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Neuro-Identification of Some Commonly Used Volatile Organic Compounds Using Electronic Nose

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Abstract

Electronic nose system comprising of three Figaro sensors (TGS2602, TGS832 and TGS816) arrayed in a chamber interfaced through PICO ADC11/10 card to a computer system loaded with artificial neural network (ANN) was used to identify three volatile organic compounds (Formaldehyde, Acetone and Chloroform). The back propagated ANN had four layers having positive linear, logsigmodal, logsigmidal and tansigmodal transfer functions with 10, 20, 20, 1 neurons, respectively. 60% of the acquired data was used for training and 20% each for testing and validation.TGS832 had the highest average sensitivity (1.3639 volts) while TGS816 had the least (0.0420 volts) for formaldehyde with similar trend for chloroform and acetone. Sensors' sensitivities were significantly different from the control at $p < 0.05$. Mean square error of 0.0006, 0.0001 and 0.0003(R^2:0.996, 0.997 and 0.996) were obtained for the ANN training of formaldehyde, chloroform and acetone respectively. Validation run gave correct identification of the VOCs.

Key Words: Sensors, Neurons, Normalization, Electronic nose, Data card

1.0 Introduction

The use of artificial intelligence devices is fast gaining ground in the nations of the world. Prominent among these are the electronic noses (e- nose) that are array of sensors that can detect materials through smell (Kwon, *et al.*, 1995, Hong, *et al*, 2000). Combinations of these with other computer-based software have proofed to be excellent devices in chemical analysis. The e-noses were engineered to mimic the mammalian olfactory system within an instrument designed to obtain repeatable measurements (Shurmer,, 1990). The two main components of an e- nose are the sensing system that can be an array of chemical sensors or a single sensing device and the automated pattern recognition system (Patrash & Zellers, 1993; Hong, *et al*, 2000). They are able to identify mixtures of organic samples, measure and characterize volatile aromas released from a multitude of sources for numerous applications (Persaud *et al.*, 1993, Davide *et al.*, 1995).

Advances in electronic noses have improved product attributes, uniformity and consistency because of increases in quality control capabilities afforded by e-nose monitoring of all phases of industrial manufacturing process (Dalton *et al*, 2004, Wilson & Baietto, 2009). They are used for quality control of raw materials, manufactured products, process design, freshness and maturity monitoring (Gomez , *et al*, 2006; Pathange, *et al*, 2006), shelf life investigations (Riva, *et al*, 2004), classification of scents and perfumes, microbial pathogen detection and environmental assessment studies (Stetter, 1992). It is a non destructive technique used to assess fruit quality based on aroma characteristics that are highly correlated with all the factors that affect shelf – life and future marketability (Schaller, *et al,* 1998). Electronic noses have been used to identify and classify different wood and tree species and in the investigation of a problem relation to the quality of pulp and paper (Cordeiro, *et al.,*2012).

Arshak *et al* (2004) reviewed the range of sensors used in electronic (e- nose) systems to date. The operating principles and fabrication methods of each sensor type as well as the applications in which the different sensors have been utilized and, the advantages and disadvantages of each type for application

in a cost – effective, low–power hand held – e nose system were outlined. The noninvasive, rapid and relatively inexpensive nature of the technology makes it extremely attractive for further development in a variety of medical application hence, the wide application in medicine.

In medicine, the potential to assist in diagnosis has been found to be promising (Thaler *et al*, 2001). It has been identified as a novel method to identify potential upper respiratory infections and to discriminate among common upper respiratory bacterial pathogens (Lai, *et al*, 2002; Philips, *et al*, 2003 Aronzon , *et al*, 2005). The use of electronic nose to detect, and subsequently control the emission of hazardous gaseous substances in the environment has shown great potential to complement sensory analysis and augment the gas chromatography analysis method currently used because, it helps to maintain a pollution free environment and to reduce all such emissions to the barest minimum (Cai & Levy, 2006).

