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Electronic nose simulation tool centred on PSpice

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Abstract

Electronic noses consist of an array of non-selective gas sensors with a pattern recognition engine. The sensors and pattern recognition methods depend on the specific application. The design process of electronic noses usually involves time-consuming measurements in a non-standard trial and error process. This paper addresses the problem by using an electronic nose simulation tool centred on PSpice. Using previously developed generic PSpice models for the response of gas sensors, a four-element tin oxide sensor array was simulated. The sensor model parameters were adjusted using calibrated response data from ethanol, methane and their mixtures, detected with real tin oxide sensors. To study the performance of the array, statistical error modelling and PSpice simulations were used in a Monte Carlo analysis coupled with principal component analysis. The results show that this simulation strategy is useful for analysing the effects of sampling errors, the changes in operation temperature, random errors and sensor drift. The importance of these errors is discussed in terms of the array discrimination ability. We conclude that this simulation strategy can help to systematise the design of electronic noses.

Keywords: Resistive gas/odour sensors; PSpice analog behavioural models; Sensor array; Electronic nose simulation; Statistical error model

1. Introduction

The identification of gases and odours is of major interest because it has a considerable number of potential applications, some of which are related to quality control in the food or cosmetic industries and to monitoring air quality. In the past 10 years, electronic noses — electronic instruments that mimic the human olfactory system — have developed rapidly. More than 10 companies have now developed commercial instruments, which consist of an array of non-selective gas/odour sensors with a pattern recognition engine [1,2]. To date electronic noses are application-specific and their design (e.g. selecting appropriate sensors and suitable pattern-recognition techniques) is a non-standard empirical process [3]. The design is generally a trial and error process via which the number and type of odour sensors and the pattern-recognition tools are selected under the constraints determined by each application. This means that the design process may require time-consuming measurements to be made. Furthermore, it is not always straightforward to obtain the feedback necessary to optimise the sensor array and to select the best pattern recognition methods from these measurements. Even when estimates of sensor responses are accurate, other questions arise about the performance of the sensor array: are the patterns different enough to discriminate between any gases (or complex aromas) that might be encountered? Which gases or aromas will be the most difficult to distinguish? How do systematic and random errors in sensor responses influence the analysis? How does sensor drift affect performance? Some of these questions can be answered by pattern recognition analyses but most of them can only be answered by data collection. When more than just a few gases or aromas are considered, the latter can be intractable and other approaches are needed [3,4]. Recently, generic equivalent PSpice models for metal oxide, conducting polymer and gravimetric sensors have been developed [5–7]. These models can depict the response of the odour sensors under different operating conditions (e.g. different working temperatures and humidity contents in air). Because PSpice behavioural models of sensors are easy to construct, it should be easy to develop simulation tools for sensor arrays and electronic noses. Using simulated sensor responses there is less need to run time-consuming trial and error tests to validate the electronic nose. Furthermore, the data required to determine which pattern recognition method is best fitted

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to a specific application and to provide statistical estimates of odour recognition/quantification success rates, can be easily and rapidly gathered using simulated instead of real data.

In this article, we report the development of a simulation tool, which is based on PSpice, to systematise the design of electronic noses. After a brief description of the electronic nose model, details are given about the statistical error models used for simulation. The PSpice simulation tool is used to study how errors (e.g. statistical errors, sensor drift, changes in ambient conditions, etc.) affect the performance of an electronic nose.

2. Electronic nose simulation tool

The electronic nose consists of a four-element tin oxide sensor array (e.g. Taguchi type tin oxide sensors) and a pattern recognition engine. The core of the simulation tool is made up of the PSpice models, which are used to emulate the responses of the sensors in the array. The PSpice models used are able to accurately depict the response of metal oxide sensors to multicomponent gas/odour mixtures under different operating conditions, and are described elsewhere [6]. However, a short overview is given here. According to our previous modelling, the static electrical conductance of metal oxide gas sensors in the presence of a binary mixture of gases follows the equation:

$$G_s = G_{0T}e^{-EA_0/KT} + k_{1T}e^{-EA_1/KT}C_1^{n_1KT} + k_{2T}e^{-EA_2/KT}C_2^{n_2KT} + \cdots + k_{mixT}e^{-EA_{mix}/KT}C_1^{n_1KT}C_2^{n_2KT} \quad (1)$$

where C_1 and C_2 are the concentrations of species 1 and 2, respectively, k_{1T} and k_{2T} the pre-exponential factors of the sensitivities to species 1 and 2, n_1 and n_2 the pre-factors of the power law exponents for oxides, k_{mix} is the pre-exponential factor of the change in conductance caused by the interaction of the two species, G_{0T} the pre-exponential factor of the baseline conductance, EA_i's are the activation energies, T is the absolute temperature and K the Boltzmann's constant. The response model described by Eq. (1) assumes a quasi-linear interaction between the gases in the binary mixture, which is the case when gases are chemically independent. The dependence of the baseline and the power-law factors on the temperature has been studied elsewhere [8,9].

Block diagrams of the electronic nose simulation tool and a generic PSpice sensor model are shown in Fig. 1. The experimental data set contains calibration data which were collected as part of a previous study that developed a domestic appliance for measuring methane in the presence of ethanol [10]. These data were used to adjust the values of the parameters of the PSpice sensor models, by applying a standard fitting procedure in Matlab. Table 1 shows the values of the static model parameters for the four tin oxide sensors.

