Mixed Odor Classification for QCM Sensor Data by Neural Network

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KEYWORD

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ABSTRACT

Compared with metal oxide semiconductor gas sensors, quarts crystal microbalance (QCM) sensors are sensitive for odors. Using an array of QCM sensors, we measure mixed odors and classify them into an original odor class before mixing based on neural networks. For simplicity we consider the case that two kinds of odor are mixed since more than two becomes too complex to analyze the classification results. We have used eight sensors and four kinds of odor are used as the original odors. The neural network used here is a conventional layered neural network. The classification is acceptable although the perfect classification could not been achieved.

1 Introduction

Over the last decade, odor sensing systems (so-called electronic nose (EN) systems) have undergone important development from a technical and commercial point of view. The EN refers to the capability of reproducing human sense of smell using sensor arrays and pattern recognition systems[MILKE, J. 1995].

We have presented a type of an EN system to classify the various odors under the various densities of odors based on a competitive neural network by using the learning vector quantization (LVQ) method in [CHARUMPORN, B. *et al*. 2003]. The odor data were measured by an odor sensor array made of MOGSs. We used fourteen MOGSs of FIGARO Technology Ltd in Japan. We considered two types of data for classification in the experiment. The first type was a set of four kinds of tees and the second one was a set of five kinds of coffees of similar properties. The classification results of tees and coffees were about 96% and about 89%, respectively, which was much better than the results in [FUJINAKA, T. *et al*. 2008], [OMATU, S. *et al*. 2011].

In this paper, we will consider the classification of mixed odors based on the sensing data by using quarts crystal microbalance (QCM) sensors. QCM sensors are sensitive to odors and we can measure the odor data precisely. Using many QCM sensors, we will try to separate the odors being mixed with two kinds of odor into the original odors based on the neural network classifier.

2 Principle of QCM Sensors

The QCM has been well-known to provide very sensitive mass-measuring devices in nanogram levels, since the resonance frequency will change sensitively upon the deposition of a given mass on the electrodes. Synthetic polymer-coated QCMs have been studied as sensors for various gasses since QCM coated with a sensing membrane works as a chemical sensor. The QCM sensors are made by covering the surface with several kinds of a very thin membrane with about 1 mm as shown in Fig. 1.

Since the QCM oscillates with a specific frequency depending on the cross section corresponding to three axis of the crystal, the frequency will change according to the deviation of the weight due to the adsorbed odor molecular (odorant). The membrane coated on QCM has selective adsorption rate for a molecular and the frequency deviation show the existence of odorants and their densities. Odorants and membrane are tight relation while it is not so clear whose materials could be adsorbed so much.

In this paper we have used the following materials as shown in Table 1. The reason why fluorine compounds are used here is that the compounds repel water such that pure odorant molecules could be adsorbed on the surface of the membrane. To increase the amount of odorants to be adsorbed it is important to iron the thickness of the membrane. In Table 1, we have tried to control the density of the solute in the organic solvent. The basic approach used here is a sol-gel method. The sol-gel process is a wet-chemical technique used for the fabrication of both glassy and ceramic materials. In this process, the sol (or solution) evolves gradually towards the formation of a gel-like network containing both a liquid phase and a solid phase. Typical precursors are metal alkoxides and metal chlorides, which undergo hydrolysis and polycondensation reactions to form a colloid. The basic structure or morphology of the solid phase can range anywhere from discrete colloidal particles to continuous chain-like polymer networks.

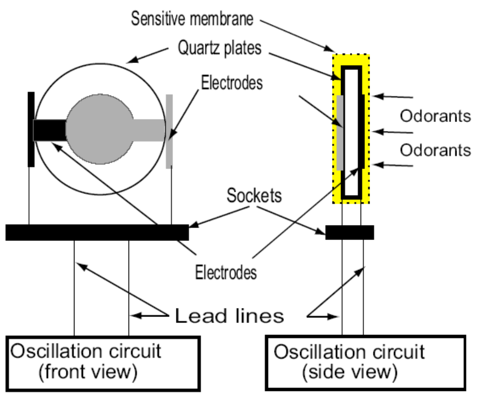

Fig.1. Principle of QCM. The odorants attached on sensitive membrane will make the weight of quartz plane. Thus, the original frequency of the crystal oscillation will become smaller according to the density of odorants.

