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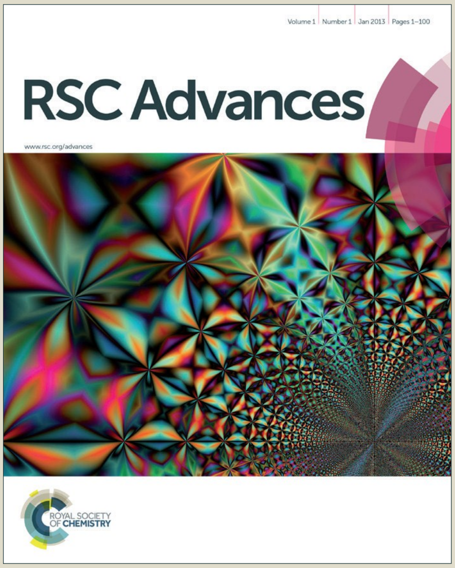

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A novel electronic nose for simultaneous quantitative determination of concentrations and odor intensity analysis of benzene, toluene and ethylbenzene mixtures

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ABSTRACT

Aromatic hydrocarbons (benzene, toluene, ethylbenzene et al.) are part of main components of air pollution and odor nuisance. However, previous studies on simultaneous detection of aromatic mixtures and analysis of odor intensity by electronic nose (E-nose) were limited. The aim of this study is to develop a novel E-nose system to simultaneously determine chemical concentrations and odor intensity of benzene, toluene and ethylbenzene mixtures . The system consists of a sensor array with 5 gas sensors, a signal converter and a pattern recognition system which based on Back Propagation (BP) neural network. 300 groups of aromatic hydrocarbons mixtures (benzene, toluene and ethylbenzene) with different concentrations were determined by sensor array and gas chromatography (GC) to build, test and optimize the BP neural network. Then the optimum structure and functions of the BP network were verified by about 50 times of contrast tests. Results showed that the average relative error of concentrations measured by the E-nose system was 9.71% relative to the results of GC. Furthermore, six odor intensity prediction models were used to convert the concentrations of the aromatic mixtures to their odor intensity. Based on the comparison with sensory analysis, Weber-Fechner law model, Vector model and Simplified Extended Vectorial model were adopt to predict the odor intensity of single, binary and ternary compounds respectively.

Keywords: Aromatic hydrocarbons, Electronic nose, Artificial neural network, Odor intensity, Gas sensor

1. Introduction

Aromatic hydrocarbons (benzene, toluene, ethylbenzene et al.) form an important group of volatile organic compounds (VOC) and have been confirmed as part of the most malodorous components[1, 2]. Previous studies showed that the emission of aromatic hydrocarbons may occur in both indoor (living room, plants et al.) [3, 4] and outdoor (landfill, industrial area, oil refineries et al.) environments [5, 6] which may cause leukemia, lung tumors, myelitis, epilepsy and other occupational health problems to residents nearby[7, 8]. With the increase of public concern, monitoring aromatic hydrocarbons became vital and the analysis methods as well as the apparatus have attracted much attention.

Since the 21st century, there has been increasing researches in order to achieve more objective and faster methods to analyze VOC, which led to the development of E-nose system. An E-nose system is a gas monitor instrument that mainly comprises a sensor array and an appropriate pattern-recognition system capable of recognizing simples[9-11]. At present, pattern-recognition system was the key part because it affected analysis results greatly. For example, principal component analysis (PCA), support vector machines (SVM) and partial least square (PLS) were most used for qualitative analysis of multiple VOC [12-14], independent component analysis (ICA) and singular value decomposition (SVD) were most applied in quantitative analysis of single gas[12, 15-17] while the most common method for odor identification and determination of odor intensity were artificial neural network (ANN) [9, 17-19].

However, to the best of our knowledge, most existing E-noses always failed to achieve precise quantitative analysis of mixture gases. In addition, most E-noses associated the sensors response values with odor intensity directly and used odor sensory method to test the odor intensity[20-22]. Once the target compound was changed, the whole E-nose system had to be rebuilt, requiring more efforts. In previous studies, odor intensity prediction models which can convert chemical concentrations to odor intensity by mathematical formulas had been applied in odor determination[17, 23-25]. The formulas can be compiled to code and written into ANN that expanded the scope of application. Meanwhile, air quality need to be evaluated by both odor intensity and chemical concentrations of VOC[26]. Taking the complicated sources of aromatic hydrocarbons into account, it is necessary to develop a novel E-nose system to analyze concentrations and odor intensity of aromatic hydrocarbons.

In this study, a novel E-nose system which included a sensor array, a signal converter and a pattern recognition system was developed to simultaneously determine chemical concentrations and odor intensity of benzene, toluene and ethylbenzene mixtures. The sensor array was equiped with 5 selected sensors, the signal converter converted electrical signals to response values and back propagation (BP) neural network was chosen as the pattern recognition system which converted response values of component in mixtures to individuals' concentrations. Then the concentrations determined by the E-nose were correlated to the results of gas chromatography-flame ionization detector (GC-FID)[27]. Furthermore, six prediction models were adopted to convert the concentrations to odor intensity of mixtures and the results were verified by the comparison with sensory analysis.