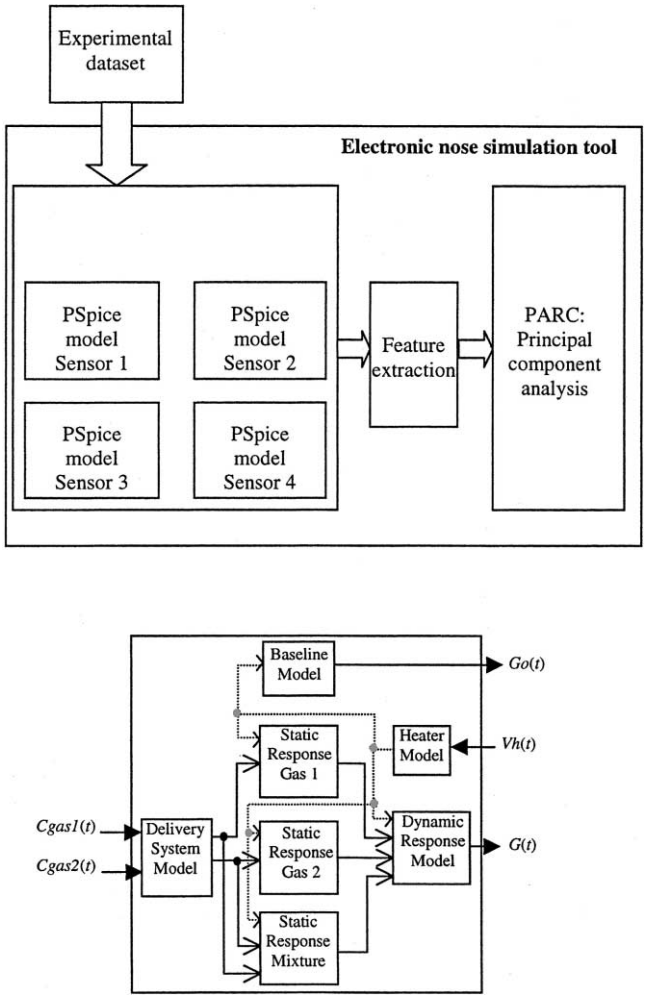

Fig. 1. Top: block diagram of the electronic nose simulation environment. Bottom: block diagram of a metal oxide sensor PSpice model.

Once the parameters of the sensor models were set, the simulation procedure was as follows.

1. Random and systematic errors were applied to alter the values of the parameters in the PSpice models. Random errors were assumed to have a Gaussian distribution.
2. By iteratively running PSpice simulations with altered model parameters, a large response data set was obtained. Features were extracted from the sensor responses.
3. These features were input to a PARC recognition engine (principal component analysis), which was simulated with Matlab in order to discuss system performance in terms of the electronic nose discrimination ability.

The usefulness of this simulation method as a diagnostic tool for studying the effect of both random and systematic errors on the instrument performance is shown in the section below. The success of the Monte Carlo simulation depends

Table 1
Values of the PSpice static model parameters for the four tin oxide gas sensors in the presence of ethanol, methane and their binary mixtures

Parameter	Sensor 1	Sensor 2	Sensor 3	Sensor 4
G_0	0.16	0.32	0.12	0.23
E_{a0}	5×10^{-3}	4.3×10^{-3}	3.9×10^{-3}	5.6×10^{-3}
k_1	6.14×10^{-4}	3.14×10^{-3}	8.3×10^{-3}	1.7×10^{-3}
EA_1	5.31×10^{-3}	2.31×10^{-2}	2.1×10^{-2}	2.23×10^{-2}
n_1	13.95	11.03	5.97	10.26
k_2	9.8×10^{-5}	2.8×10^{-4}	1.6×10^{-4}	1.72×10^{-3}
EA_2	6.2×10^{-3}	9.21×10^{-3}	3.11×10^{-3}	1.02×10^{-3}
n_2	6.83	7.55	6.54	4.05
k_{mix}	-5.2×10^{-6}	-1.2×10^{-6}	-2.5×10^{-5}	-1×10^{-5}
EA_{mix}	3.31×10^{-3}	2.87×10^{-3}	4.35×10^{-2}	2.19×10^{-3}

on the accuracy with which response errors encountered in actual sensor operation are portrayed in the models used. The following section describes the various error models used.

3. Description of the error models

Various error models were used to simulate the effect of errors on both the static and dynamic response of the electronic nose studied.

The first model simulated the effect of random errors in the concentration of the measured species (e.g. the occurrence of sampling errors). The concentrations of ethanol and methane were generated according to the following equations:

$$C'_{eth} = C_{eth}(1 + k_{eth}\alpha_{eth}) \quad (2)$$

$$C'_{met} = C_{met}(1 + k_{met}\alpha_{met}) \quad (3)$$

where k_{eth} and k_{met} are the relative standard deviations (R.S.Ds.) of the concentrations of ethanol and methane, respectively, and α_{eth} and α_{met} the independent normally distributed variables with zero mean and standard deviation (S.D.) of 1. This model applied different concentrations of the two species for each simulated exposure.

The second model is useful for analysing the occurrence of errors in the operating temperature of the sensors. The operating temperature of metal oxide resistive sensors is usually set by applying a constant voltage (V_h) to a heating resistor. In this model, the heating voltage was set according to the following equation:

$$V'_h = V_h(1 + k_h\alpha_h) \quad (4)$$

where, like the first error model, k_h is the R.S.D. of the heating voltage and α_h is a normally distributed variable with zero mean and S.D. of 1. This model applied the same heating voltage to all the sensors in the array for one simulation and different heating voltages for different simulations.

