGS 823	Acetone, Ethanol, Benzene
TGS 832	Chlorofluorocarbon (CFC), Ethanol, Ethane

3. Experimental Setup And Measurements:

In this study, two experiments were setup in order to fulfil the proposed objective. The gas chromatography mass spectrometry test was arranged purposely to find volatile chemical compound of the sample herbs. The potential gas sensor is then choose based on volatile chemical compound found from GCMS test result Next, one to five feature analysis of e-nose signal was accomplished for the intention of designate the best gas sensor among the potential gas sensor and thus to build up array of gas sensor for e-nose herbs recognition.

3.1 Gas Chromatography Mass Spectrometry Test:

The election of gas sensors for developing the E-nose system are decided through the chemical compound analysis. The extraction of gas compounds for each herbs can be performed through the experiment setup as as shown in Figure 4.

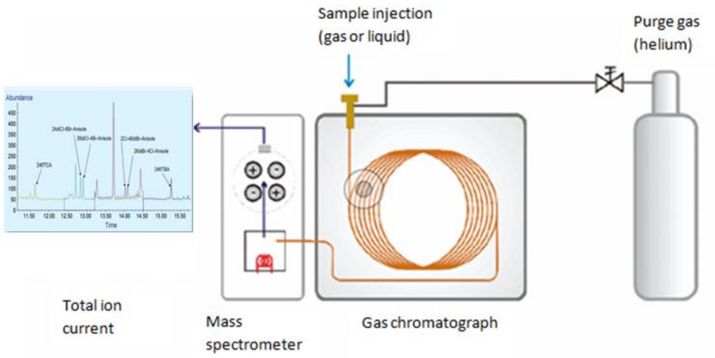

Fig. 4: Experimental setup for GCMS

The sample need to be volatilized or extracted from the matrix by injection techniques. After injection of a mixture, separation is achieved in the capillary column. This column is coated with a fluid or a solid support, the stationary phase. An inert gas, also called the mobile phase, is flowing through the column. Depending on the phase equilibrium between the stationary and mobile phase, compounds travel with different velocities through the column. The mixture becomes separated, and as a result, individual compounds reach the detector with a different retention time. By choosing a column, which separates on boiling point, polarity, size or stereochemistry, a wide range of compounds can be separated. The mass spectrometer combines a high sensitivity with the unique property of being able to determine the molecular composition. Finally, the output is in the form of abundance versus retention time graph.

3.2 Electronic Nose Experiment:

The E-nose development in this project consists of five Figaro metal oxide sensors used to evaluate five different types of herbs namely Curry *(Murraya Koenigii)*, Lemongrass *(Cymbopogen Citrates)*, Kaffir Lime/Limau Purut *(Citrus Hystrix)*, Pandan Leaves *(Pandanus Amaryllifolius)* and Golden Lime/Limau Kasturi *(Citrus Microcarpa)*. The leaves are crumpled before being tested with the E-nose sensor as shown in Figure 5 so that the odor will be completely released from the herbs for better recognition. The sensor arrays sense the odor and generate data to be used in feature analysis.

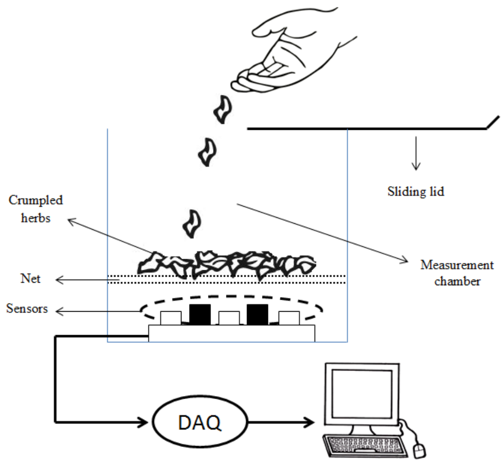

Fig. 5: Experimental setup for e-nose

Throughout the analysis, the gas sensors are represented by sensor 1 to 5 for simplification as in Table 3.

Table 3: Representation of TGS series sensors

Sensors	Synonyms
TGS 2611	Sensor 1
TGS 2610	Sensor 2
TGS 2620	Sensor 3
TGS 823	Sensor 4
TGS 832	Sensor 5

RESULT AND DISCUSSIONS

In this section, the GCMS analysis and major chemical compound in herbs are listed. Meanwhile, average voltage values obtained from each e-nose gas sensor are plotted based on the features. One to five features analysis are done in order to find the most suitable sensor for e-nose and the best combination of gas sensor array if it is needed.