Volatile Organic Compounds (VOCs) are chemical compounds that have high enough vapour pressures under normal conditions to significantly vaporise and enter the air resulting in air pollution (Rinnan, *et al*, 2005). There are a wide range of carbon-based molecules that are considered VOCs such as aldehydes, ketones, and hydrocarbons. Health effects from VOCs are usually temporary and improve once the source of the exposure is identified and removed. These health effects can include irritation of the eyes, nose, throat and skin. Headache, nausea and dizziness may occur, as well as fatigue and shortness of breath. Health effects vary depending on the chemicals involved and the duration of the exposure (Kesselmeier & Staudt, 1999; Rinnan, *et al*, 2005). Formaldehyde and pesticides are considered probable carcinogens. Benzene can affect the bone marrow by decreasing red blood cells (anemia) or by decreasing platelets, which causes excessive bleeding; acute inhalation exposure of chloroform affects the central nervous system, cardiovascular system, and liver function. Exposure to acetone inhibits the metabolism and elimination of ethyl alcohol thereby potentially increasing the toxicity in the body (USDHHS, 1993; CDPHE,2000)

This study is to design and implement an artificial intelligence system (comprising of electronic nose device and artificial neural network (ANN)) to identify and classify some commonly used volatile organic compounds in the laboratory (formaldehyde, acetone and chloroform) that can constitute air pollutants.

2.0 Methodology

2.1 Materials

Three major set of materials that were involved in this study are Computer Hardware / Software **(** Personal computer, Data acquisition card(ADC 11/10), Matlab 6.5 version and SPSS package); Series of Gas Sensors **(** Figaro TGS 2602, Figaro TGS 832 and Figaro TGS 816) and Chemicals **(** Formaldehyde, Chloroform and Acetone)

2.2 Process Description

The gas sensing process setup (Figure 1) was designed as a test used for the experimental evaluation of ANN identification of organic gases. A sample of each chemical sensed was placed in a gas chamber already arrayed with the series of Figaro sensors. Two of each Figaro TGS 2602, Figaro TGS 832 and Figaro TGS 816 were arrayed to Acquire data in replicates so as to establish the uniformity of the process. Each sensor was powered by 8.0-volt power pack affixed on a voltage-regulated circuit according to their power requirements. An 11 channel ADC data acquisition card interfaced the computer system and the gas chamber through the connection of six channels to the six sensors and a channel without sensor to serve as control. As each sensor sensed any gas, its reading was acquired and simultaneously recorded into the system through the card. Acquisition of each data for respective gas film was allowed to run for 500 seconds. This was done to allow the gas film to saturate the entire chamber. The steady reading of the sensors to each gas film served as an indication that there has been recognition of such a gas. All the readings were then transferred into an ANN environment in Matlab 6.5 version where they were trained to match each of the gas.

2.3 Analysis of the Data and Neuro-Predictive Model of the process.

Significant differences in the data acquired by the sensors arrayed were compared using analysis of variances (ANOVA) for each gas at $p < 0.05$.

About 60% of all data acquired by the three sensors for each gas were randomly assigned to the training set, while 20% went to testing and the remaining 20% were assigned to the validation set. The network training was carried out using the standard back propagation method. The positive linear was used as the transfer function in the input having 10 neurons, logsigmodal as the transfer function in the first layer having 20 neurons, another logsigmodal as the transfer function in the second layer also having 20 neurons and finally, tansigmodal as the transfer function in the output having one neuron. Also, the levenberg-Marquardt (trainlm) training function was used in each case because of its speed of convergence and accuracy. The stop criteria were based on the mean square error (MSE). This ANN network composed of four layers. The input variables were preprocessed using the normalization technique; before they were fed to the back propagated ANN. In order to validate the normalized –ANN model obtained, the input/output data of the untrained data were presented to the trained network to see how well the network model predicts the corresponding output data. A generalization test with both familiar and unfamiliar data set was also conducted on the network. The software implementation of this model was carried out on MATLAB 6.5 version.