The third model applied a random error in the parameters that set the static response of the sensors. This error model altered the values of all the parameters in Eq. (1) except gas concentration and temperature of operation. The value of a given parameter p_i was altered according to the equation:

$$p'_i = p_i(1 + k\alpha_i) \quad (5)$$

where k is the R.S.D. of all the parameters whose values are altered by the third error model and the α_i's are independent, normally distributed variables with zero mean and S.D. of 1. For every simulation and sensor, this model applied different parameter values.

The fourth model applied a random error in the parameters that set the dynamic response of the sensors to a temperature modulation. The dynamic response to a temperature modulation is set, in the PSpice model, by a Laplace block that simulates the thermal inertia of the sensor [6]. This error model alters the values of the poles that account for the thermal inertia of every sensor. The strategy of altering these poles is the same as the one described in the error model in Eq. (5) above.

Finally, the fifth error model applied an offset error in the parameters that set the static response of the sensors. The offset error in all these parameters is useful so that the effect of sensor drift can be analysed. The value of a given parameter p_i was altered according to the equation:

$$p'_i = p_i(1 + d) \quad (6)$$

where d is the percentage of the systematic drift of the parameters.

4. Results and discussion

The aforementioned error models were applied to perform a Monte Carlo simulation, coupled with principal component analysis, of a four-element tin oxide sensor array to detect methane and ethanol. Three different situations were simulated: the measurement of 100 ppm of ethanol, 10 000 ppm of methane and a binary mixture of ethanol (100 ppm) and methane (10 000 ppm).

4.1. Error-enhanced static responses

The three error models for the static response take into account errors in sampling, errors in setting the temperature of operation of the sensors and random errors in the parameters of the PSpice sensor models.

For every response of a sensor in the array, the feature extracted was the conductance change defined as

$$\Delta G = G_s - G_0 \quad (7)$$

where G_0 is the sensor baseline conductance and G_s the steady-state value of the sensor conductance in the presence of the gas/odour.

4.1.1. Sampling errors

Eleven replicates (with sampling errors) of every situation were simulated, giving a total of 33 simulations.

The values of the R.S.D., k_{eth} and k_{met}, were set to 0.1 (see Eqs. (1) and (2). When the measurement of ethanol was simulated, C_{eth} and C_{met} were set to 100 and 0, respectively. When the measurement of methane was simulated, C_{eth} and C_{met} were set to 0 and 10 000, respectively. Finally, when the binary mixture of ethanol and methane was simulated, C_{eth} and C_{met} were set to 100 and 10 000, respectively. A principal component analysis was performed on the simulated data. The score plot of this analysis is shown in Fig. 2. Since the sensors in the array were similar, the data were mean centred. The first two principal components accounted for 98.32% of the variance in data. This high degree of variance captured by the two first principal components is as expected because the responses of tin oxide sensors are generally highly correlated. Fig. 2 shows that a linear method like PCA is able to correctly separate the clusters associated with ethanol, methane, and their binary mixture, even when there are errors (10% R.S.D.) in the sampling method. To establish a measure of the dispersion within each cluster, the scores of the centres of the clusters were found. Then, the average Euclidean distance of all the measurements within a cluster, from their cluster centre were computed. The lower this number, the lower the dispersion is within a cluster. Table 2 shows the results computed from the data shown in Fig. 2. Since the distances between cluster centres are considerably higher than dispersions within clusters, the discrimination ability of the sensor array is high. To quantify the discrimination ability a figure of merit was defined as

Table 2
Discrimination ability of the sensor array (with 10% R.S.D. sampling errors)[a]

Cluster	a	b	c
a	1.89	27.31	7.89
b		0.71	30.14
c			1.77

[a] The main diagonal elements are the dispersions within each cluster and the off diagonal elements are the distances between cluster centres.

$$\mathrm{RP}_{ij} = \frac{d(\mathrm{c}_i, \mathrm{c}_j)}{D(i) + D(j)} \quad (8)$$

where RP_{ij} is the discrimination between clusters i and j, $d(\mathrm{c}_i, \mathrm{c}_j)$ the Euclidean distance between cluster centres and $D(i)$ and $D(j)$ are the dispersions within clusters i and j, respectively. According to results shown in Table 2, $\mathrm{RP}_{ab} = 10.50$, $\mathrm{RP}_{ac} = 2.16$ and $\mathrm{RP}_{bc} = 12.15$.

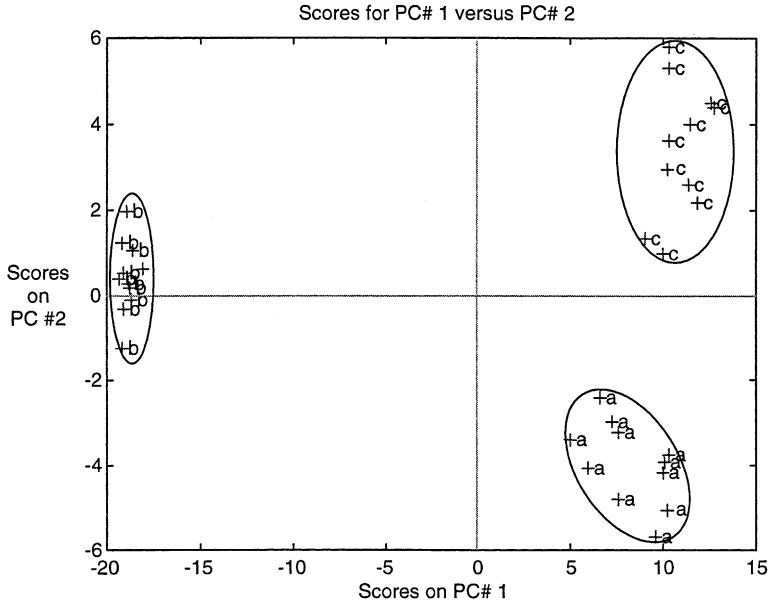

Fig. 2. Simulation of a four-element tin oxide gas sensor array. Occurrence of sampling errors (10% R.S.D.). Cluster a corresponds to ethanol 100 ppm, b to methane 10 000 ppm and c to a binary mixture of ethanol 100 ppm + methane 10 000 ppm.