2. Materials and methods

2.1. Sensors array for E-nose

The most significant component of an artificial olfaction system is sensor array. The signal of the sensor array is interpreted by some computational methods to present the measuring results of gas concentrations or other characteristics. Among most of E-noses, metal oxide type of sensor was used due to its long-term stability [28]. Catalytic combustion type and electrochemical type were also selected occasionally [29]. In this study, 12 sensors, which belonged to above three types and were from three manufacturers, were selected to compose the sensor array. The basic data of them was shown in **Table 1**.

2.2 E-nose system setup

A customized E-nose has been developed and used for determining concentrations of aromatic hydrocarbons gases in this study and the schematic was presented in **Fig.1**. A cylindrical glass container (volume of 17.3 L) with a hole (diameter of 4 cm) on its lid worked as the gas vessel. A simple plug was just used to seal the vessel while another one was applied to seal and connect to the sensor array. Therefore, when the latter was used, the hole was plugged up and the gas in the sealed vessel would have full contact with the array at the same time. The whole gas vessel was kept in a constant temperature and humidity instrument, the temperature was 25 ± 0.5 °C and the relative humidity was 45% to 50%.

Originally, the sensor array was composed of 12 gas sensor, a temperature sensor and a humidity sensor, as the experiments proceeded, the unsuitable sensors were removed while the suitable sensors were retained (the select method was shown in Section 2.4). The response values of the sensor array were converted from electrical signals to digital signals by the signal converter and recorded by the pattern recognition system. The method of pattern recognition used in this study was BP neural network [30] and its procedure code was compiled by Matlab (Matrix & Laboratory, programming software).

2.3 Databases measurement method

2.3.1 Preparation of working gases

In this study, the working solutions were benzene, toluene and ethylbenzene with purity > 99.9% (J & K Chemical Technology, China). A certain volume of working solutions was injected to the gas vessel by a micro-injector, and then the plug without sensors was plugged immediately to seal the gas vessel. After that the electric fan was turned on and kept for ten minutes to make the solution evaporate rapidly and uniformly to form aromatic hydrocarbon gaseous mixture with target concentration. The plug was replaced by the one with sensor array to make the sensor array contact with the gas completely.

2.3.2 GC-FID analysis procedure

After gaseous mixture reached target concentration, 1 mL gas was extracted by a micro-injector through the gas export (shown in Fig.1). The chemical concentration of the gas was measured by a gas chromatography (GC-2014, Shimadzu, Japan) with a flame ionization detector and a Rtx-5 capillary column (30 m × 0.25 mm ID, 0.5 μm film thickness). The carrier gas (nitrogen) was operated at 1.0 mL min^{-1} and the flow rate of hydrogen and air was 20 mL min^{-1}. The inlet temperature was 200 °C and the split ratio was 1:10. The column oven temperature was set at 60 °C for 3 min and up to 150 °C at 10 °C min^{-1} and held for 3 min.

2.3.3 E-nose preheating

After the E-nose was turn on, it needed 2 hours to preheat the sensor array, making all sensors stable to prevent any baseline drift in the experiment.

2.3.4 E-nose response

After the E-nose was turned on, the computer began to record the response values of sensor array. The response values increased gradually as the sensor array contacted with the gas in the gas vessel (after 2.3.2). After a period of time the values became stable, these data were the response values of the tested gas[31]. The response values and the response time were recorded in the computer.

2.3.5 E-nose recovery

After the determination was finished, the lid of the gas vessel was opened. With the rotation of the electric fan, the gas spread to the fuming cupboard gradually. Meanwhile, the response values began to decrease and returned to the baseline after some time. The recovery time was recorded in the computer[31]. The above was a complete gas determination process.

GC-measured concentrations and E-nose response values composed the databases used to build, test and optimize the BP network.

2.4 Selection and characterization of sensor array

In accordance with the method in Section 2.3, 0.4 μL working solution of benzene was injected into the vessel. After completely volatilizing, the concentration of gaseous benzene in the vessel was 20 mg m^{-3}. If the response value of a sensor remained on the baseline, this meant that the sensor was not suitable for measuring benzene. The same procedure was used to select the suitable sensors for toluene and ethylbenzene. Finally, the sensors unsuitable for all three compounds were weeded out and the rest of the sensors composed the array of the E-nose.

2.5 Concentrations determination

2.5.1 Databases measurement

In order to build a complete E-nose system, a database composed of response values and corresponding chemical concentrations was needed. That database was called training database and the data in it were called training data [32]. In the national standard of China, the concentrations of aromatic compounds in the workplace have strict standards. The maximum permissible concentration-time weighted averages (PC-TWA) of benzene, toluene, ethylbenzene were 6 mg m^{-3}, 50 mg m^{-3}, 100 mg m^{-3} respectively [33]. Therefore, the testing range of concentration of aromatic hydrocarbons was 5 to 200 mg m^{-3} in this study. Specifically, the training database contained 210 groups of data which included benzene, toluene and ethylbenzene in the scope of 5 mg m^{-3} to 200 mg m^{-3}. In the training database, 60 groups were single compounds, 45 groups were binary mixtures, and 105 groups were ternary mixtures.

