The Implementation of Preconcentrator in Electronic Nose System to Identify Low Concentration of Vapors Using Neural Network Method

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The Implementation of Preconcentrator in Electronic Nose System to Identify Low Concentration of Vapors Using Neural Network Method

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***Abstract*— Vapor identification system having high sensitive and discriminative capabilities is much needed in various applications such as in monitoring of environmental condition, detecting of hazardous substances, and producing of flavored foods or drinks and others. Nowadays, electronic nose technology which consists of gas sensor array and neural network pattern recognition could not recognize well for the low concentration vapors. In this research, the implementation of a preconcentrator was used to increase the vapor concentration allowing the electronic nose system to gain its high sensitivity and selectivity. The experimental result showed that the electronic nose system equipped with the preconcentrator could distinguish ethanol, benzene and acetone vapors in low concentrations successfully.**

Keywords—electronic nose, preconcentrator, selectivity, sensitivity

I. INTRODUCTION

Recently, an objective instrument such as spectrophotometer and gas chromatography has become one of the most widely used analytical detectors for liquid or gas analysis. However, these analytical instruments are large, expensive, time consuming and require trained operators, which has limitations on their potential applications. It has, therefore, being developed a new analytical instrument based on mimicking the human olfactory due to its ability to be a rapid, non-invasive, simple, cheap, and easily operated tool which is known as "electronic nose". An electronic nose is a device which consists of an array of chemical sensors with different selectivity and a pattern recognition system. The interaction between the sensor array and volatile organic compounds generates a specific fingerprint or pattern which can be classified by the recognition system.

The electronic nose system has developed significantly along with advances in sensor technology. The commonly used sensors for electronic noses include metal oxide semiconductor, conducting polymer, quartz crystal microbalance, surface acoustic wave, and optical sensors [1]. The metal oxide semiconductors are one of the most common materials of sensor systems as they possess a broad range of electronic, chemical, optical and physical properties that are often stable to vary with the chemical composition of ambient air [2].

The multivariate responses of gas sensor array with partially overlapping sensitivities can be used to characterize volatile compounds by pattern recognition means. There are several classification techniques which are usually applied in the electronic nose including principal components analysis, Fisher's linear discriminant analysis, k nearest neighbor, radial basis function, and multilayer perceptron neural network. The latter method is an algorithm that has been commonly developed for many years in the electronic nose technology which can handle both linear and nonlinear problems [3,4]. Moreover, the addition neurons in hidden layers may allow the network to perform a more efficient approximation as pattern recognition [5].

Currently, the development of the electronic nose technology has been carried out in wide field of applications such as environment monitoring [6], quality control [7], and disease diagnosis [8] which human exhaled breath contains a large number of volatile organic compounds. The vapor concentration level of most gas sensors are in part per million (ppm) order, however the concentration of marker gas contained in human breath and also gaseous pollutants in atmosphere are in parts per billion (ppb) [9,10]. A vapor preconcentrator is, therefore, essentially applied to the electronic nose system in order to be able to diagnose the low concentration vapor under current precision levels of gas sensors.

II. LITERATURE REVIEW

A. Metal Oxide Semiconductor Sensor

The materials of metal oxide semiconductor are used as gas sensors based on the principle of the variability of electrical conductivity of metal oxides when exposed to gases, such as O_2, CO_2, H_2, and volatile organic compounds. The metal oxide semiconductor sensor technology is based on the change in resistance of a sensitive metal oxide layer

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which depends on the gases that interact with the adsorbed oxygen on the semiconductor, the metal oxide grain size and the working temperature. This type of sensor demonstrates good sensitivity, robustness and the ability to work at high temperatures [11], this sensor is, therefore, commonly used to monitor a variety of gases in air pollution monitoring systems, the drinks or food industry, medical diagnosis equipment and toxic or inflammable gas leak detectors.

Fig. 1 shows typical gas sensor structure based on metal oxide semiconductor. The metal oxide semiconductor sensor is consisted of sensor cap, sensing element, and sensor base. The sensing element is composed of sensing material and heater to heat up sensing element (eg. 400 °C). Depending on the target gas, the sensing element will utilize different materials such as Tin dioxide (SnO_2), Tungsten oxide (WO_3), etc. Fig. 2 represents typical sensitivity characteristics of the commercial gas sensor based on metal oxide semiconductor. It indicates that gas concentration level of semiconductor gas sensor is in part per million orders.