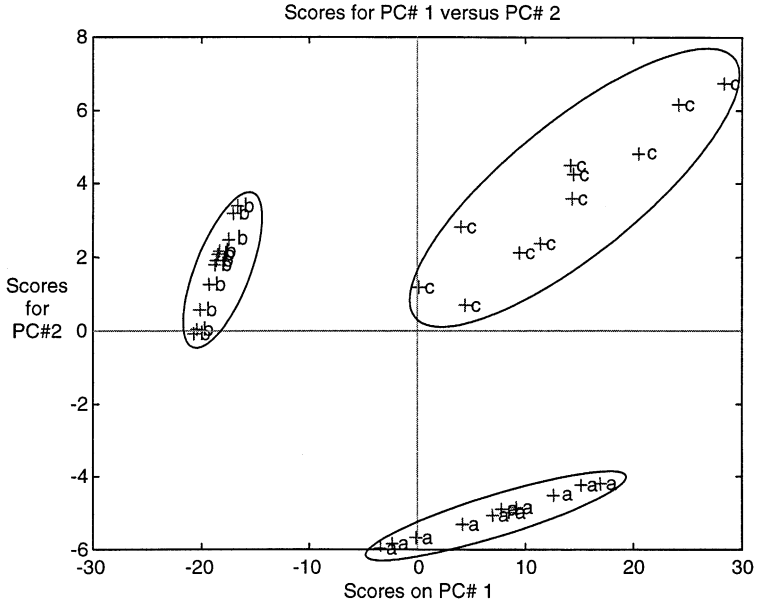

Fig. 3. Simulation of a four-element tin oxide gas sensor array. Occurrence of errors in the temperature of operation (10% R.S.D.). Cluster a corresponds to ethanol 100 ppm, b to methane10 000 ppm and c to a binary mixture of ethanol 100 ppm + methane 10 000 ppm.

4.1.2. Errors in the temperature of operation

Errors can occur in the temperature of operation if there is a change in the voltage applied to the heating resistors of the sensors. Once again three different measurements (only ethanol, only methane and ethanol and methane together) were simulated. Eleven replicates of every measurement (assuming random errors in the heating voltage) were obtained, giving a total of 33 simulations. The value of the R.S.D. k_h was set to 0.1 (see Eq. (3). A PCA was performed on the simulated data. Once again the data were mean centred. The first two principal components accounted for 98.9% of variance in the data. The score plot of this analysis is shown in Fig. 3. Table 3 shows that errors (with 10% R.S.D.) in the heating voltage of the sensors lead to a higher dispersion within the clusters than errors in the sampling. A 10% error in the heating voltage of the sensors leads to a 4.6% change in absolute operating temperature of the sensor (e.g. when $V_h = 5$ and 5.5 V, the operating temperatures are 543 and 568 K, respectively). Therefore, errors in setting the heating voltage of the sensors are more critical than sampling errors in terms of the discrimination ability of the array. According to the results shown in Table 3, $RP_{ab} = 3.84$, $RP_{ac} = 0.86$ and $RP_{bc} = 3.80$.

Table 3
Discrimination ability of the sensor array (with 10% R.S.D. errors in the temperature of operation)[a]

Cluster	a	b	c
a	5.38	26.08	10.56
b		1.40	31.45
c			6.87

[a] The main diagonal elements are the dispersions within each cluster and the off diagonal elements are the distances between cluster centres.

4.1.3. Errors in the parameters that set the static response of the sensor

The parameters that set the static sensor response were altered in accord with the third error model. Two different cases with 10 and 20% R.S.Ds. were considered. For each case 11 replicates of each species (ethanol, methane and ethanol + methane) were simulated, giving a total of 66 simulations. Four principal component analyses were performed (one for each case with mean centred and autoscaled data). Fig. 3 shows the two score plots when the static model parameters were considered to have a 10% relative standard error (R.S.E.). The first two components accounted for 98.7 and 98.9% of the variance when the data were mean centred and autoscaled, respectively. Fig. 4 shows that autoscaling the data led to a better separation between the clusters. Table 4 shows the dispersions within the clusters and the distances between them. To better compare the effects of mean centring and autoscaling the data, the discrimination ability, as defined by Eq. (7), was calculated. For mean

Table 4
Discrimination ability of the sensor array (with 10% R.S.D. errors in the static model parameters)[a]

Cluster	a	b	c
a	5.64	27.65	5.17
	0.50	*1.28*	*1.91*
b		1.29	31.89
		0.32	*4.03*
c			6.13
			0.48

[a] The main diagonal elements are the dispersions within each cluster and the off diagonal elements are the distances between cluster centres (plain font is for mean centred data and italics is for autoscaled data).

