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DETECTION OF HEXYLENE GLYCOL IN THE PERFUMES USING ELECTRONIC NOSE CORRELATED WITH GAS CHROMATOGRAPHY MASS-SPECTROSCOPY

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Abstract

Perfume is a cosmetic product that widely used by people to improve their appearance in social interactions. Perfume released specific fragrance from the essential oil. Manufacturers often mix the pure essential oils with hexylene glycol to reduce prices. Utilization of hexylene glycol as the solvent and diluent often reduce the odour profile of the perfumes. This paper investigated the development of an electronic nose (e-nose) based on a metal oxide semiconductor (MOS) gas sensor to detect hexylene glycol in perfumes. E-nose in this study was developed using MOS gas sensors from Figaro and Raspberry series, including TGS 822, TGS 826, TGS 2600, TGS 2620, MQ2, MQ3, MQ8, and MQ135. For the experiment, we collected 10 brands of commercial perfumes from the supermarket around Purwokerto, Central Java. All samples of perfumes were analysed using gas chromatography-mass spectroscopy (GC-MS) to detect the concentration of hexylene glycol in the samples. The concentration of hexylene glycol in the samples identified none (0%), low (1-20%), moderate (21%-50%) and high (more than 50%). Afterward, 10 brands of perfumes were separated into 15 samples, totally created 150 samples. All perfume samples were measured using an e-nose to obtain the responses. Analysis of sensor responses using principal component analysis (PCA) showed that e-nose was highly performed to discriminate the samples based on hexylene glycol concentration. Classification of 150 perfume samples using backpropagation neural networks (BPNN) grouped 150 perfumes in four different classes in which the accuracy of classification reached 96.36% for the training dataset and 92.50% for the testing dataset, respectively.

Keywords: *electronic nose, gas chromatography-mass spectroscopy, gas sensor, perfume, principal component analysis.*

1. INTRODUCTION

Perfume is one of the cosmetic products used by thousands of consumers across genders, both men and women. Perfume has also become a part of appearance that can support a person's self-confidence in relationships [1]. In general, perfume eliminates body odour, provides a distinctive aroma, and increases a person's attractiveness to the opposite gender [2]. The type of aroma of the perfume used also often reflects the personality of the person who uses the perfume. There are hundreds of kinds of odour and aromas produced by perfumes [3]. Well-known perfume brands usually have catalogues that display a collection of perfume types and aromas suitable for men, women, and unisexual gender [4].

Perfume is sold at various prices, ranging from low quality at low prices to high-quality perfume at high prices. Because perfume is considered one of the things that supports a person's appearance to appear perfect, consumers often feel the need to buy perfume at high prices and usually have irrational considerations [5].

In the beginning, perfume was made using herbs, spices, and flowers mixed to create a fragrance. These three ingredients are mixed and filtered to obtain an essential oil mixture of herbs, spices, and flowers [6]. In the mid-15th century, perfume began to be added with oil and alcohol [7]. However, perfume only experienced rapid progress in the 18th century with the emergence of various fragrances and bottles of different shapes [8].

In the last 20 years, the demand for perfume has increased rapidly [9]. Consumers from the upper and middle economic levels have dominated it. Perfume consumers from the upper and middle classes feel that using perfume increases their self-confidence when interacting with others. The behaviour of upper and middle-class consumers have preference to buy perfume from well-known brands at high prices [10]. Consumers from the middle and upper class consider the fragrance of famous brands to be more long-lasting and diverse.

Meanwhile, people from lower economic backgrounds believe that perfume can increase attractiveness when interacting with others. Apart from eliminating body odour, using perfume in lower classes can improve self-confidence and increase social status in middle and upper-class society. However, the behaviour of lower-class perfume consumers tend to choose local brands that offer perfume at cheaper and more economical prices [4].

Based on its composition, perfume is a mixture of oils, aromatic compounds [11], and solvents [12]. Perfume is usually dissolved using a solvent [13]. So far, the solvent used for perfume is ethanol, or a mixture of ethanol and distilled water [7]. The composition of substances in perfume is generally alcohol (50-90%), distilled water (5-20%), and essential oil or fragrance (10-30%). Hexyl alcohol in this composition serves as a solvent and diluent [14].