Another database composed of different response values and the corresponding chemical concentrations was needed to test and optimize the E-nose system, which was called test database and the data in it were called test data. The test database included 80 groups of data which were also uniformly distributed in the range of 5 mg m^{-3} to 200 mg m^{-3}. All test data were different from training data and were measured by the method in Section 2.3.

2.5.2 BP network structure design

Five sensors were selected and composed the sensor array of the E-nose system. Due to the cross-sensitivity, selection differences and stability differences of gas sensors[34], when a single sensor is used to measure gas mixtures, it may have response to more than one kind of gas, so it is difficult to use general mathematical method to analyze the response values. The problem can be solved by pattern recognition technique which employs computer to recognize the sample from the sample library[9]. BP neural network algorithm has been one of the most frequently-used pattern recognition techniques in the field of E-nose because it is powerful, easy to understand and simple to train[30]. Thus BP neural network was chosen to build E-nose software system and Matlab was used to write program code.

BP neural network is a nonlinear and self-adaptive information processing system and consists of a large number of processing unit[30]. The basic structure includes input layers, hidden layers and output layers. Each layer is composed of neurons and transfer function. In this study, the dimensions of input and output vector were consistent with that of input and output layer and were determined by the number of the sensors and the types of the measured gases. The number of input layer neurons was five and the number of output layer neurons was three. The hidden layers had a most important influence on BP neural network's results, so the amount of the hidden layers and neurons in each layer as well as the transfer function types need to be tested and optimized.

The BP neural network can be built with the simplest hidden layer structure, but the training failed to converge with too few hidden layers or neurons. Therefore, the system began with only one hidden layer and added one each time until the convergence started.

Before the training, the training data were normalized [35], the normalization formula was

$$B = \frac{(A - \mathrm{Min})}{(\mathrm{Max} - \mathrm{Min})} \quad (1)$$

Where A is original training data, B is normalized training data, Min is the minimum of all the original training data, and Max is the maximum of all the original training data.

After normalization and training convergence, the BP network was built. Since the result of each training was different, in order to reduce the random error, the data were trained three times, and every result was stored respectively. These three same networks were called parallel networks.

After training completion, each parallel neural network was invoked again, and the 80 groups of test data (which were normalized by the same method) were led in, the measuring results were calculated by Matlab. Because of the simple structure of the network, the results were of low accuracy, so the BP neural network need be tested and optimized. Firstly, the transfer function and training function were tested in sequence to make the measuring more accurate. Then, the number of hidden layer was added from the minimum to the number which could make the measuring result achieve best accuracy. The same method was used for testing and optimizing the number of neurons in each hidden layer. The whole process of modification was single variable experiment and all tests were repeated three times.

2.5.3 Comparison with GC-FID

The GC-FID technology for aromatic hydrocarbons determination was already well-developed, so the concentrations measured by GC-FID were used as the true values while the results of E-nose were used as treated measured values [16]. Those two kinds of values were compared, and the average relative errors (ARE) of test data were calculated as the criterion of accuracy. Through the modification, the best parameters of the neural network were ascertained and the codes of them were written into the final software system.

2.6 Odor intensity determination

Till date, many prediction models have been proved its ability to convert concentrations to odor intensity[24]. In this study, the optimum models for aromatic hydrocarbons were selected and the constants of each of model were also calculated. The odor intensity of a series of aromatic hydrocarbons gases of different concentrations (5 mg m^{-3} to 200 mg m^{-3}) were measured by odor sensory method. Then linear regression and nonlinear regression were used to calculate constants. Detailed measurement method was as follow: each tested compound was respectively injected into an olfactory-bag (3 L volume and full of clear air), when all the compounds had completely evaporated, odor sample was prepared through transferring a certain quantity of gas from the previous olfactory-bag to a new bag by injector. Then 6 sniffing panelists evaluated the testing gas according to the odor intensity referencing scale (OIRS, from level 1 (aqueous solution of 1-butanol of 12 mg m^{-3}) to level 8 (1550 mg m^{-3}) with a geometric progression of two) [23], the mean results were calculated as the final odor intensity.

After all the constants were confirmed, the odor intensity of the gases whose concentrations were same as the test database was measured by odor sensory method. The prediction models were employed to predict the odor intensity and the results were compared with sniffed values, then the optimum models were determined.

3. Results and discussion

3.1 The sensor array

After selecting all sensors, the suitable sensors MC119, MQ6 and TGS2610 were responded to benzene, toluene and ethylbenzene. Sensor 2M008 was responded to toluene and ethylbenzene. Sensor WSP2620 was only responded to ethyl benzene.

For E-nose, the very short measuring time is one of the significant advantages, while the response and recovery time are the main restricting factors. So in accordance with the method in Section 2.3, the response values of 100 mg m^{-3} benzene, toluene and ethylbenzene were measured respectively. As shown in **Fig.2,** **t**he response values, response time and recovery time were all recorded and the response recovery curve was drawn. The values of MC119 were not very stable, so the average of 15 continuous tested values was defined as the its response value[36]. The response time of all sensors was less than 4 minutes and the recovery time was less than 2 minutes. The rapid measuring speed made the determination process finish in 10 minutes, compared with the traditional method, the determination time was greatly shortened.