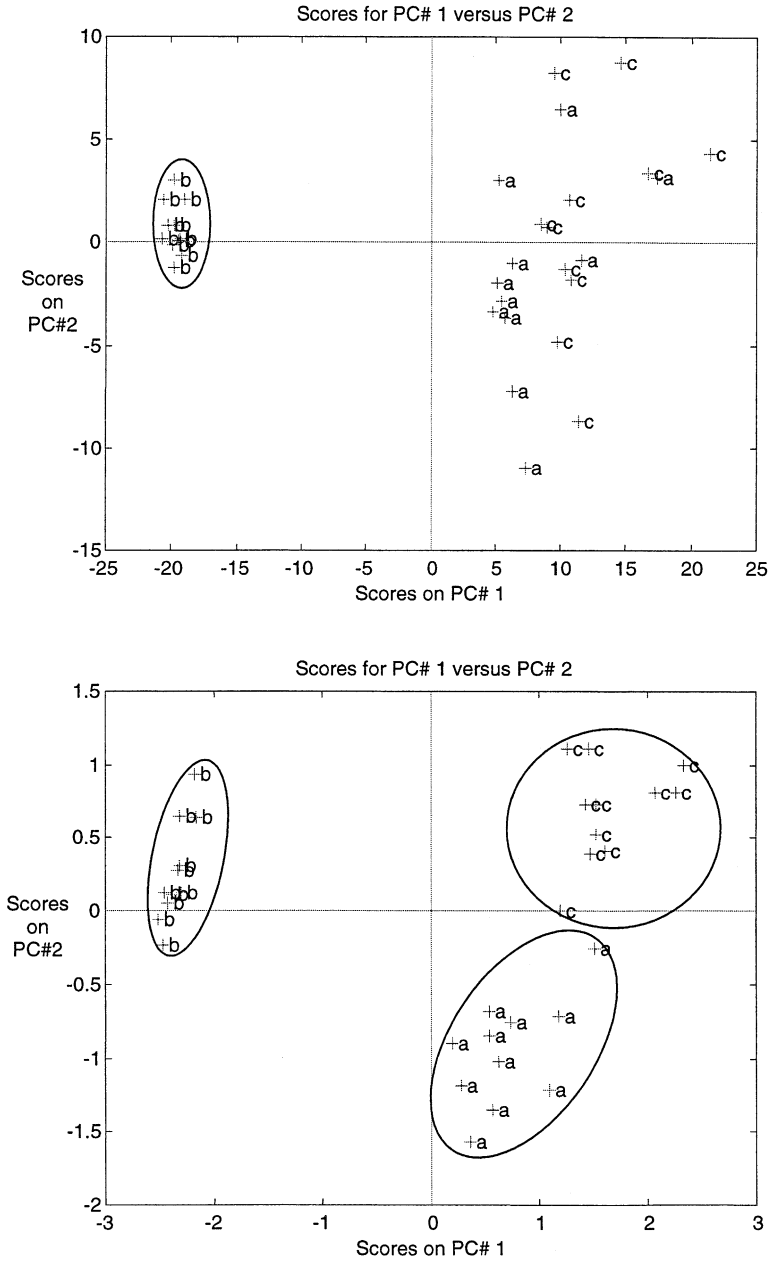

Fig. 4. Simulation of a four-element tin oxide gas sensor array. Occurrence of errors in the static response model parameters (10% R.S.D.). Top: data are mean centred. Bottom: data are autoscaled. Cluster a corresponds to ethanol 100 ppm, b to methane 10 000 ppm and c to a binary mixture of ethanol 100 ppm + methane 10 000 ppm.

centred data, $RP_{ab} = 3.99$, $RP_{ac} = 0.44$ and $RP_{bc} = 4.30$. For autoscaled data, $RP_{ab} = 1.56$, $RP_{ac} = 1.95$ and $RP_{bc} = 5.04$. The autoscaling procedure significantly improved the discrimination between clusters a (ethanol) and c (binary mixture of ethanol and methane).

Fig. 5 shows the two score plots when a 20% R.S.E. in the static model parameters was considered. The first two components accounted for 96.9 and 97.4% of the variance when the data were mean centred and autoscaled, respectively. In this case autoscaling the data did not lead to a linear separation between the species a and c. Table 5 shows the dispersions within the clusters and the distances between them. To compare the results of autoscaling or mean centring the data, the discrimination ability of the array was calculated using data shown in Table 5. For mean centred data $RP_{ab} = 2.12$, $RP_{ac} = 0.14$ and $RP_{bc} = 2.33$. For autoscaled data $RP_{ab} = 1.96$, $RP_{ac} = 0.76$ and $RP_{bc} = 2.62$.

4.2. Error-enhanced dynamic responses

Previous works have shown that important information for gas identification can be extracted through thermal