Sensor number	Materials of membrane
Sensor 1	Tms, en(4ml), dna(0.023ml)
Sensor 2	Tms, wt(3.13ml), en(4.0ml), dna(0.023ml), ea(0.043ml)
Sensor 3	Tms, wt(3.13ml), en(4ml), dna(0.014ml), ea(0.014ml)
Sensor 4	Tms, wt(3.13ml), en(4.0ml), dna(0.015ml), ea(0.015ml)
Sensor 5	Tms, wt(3.0ml), en(4.0ml), dna(0.043ml), ea(0.043ml)
Sensor 6	Tms, wt(0.05ml), en(3.0ml), dna(0.043ml), ea(0.043ml)
Sensor 7	Tms, wt(0.03ml), en(3.2ml), dna(0.043ml), ea(0.043ml)
Sensor 8	No membrane

Table. 1. Chemical materials used as the membrane. Here, Tms is Triethoxymethylsilane, wt is water, en is ethanol, dna is dilute nitric acid, and ea is ethylacrylate

3 Odor Sensing System

Generally, it is designed to detect some specific odor in electrical appliances such as an air purifier, a breath alcohol checker, and so on. Each of QCM membranes has its own characteristics in the response to different odors. When combining many QCM sensors together, the ability to detect the odor is increased. An EN system shown in Fig. 2 has been developed, based on the concept of human olfactory system. The combination of QCM sensors, listed in Table 1, are used as the olfactory receptors in the human nose.

The odors used here are shown in Table 2. Note that the chemical properties of these odors are very similar and it has been difficult to separate them based on the measurement data by using MOGS sensors.

Symbols	Kind of odors
A	Ethanol
B	Water
C	Methyl-salicylate
D	Triethylamine

Table. 2. Kinds of odors measured in this experiment.

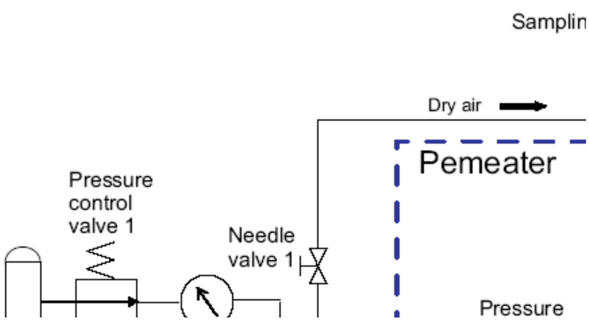

Fig. 2. Odor sensing systems. The air will be emitted from the dry air cylinder. Air flow is controlled by pressure control valves 1 and 2. By using the needle valve 2, more precise folow rate of

4 Classification Method of Odor Data

In order to classify the odors we adopt a three-layered neural network based on the error back-propagation method as shown in Fig. 3.

The error back-propagation algorithm which is based on the gradient method is given by the following steps.

Step 1. Set the initial values of $w_{ji}, w_{kj}, \theta_j, \theta_k$ and $\eta > 0$.

Step 2. Specify the desired values of the output d_k, k = 1,2, . . . ,K corresponding to the input data x_i, i = 1,2, . . . , I in the input layer.

Step 3. Calculate the outputs of the neurons in the hidden layer and output layer by

$$\mathrm{net}_j = \sum_{i=1}^{I} w_{ji} x_i - \theta_j,\ O_j = \sum_{i=1}^{I} w_{ji} x_i - \theta_j$$

$$\mathrm{net}_k = \sum_{j=1}^{J} w_{kj} O_{ji} - \theta_k,\ O_k = f(\mathrm{net}_k)$$

where

$$f(x) = \frac{1}{1+e^{-x}}.$$

Step 4. Calculate the error e_k and the generalized error δ_k by

$$e_k = d_k - O_k,\ \delta_k = e_k O_k (1 - O_k)$$

$$\delta_j = \sum_{k=1}^{K} w_{kj} \delta_k O_j (1 - O_j)$$

Step 5. Stop if e_k is sufficiently small for all k. Otherwise, calculate the following relations:

$$\Delta w_{kj} = \eta O_j \delta_k,\ w_{kj} \Leftarrow w_{kj} + \Delta w_{kj}$$

$$\Delta w_{ji} = \eta O_i \delta_j, \; w_{ji} \Leftarrow w_{ji} + \Delta w_{ji}$$

Step 6. Go to *Step* 3.

Using the above recursive procedure, we can train the odor data. The measurement data is an eight-dimensional vector which is obtained with eight sensors stated in Table 1.

5 Measurement of Odor Data

We have measured four types of odors as shown in Table 2. The sampling frequency is 1 [Hz], the temperatures of odor gases are 24–26 [◦ C], and the humidity of gases is 6–8 [%]. To control the density of gases, we use the diffusion tubes. Odor data are measured for 600 [s]. They may include impulsive noises due to the typical phenomena of QCM sensors. To remove these impulsive noises we adopt a median filter which replaces a value at a specific time by a median value among neighboring data around the specific time. In Fig. 4 we show the measurement data for the symbol A(ethanol) where the horizontal axis is the measurement time and the vertical axis is the frequency deviation from the standard value (9 [MHz]) after passing through a five-point median filter.