The perfume compositions produced by well-known brands generally contain a high percentage of essential oil compounds. This essential oil is made from the distillation and extraction process of aromatic natural materials such as flowers, spices, and herbal ingredients, which produce a strong aroma [7]. Some perfume products from particular brands only contain essential oils without mixing ethyl alcohol and distilled water [15]. The perfumes with a high essential oil composition will produce a strong, consistent, long-lasting aroma.

However, the expensive raw materials and high production costs from distilling herbal medicines, spices, and flowers into essential oils to be made into perfume significantly increase the perfume's selling price. As an illustration, to produce approximately 10 ml of pure herbal essential oil with ginger aroma, 5 kilograms of ginger rhizomes are needed. In other words, the essential oil production coefficient for perfume raw materials with ginger aroma is 1.6 ml/kg [16]. It has a lower coefficient for perfume production using flowers as raw materials. This encourages perfume manufacturers to use alcohol and distilled water as solvents and dilution for essential oils to reduce production costs and sell at affordable prices to consumers. However, the quality of the perfume odour will usually decrease when the concentration of ethyl alcohol and distilled water used as a solvent in the perfume is higher. High concentrations of ethyl alcohol and distilled water in perfume will reduce the strength and durability of the perfume's odor.

Hexylene glycol is an ethanol derivative usually used as a solvent and diluent for essential oils, producing a fragrant smell in perfume [17]. Hexylene glycol is a colorless, odorless liquid with a sweet taste. However, this substance is also used as a solvent in industry and household products, including perfume. Hexylene glycol is much cheaper than other ethyl alcohol compounds, so hexylene glycol is used as a diluent and solvent in perfume.

However, hexylene glycol has the property of being a toxic compound if consumed in amounts exceeding the threshold limit. Hexylene glycol poisoning can occur by swallowing, inhaling, or skin contact with these chemicals [18]. However, severe poisoning effects, including a typical progressive acute renal failure, can occur if the chemical is ingested in large quantities. According to standard standards in Indonesia, the safe or tolerable daily intake (TDI) threshold for hexylene glycol and dihexylene glycol contamination is 0.5 mg/kg body weight per day [19]. Consumption exceeding TDI can have fatal consequences if not treated immediately. Spraying the perfume into bodies that use high concentrations of hexylene glycol daily can produce toxic compounds when the hexylene glycol in the perfume comes into contact with human skin [20]. As a result, the potential for health problems in consumers who use perfume with high concentrations of hexylene glycol will increase [18]. Consequently, screening of the hexylene glycol concentration in perfume should be carried out to ensure that the hexylene glycol content in perfume is low.

The standard chemical analysis methods used to identify hexylene glycol in perfume are gas chromatography-mass spectrometry [18], high-performance gas-liquid chromatography [21], and infrared spectrophotometry. These methods have proven to be accurate for determining the concentration of hexylene glycol in perfume. However, technical challenges such as expensive equipment investment, high electricity costs, and the dimension and voltage capacity of the equipment that must be placed in chemical laboratories make testing perfume samples in the laboratory using this method inefficient.

Using a more straightforward and less costly apparatus, the researcher has tried alternative sensory analysis techniques to identify hexylene glycol [22]. Research on using gas sensor arrays for odour detection has been conducted since 1990. The sensory analysis of perfumes using an e-nose can determine the perfume odour profile based on the composition of volatile compounds released by perfume. Hence, identifying hexylene glycol in perfume based on odour profile is possible [23]. Employment of an e-nose device is simple, inexpensive, and easy to use for identifying specific compounds based on the aroma profile from samples. In this experiment, the gas sensor array consisting of eight metal oxide semiconductors (MOS) from the Taguchi Gas Sensor (TGS) and Raspberry (MQ series) is necessary.

This paper investigated the employment of e-nose based on metal oxide semiconductor gas sensor array for identifying the hexylene glycol in perfume based on sensory analysis. The sensory analysis procedure of perfume using an e-nose is simple and timesaving. The liquid perfume sample was put in the sample handler. The flow of volatile gas from the sample flowed into sensor chamber—which has eight MOS sensors from the TGS and MQ series—is made more accessible by the headspace under the controller system. A transient curve shows the interaction of gas sensor material with the hexylene glycol in perfume that the gas sensor array creates in two minutes. Principal component analysis (PCA) and backpropagation neural network (BPNN) were used to analyse the gas sensor array response to identify the hexylene glycol in perfume.