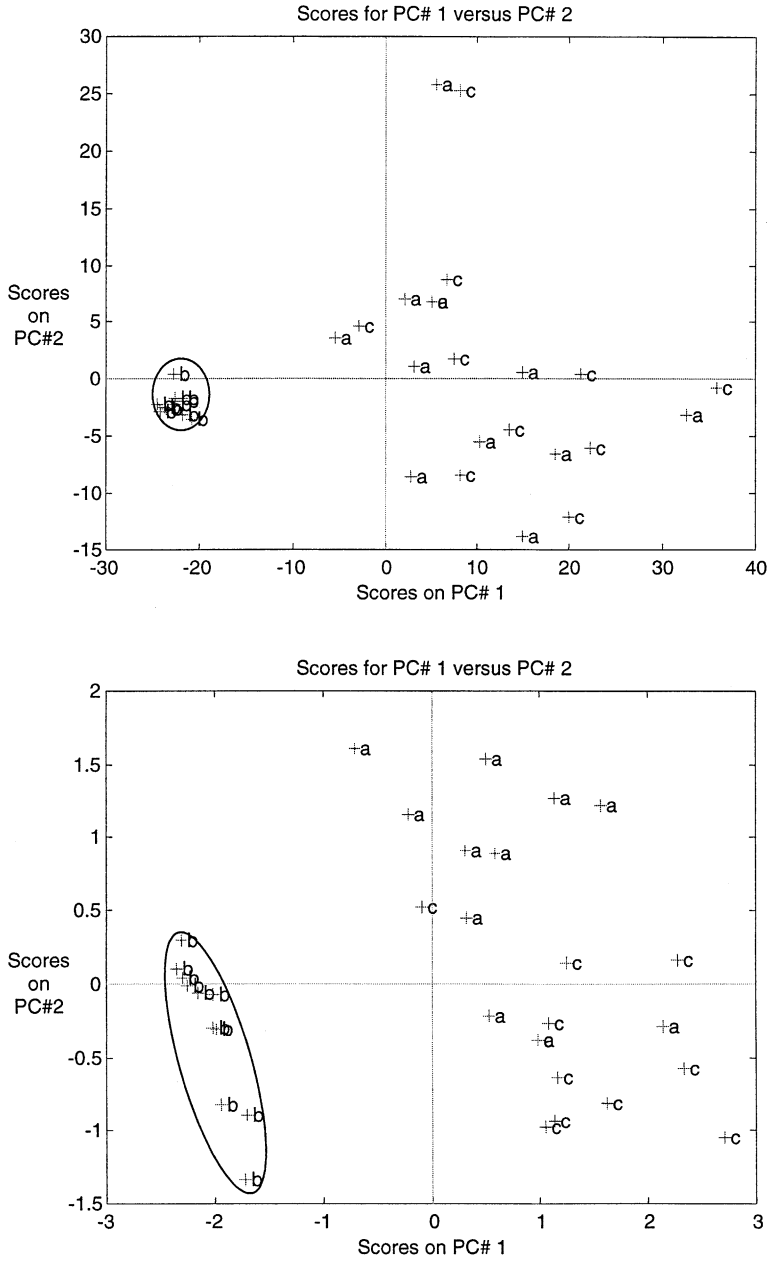

Fig. 5. Simulation of a four-element tin oxide gas sensor array. Occurrence of errors in the static response model parameters (20% R.S.D.). Top: data are mean centred. Bottom: data are autoscaled. Cluster a corresponds to ethanol 100 ppm, b to methane 10 000 ppm and c to a binary mixture of ethanol 100 ppm + methane 10 000 ppm.

Table 5
Discrimination ability of the sensor array (with 20% R.S.D. errors in the static model parameters)[a]

Cluster	a	b	c
a	13.78	32.34	3.78
	1.01	*2.92*	*1.41*
b		1.45	36.09
		0.48	*3.49*
c			14.04
			0.85

[a] The main diagonal elements are the dispersions within each cluster and the off diagonal elements are the distances between cluster centres (plain font is for mean centred data and italics is for autoscaled data).

modulation of metal oxide gas sensors [11]. The error model for the sensor dynamic response considers the occurrence of random errors in the parameters that set the response to a temperature modulation.

The parameters that set the thermal inertia of the sensors to a change in the voltage applied to their heating elements were altered in accord with the fourth error model. This model can be used to analyse the effects of membrane fatigue in micro-hotplate sensors. A 10% R.S.D. was considered. Eleven replicates of each species (ethanol, methane and ethanol + methane) were simulated, giving a total of 33 simulations. Fig. 6 shows a typical PSpice simulation with