In order to test the stability of the sensor array, twenty groups of response values of single gas of benzene, toluene and ethylbenzene were measured respectively. The concentrations ranged from 5 mg m^{-3} to 200 mg m^{-3} and the interval was 10 mg m^{-3}. All the data were measured three times and the relative standard deviations (RSD) of response values were calculated, the results were shown in **Fig.3**. All RSD values were less than 7%, which showed the experiment had good precision.

3.2 BP network test and optimization

The purpose of this section is to get the minimum error results by testing and optimizing BP network structure. As the method in 2.5, transfer function, training function, number of hidden layers and number of neurons in each hidden layer all needed to be modified. The functions 'logsig', 'purelin' and 'trainbfg' were set as default, and the minimum number of hidden layers and neurons which can make training convergent were 3 and 16 respectively. Other parameters would be discussed then.

3.2.1 Function

Six kinds of transfer functions named 'logsig', 'dlogsig', 'tansig', 'dtansig', 'purelin' and 'dpurelin' were tested. The former four ones were hidden layer functions and ‘logsig’ was considered as the best one since the normalized training data were all smaller than 1. The last two functions were output layer functions and only ‘purelin’ could make the training converge, so ‘purelin’ was adopted.

Relative to the transfer function, the training function have a greater significanc. In Matlab, fifteen kinds of training functions were provided. With ‘logsig’ and ‘purelin’, 3 hidden layers and 16 neurons as parameters, all training functions were used to train the network. The AREs of all funtions were calculated and the results showed that ‘trainlm’ had the smallest error and the value was 12.77%.

3.2.2 Hidden layer

The network with less than 3 hidden layers can’t converge. Therefore, only 3 hidden layers were employed in the first training process. Then the process was repeated with increasing one layer at a time until the ARE reached the minimum. Through 6 times training (3 layers to 8 layers), ultimately, the optimum number of hidden layers was 6 and the ARE was 11.62%.

3.2.3 Neurons

The first training process was carried out with 16 neurons in each layer and repeated with increasing one neuron at a time to modify. Through 7 times training (16 neurons to 22 neurons), 20 neurons had the samllest ARE and the value was 9.71%.

Discussed above, the BP neural network used ‘logsig’ and ‘purelin’as transfer function and 'trainlm' as training function and was composed of 210 groups of training data, 5 dimensions input layer and 3 dimensions output layer, 6 hidden layers and 20 neurons in every layers.

3.3 Comparative analysis of E-nose and GC-FID

Through measurement of 80 groups of test data, the results showed that the network could measure the chemical concentrations of benzene, toluene, ethylbenzene in the scope of 5 mg m^{-3} to 200 mg m^{-3}. The test set was used to validate the determination capabilities of the E-nose (**Fig.4**). The Pearson correlation coefficient, the Significance of paired-sample T-test with 95% confidence interval, the ARE of the predicted results and the correlation coefficient between E-nose and GC-FID measured values were shown on **Table 2.** The results showed that the E-nose system could determine respective concentrations of aromatic hydrocarbon mixtures simultaneously and it had a high accuracy relative to GC-FID.

3.4 Odor intensity analysis

Odor pollution has been one of the seven major environmental pollution hazards and aromatic hydrocarbon is one of the most common causes of odor pollutants. After years of experimental researches, a conclusion had been found that for a single material, the odor intensity increased with the increasing of chemical concentration, but it was not a simple linear relationship. Furthermore, due to the interaction between odor compounds，the total odor intensity of multiple mixtures is not simply the sum of all the components which let the prediction become difficult.

3.4.1 Prediction models review

In the recent researches, some prediction models have been proved to have high prediction accuracy, such as Weber-Fechner law, Power Law Model and Linear Model for single compounds, the Vector Model for the binary compounds, Extended Vectorial Model (EV Model) for ternary compounds and Strongest Component Model (SC Model) and Euclidean Additivity Model (EA Model) for both of binary and ternary[25, 37-39]. Their formulas were shown in **Table 3**.

3.4.2 Prediction models simplification

The EV model was used to predict the odor intensity of ternary compounds, the formula of which contains 3 constants. When one of the compounds changed, all the three constants would change accordingly. So model simplification was significant.

Through the study of the interaction of odor, for the ternary mixtures, there was a linear relationship between the sum of the odor intensity of the entire single compound (sum intensity, I_s) and the odor intensity of the mixture (total intensity, I_t). If the odor intensity of each single compound (single intensity, I_A) is approximately equal, the degree of interaction of the compounds remains the same[24]. For the benzene, toluene and ethylbenzene, through sniff and calculation, the formula was

$$I_t = 0.36815 \cdot I_s = 0.36815 \cdot (3 \cdot I_A) = 1.10445 \cdot I_A \quad (2)$$

the R^2 was 0.996.