3.0 Results and Discussion

3.1 Statistical Analysis of Data

The descriptive statistics of the data captured by the acquisition card that interfaced the three sensors (TGS2602, TGS 832, TGS 816), the control (no sensor) with the computer system is as shown on Table 2. The control gives the data pattern for the channel without any sensor inserted. The three sensors were arranged in array to the odour from each of the three organic chemicals (formaldehyde, chloroform and acetone) and their data is as shown against each chemical. It is clear from this data that each of the sensors responded differently for each of the chemicals, which is an indication of their applicability to chemical classification. The TGS832 had the highest average sensitivity (1.3639 volts), followed by TGS2602 (0.2308volts) while TGS816 had the least (0.0420 volts) for formaldehyde. This pattern is similar for chloroform and acetone.

In addition, Table 3 shows the analysis of variance of each category of data acquired through each of the three sensors for the three chemicals as compared with the control. As shown on the last column of the Table 3, all the p-values are lass than 0.05, which signifies that there are significant differences among the data acquired. The difference in the variance of all these data are essential due to the fact that it is always required that any data that will be used for ANN analysis must possess some degree of variability in order to develop a stable Network. Therefore, as obtained from the ANOVA of this data set, it is than convenient to use the data set for ANN training and validation. The implication of the significant differences in the data obtained is that each sensor exhibits unique sensitivity to the various chemicals.

3.2 Neuro-Predictive Model of the Process

The 60% of the 500 data set obtained for each of the chemicals were used for training, 20% for testing and 20% for validation of the neural network model built. The general performance of the artificial neural networks built for each of the three data set is presented in Table 4. The performance of training of the neural networks is presented on Figure 2 to Figure 4 for formaldehyde, chloroform and acetone respectively. The best result was obtained for the ANN, which composed of 10 neurons in the input layer,20 neurons in each of the 2 hidden layers and 1 neuron at the output layer. In order to improve the result and to prune the ANN structure, the input variables were preprocessed using the normalization technique before they were fed to the back propagated ANN.

Likewise, the trend of performance shown on Figure 2 to Figure 4 for training, validation and testing is an indication of the stability of the network in predicting and identifying future data set of chemicals. The implication of this result obtained is that, in future once any gas fume that is among these ones that have been used to train the ANN is contained in the chamber, the data acquired by the sensor will be passed to the ANN already trained and instantly the ANN will give a coded output that can be interpreted from Table 1. For instance if the output is 0,then none of them is present, if 1,then formaldehyde; if 2 then acetone and finally, if 3 it is then chloroform. This is particularly important when one considers the nature and complexity of most gas fume and air pollutants evolving from reactions in industries exhaust from vehicles, generators, boilers, aircrafts and gases generated from domestic activities e. t. c. Figure 5 to Figure 7 show the graphical representation showing how the actual data and the model predicted data were closely related at various time intervals.

4.0 Conclusion

In this work, the application of Artificial Intelligence unit for gas identification and environmental monitoring in general was discussed and analysed. It can be concluded that the three sensors in the electronic nose exhibited significantly different sensitivity to the gases with TGS832 being the highest and TGS816 the least for the three gases. The combined use of the gas sensors arrayed in the gas chamber , data acquisition card and computer softwares proved to be a faster and effective accurate measure of gas identification. In effect, this method of gas identification is a potential substitute for the conventional methods.

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Table 1: Output code for each of the gases

Chemicals	**Output Identification Code**
None	0
Formaldehyde	1
Acetone	2
Chloroform	3

Table 2: Descriptive statistics of captured data.

Chemical	Sensor Type	N	Mean	Maximum	Minimum	Standard Deviation
None	**Control**	500	1.8558	1.8330	1.8750	0.0069
Formaldehyde	**TGS2602**	500	0.2308	0.2200	0.2340	0.0039
	TGS832	500	1.3639	0.0020	1.6180	0.2014
	TGS816	500	0.0420	0.0420	0.0430	0.0000
Chloroform	**TGS2602**	500	0.1558	0.1410	0.1610	0.0056
	TGS832	500	0.7056	0.3980	0.9460	0.1581
	TGS816	500	0.0300	0.0200	0.0490	0.0093
Acetone	**TGS2602**	500	0.1695	0.1470	0.1880	0.0126
	TGS832	500	1.4636	0.8670	1.6780	0.1989
	TGS816	500	0.1003	0.0730	0.1590	0.0181

