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Identification of paper quality using a hybrid electronic nose

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Abstract

A hybrid intelligent gas array sensor (or electronic nose) has been constructed, which comprises 10 CHEMFET devices, four Taguchi gas sensors (TGS), one infrared CO_2 sensor and a microcomputer in order to examine the odours from five cardboard papers from commercial manufacturers. Four of the papers came from two different production lines of the same Swedish manufacturer; the duplicate paper from each line was processed further to reduce the odour from this packaging material. The fifth paper came from another manufacturer. The sensor array data was screened using both principal component analysis (PCA) and cluster analysis (CA), and predictively classified using a back-propagation neural network. It was discovered using PCA/CA that only four of the 15 sensors were necessary to discriminate totally between the five classes of paper when air, which was initially classified separately, was used as a reference. Thus we have shown that the olfactory quality of cardboard papers can be recognized using a simple hybrid CHEMFET/TGS electronic nose.

Keywords: Gas array sensor; Electronic nose; Principle components analysis; Cluster analysis

1. Introduction

There has been considerable interest in the development of electronic noses in the past few years [1]. In general these electronic noses have exploited a single class of active sensor material, such as semiconducting oxides, conducting polymers, phthalocyanines or catalytic gate metals (in a MOSFET). However, this limits the capability of each monoclass [1] electronic nose to certain classes of reducing and oxidizing gases which may be inadequate in more challenging applications. Consequently, we report on the use of a hybrid (multi-class) sensor electronic nose [2] which combines three sensor types: metal gate MOSFETs, doped semiconducting oxide chemoresistors and an optical infrared carbon dioxide sensor which has been employed to analyze the odours from several cardboard papers of importance in the packaging industry where it is essential that the packaging material does not introduce unwanted odours into the foodstuffs or other products that are packaged.

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[1] Class refers here to the basic chemical sensing principle of the sensor.

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2. Electronic nose system

The hybrid 15 sensor array comprises three different class of gas sensors with the details given in Table 1. Ten of the sensors were metal oxide semiconductor field-effect transistors (MOSFETs) [3]. The MOSFETs

Table 1
Details of sensors used in the hybrid nose

Sensor no.	Sensor class	Device type	Operating temperature (°C)
1**	MOSFET	Thin Pd gate	150
2*	MOSFET	Thin Pt gate	160
3	MOSFET	Thick Pd gate	170
4*	MOSFET	Thin Pd gate	180
5	MOSFET	Thin Ir gate	190
6	MOSFET	Thin Ir gate	150
7*	MOSFET	Thin Ir/Pt gate	160
8	MOSFET	Thin Pt/Pd gate	170
9**	MOSFET	Thin Ir gate	180
10	MOSFET	Thin Pd gate	190
11	Chemoresistor	TGS 813	~400
12**	Chemoresistor	TGS 800	~320
13	Chemoresistor	TGS 881	~400
14**	Chemoresistor	TGS 825	~320
15	Optical absorption	CO_2	~20

The asterisks denote the importance of the sensors.

possessed gates of different catalytic metals (that is, Pd, Pt and Ir) of different thicknesses and were operated at different temperatures (150 to 190 °C) to provide selectivity. The drain current of each MOSFET was measured at a constant forward bias gate voltage when exposed to the head space. Four of the sensors were TGS, (doped) semiconducting oxide chemoresistors where resistances were determined from the output of a potential divider circuit. The third class of sensor was a CO_2 sensor which was a commercial infrared absorption instrument with an analog voltage output.

50 g samples of each of the five papers were placed in an air tight 200 ml glass vessel and stored at room temperature for 6 h to equilibrate. The measurement procedure consisted of pumping the head space of paper through the sensor chamber at 30 ml/min for 2 min and then waiting 5 min for recovery. The signal from the hybrid array was recorded for each paper in turn (paper 1, 2, 3, 4 and 5) followed by ambient air (reference). This procedure was repeated until each paper (and air) had been measured a total of 16 times. The reference air was measured so that the effect of ambient atmospheric conditions could be reduced by pre-processing if desirable.

3. Multivariate analysis

Principal component analysis (PCA) and cluster analysis (CA) [4] were used to examine the array data and test the effectiveness of various pre-processing algorithms [5] and sensor combinations. A Euclidean metric was used in the CA with an 'average between groups'

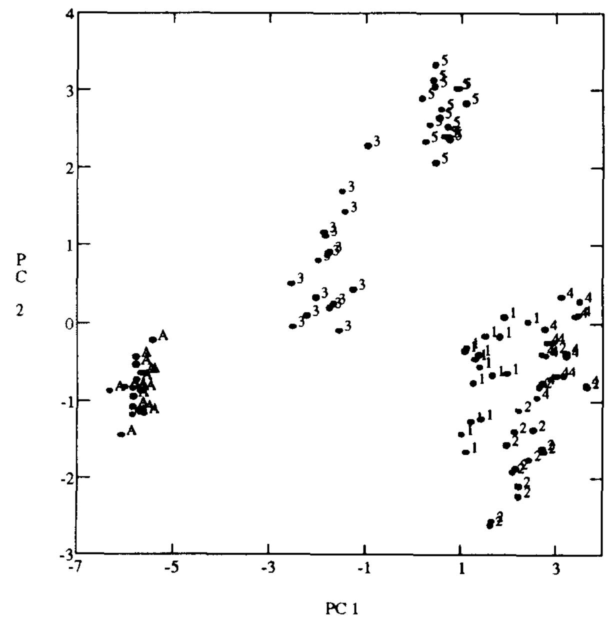

Fig. 1. PCA of the response of a 15-element hybrid electronic nose to the head space of five different papers (labelled 1 to 5) and air (labelled A).