When the single intensity was approximately equal, the formula of EV model was

$$I_t^2 = 3 \cdot I_A^2 + 2 \cdot I_A^2 \cdot (\cos\alpha_{AB} + \cos\alpha_{AC} + \cos\alpha_{BC}) \quad (3)$$

For this study, the constants were confirmed, so set

$$\cos\alpha_{AB} + \cos\alpha_{AC} + \cos\alpha_{BC} = 3 \cdot \cos\alpha \quad (4)$$

The formula was changed as

$$I_t^2 = 3 \cdot I_A^2 + 6 \cdot I_A^2 \cdot \cos\alpha = 3 \cdot I_A^2(1 + 2\cos\alpha) \quad (5)$$

The formula (2) was put into the formula (5), the formula was changed as

$$(1.10445 \cdot I_A)^2 = 3 \cdot I_A^2(1 + 2\cos\alpha) \quad (6)$$

Then, the $\cos\alpha$ was calculated, the result was -0.30, the formula of simplified Extended Vectorial (SEV) model was

$$I_t^2 = I_A^2 + I_B^2 + I_C^2 - 0.60 \cdot (I_A \cdot I_B + I_A \cdot I_C + I_B \cdot I_C) \quad (7)$$

3.4.3 Prediction of the odor intensity

For each single compound in aromatic hydrocarbons，the constants of every models were calculated by linear regression or non-linear regression，the results were shown in **Fig.5** and the formulas and the correlation coefficients (R^2) of each model were shown in **Table 4**, all of R^2 were higher than 0.97.

The measuring method in Section 2.5 was used to measure the chemical concentrations of test database by the E-nose, then the prediction models were used to convert the chemical concentrations to the odor intensity, the results were called predicted results. The method in Section 2.7 was used to measure the odor intensity of all samples, the results were called measured results.

These predicted results and measured results were compared and the best models were applied in E-nose system. The Pearson correlation coefficient, the Significance of paired-sample T-test with 95% confidence interval and the ARE of the predicted results were shown on **Table 5**. As shown in the results，the Weber-Fechner law model, the Vector model and the SEV model had the smallest average relative error which meant the best precision and accuracy. So the three models were used to predict the odor intensity, the total ARE was 5.31%, Pearson correlation coefficient was 0.947 and Significance of paired-sample T-test was 0.175.

Finally, the Matlab was used to edit code and the formula of each best prediction model was written into the program to realize the function that can simultaneously determines the chemical concentrations and the odor intensity.

3.5 Comparison with previously reported E-noses

Compared with previously reported E-noses, the testing time for one test was less than ten minutes, which kept the advantage of fast determination.

On the analysis of the error, the relative errors of chemical concentrations and odor intensity were 9.71% and 5.31% respectively. Therefore, the accuracy of the novel E-nose maintained a similar level in comparison to previously reported E-noses.

In the field of environmental research, the application of previously reported E-noses focused on qualitative analysis single or mixed gases, quantitative determination of concentrations of single gas or odor analysis. However, there has been few study on the simultaneously quantitative analysis of mixed gas, so it was still a problem needed to be solved. The E-nose in this paper could quantitatively determine the chemical concentrations and measure odor intensity of aromatic hydrocarbon mixed gases simultaneously, which extended the range of application.

4. Conclusion

In the present study, an E-nose system which is based on the BP neural network was designed. It could rapidly, conveniently and accurately determine the chemical concentrations and odor intensity of the mixtures of benzene, toluene, ethylbenzene in the scope of 5 mg m^{-3} to 200 mg m^{-3}, the average relative error of concentrations and odor intensity were 9.71% and 5.31% respectively. The concentrations were measured by BP neural network while the odor intensity was measured by model prediction. The different models for single, binary and ternary compounds were Weber-Fechner law model, Vector model and Simplified Extended Vectorial model respectively. The overall results of the study suggest the potential of E-nose as a device for determination of the chemical concentrations and odor intensity of aromatic hydrocarbon mixtures.

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Figure caption

Fig.1. The basic structure of the E-nose system

Fig.2. The sensor array response recovery curve

Fig.3. The relative standard deviation of the benzene, toluene and ethylbenzene

Fig.4. The relationship of CG-FID versus E-nose results from linear regression

Fig.5. The results of regression of Weber-Fechner law, Power Law Model and Linear Model

Table.1 The basic data of the sensor array

Name	Manufacturer	Type
2M008	Guotaihengan	metal oxide
TGS2610	Figaro	metal oxide
TGS822	Figaro	metal oxide
TGS823	Figaro	metal oxide
TGS825	Figaro	metal oxide
TGS826	Figaro	metal oxide
MQ6	Winsen	metal oxide
WSP2620	Winsen	metal oxide
MC115	Winsen	catalytic combustion
MC119	Winsen	catalytic combustion
ME3-C6	Winsen	electrochemical
ME3-C7	Winsen	electrochemical

Table.2 The comparative result of E-nose and GC-FID

	Pearson	Significance	ARE/%	R^2
Single	0.996	0.911	4.90	0.992
Binary	0.991	0.982	7.13	0.982
Ternary	0.984	0.559	12.34	0.982
Total	0.990	0.622	9.71	0.986