Table 3: Anova of enose data for the gases as compared with the control

Chemical	Sensors		Sum of Squares	df	Mean Square	F	p-Value.
Formaldehyde	TG2602	Between Groups	1.267E-03	37	3.425E-05	2.432	.000*
		Within Groups	6.505E-03	462	1.408E-05		
		Total	7.772E-03	499			
	TGS832	Between Groups	4.658	37	.126	3.735	.000*
		Within Groups	15.573	462	3.371E-02		
		Total	20.231	499			
	TGS816	Between Groups	4.980E-07	37	1.346E-08	12.437	.000*
		Within Groups	5.000E-07	462	1.082E-09		
		Total	9.980E-07	499			
Chloroform	TG2602	Between Groups	2.522E-03	37	6.817E-05	2.393	.000*
		Within Groups	1.316E-02	462	2.848E-05		
		Total	1.568E-02	499			
	TGS832	Between Groups	1.860	37	5.027E-02	2.189	.000*
		Within Groups	10.611	462	2.297E-02		
		Total	12.471	499			
	TGS816	Between Groups	8.014E-03	37	2.166E-04	2.848	.000*
		Within Groups	3.514E-02	462	7.605E-05		
		Total	4.315E-02	499			
Acetone	TG2602	Between Groups	1.209E-02	37	3.268E-04	2.231	.000*
		Within Groups	6.768E-02	462	1.465E-04		
		Total	7.977E-02	499			
	TGS832	Between Groups	2.832	37	7.653E-02	2.091	.000*
		Within Groups	16.908	462	3.660E-02		
		Total	19.739	499			
	TGS816	Between Groups	2.091E-02	37	5.652E-04	1.823	.003*
		Within Groups	.143	462	3.100E-04		
		Total	.164	499			

* Significant at $p < 0.05$.

Table 3: General performance for ANN models

Chemical	MSE	R^2
Formaldehyde	0.0006	0.996
Chloroform	0.0001	0.997
Acetone	0.0003	0.996

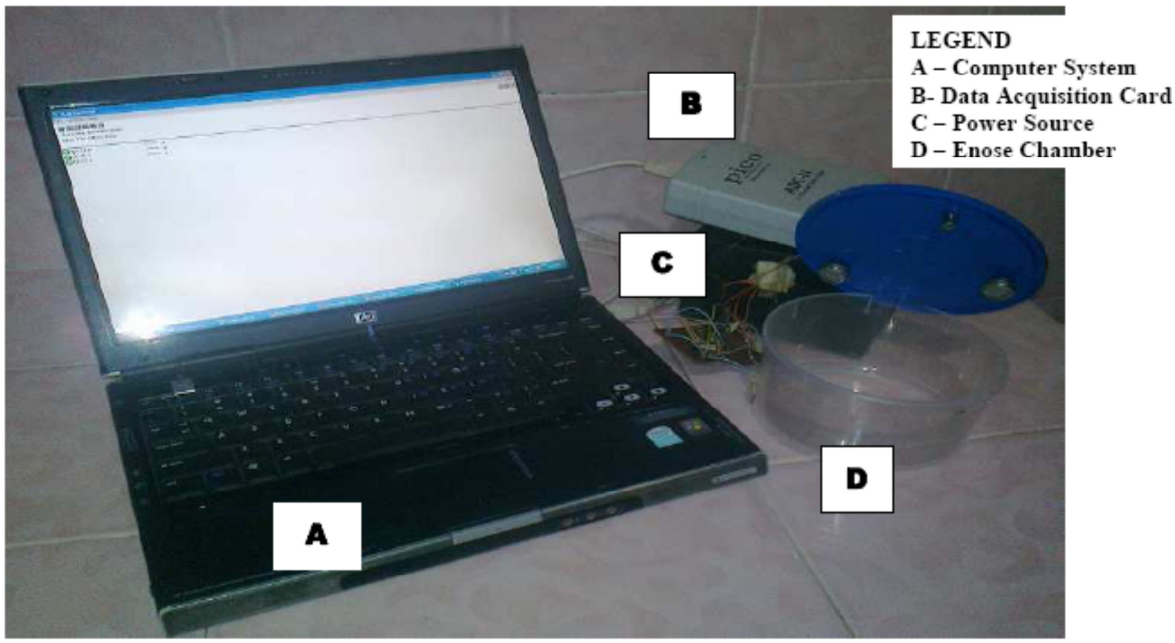

Figure 1: Gas sensing process laboratory setup.