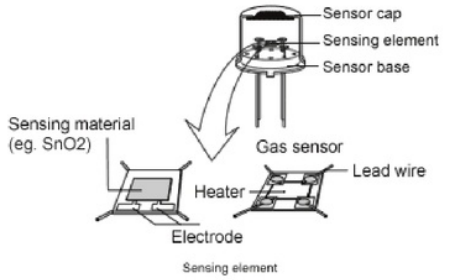

Fig. 1. The structure of metal oxide semiconductor sensor.

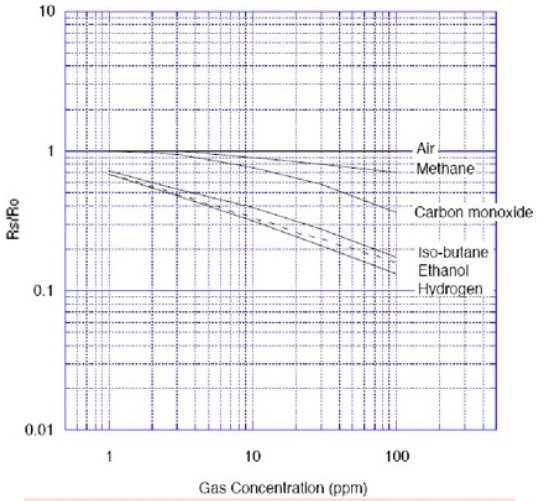

Fig. 2. A typical responses of the metal oxide semiconductor sensor.

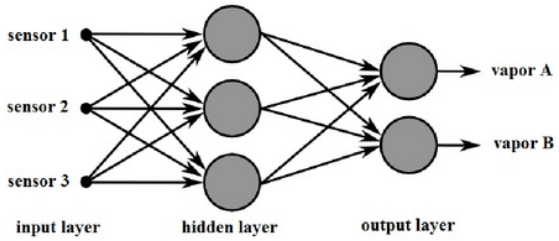

Fig. 3. A typical artificial neural network implemented in an electronic nose system.

B. Neural Network Pattern Recognition

An Artificial Neural Network is an information processing paradigm inspired by the biological nervous systems, such as the brain. It is composed of a large number of interconnected processing elements of neurons working in unison to solve specific problems. This method is purposed for specific applications, such as pattern recognition or data classification through a learning process [12]. The learning process involves adjustments to the synaptic connections or weights among the neurons. Fig. 3 shows three layer neural network architecture as pattern recognition in an electronic nose system.

The backward propagation of errors- abbreviated with back propagation- is a common algorithm of training phase in artificial neural networks which learns by example. An optimization method such as gradient descent calculates the gradient of a loss function with respects to all the weights in the network. The gradient of the loss function is fed to the optimization method to update the interconnection weights to minimize the overall error. This method is expressed as below:

Initially, the weights will be set randomly. The weighted sum of all its hidden neuron is:

$$neth_j = \sum_i wh_{ji}\, i_i \tag{1}$$

where wh is the weight on the connection from the input units i to the hidden unit h. A commonly used activation function is the logistic function. The output for each hidden neuron is defined as:

$$h_j = \frac{1}{1+e^{-\lambda neth_j}} \tag{2}$$

The weighted sum of all its output neuron is:

$$neto_k = \sum_j wo_{kj}\, h_j \tag{3}$$

The output for each output neuron is expressed as:

$$o_k = \frac{1}{1+e^{-\lambda neto_k}} \tag{4}$$

The overall error is defined as:

$$\underline{e}^p = \underline{t}^p - \underline{o}^p \tag{5}$$

where t is the target output and o is the actual output. The squared error function is:

$$E^p = \frac{1}{2}\left(e^p\right)^T e^p = \frac{1}{2}\sum_j \left(t_j^p - o_j^p\right)^2 \quad (6)$$

The change in output weight is:

$$\Delta wo_{kj} = -\frac{\partial E}{\partial wo_{kj}} = -\frac{\partial E}{\partial o_k}\frac{\partial o_k}{\partial neto_k}\frac{\partial neto_k}{\partial wo_{kj}} = \lambda(t_k - o_k)o_k(1-o_k)h_j \quad (7)$$

$$\Delta wo_{kj}(n+1) = \varepsilon \Delta wo_{kj} + \alpha \Delta wo_{kj}(n) \quad (8)$$

where ε and α are the learning rate and momentum constant, respectively. The learning rate controls the size of weight during learning while the momentum parameter is used to prevent the system from converging to a local minimum or saddle point.