Table 2
Confusion matrix for the performance of a 15:7:6 neural network on 5 papers and air

Predicted class	True class					
	Paper 1	Paper 2	Paper 3	Paper 4	Paper 5	Air
Paper 1	15	0	0	0	0	0
Paper 2	0	15	0	0	0	0
Paper 3	0	0	16	0	0	0
Paper 4	1	1	0	16	0	0
Paper 5	0	0	0	0	16	0
Air	0	0	0	0	0	16

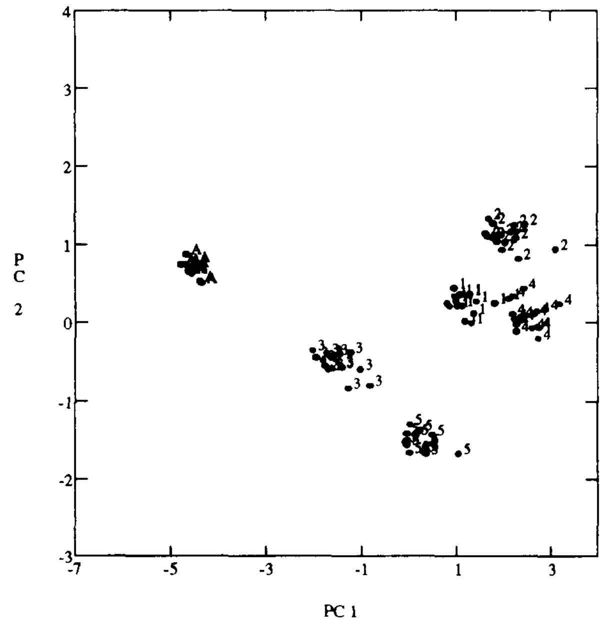

Fig. 2. PCA of the response of a seven-element hybrid electronic nose to the head space of five different papers (labelled 1 to 5) and air (labelled A).

Table 3
Confusion matrix for the performance of a 7:7:7:5 neural network on 5 papers

Predicted class	True class				
	Paper 1	Paper 2	Paper 3	Paper 4	Paper 5
Paper 1	16	0	0	0	0
Paper 2	0	15	0	0	0
Paper 3	0	0	16	0	0
Paper 4	0	1	0	16	0
Paper 5	0	0	0	0	16

method of linkage. No significant improvement was found in using either a non-Euclidean metric or a more sophisticated linkage method. Multivariate analyses were performed using Unistat Version 1.14 (Unistat Ltd, UK).

The individual sensor responses x_{ij} were normalized between -1 and $+1$:

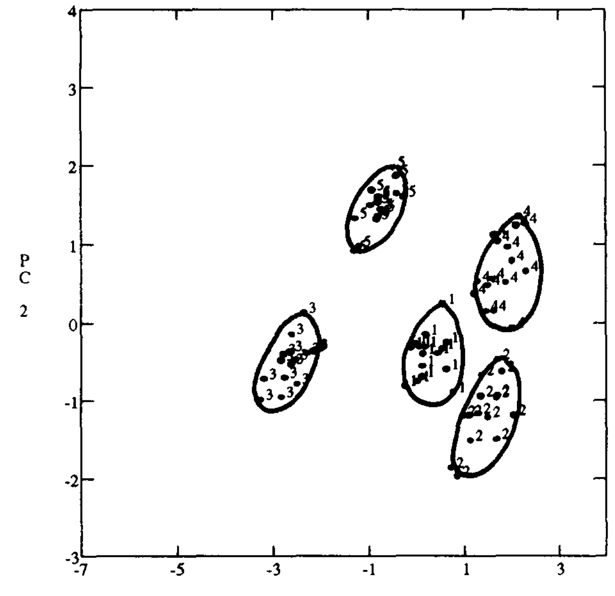

Fig. 3. PCA of the response (relative to air) of a four-element hybrid electronic nose to the head space of five different papers (labelled 1 to 5).

$$x_{ij}^{\text{norm}} = \frac{2[x_{ij} - \min_i\{x_{ij}\}]}{[\max_i\{x_{ij}\} - \min_i\{x_{ij}\}]} - 1 \quad (1)$$

where the subscript i is the sensor number (up to 15) and the subscript j is the paper class (up to 6), so that they could be efficiently trained by a back-propagation Rumelhart network with an initial weight range of $[-1, +1]$.