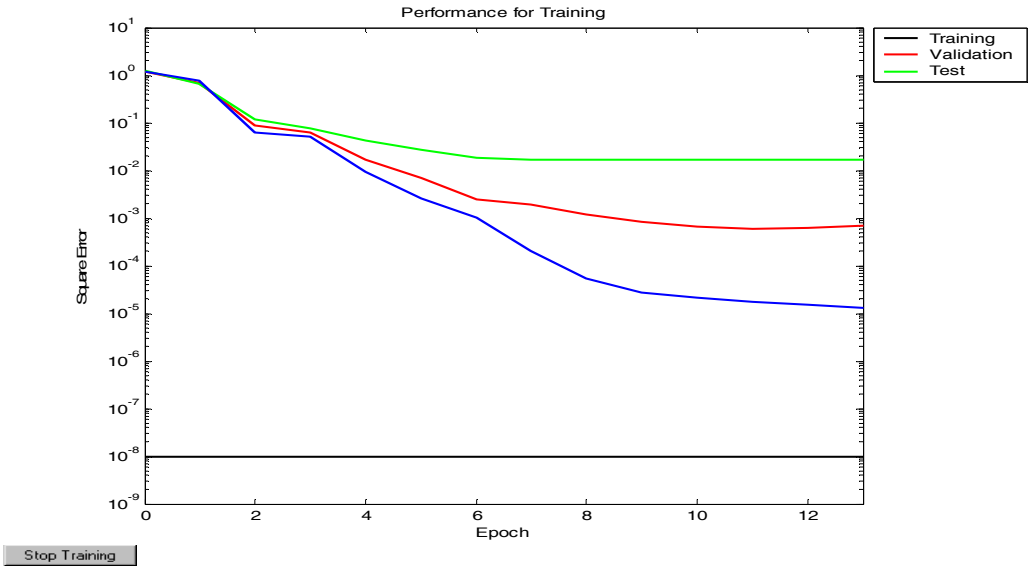

Figure 2: Training performance for formaldehyde

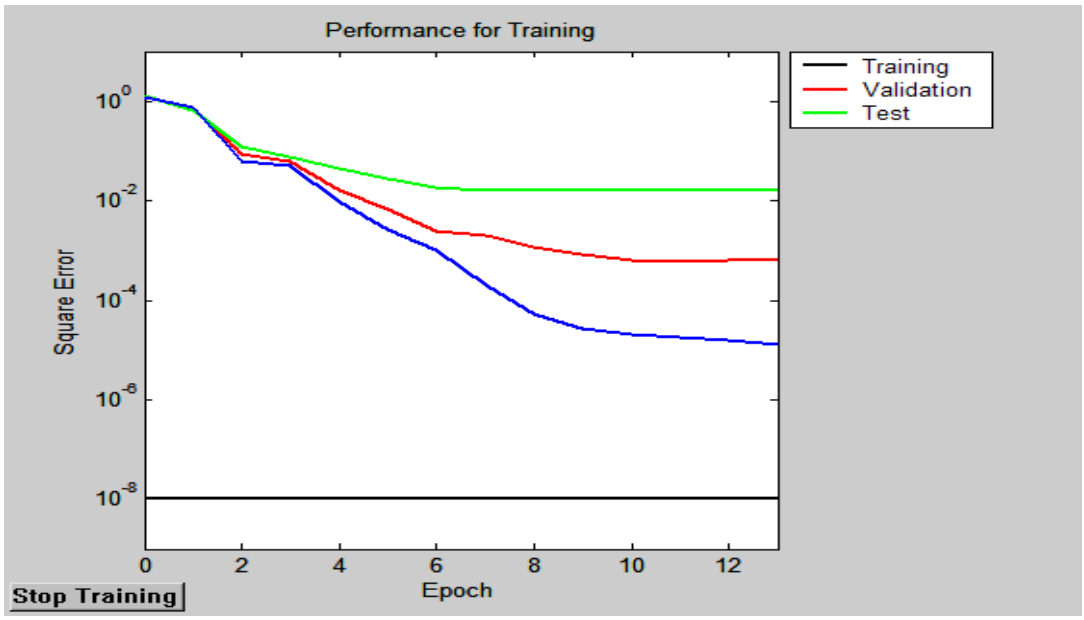

Figure 3: Training performance for chloroform