The updated output weight is:

$$wo_{kj}(n+1) = wo_{kj}(n) + \Delta wo_{kj}(n+1) \quad (9)$$

The change in hidden weight is:

$$\Delta wh_{ji} = -\frac{\partial E}{\partial wh_{ji}} = -\frac{\partial E}{\partial o_k}\frac{\partial o_k}{\partial neto_k}\frac{\partial neto_k}{\partial h_j}\frac{\partial h_j}{\partial neth_j}\frac{\partial neth_j}{\partial wh_{ji}} = \sum_k \lambda h_j(1-h_j)\lambda(t_k - o_k)o_k(1-o_k)wo_{kj}.i_i = \lambda h_j(1-h_j)\left\{\sum_k \lambda(t_k - o_k)o_k(1-o_k)wo_{kj}\right\}i_i \quad (10)$$

$$\Delta wh_{ji}(n+1) = \varepsilon \Delta wh_{ji} + \alpha \Delta wh_{ji}(n) \quad (11)$$

The updated hidden weight is:

$$wh_{ji}(n+1) = wh_{ji}(n) + \Delta wh_{ji}(n+1) \quad (12)$$

This sequence of events is usually repeated until an acceptable error has been reached or until the network no longer appears to be learning.

III. Material And Method

A. Preconcentrator

The preconcentrator unit is a sample collection or concentration stage that samples and collects analytes from an inlet gas sample stream and ejects them on command into the separation stage. Preconcentrating is a well known method based on the collection of an analyte during a fixed period [13]. In this study, the preconcentrator consists of a 3.5" long glass tube with a 0.25" inner diameter packed with 60-80 mesh Tenax GR for trapping volatiles shown in Fig. 4. Tenax is a porous polymer resin based on 2,6-diphenyleneoxide which is widely used for trapping volatile organic compounds from air and liquids. The Tenax GR is a composite material of Tenax TA and 30% graphite giving a higher breakthrough volume for most volatile organics at the temperature stability to 350 °C. These properties, therefore, make this material an ideal adsorbent for the trapping of volatiles from air, water and solid samples. Using thermal desorption techniques, detection of volatile organics in the ppb and ppt level is feasible.

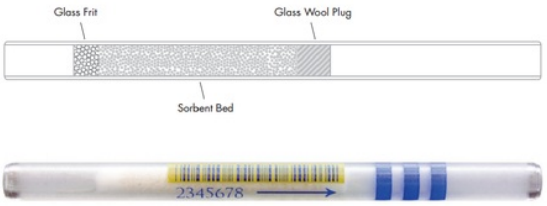

Fig. 4. A glass tube preconcentrator.

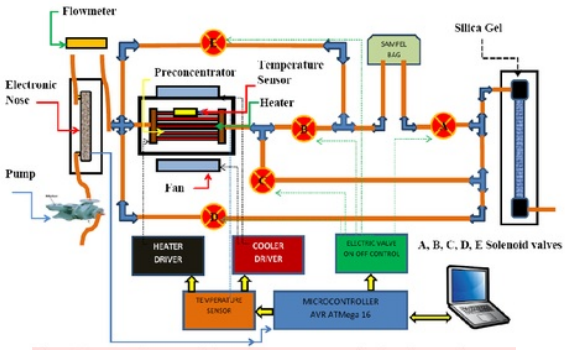

Fig. 5. System layout of the preconcentrator for the electronic nose.

According to the trapping theory, the cooler the system, the stronger the trapping capability is. It means that the trap capability between the sorbents and the volatile compounds decreases at increasing temperature. The trapping efficiency tends to increase exponentially with a decrease in temperature.

Figure 5 describes the system architecture of the preconcentration system for the electronic nose. In the sample collection or adsorption phase, a 12V dc cooling fan driven with pulse width modulation method was used to provide the temperature of preconcentrator at about 20 °C. While in the sample desorption phase, a 220V ac heating element of nickel-chromium material was used to provide the temperature up to 250 °C. A resistance temperature detectors PT100 was used to measure temperature the preconcentrator in both the adsorption and desorption phases The sensor element is made of a fine coiled wire of pure material, typically platinum, nickel or copper wrapped around a ceramic or glass core. The material has a predictable change in resistance as the temperature changes that is used to determine temperature. This type of temperature sensor is slowly replacing the use of thermocouples in many applications below 600 °C, due to higher accuracy and repeatability. Because it could be influenced by environmental temperature, the proportional controlling method was used in this experiment to maintain the desired temperature of the preconcentrator.