Table.3The formulas of prediction models

Models	Formula
Weber-Fechner law	$I = \mathrm{K} \cdot \log C + \mathrm{n}$
Power Law Model	$I = \mathrm{K} \cdot C^{n}$
Linear Model	$I = \mathrm{K} \cdot \ln(\mathrm{OAV}) + \mathrm{n}$
Vector Model	$I_t^2 = I_A^2 + I_B^2 + 2 \cdot \cos\alpha \cdot I_A \cdot I_B$
EV Model	$I_t^2 = I_A^2 + I_B^2 + I_C^2 + 2 \cdot I_A \cdot I_B \cdot \cos\alpha_{AB} +$ $2 \cdot I_A \cdot I_C \cos\alpha_{AC} + 2 \cdot I_B \cdot I_C \cos\alpha_{BC}$
EA Model	$I_t^2 = \sum_{I}^{P} I_i^2$
SC Model	$I_t = \mathrm{MAX}(I_i)$

I: odor intensity

C: odorant concentration (mg m^{-3})

$\mathrm{I_t}$: the total odor intensity

$\mathrm{I_i}$, $\mathrm{I_A}$, $\mathrm{I_B}$ and $\mathrm{I_C}$: independent odor intensity of every component

p: the number of gases

k, n and cosα: constant specific to the odorant

OAV: the result of concentration value divided by odor threshold.

Table.4 The formulas of prediction models for aromatic hydrocarbons

Compound	Weber-Fechner Law	R^2	Power Law	R^2	Linear Model	R^2
Benzene	$I= 2.6704 \cdot \log C + 0.1531$	0.9893	$I=1.5040 \cdot C^{0.2765}$	0.9803	$I=1.1598 \cdot \ln(OAV)-5.1174$	0.9871
Toluene	$I= 2.8372 \cdot \log C + 0.9766$	0.9823	$I=2.1482 \cdot C^{0.2459}$	0.9845	$I=1.2322 \cdot \ln(OAV)-5.5470$	0.9787
Ethylbenzene	$I= 2.5710 \cdot \log C + 1.7742$	0.9875	$I=2.6727 \cdot C^{0.2098}$	0.9798	$I=1.1166 \cdot \ln(OAV)-6.6476$	0.9851

I: odor intensity

C:odorant concentration (mg m^{-3})

OAV: the result of concentration value divided by odor threshold.

Table.5 The correlation analysis and average relative error of each prediction results

	Sample quantity	Models	Pearson	Significance	ARE
Single	24	Weber-Fechner law	0.971	0.468	4.96%
		Power Law Model	0.971	0.524	6.10%
		Linear Model	0.971	0.089	6.67%
Binary	27	Vector Model	0.929	0.596	5.21%
		SC Model	0.818	0.255	8.37%
		EA Model	0.934	0	20.58%
Ternary	29	SEV Model	0.909	0.301	5.86%
		SC Model	0.731	0.025	9.98%
		EA Model	0.884	0	53.85%

15x3mm (600 x 600 DPI)