4.1 Phytochemical of the Herbs from GCMS Analysis:

From analysis of GCMS, it shows all the herbs contain compounds with suffix-ol which is used in organic chemistry to represent alcoholic compounds. Ethanol from alcohol group of chemical compound shows positive relations with gas detected by the sensor arrays. Therefore, five metal oxide gas sensor can be used for E-nose due to ability of gas sensor to detect chemical compound in sample herbs.

Table 4: GCMS-Analysis and major chemical compound in herbs

Herbs	Chemical Compound	Area Peak (%)
Curry *(Murraya Koenigii)*	- Pinene <alpha-> - Terpinen-4-ol - Caryophyllene (E-) - Sabinene - Selinene <alpha->	- 14.80 - 3.84 - 11.44 - 24.72 - 3.90
Lemongrass *(Cymbopogen Citrates)*	- Myrcene - Neral - Geranial - Intermedeol <neo-> - Valencene	- 2.57 - 24.50 - 37.56 - 9.26 - 4.31
Kaffir Lime *(Citrus Hystrix)*	- Sabinene - Linalool - Citronellal - Citronellol - Citronellyl propanoate	- 3.40 - 4.86 - 66.19 - 9.27 - 2.73
Pandan Leaves *(Pandanus Amaryllifolius)*	- Sabinene - Tetradecanal - Methol <iso-> - Isophytol - Phytol acetate <E->	- 3.26 - 4.18 - 2.27 - 80.78 - 3.49
Golden Lime *(Citrus Microcarpa)*	- Pinene <beta-> - Germacrene D - Hedycaryol - Eudesmol <gamma-> - Eudesmol <beta->	- 16.61 - 8.92 - 16.68 - 8.84 - 17.96

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4.2 One Feature Analysis of E-nose Signal:

Gas sensor signal from E-nose for one feature analysis was captured as in Figure 6a-6e. From the figures, the observation of e-nose signal from gas sensor is overlapped and not significant to classify the herbs. From one feature analysis, it can be conclude that single sensor was not convenient for e-nose to be well functional and the best gas sensor array has been considered for the next step through further studies of feature analysis.