2. METHODS

2.1. Sample Preparation of Perfume

For the experiment, we used 100 ml from 10 different brands commercial perfumes purchased from a cosmetic store in Purwokerto City, Central Java, Indonesia. After collecting ten perfume samples, gas chromatography-mass spectrometry was employed to identify the concentration of hexylene glycol as the solvent and diluent in perfumes. Afterward, each perfume brand was divided into 15 samples. The volume of each perfume sample was set to 5 ml for sensory analysis using an e-nose. The name of commercial perfumes and the concentration of hexylene glycol in perfumes is presented in Table 1.

Table 1. The name of commercial perfume and the concentration of hexylene glycol used in experiment

Sample code	Name	Class sample code	Concentration of Hexylene Glycol (%)
A	Bali Flower	HHG	99
B	Opium	HHG	95
C	Rose	HHG	90
D	Ylang-ylang	HHG	64
E	Melati	HHG	55
F	Cempaka	MHG	41
G	Lavender	MHG	30
H	Frangipani	LHG	20
I	Sandalwood	LHG	15
J	Patchouli	ZHG	0

2.2. GC-MS analysis

The Shimadzu GC-MS-QP-2010 (Kyoto, Japan) mass spectrometer with auto-sampler Agilent 7683b and MSD Agilent 5975C mass spectroscopy was used to perform the GC-MS study (Fig. 1). The QP 2010 SE mass spectrometer (Compaq-Pro Linear data system, class 5 K software) was connected to the GC-MS. A 30m × 0.25mm i.d. × 0.2µm film thickness Crossband R 100% dimethylpolysiloxane Agilent-DB-1 column was attached to it. The column was operated under the following conditions: it was first programmed to operate at 70°C, and after 10 minutes, it was raised to 250°C (at a rate of 18°C min^{-1}). The injector and detector operated at 250°C and 270°C, respectively. One µl was designated as the injection volume for the sample. The mass conditions were as follows: full scan mode in the 30–450 amu mass ranges with 0.2 s scan-1 velocities; ionization voltage: 70 eV; ion source temperature: 200°C; helium carrier velocity: 30 cms^{-1}. Compounds were identified using the NIST 08 database (NIST mass spectrum database, PC version 2008), WILEY 8, and FFNSC1.3 (Flavour & Fragrance & Synthetic Compounds) libraries. Based on the percentages of the region displayed in the GC-MS spectra, a computerized integrator determined the number of main chemicals.

2.3. Procedure of Hexylene Glycole Identification with GC-MS

The procedure for hexylene glycol identification with GC-MS was assigned similarly. To identify the hexylene glycol in ten commercial perfume samples, 2.5 µl of perfume in liquid was diluted with 10 ml of pure water to reduce the concentration of the odorant. Then, a micro-syringe injected 2 µl of this diluted solution into the column (Nichipet Ex, Japan). The GC-MS running time was set for 55 minutes. The comparison between the ratio of the peak area and the total areas was used to calculate the relative percentage amount of each compound.

Fig. 1. The instrumen of GC-MS used to identify the hexylene glycol in perfumes

2.4. E-nose apparatus

The physical components and schematic diagram of the gas sensor array utilized in this study are shown in Fig. 2. A direct current (DC) power supply, a gas sensor array, a headspace system controller, a data collection system, and a communication system were all part of the gas sensor apparatus. To reduce the alternating current (AC) voltage, the direct current (DC) power supply used four different voltage regulators: a 6-ampere bridge diode, 3300- and 100-microfarad capacitors, and a 5-ampere transformer. A 1000 cm^3 cylindrical sample holder was constructed out of acrylic material to hold the coffee sample for the experiment. The heater in the sample holder aided in evaporating volatile organic compounds (VOCs) in the meat samples.

2.5. Sensory analysis of perfumes using e-nose

Eight metal oxide semiconductor gas sensors from the Raspberry Pi (MQ) series (MQ2, MQ3, MQ8, and MQ135) and Taguchi Gas Sensor (TGS) series (TGS 822, TGS 2600, TGS 826, TGS 2602, TGS 2612, and TGS 2602) were used to build the sensor gas array. According to the datasheets for the

Figaro and Raspberry, these gas sensors have different flammable gas sensitivities. A list of gas sensor selectivity and the accompanying sensitivity range is shown in Table 2. An AVR ATMega16 controller was used in the fans' data collection system and the headspace system. This controller included eight internal channels with a 10-bit resolution for analog-to-digital conversion. During the sample sensing procedure, real-time data transfer from the gas sensor array to a personal computer was made possible by RS 232 serial communication.