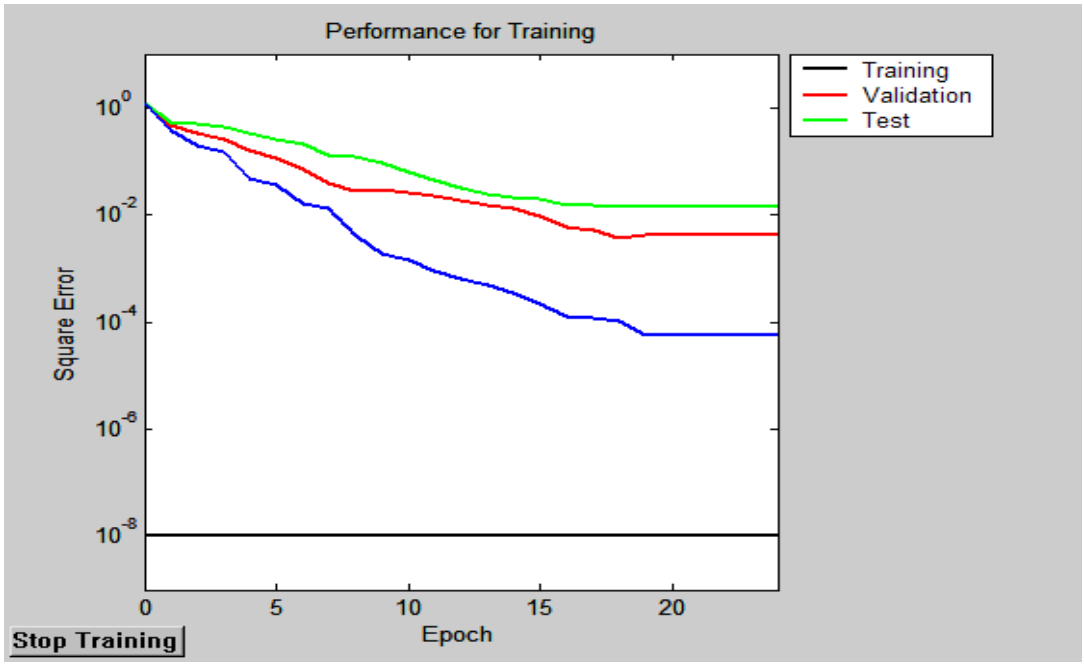

Figure 4: Training performance for acetone

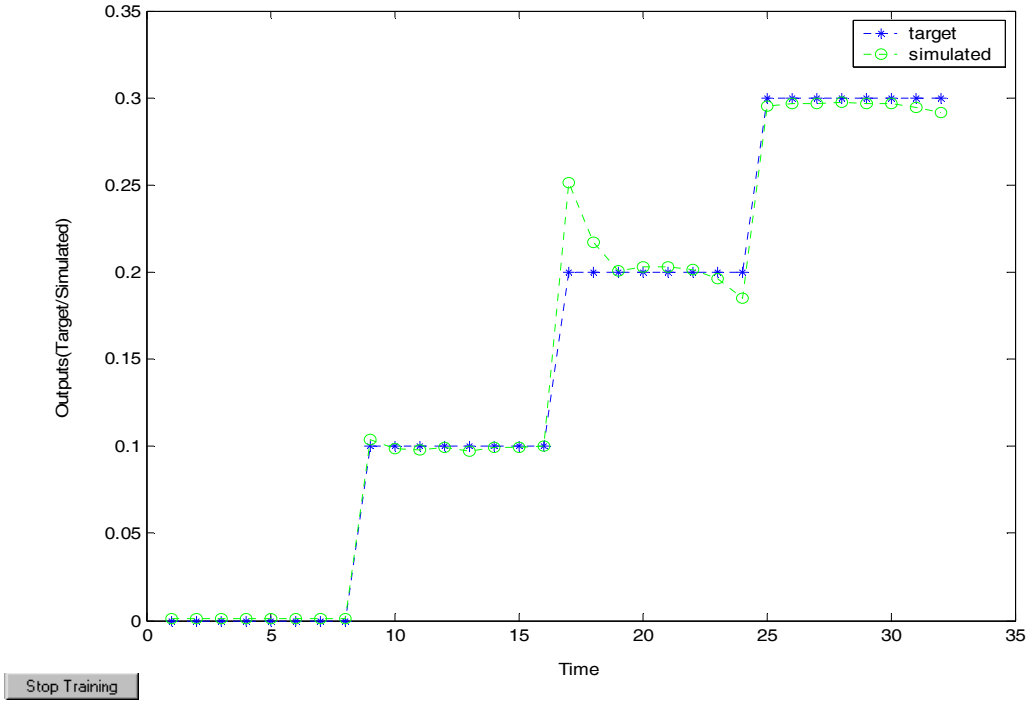

Figure 5: Relationship between