THE APPLICATION OF NEURAL NETWORK OF MULTI-CHANNEL QUARTZ CRYSTAL MICROBALANCE FOR FRAGRANCE RECOGNITION

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ABSTRACT

Detection of fragrances or odorous compounds that can readily evaporate at room temperature, has gained considerable attention. A multi-channel quartz crystal microbalance sensor coated with different sensing materials was employed in the present study to detect the odorous compounds. Principle Component Analysis method was used to visualize the classification of each fragrance in two-dimensional space. Back propagation neural network was used to distinguish the species of fragrances implemented in the personal computer. All-digital interface was implemented on the Field Programmable Gate Array. The results show that the sensor array could produce a specific response pattern for each fragrance and the neural network can be taught to recognize seven fragrances of perfume and four fragrances of Indonesia local tea with the identification rate of 93%.

Keywords: fragrance, response pattern, neural network

1 INTRODUCTION

Electronic Nose is an instrument that is designed to detect and identify among complex odors using a sensor array. The sensor array consists of a number of non-specific sensors coated with a variety of odor-sensitive materials. An odor stimulus produces a characteristic fingerprint from this sensor array. Patterns or fingerprints from known odors are used to construct a database of a pattern recognition system so that unknown odors can be classified. A major problem in odorous vapor identification is the substantial similarity of patterns obtained for different vapors, a phenomenon attributed to low selectivity of the sensing system [1].

Piezoelectric quartz crystal, a well known as quartz crystal microbalance, is a material with very sensitive response for the changes in mass. The frequency of the crystal will decrease by adsorbing targets on the crystal's surface. For sensing applications, a sensitive sensing film is cast on the surface of the quartz crystals. This film can bind the molecules of the vapor of interest, altering the resonant frequency of the device in proportion to the added mass. The odor sensor system typically consists of an array of several crystals, each coated with a different sensing film. The response pattern of such an array then serves as the fingerprint for a given vapor. The absorption rate is affected by the size and polarity of both the vapor and the sensing film [2].

Principal component analysis (PCA), a well-known technology of statistics, is useful in selecting the classic independents of all materials. The method can distinguish the different species by taking a view of the profile discrimination with the responses of several channels in a plot [3]. PCA contains an orthogonalization procedure such as singular-value decomposition that decomposes the primary data matrix by projecting the multi-dimensional dataset onto new coordinates base formed by the orthogonal directions with data maximum variance. The data matrix consists of a number of experiments, each consisting of a number of variables. The eigenvectors of the data matrix are called principal components and they are uncorrelated among them. Sensor signals can be expressed as the linear combination of eigenvectors. Generally, the k-th principal component, \(PC_k\), is a linear combination of the n response vectors \(X_n\) for the fragrances under study, where n is the number of the variables, j indicates different samples and the coefficients \((a_{nk})\), expressed by:

\[
P_C^k = \sum_{n=1}^{n} a_{nk} X_n^j \tag{1}
\]
The magnitude of each eigenvector is expressed by its own eigenvalue, which gives a measure of the variance related to that principal component. The variance is related to the quantity of information which is supplied by the component. By elimination of the less important eigenvectors, it is possible to achieve fewer vectors without any considerable information loss. During data processing, the results are transformed in a plane or in a space of the first two or three eigenvectors. The coordinates of the data in the new base are called their score. The scores plot is usually used for the classification of the data clusters.

Artificial neural network capacitates a computer the ability of learning and thinking. The application of neural network method proved to be particularly advantageous if the measured property is not connected exactly to the signal of the sensors. The optimum structure of neural network is determined by a trial and error method. One way to generalize the linear discriminant function, so as to permit a much larger range of possible decision boundaries, is to transform the input vector \( x \) using a set of predefined nonlinear basis function \( \Phi \) and represent the output as a linear combination of this function:

\[
y_k = \sum_{j=1}^{M} w_{kj}x_j + w_{k0} \quad (2)
\]

The basis function can be given by logistic activation function:

\[
\Phi_k = \frac{1}{1 + e^{-y_k}} \quad (3)
\]

The neural is trained to minimize the entropy cost function. Back propagation neural network is the most popular technology of the chemical sensor array [4]. Being one of the most popular neural networks in electronic noses, back propagation neural network has become the de facto standard for pattern recognition of signals from a chemical sensor array. This method is a supervised learning algorithm based on the generalized delta rule, usually using gradient descent for minimizing the total squared output error between the desired and the actual net outputs. The performance of back propagation neural network is dependent on several factors, e.g., the number of hidden layers, learning rate, momentum and training data [5].

In this paper, qualitative analysis of the fragrances was done by using quartz crystal microbalance sensor array and three layers network structure with back propagation method. PCA was used to visualize the classification of each fragrances detected by the sensor array.