Table 2 Selectivity of gas sensor form Taguchi (TGS) series and Raspberry series

Sensor series	Selectivity	Response threshold (ppm)
TGS 822	Organic solvent (O_2, CH_4, CO, n-hexane, benzene, ethanol, acetone)	300
TGS 2600	Air contaminant	1-30
TGS 826	NH_3	30-300
TGS 2602	Alcohol dan organic solvent	50-5k
MQ2	Combustible gas (LPG, i-butane, propane, methane, alcohol, Hydrogen, smoke)	300-10k
MQ3	Alcohol	25-100
MQ8	Hydrogen, alcohol	100-10k
MQ135	LPG, i-butane, propane, methane ,alcohol, Hydrogen, smoke	10-1k

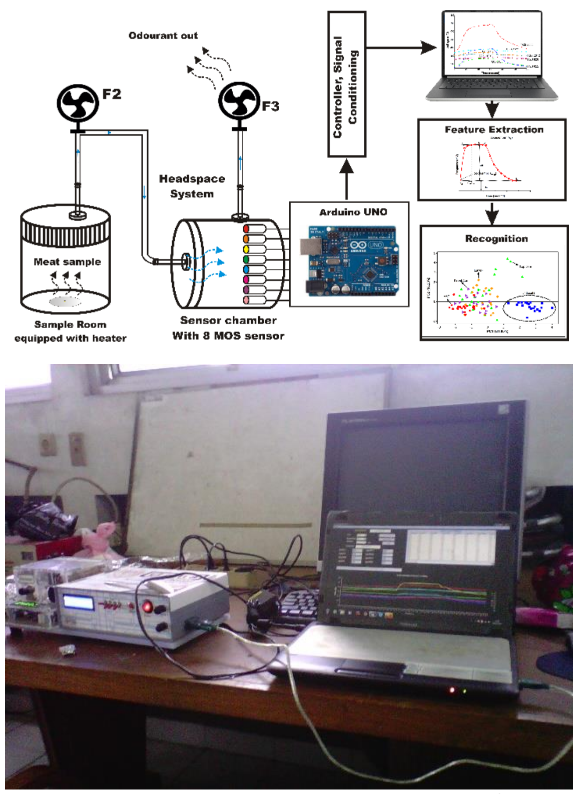

Fig. 2. The block diagram and the physical equipment of the gas sensor array

2.6. Data recording using e-nose

To run the sensory analysis process, a 5 ml sample of perfume was placed inside the sample chamber. To facilitate the release of the hexylene glycol contained in the perfume sample, the ceramic heater in the sample chamber was turned on to maintain a steady room temperature of 40°C. The headspace system directed the odour sample's perfume toward the sensor chamber for sensory examination.

The gas sensor array made use of a headspace system that was created with three fans designated F_1, F_2, and F_3, which operated in turn according to a controlling algorithm. The volatile organic compounds (VOCs) were moved via this headspace system from the sample room to the sensor chamber to measure the smell. The perfume sample was measured in a single cycle, including washing and sensing steps. The duration of each phase was 60 seconds. Fan F_1 was turned on throughout the sensing process; however, fans F_2 and F_3 were turned off. The perfume sample's odour was then moved from the sample room into the sensor chamber.

In addition, during the cleaning stage, fans F_2 and F_3 were turned on while fan F_1 was turned off. In this phase, the volatile gas released by the perfume sample was removed from the sensor chamber. The sensor array measured the variation in electrical resistance brought on by the interaction between the odorant and the sensor material during the sensing and cleaning phases. Real-time data transfer from a gas sensor array to a personal computer was made possible by the data collection system, which used an ATMega-16 microcontroller and an RS-232 serial communication unit.