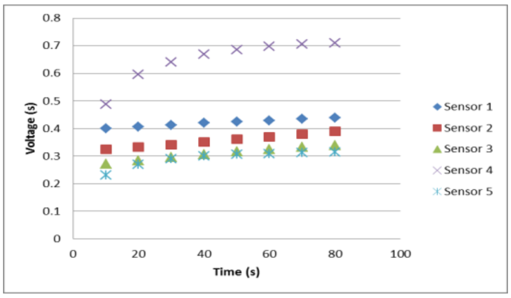

Fig. 6a: Sensors voltage against time for Curry sample

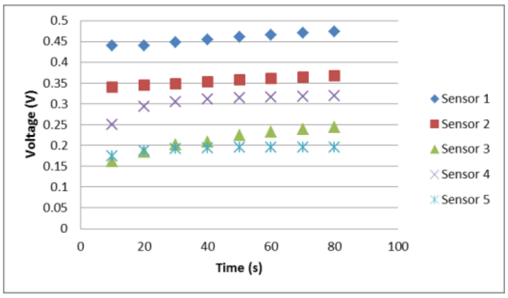

Fig. 6b: Sensors voltage against time for Lemongrass Sample

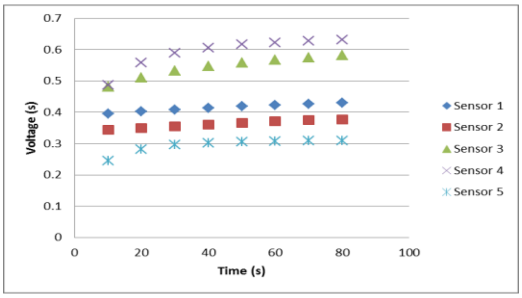

Fig. 6c: Sensors voltage against time for Kaffir Lime sample

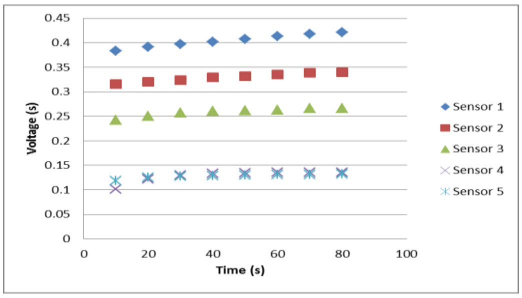

Fig. 6d: Sensors voltage against time for Pandan Leaves sample

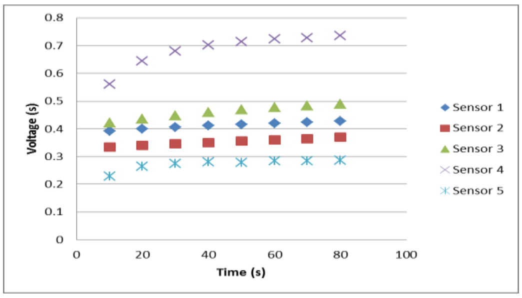

Fig. 6e: Sensors voltage against time for Golden Lime sample

4.3 Two Feature Analysis of E-nose Signal:

Two feature analysis of e-nose signal was figured out to enhance the ability of the sensor for better recognition of the herbs. Figure 7a-7d shows the most significant combination of gas sensor for herbs recognition in two features analysis. Unfortunately, the other combination sensors for the two features plot was not successful in classifying the herbs, hence three-feature analysis which involved three dimensional plot was carried out.

4.4 Three Feature Analysis of E-nose Signal:

In three features analysis, there are two combinations of gas sensor gives the best classification for the samples. Figure 8a shows the combination of sensor 2, sensor 3 and sensor 4 as well as in Figure 8b which is combination of sensor 3, sensor 4 and sensor 5 shows significant results for three feature analysis.

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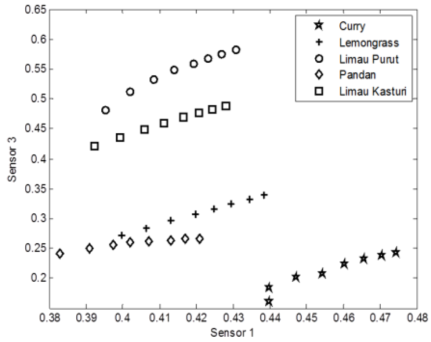