2 EXPERIMENTAL

Quartz crystal microbalance sensors were AT-cut spherical quartz crystals, with a basic resonant frequency of 20 MHz and were provided with gold electrodes on both sides. The crystals were coated with the prepared sensing film materials of squalane, apiezone-L, ethyl cellulose, silicone OV-17, silicone OV-25 and polyethylene glycol (PEG) 1540 via ultrasonic atomizer. Among other methods for depositing sensing films, this method offers better the surface stability and the reproducibility of sensor responses [6]. The sensors were mounted in a sealed test chamber, shown in Figure 1. The fragrance generation system consisted of calibrated mass flow controllers, conventional gas bubblers containing the liquid sample, and a pair of three-way electronic valves. The fragrance was generated by flowing of 50 mL/min carrier gas of dry nitrogen (N\(_2\)), through the bubbler within forty seconds. The electronic valves were computer controlled to automatically expose the sensor array to various sort of fragrances. The frequency response was monitored using a multi channel frequency counter interfaced to Personal Computer via RS232 serial communication. All digital interface was implemented on the Field Programmable Gate Array (FPGA) Xilinx XC3S500E Spartan-3E and software Xilinx ISE Webpack 9.2i, shown in Figure 2. Real time data were displayed and analyzed to obtain frequency shifts between before and after fragrance exposure. All experiments were performed at the temperature of 32±2 °C.

![Figure 1. The experimental setup of fragrance identification system](image)
Sensors were exposed to seven fragrances of perfume liquid, namely apple, frangipani, jasmine, melon, rose, sandalwood, and vanilla and also exposed to four fragrances of Indonesia local tea, namely Balap Sepeda, Gopek, Hijau Daun, and Poci. After fragrance exposure, the sensor array was purged with dry N\textsubscript{2} to flush the vapor molecules. At each sample, the frequency shifts of each sensor within forty seconds after sample injection were recorded to obtain a six dimensional pattern, representing the exposed fragrance.

The multilayer neural network was applied to the sensor array to recognize fragrances automatically. The number of input nodes was six correspond to the number of sensors, and the number of output neurons was eleven equal to that of the sort of fragrances, shown in Figure 3. The number of hidden neurons was twenty to accelerate and improve the convergence in training phase. Both learning rate and moment constant were empirically determined to be 0.01.

The sensitivity of the sensor is linearly proportional to the vapor concentration \([7]\). Since the concentration for an unknown fragrance is also unknown, the identification must be based on signature patterns, and not on the concentration dependent amplitudes. Therefore the concentration information was removed by normalizing each pattern by dividing of each sensor response with sum of all of the sensor responses. The normalized frequency shifts of the sensor array for each perfume fragrance is shown in Figure 5.

3 RESULT

The first experiment was carried out with the sample of perfume fragrances. The baseline value was obtained when the dry N\textsubscript{2} gas was flowed into the sensor chamber. During in the sample injection, the frequency is decreasing due to the acoustic losses, shown in Figure 4.

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Figure 3. The sensor array combined with Neural Network pattern recognition

Figure 4. The time response of the sensor array to perfume fragrances

Figure 5. The signatures of perfume fragrance resulted by the sensor array

Figure 6. The scattering diagram of perfume fragrances visualized by PCA
The measurement data are six-dimensional, since six sensors were used. The mapping method is required to find a low dimensional vector that preserves most of the information in the original feature vector. Scattering diagram by PCA with two of the most significant components is shown in Figure 6. The seven clusters formed match with the seven types of perfume fragrances so that the fragrance were completely separated in the principal component space, with the cumulative sum of the variances:

<table>
<thead>
<tr>
<th>Cumulative Variance</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>81.2134</td>
<td>81.2134</td>
</tr>
<tr>
<td>95.5357</td>
<td>95.5357</td>
</tr>
<tr>
<td>98.5908</td>
<td>98.5908</td>
</tr>
<tr>
<td>99.6982</td>
<td>99.6982</td>
</tr>
<tr>
<td>100.0000</td>
<td>100.0000</td>
</tr>
</tbody>
</table>

This shows that almost 95% of the variance is accounted for by the first two principal components.

The second experiment was carried out with the samples of Indonesia local tea fragrances. The typical response and the normalized frequency shifts of the sensor array to the tea fragrances are shown in Figure 7 and Figure 8, respectively. The four tea fragrances were also completely separated in the principal component space, shown in Figure 9, with the cumulative sum of the variances:

<table>
<thead>
<tr>
<th>Cumulative Variance</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>92.8409</td>
<td>92.8409</td>
</tr>
<tr>
<td>99.1536</td>
<td>99.1536</td>
</tr>
<tr>
<td>99.6980</td>
<td>99.6980</td>
</tr>
<tr>
<td>99.9898</td>
<td>99.9898</td>
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<tr>
<td>100.0000</td>
<td>100.0000</td>
</tr>
</tbody>
</table>

The multilayer neural network was applied to the sensor array to recognize all fragrances automatically. In the training phase, 55 data sets were fed into the neural network. The neural can be taught to discriminate each fragrance with the error rate of 1% taking 27,390 epochs, shown in Figure 10. In the running phase, the others 55 data sets were fed into the neural network. The network can recognize all fragrances tested in the experiment with the identification rate of 93%. The activation rates of the output neurons were shown in Fig. 11.
The Application Of Neural Network Of Multi-Channel Quartz Crystal Microbalance For Fragrance Recognition - Muhammad Rivai

CONCLUSION AND DISCUSSION

It has been investigated that the electronic nose comprising six quartz crystal microbalance sensor and back propagation neural network was able to distinguish several samples of fragrances. This system has been shown to resolve the fragrances, including fragrances of different classes (i.e. apple, frangipani, jasmine, melon, rose, sandalwood, and vanilla) as well as those within a particular class of Indonesia local tea (i.e. Balap Sepeda, Gopek, Hijau Daun, and Poci). The neural network can be taught to recognize all of the fragrances with the identification rate of 93%.

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REFERENCES

Figure 12. The time response of the sensor array to fragrances