Graphical Abstract

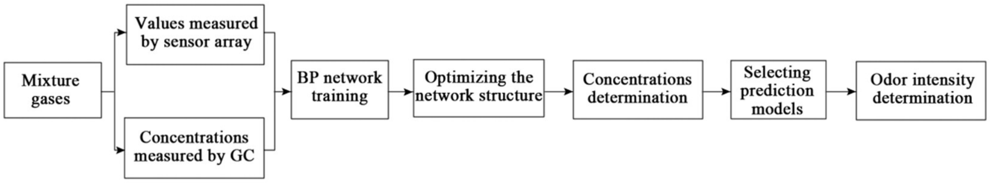


Fig.1. The basic structure of the E-nose system

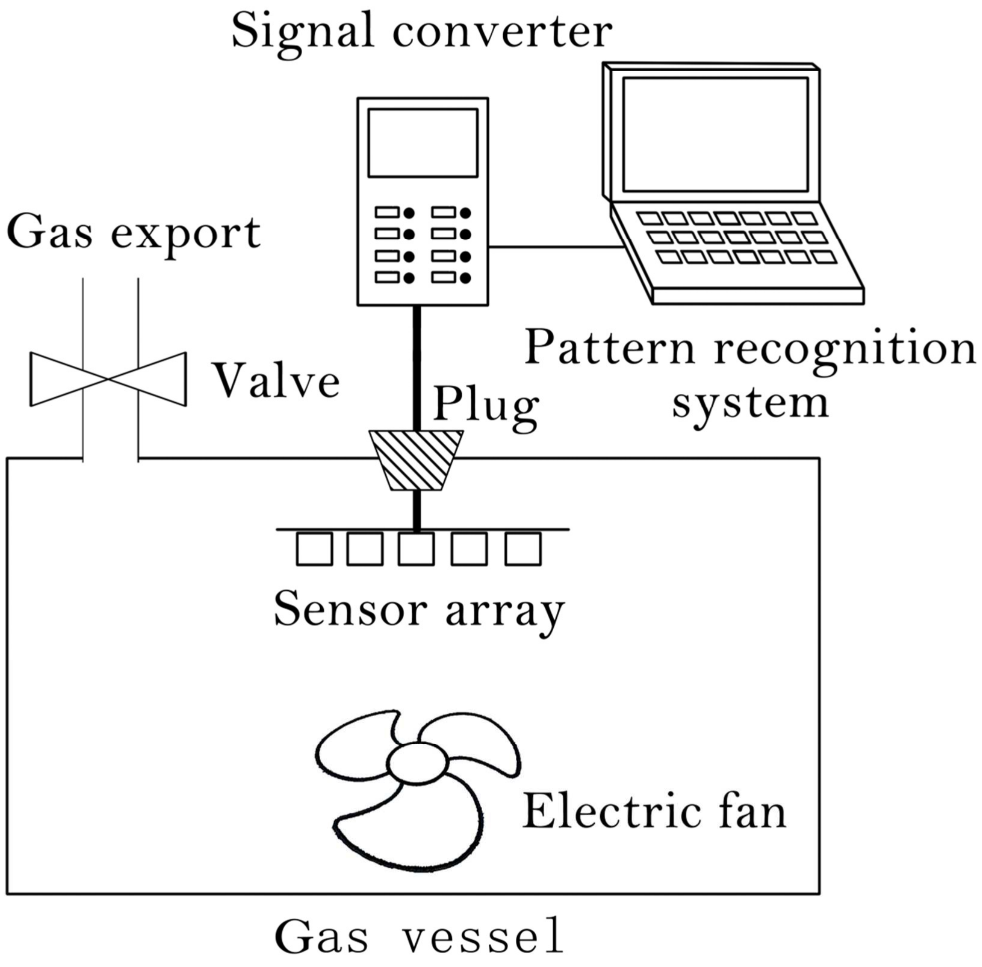
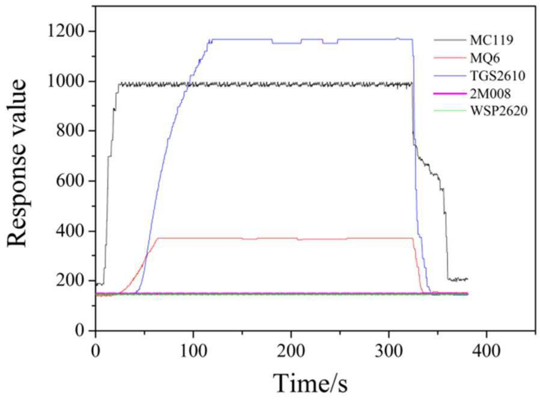
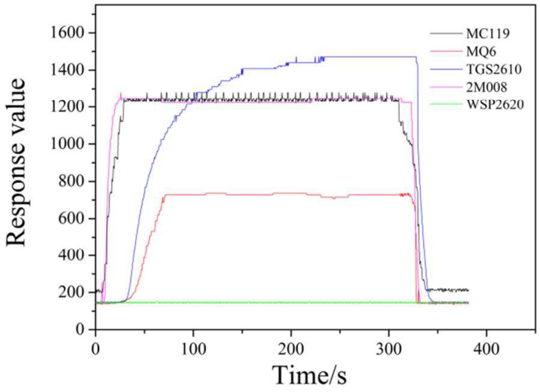


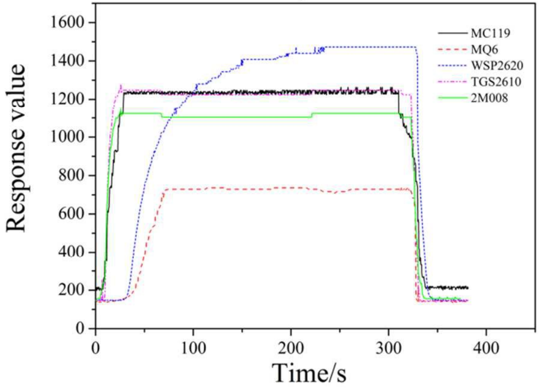
Fig.2. The sensor array response recovery curve