The back-propagation networks were trained and tested using the well-known 'leaving one out' method in which each one of the 16 duplicate samples were removed in turn prior to training and then used to test the network performance. The performance of the network was evaluated from the confusion matrix and the total sum squared output error. A variety of network architectures were systematically investigated with different numbers of elements in the hidden layers, and different neural connectivities [6]. All the neural analyses were carried out using Neural Works Explorer (Neuralware Inc., USA) on a personal computer with a 33 MHz 486 microprocessor.

4. Results

Fig. 1 shows a PCA of the response of the array of 15 sensors to the 6 classes of 5 papers and air (96 measurements). As can be seen, it is only possible to separate out all the samples of paper 3, paper 5 and reference air from the other three papers. This suggests that a neural network should predict easily the classes of paper 3, paper 5 and air, but it would find it harder to predict the rest of the data. Initially, a network architecture of 15:7:6 was used with the six output classes corresponding to the five papers and reference air. Table 2 shows the confusion matrix, where there is some overlap between classes 1, 2 and 4, and so two samples near the boundaries are misclassified.

A closer examination of the sensor correlation matrix and a CA of the transposed response matrix revealed that many of the sensors were strongly correlated and so contributed little to the discrimination process. From these analyses, a subset of seven key sensors was identified, namely five MOSFET and two TGS (see Table 1). Fig. 2 shows the PCA performed on this seven-element electronic nose where it is now possible

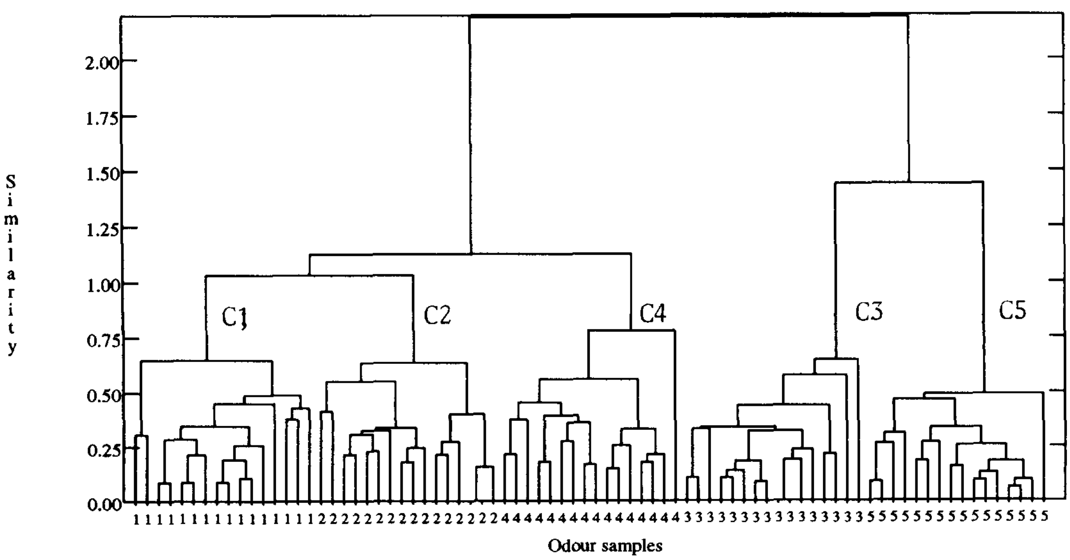

Fig. 4. CA (Euclidean metric, average between groups) of the response (relative to air) of a four-element hybrid electronic nose to the head space of five different papers (labelled 1 to 5). All the samples have been correctly assigned to five separate clusters (labelled C1 to C5).

to separate out paper 2 from the rest, but there is still some overlap between papers 1 and 4. A number of different network architectures and training parameters were then tested. The best result came from a 7:7:7:5 network in which the air samples were removed from the training data-set to try and get better separation between the different paper classes. This was partly successful as shown by the confusion matrix in Table 3 where one paper 2 sample is wrongly predicted as paper 4.

Finally, the response of the array to paper was redefined in terms of its response relative to the sampled reference air. The pre-processed data-set was then reanalyzed using PCA and CA and it was found that good results could be achieved with only four sensors: two MOSFETs (1 and 9) and two TGS (12 and 14). The results are shown in Figs. 3 and 4. Good distinction is now seen between all of the paper classes (for example, all 96 samples are correctly assigned to clusters C1 to C5 in the dendrogram), and the back-propagation achieved 100% prediction using either a 4:7:5 network (with four sensors) or a 7:7:7:5 network (with seven sensors).

5. Conclusions

A hybrid electronic nose can be used to analyze the olfactory quality of different commercial cardboard papers. However, success of such an application depends critically upon the way in which the gas samples are gathered, the choice of sensors and the pre-processing algorithms. The quality of five papers has been determined successfully by a hybrid electronic nose which comprises only four of the 15 gas sensors initially utilized. It was found that 100% prediction was achieved when the sensor signals were referenced to a set of air samples taken periodically. This was due to a reduction in the effect of temporal drift in the sensor signals during the sampling period. This paper shows that the class of sensor (such as semiconducting oxide or MOSFET) used in an electronic nose is just as important as the type of sensor used (for example oxide dopants or gate material).

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