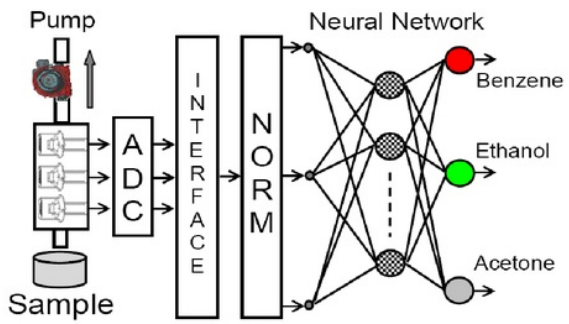

Fig. 6. The electronic nose system.

The carrier gas is from ambient air purified by the silica gel. The dry air was then flowed through the electric valve of D to clean the sensor chamber. In the adsorption phase, the dry air was directed through the valves of A and B. While in the desorption phase, the dry air was directed via the valve of C. Ignoring the preconcentrator role, the solely response of the electronic nose was achieved when the dry air was flowed through the valves of A and E.

B. Electronic Nose

Figure 6 expresses the electronic nose system consisted of gas sensor array and neural network pattern recognition. The sensor array is composed of three metal oxide sensors, namely MQ-131, MQ-136, and MQ-137. To improve the preconcentrator effects, the sensor chamber of the electronic nose needs to be made as small as possible. The signals of gas sensors are sampled into a computer through a 10-bit analog-to-digital converter. The normalization technique reduces the short term instability of the sensor response without losing the quantitative information of the samples [14]. The input layer of neural network is comprised of three nodes corresponding with the number of sensors, the hidden layer is composed of twenty neurons to accelerate and improve the convergence in learning phase and the output layer is consisted of three neurons with respect to the number of gases.

IV. Result And Discussion

Fig. 7 shows a photo of the electronic nose in conjunction with a preconcentrator unit used in the experiments. Due to the slow response of the gas sensor, the dry air was flowed at 500 and 50 mL/min at the adsorption and desorption phases, respectively. Table I indicates that the desired temperature was achieved at only several seconds.

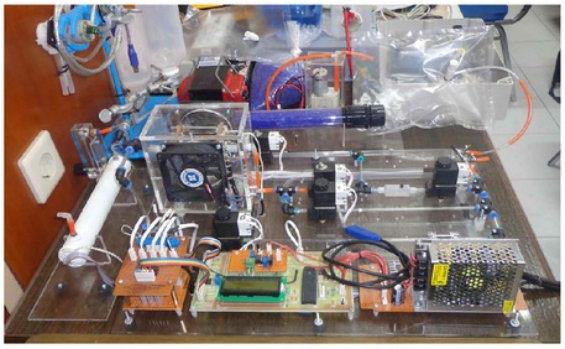

Fig. 7. The electronic nose system.

TABLE I. The settling time of temperature controlling.

No.	Temperature (°C)	Time (sec.)
1.	50	04.23
2.	100	06.57
3.	150	08.46
4.	200	09.94
5.	250	11.34
6.	300	12.46

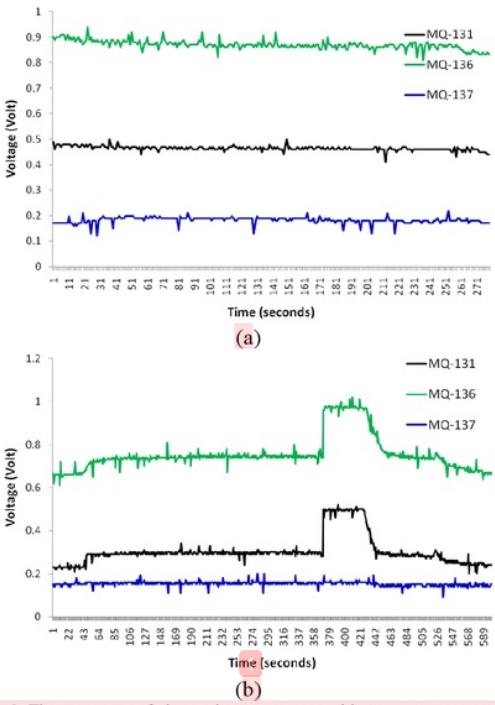

Fig. 8. The responses of electronic nose system without preconcentrator to (a) ethanol and (b) benzene vapors.