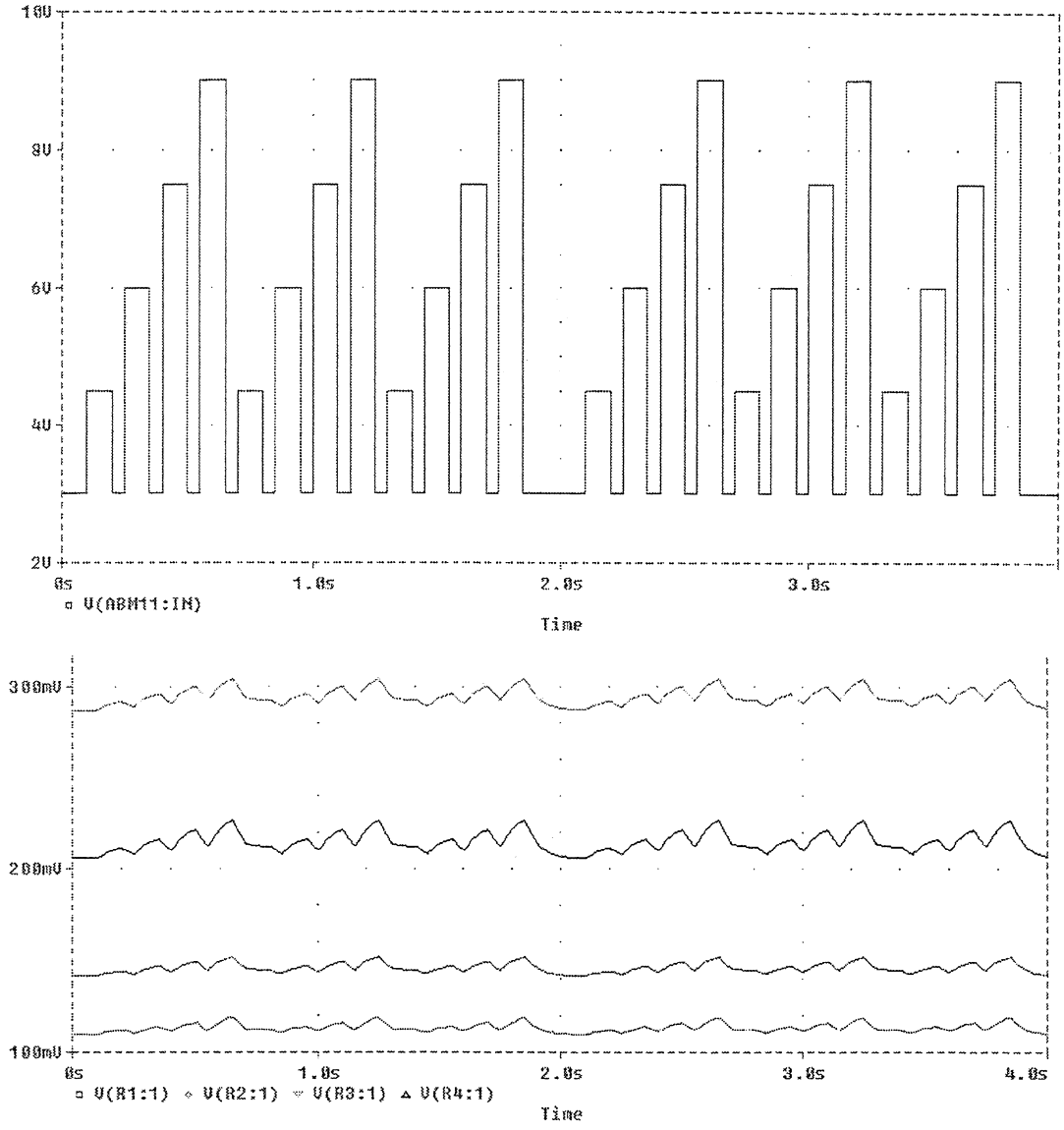

Fig. 6. PSpice simulation of the dynamic response of a four-element sensor array to a temperature modulation. Top: signal input to the heating elements of all sensors. Bottom: typical dynamic response of the sensors (the outputs in mV are equivalent to conductance in μS).

the signal input to the heating elements of the sensors and their dynamic response. To extract features from the dynamic sensor responses, a Fourier analysis was enabled during the PSpice simulations. For every sensor signal, the dc component and the first five harmonics were extracted. This gave a total of six features per sensor (24 features from the four-element array) and simulation. To give the same importance to all the Fourier coefficients, the data were autoscaled before a PCA was performed. The first two principal components accounted for 97.3% of variance in data, which shows the high correlation between the Fourier coefficients. Therefore, another PCA was performed using only the first and second harmonics (8 features from the array instead of 24). The results were equivalent. Fig. 7

Table 6
Discrimination ability of the sensor array (with 10% R.S.D. errors in parameters that set the dynamic response to a temperature modulation)[a]

Cluster	a	b	c
a	0.94	9.30	4.30
	0.64	*5.42*	*2.35*
b		0.47	10.30
		0.35	*6.00*
c			1.00
			0.70

[a] The main diagonal elements are the dispersions within each cluster and the off diagonal elements are the distances between cluster centres (plain font is for six Fourier coefficients per sensor and italics is for two Fourier coefficients per sensor).