Fig. 7a: Sensor 3 against sensor 1 for five types of herbs

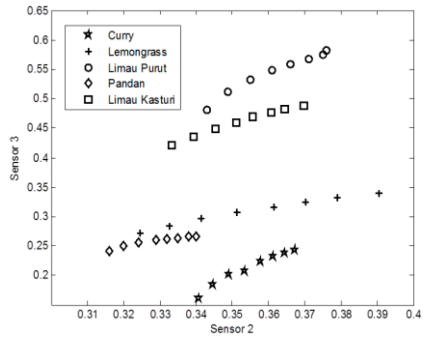

Fig. 7b: Sensor 3 against sensor 2 for five types of herbs

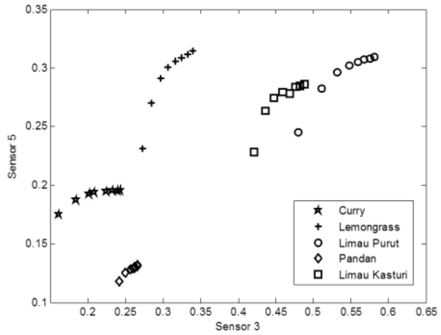

Fig. 7c: Sensor 5 against sensor 3 for five types of herbs

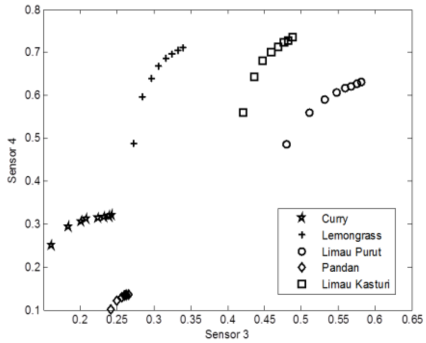

Fig. 7d: Sensor 3 against sensor 2 for five types of herbs

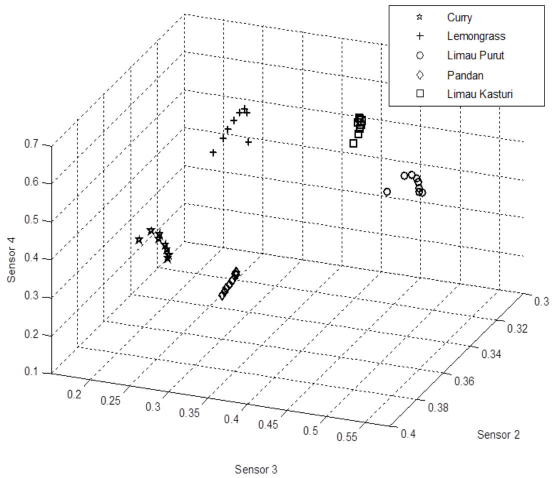

Fig. 8a: Sensor 2, sensor 3 against sensor 4 voltages for five types of herbs sample

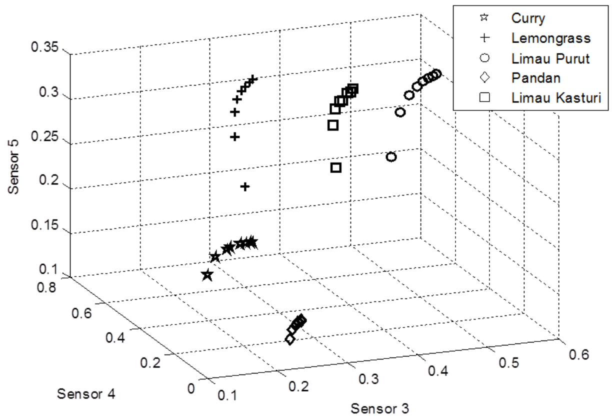

Fig. 8b: Sensor 3, sensor 4 against sensor 5 voltages for five types of herbs sample

The other sensor combinations show some confusion in classifying the herbs due to overlapped and close to adjacent signal from other sensor. However, conclusion can be made was the ability of sensors to classify herbs increases as the number of sensors is increased.

4.5 Five Feature Analysis:

In five feature analysis, array of five gas sensors has been demonstrated the highest capability in classifying herbs sample. Data obtained from sensors array are classified using Artificial Neural Network techniques. The comparison of five feature analysis with two and three feature analysis for two set of data was provided in Table 5a-5b. Accuracy achieve to 90% in five feature analysis for test set 1 proves the high capability of the gas sensor in classifying the correct herbs with combination of five gas sensor array.

Table 5a: Comparison between the training set and test set 1

Features-Analysis	Five Features	Three Features	Two Features		
Sensors Involved	All	2, 3 and 4	2 and 3	2 and 4	3 and 4
Curry	8/8	7/8	6/8	7/8	7/8
Lemongrass	8/8	6/8	3/8	7/8	4/8
Kaffir Lime	6/8	7/8	4/8	3/8	6/8
Pandan Leaves	6/8	7/8	5/8	4/8	8/8
Golden Lime	8/8	7/8	7/8	4/8	4/8
Total	36/40	34/40	25/40	25/40	29/40
Accuracy	90 %	85%	62.5%	62.5%	72.5%

Table 5b: Comparison between the training set and test set 2

Features-Analysis	Five Features	Three Features	Two Features		
Sensors Involved	All	2, 3 and 4	2 and 3	2 and 4	3 and 4
Curry	7/8	7/8	6/8	7/8	7/8
Lemongrass	8/8	6/8	3/8	7/8	4/8
Kaffir Lime	6/8	7/8	4/8	3/8	6/8
Pandan Leaves	6/8	7/8	5/8	4/8	8/8
Golden Lime	8/8	7/8	7/8	4/8	4/8
Total	35/40	34/40	25/40	25/40	29/40
Accuracy	87.5 %	85%	62.5%	62.5%	72.5%

Conclusions:

In this project, GCMS test was succeed to give the phytochemical of the five herbs samples. From the phytochemical of the herbs, the potential gas sensor then has been determined. Next, one to five feature analysis of the e-nose signal was performed. Based on the feature analysis, five feature analysis was demonstrated the best result for 90% accuracy compared to the other feature analysis and hence five types of gas sensor will be used as sensor array in application of e-nose for herbs classification.

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