a.Benzene



b.Toluene



c.Ethylbenzene

Fig.3. The relative standard deviation of the benzene, toluene and ethylbenzene

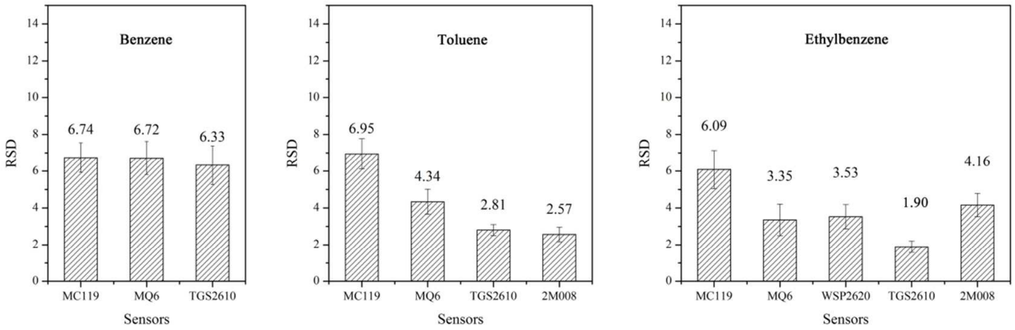


Fig.4. The relationship of CG-FID versus E-nose results from linear regression

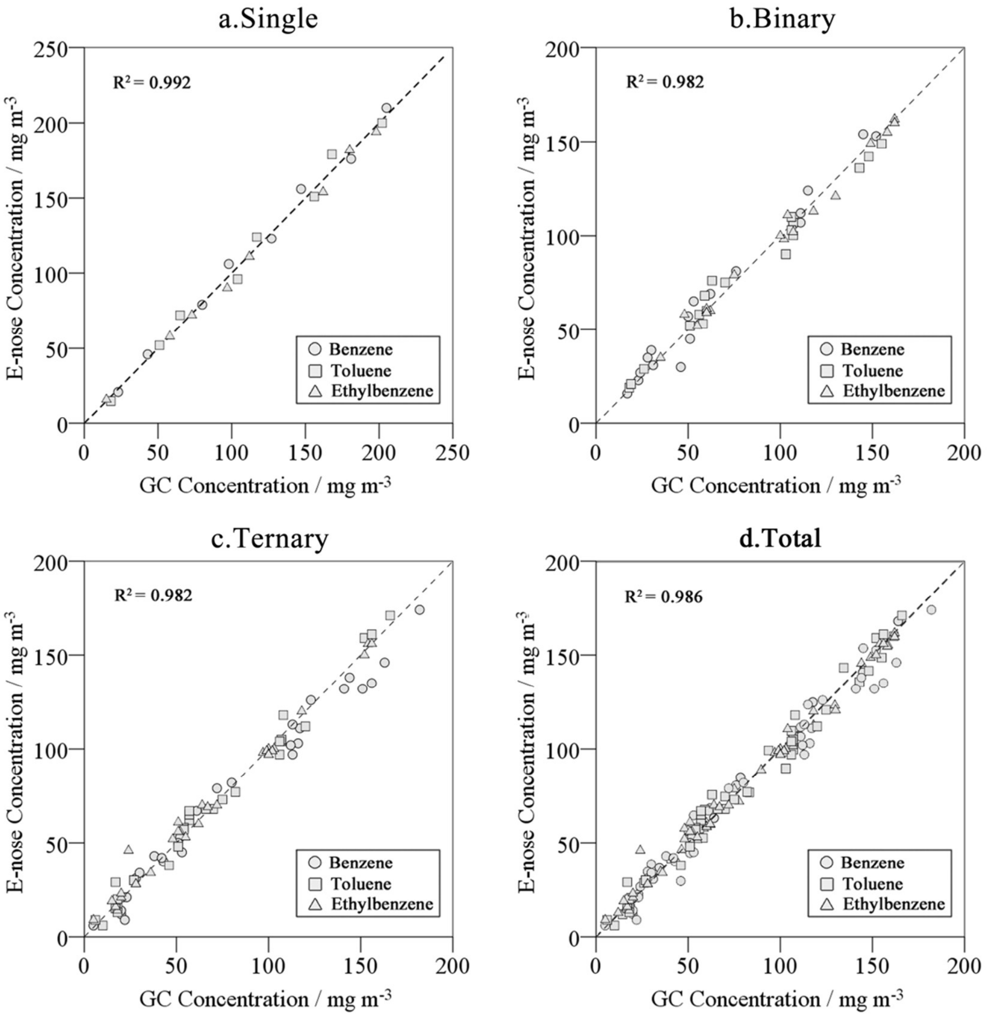
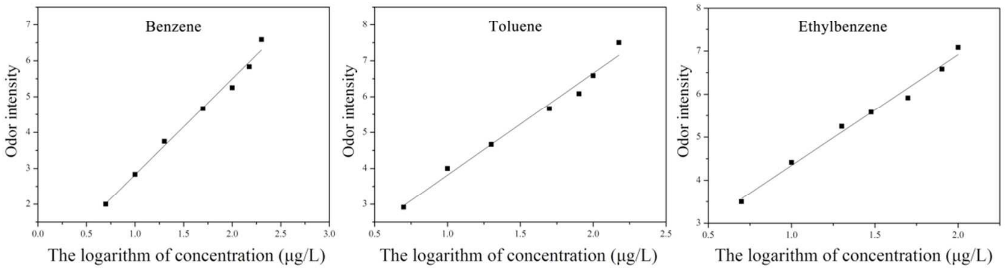
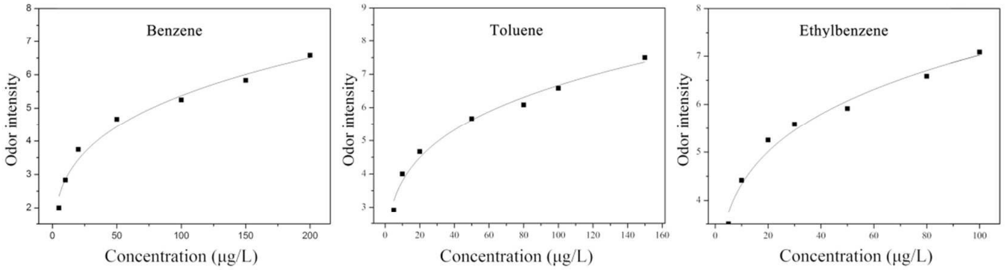


Fig.5. The results of regression of Weber-Fechner law, Power Law Model and Linear Model

a.Weber-Fechner law



b. Power Law



c.Linear Model