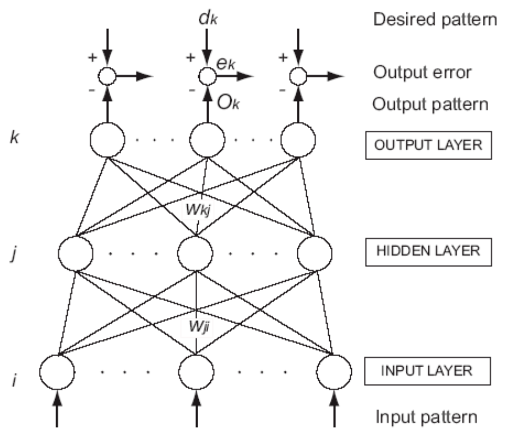

Fig. 3. Three layered neural network with the error back-propagation. The neural network consists of three layers, that is, an input layer i, a hidden layer j, and an output layer k. When the input data $x_i, i = 1,2,\ldots,I$ are applied to the input layer, we can obtain the output O_k at the output layer which is compared with the desired value d_k assigned in advance. If the error $e_k = d_k - O_k$ occurs, then the weighting coefficients w_{ji}, w_{kj} are corrected such that the error becomes smaller based on the error back-propagation algorithm.

6 Training for Classification of Odors

In order to classify the feature vector, we allocate the desired output for the input feature vector where it is nine-dimensional vector as shown in Table 3 since we have added the coefficient of variation to the usual feature vector to reduce the variations for odors. The training has been performed until the total error becomes less than or equal to 5×10^{-2} where $\eta = .3$.

Symbols	Output A	Output B	Output C	Output D
A	1	0	0	0
B	0	1	0	0
C	0	0	1	0
D	0	0	0	1

Table. 3. Training data set for ethanol (A), water (B), methyl-salicylate (C), and triethyl-amine (D).

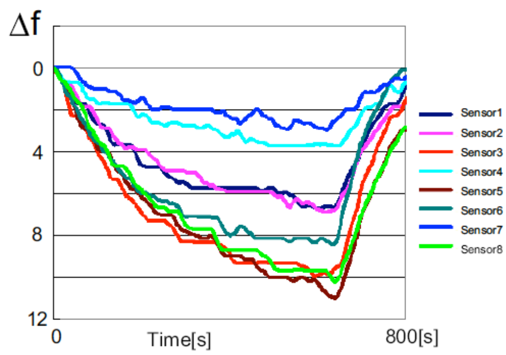

Fig. 4. Measurement data. Here, eight sensors are used and the data were measured for 600 [s]. The maximum value for each sensor among eight sensors is selected as a feature value for the sensor. Therefore, we have eight sensor values for an odor and they will be used for classification.

7 Testing for Classification of Odors

After training the data we have tested other data sets in which two kinds of odors are mixed with the same rate. The classification results are shown in Table 4 where the underlined numerals denote the top case where the maximum output values are achieved. The maximum values show one of the mixed odors. But some of them do not show the correct classification for the remaining odor. Thus, we have modified the input features such that

$$z = x - 0.9y$$

where x is the feature, y denotes the top value of each row in Table 4, and z is a new feature. Using the new feature vector, we have obtained the classification results as shown in Table 5. By changing the features according to the above relation, better classification results have been obtained. But the coefficient .9 used in the above equation is not considered so much. The value might be replaced by the partial correlation coefficient in multivariate analysis.

Symbols	Output A	Output B	Output C	Output D
A&B	.673	.322	.002	.001
B&C	.083	.696	.174	.001
C&D	.001	.004	.016	.992
D&A	.003	.003	.002	.995
A&C	.992	.006	.002	.000
B&D	.003	.003	.003	.995

Table. 4. Testing the mixed odors where the top and the second from the top are the classification results.

Symbols	Output A	Output B	Output C	Output D
A&B	.263	.290	.166	.066
B&C	.358	.029	.631	.008
C&D	.002	.071	.644	.163
D&A	.214	.004	.037	.230
A&C	.031	.020	.527	.026
B&D	.108	.010	.039	.325

Table. 5. Testing the mixed odors where except for the largest value the top is selected as the second odor among the mixed odors.

7 Conclusions

We have presented the reliability of a new EN system designed from various kinds of QCM sensors. It has been shown that after training the neural network for each odor, we can classify the original odor from the mixed odors in case of two odor case. The case of mixing More than two odors is open for the future research.

8 Acknowledgment

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