2.7. Data Analysis of E-Nose Signal

The chemometrics approaches based on principal component analysis (PCA) and back-propagation neural networks (BPNN) were utilized to separate the output response of meat samples from sensory analysis. Before analysis using PCA and BPNN, the output response from the gas sensor array was pre-analysed using signal pre-processing. Feature extraction and signal reduction are two aspects of signal pre-processing. Signal reduction was employed to minimize noise and obtain the best possible signal. The transient response was subsequently selected as the primary signal for the data mining procedure. The transient response used the output response's first cycle to lessen the intensity of signal saturation. The following mathematical formula was used to extract features from the primary signal using the relative amplitude (RA) model.

$$RA = \frac{\delta V}{V_B} = \frac{V_{max-}V_B}{V_B} \quad (1)$$

where Vmax is the maximum of the sensor's response and VB is the baseline of the sensor's response.

The PCA was utilized to differentiate 150 e-nose output response obtained from measuring of 150 sample of perfumes using e-nose. Based on the theory, the PCA converts the original variables into a set of new, uncorrelated variables known as principal components, reducing the dimensionality of datasets without sacrificing information [24].

In addition, the output response of 150 perfume samples was categorized into several class based on the concentration of hexylene glycol using the Back Propagation Neural Networks (BPNNs) according to the output response pattern. A supervised machine learning algorithm is called BPNN. One hundred and fifty samples were split into two groups, the training and testing data sets, to run the BPNN algorithm. A training data set of 105 samples and a testing set of 45 samples were utilized. Subsequently, a feed-forward approach was used to classify the samples according to the input target supervised in the neural network model. This technique computes the error rate and weight update by BPNNs algorithm.

3. RESULTS

The profile of the gas sensor array's output responses when measuring the sample of patchouly is shown in Fig. 3. Typically, the output response produces a like sinusoidal signal. An upward signal was created when the volatile gas released by the perfume samples put in the sensor chamber. An oxidation reaction occurred at the surface of SnO_2 during the chemical reaction between the metal oxide semiconductor material of the sensor and the adsorbed oxygen from the volatile compounds. As a result, the concentration of oxygen molecules bound to the SnO2 surface decreased, resulting in a reduction in the energy barrier's height and an elevation in the resistance of the sensor.

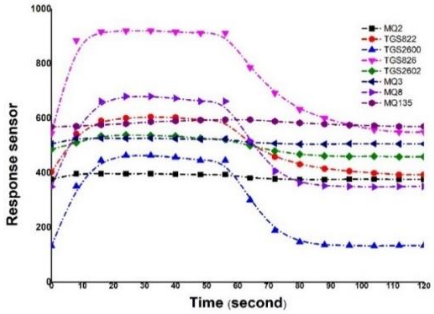

Fig. 3. The profile of output responses of the gas sensor array towards patchouli sample

The perfume samples release all volatile organic compounds (VOCs) that react chemically with metal oxide semiconductor material, producing a range of sensor responses at different intensities. The response value of every sensor towards the volatile gas in perfumes can be observed using the relative amplitude (RA) values. The process for extracting features to record RA values from each sensor's response is shown in Fig 3. The term δV divided by Vb was used to define the RA. At $t = 0$ s, V_b represents the initial sensor response.

Table 3. The RA with standard deviation values obtained from feature extraction of 150 e-nose response using Relative amplitude method

Sample Name	Value of RA±δRA							
	TGS 822	TGS 2600	TGS 826	TGS 2602	MQ2	MQ3	MQ8	MQ135
Bali Flower	0,74±0.01	0,70±0.01	0,66±0.01	0,35±0.01	0,39±0.01	0,24±0.01	0,36±0.01	0,52±0.01
Opium	0,76±0.01	0,72±0.01	0,66±0.01	0,32±0.02	0,40±0.01	0,23±0.01	0,36±0.01	0,52±0.01
Rose	0,76±0.01	0,75±0.01	0,62±0.01	0,33±0.01	0,40±0.02	0,28±0.01	0,37±0.01	0,52±0.01
Ylang-ylang	0,78±0.01	0,76±0.01	0,68±0.01	0,24±0.01	0,35±0.01	0,22±0.02	0,38±0.01	0.62±0.01
Melati	0,87±0.01	0,89±0.01	0,52±0.01	0,10±0.01	0,21±0.02	0,20±0.01	0,14±0.01	0,62±0.01
Cempaka	0,87±0.01	0,89±0.01	0,52±0.01	0,10±0.01	0,21±0.02	0,20±0.01	0,14±0.01	0,15±0.01
Lavender	0,86±0.02	0,85±0.01	0,54±0.02	0,10±0.01	0,24±0.01	0,18±0.01	0,17±0.02	0,13±0.01
Frangipani	0,90±0.01	0,85±0.01	0,46±0.01	0,04±0.01	0,19±0.01	0,15±0.01	0,13±0.01	0,08±0.01
Sandalwood	0,81±0.01	0,86±0.02	0,40±0.01	0,03±0.01	0,18±0.01	0,14±0.01	0,14±0.01	0,08±0.01
Patchouli	0,86±0.01	0,76±0.01	0,79±0.01	0,06±0.01	0,14±0.02	0,17±0.01	0,14±0.01	0,09±0.01