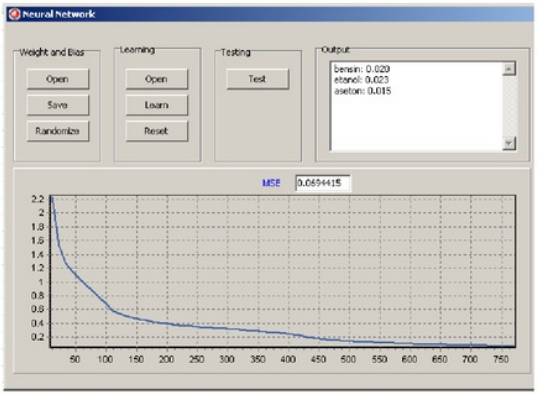

Fig. 9. The training phase of electronic nose system without preconcentrator exposed to benzene vapor.

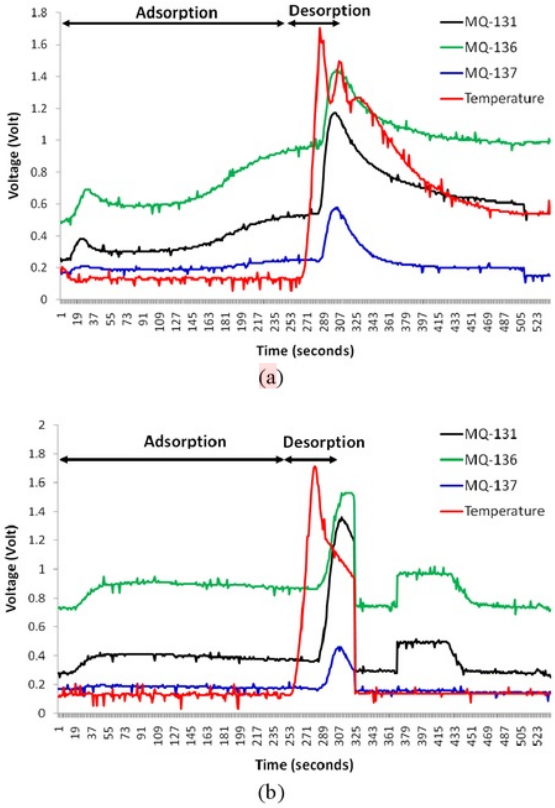

Fig. 10. The responses of electronic nose system equipped with preconcentrator to (a) ethanol and (b) benzene vapors.

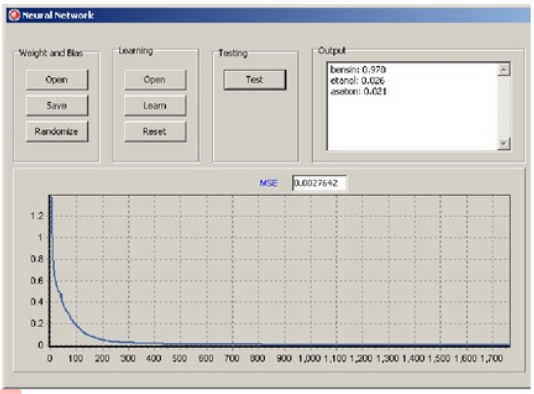

Fig. 11. The training phase of electronic nose system together with preconcentrator exposed to benzene vapor..

The first experiment was conducted with the electronic nose without preconcentrator. Fig. 8 shows the responses of sensor array to 0.01 ppm ethanol and benzene vapors. It was indicating that almost each sensor has small change in respond to these tiny samples. For the neural network training purpose, all of the sensor values were normalized as real numbers by dividing them with the highest value [15]. Nine data sets were fed into the neural network. The network is trained using the values of learning rate of 0.4 and momentum constant of 1 to achieve a target error of 0.001 or 1000 epochs. Fig. 9 describes that the network could not recognize each sample of ethanol, benzene and acetone vapor until reaching its epoch goal. It was indicating that the electronic nose without preconcentrator could not identify low concentration of vapors.

The second experiment involved the electronic nose in conjunction with preconcentrator. All parameter values of the samples materials and the neural network are the same with the previous experiment. Fig. 10 shows the responses of sensor array to ethanol and benzene vapors. In contrast to the previous one, this method exhibited that almost each sensor has significant change in respond to the vapor samples. Fig. 11 describes that the network could recognize each sample indicating that the electronic nose together with a preconcentrator unit could identify low concentration of vapors.

V. Conclusion

It has been developed an electronic nose conjunction with a preconcentrator as sample collection which extends the concentration workspaces of current gas sensors. The experiment results showed that this method could detect 0.01 ppm vapors indicating the increasing sensitivity of the current gas sensor. Moreover, the neural network could recognize each sample describing the increasing selectivity of the network. It can be concluded that the electronic nose together with a preconcentrator unit could identify low concentration of vapors. In the future work, therefore, this

equipment is a promising method to be implemented in human breath analysis containing low concentration of marker gases.

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