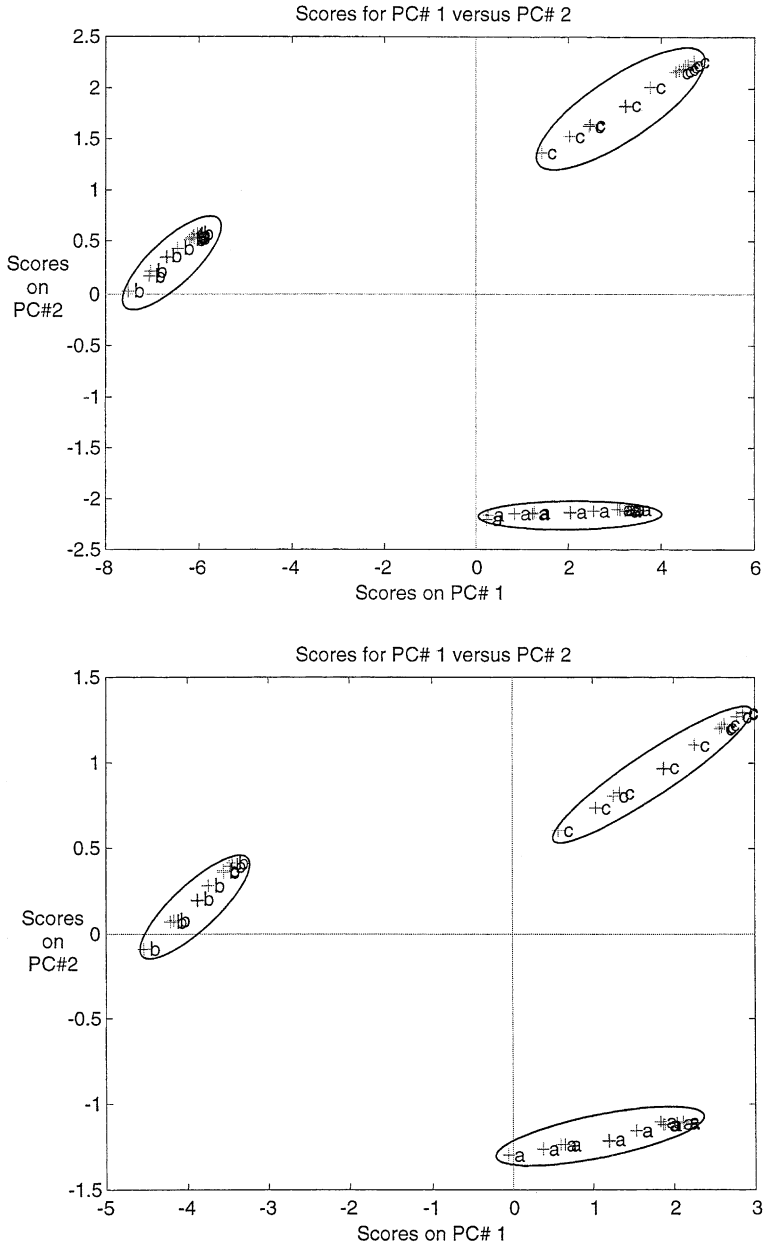

Fig. 7. Simulation of a four-element tin oxide gas sensor array. Occurrence of errors in the dynamic response model parameters (temperature modulation) (10% R.S.D.). The data (Fourier coefficients) were autoscaled. Cluster a corresponds to ethanol 100 ppm, b to methane10 000 ppm and c to a binary mixture of ethanol 100 ppm + methane 10 000 ppm. Top: using the dc component and the first five harmonics. Bottom: using the first two harmonics only.

shows the score plots of these analyses. The separation between the simulated species was good. Table 6 shows the dispersions within the clusters and the distances between cluster centres. The discrimination ability of the array was calculated to compare the effects of using six or two Fourier coefficients per sensor. Very similar results were found, $RP_{ab} = 6.60$, $RP_{ac} = 2.22$ and $RP_{bc} = 7.01$ when six coefficients were used and, $RP_{ab} = 5.47$, $RP_{ac} = 2.37$ and $RP_{bc} = 5.71$ when two coefficients were used.

4.3. Sensor drift

The fifth error model was applied to investigate the effect of drift on the four-element array. In this case, an offset error in the parameters that set the static response of the sensors was introduced. Five simulations (no drift, 1, 5, 10 and 20% drift) for each species (ethanol, methane and ethanol+ methane) were performed, giving a total of 15 simulations. A PCA was used to show the effects of drift. Data were mean

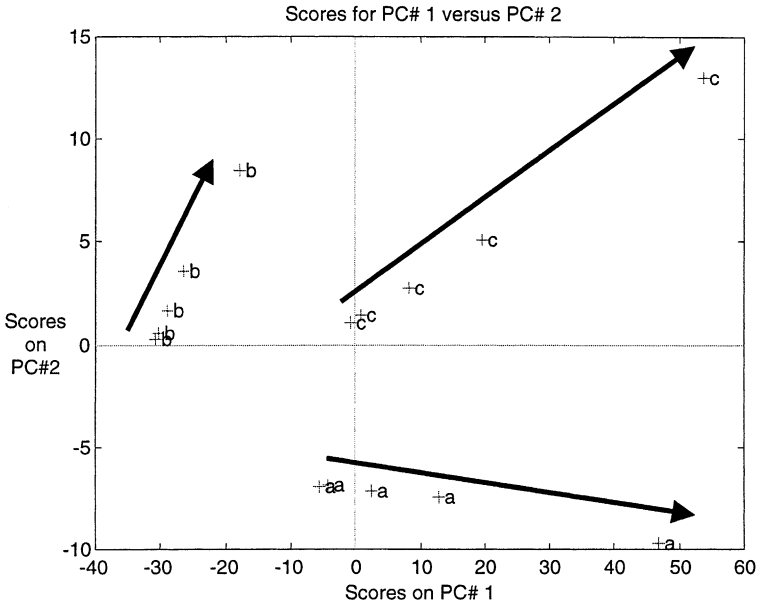

Fig. 8. Simulation of a four-element tin oxide gas sensor array. Effects of sensor drift. Cluster a corresponds to ethanol 100 ppm, b to methane10 000 ppm and c to a binary mixture of ethanol 100 ppm + methane 10 000 ppm. The data were mean centred. The arrows indicate the sense of increasing drift (from 0 to 20%).

centred and the first two principal components accounted for 98.7% of variance in data. These results are shown in Fig. 8.

5. Summary and conclusions

To study the performance of a four-element gas sensor array, statistical error modelling and PSpice simulations were used in Monte Carlo analysis coupled with principal component analysis. The parameters of the PSpice sensor models were adjusted by using calibrated data from a real tin oxide sensor array. This simulation strategy was used to investigate the effect of sampling errors, changes in the temperature of operation, random errors and sensor drift on the discrimination ability of the sensor array.

The simulations considered the detection of three species — ethanol, methane and a binary mixture of ethanol and methane — in the presence of errors. The following conclusions were drawn.

- The array is tolerant to 10% R.S.D. errors in the sampling system.
- Errors in setting the temperature of operation of the sensors are critical. The ability of the array to discriminate between the species seriously deteriorates when there are 5% R.S.D. errors in the operating temperature of the sensors.
- Errors in the parameters that set the static response of the sensors seriously affect the discrimination ability of the system. In the case of small errors (up to 10% R.S.D.), autoscaling the data, rather than only mean centring them, leads to better results.
- The dynamic sensor response to temperature modulation carries useful information for species discrimination.
- The effect of sensor drift (up to 20%) seems to be less detrimental for the electronic nose discrimination ability than all the other sources of error tested.

We have shown that simulation provides information that can otherwise only be obtained by exhaustive validation testing (time-consuming measurements). The PSpice centred simulation tool can be further applied to other analyses such as finding the best pattern recognition technique for a given application, determining which species will be the most difficult to discriminate, studying the effects of adding or removing sensors from the array, etc. We believe that this simulation tool could be used to systematise the design of electronic nose instruments.

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