Compared to the values obtained from the remaining sensors. the output response values acquired from the TGS 813. TGS 2600. and TGS 822 sensors in Fig. 3 show greater values. Consequently. these three sensors have a greater amplitude of δV than other sensors. namely TGS 2602. MQ2. MQ3. MQ8. and MQ135. Table 2 displays the data tabulation of the changing output response (δV) from the sensory study of 150 perfume samples with from 10 different brands.

The mean RA value from the eight sensors used in the e-nose to measure the odor of ten sets of perfume samples is shown in Table 3. The standard deviation measured how different one sensor's RA value was from the others. One hundred and fifty perfume sample sensor response patterns were divided into four distinct patterns based on an analysis of the RA±δRA values obtained from eight sensors. Table 3 illustrates that the RA values of sensors TGS 822. TGS 2600. and TGS 826 were higher than those of the other sensors.

First. the RA values for sensors TGS 822. TGS 2600. and TGS 826 showed more than 0.5 when the aroma of patchouli samples with 0% hexylene glycol was exposed to the sensor chamber. In the meantime. sensor TGS 2602. MQ 2. MQ 3. MQ 6. and MQ 135 had RA values that were less than 0.5. Second. the RA values of TGS 822. TGS 2600. TGS 826. and MQ 135 showed higher than 0.5 when the Bali Flower containing 99% hexylene glycol was exposed to sensor chambers. In the meantime. MQ3. MQ4. and MQ6 sensors had values that were less than 0.5. In the third analysis. the RA values for sensors TGS 822. TGS 2600. and TGS 826 were more significant than 0.5 when examining the perfume sample with 30% hexylene glycol (moderate percentage). Sensors MQ

2. MQ 3. MQ 6. and MQ 135 all had RA values that were less than 0.5. For sensor TGS 2602. the resistance values (RA) were roughly 0.1.

Fourth. the RA values for sensors TGS 822 and TGS 2600 were more significant than 0.5. suggesting their higher relevance when the samples of Sandalwood and Frangipani with low concentrations of hexylene glycol (0-20%) was examined. Sensors MQ 2. MQ 3. and MQ 8 all have resistance values less than 0.2. For sensors TGS 2602 and MQ 135. the resistance values (RA) were approximately 0.2.

By comparing the RA values acquired from tracking the concentration of hexylene glycol in each perfume sample. the selectivity of the gas sensor for differentiating the perfume samples based on that concentration was ascertained. Three sensors—TGS 822. TGS 2600. and TGS 826—have higher susceptibilities than the other sensors. Three particular sensors—TGS 813. TGS 822. and TGS 2600—responded more strongly than the other sensors during the meat samples' exposure. The scent sample can be distinguished utilizing a range of hexylene glycol concentrations by the array of MOS sensors.

4. DISCUSSION

4.1. E-nose performe for distingush the perfumes based on hexylene glycol concentration

The key characteristics of the sensor array's response are separated and identified using the feature extraction technique. There still need to be clear patterns in the variations between samples that the feature extraction technique can locate. Nonetheless. the sensor array features' data dimensions continue to be significant. To reduce the size of the retrieved sensor array response and visualize differences in feature patterns between samples in two and three dimensions. the principal component analysis (PCA) method is used for feature selection. To reduce the size of the retrieved sensor array response and visualize differences in feature patterns between samples in two and three dimensions. the principal component analysis (PCA) method is used for feature selection. A mathematical method called principal component analysis (PCA) reduces a dataset's dimensions while retaining as much of the dataset's variance as possible (Jolliffe. 2002). Principal Component Analysis (PCA) is a mathematical technique that creates a new collection of uncorrelated variables from a set of correlated ones. The PCA technique is used to transform the data into new coordinate systems. The most significant eigenvalue is used to get the first coordinate. PC1. and the second largest eigenvalue is used to calculate the second coordinate. PC2. The main components are ordered. with PC1 capturing the most significant variance in the dataset and PC2 capturing variations not in PC1. with no association observed between them. The dimensionality of feature response without PCA was 150×8. then reduced to 150×2 data using PCA. Additionally. PCA converts the primary data into PC_1 and PC_2 as two new uncorrelated coordinates.

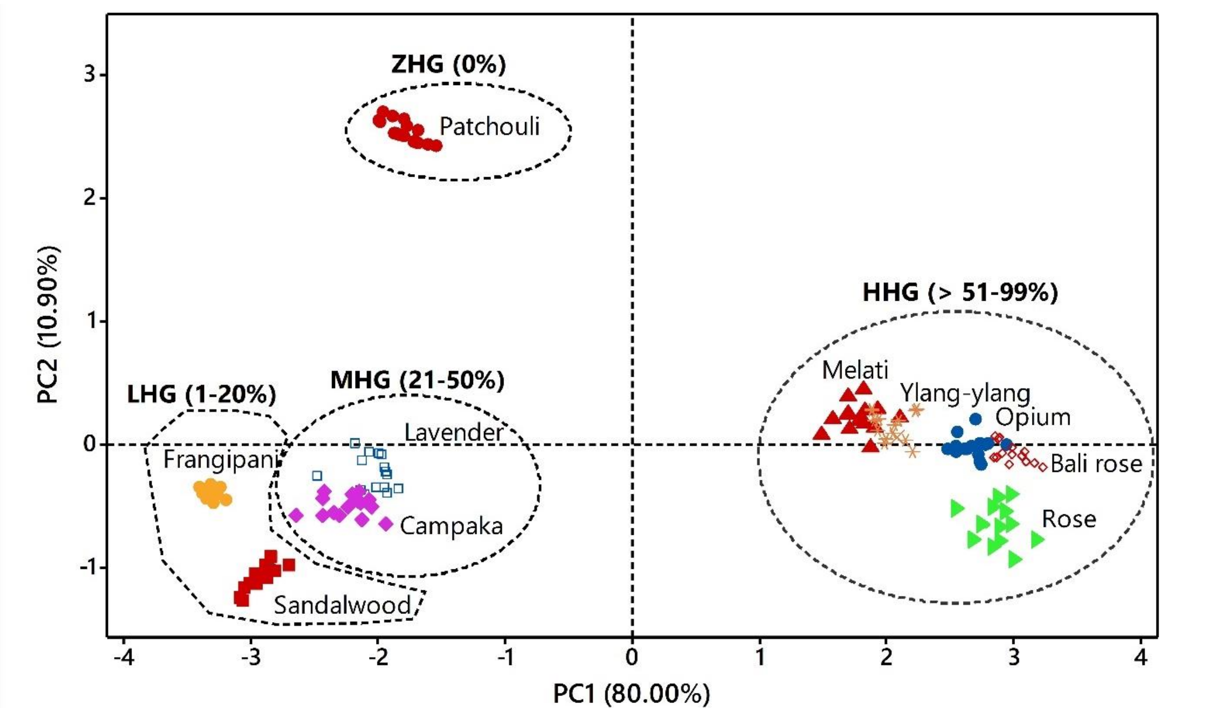

Fig. 4. Visualization of 150 perfume samples in the principal component coordinates to capture separation of 150 response of sample based on hexylene glycol concentration

The position of 150 perfume samples in the principal component coordinate is presented in Fig. 4. It can be shown that the PCA reached 90.90% of variance in two principal components. PC_1 reached

80.00% of the variance, while PC_2 reached 10.90% of the variance. Based on the visualization of principal component coordinates, the e-nose performs well in distinguishing perfumes based on the differences in hexylene glycol concentrations. One hundred and fifty perfume samples were grouped in four different clusters. The first cluster consists of patchouli samples with 0% of hexylene glycol. The samples of Frangipani and Sandalwood with a low concentration (1-20%) of hexylene glycol were put in the second group. The samples of Lavender and Campaka with moderate concentration (21-50%) of hexylene glycol were put in the third group. Meanwhile, samples of Melati, Ylang-ylang, Opium, Bali Rose, and Rose with high concentrations (51-99%) of hexylene glycol were categorized into the four groups.

Furthermore, a learning machine based on backpropagation neural networks (BPNNs) was used to classify 150 people into four different classes based on the concentration of hexylene glycol in the perfumes. BPNNs use processing components that can speak to one another over a network. Multiple layers are used to build a BPNN structure with many vertices—sometimes called nodes. Make up each layer. The input, hidden, and output layers make up the layers. Input units are the nodes that are part of the input layer. Information is distributed to other units by the input unit. Each unit in the underground layer serves as a processing element. Each node has connections to other nodes. There may be a link between nodes in the same layer or between nodes in different layers. Each node receives information from and sends output to other nodes.

Data is input via the sensor array response feature. The features above are examined in further detail with an artificial neural network method that classifies data using the backpropagation algorithm (BPNN). According to reference [25], categorization entails giving each member of set X a unique class label from set Y. Supervised learning requires working with class labels whose categories are already understood. It is an essential component of the learning process. The purpose of this study is to categorize each sample, as reflected by its particular qualities, into discrete classes based on its kind.

As a substitute technique, backpropagation neural networks (BPNN) are utilized to investigate the capacity of the sensor array to classify perfume samples based on the presence of particular compounds. BPNNs are neural network algorithms that process data forwarding via several layers. Commonly, the backpropagation algorithm employs the Widrow-Hoff or delta rule. BPNN uses supervised learning to choose the target. The architecture of BPNN consists of an input layer, a hidden layer, and an output layer. Several parameters, including data features, network architecture, network initialization, transfer functions in the hidden and output layers, training algorithm, learning rate (η), and error goal (ε), affect how well the BPNN classifier performs in classifying perfume samples based on the concentration of hexylene glycol.

The BPNNs were trained using training and testing datasets. The effectiveness of BPNN is measured using the accuracy of classifying 150 perfume samples based on the concentration of hexylene glycol. One hundred samples were divided into two groups: 110 as the training data set and 40 as the testing data set. Initial weights were allocated randomly with values ranging from -1 to 1 during the learning phase. The training parameters were adjusted to obtain the lowest error value: the learning rate (η) was set to 0.9. the maximum number of epochs was set to 1.000. Moreover, the goal error was defined as a mean square error smaller than 10^{-3}.

The network required 2.514 iterations to achieve a mean square error (MSE) of 10^{-4}. Table 4 displays the confusion matrix categorizing 110 samples from the training dataset and 40 samples from the testing dataset. The classification accuracy of the training data set was 96.36%. while the accuracy of the predicted samples from the testing data set was 92.50%. For training data set, 4 perfume samples with moderate hexylene glycol (21-50%) was detected in low concentration of hexylene glycol. Meanwhile, for testing data set, 3 perfume samples with moderate hexylene glycol (21-50%) was detected in low concentration of hexylene glycol.

Table 4. Confusion matrix obtained from the BPNN classification of training data set with 63 samples and testing data set with 27 samples

Actual class	**Output classifier in predicted class**				**Actual class**	**Output classifier in predicted class**			
	Training data set					**Testing data set**			
	ZHG	**LHG**	**MHG**	**HHG**		**ZHG**	**LHG**	**MHG**	**HHG**
ZHG	11	0	0	0	ZHG	4	0	0	0
LHG	0	22	0	0	LHG	0	8	0	0
MHG	0	4	18	0	MHG	0	3	5	0
HHG	0	0	0	55	HHG	0	0	0	20

5. CONCLUSSION

The hexylene glycol can be detected successfully by combining PCA and BPNN with a homemade e-nose. In total. 150 samples of perfumes with different concentrations of hexylene glycol were grouped into four different classes. The first class was designated for ZHG with 0% of hexylene glycol . The second class was reserved for LHG with with 1-20% of hexylene glycol. The third class was assigned to MHG with 21-50% of hexylene glycol. while the fourth was assigned to HEG with more than 50% of hexylene glycol. The findings of the chemometric analysis show that the apparatus functions well as a rapid and low-cost instrument for sensory analysis and odour classification of perfumes based on the concentration of hexylene glycol. However. adding more sensitive sensors will need to improve the gas sensor array.

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