the actual and predicted data for formaldehyde

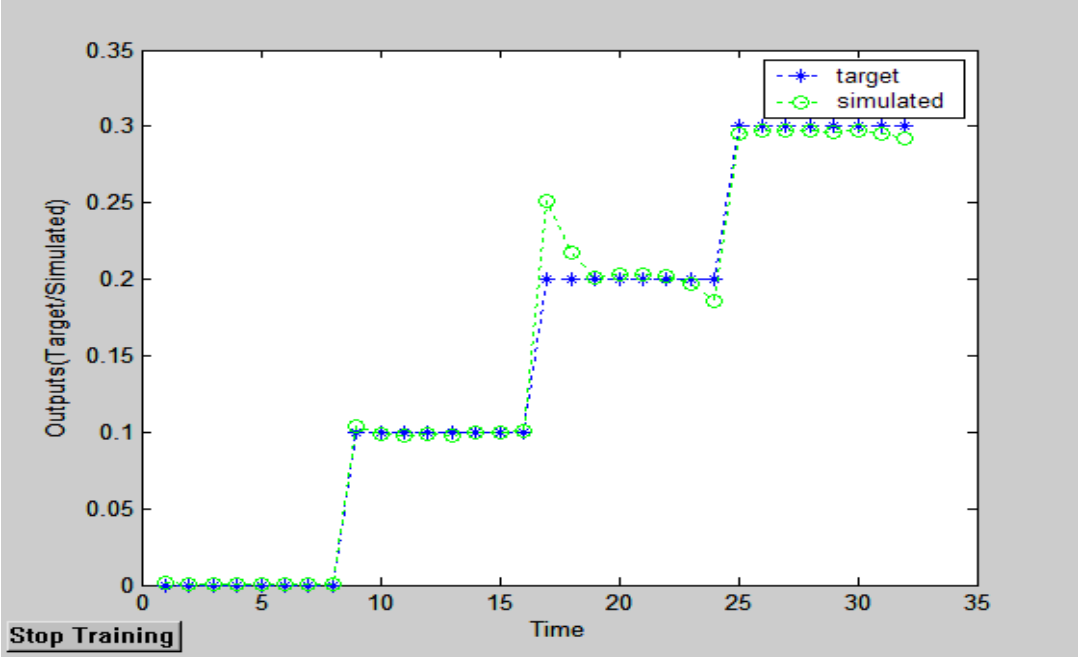

Figure 6: Relationship between the actual and predicted data for chloroform

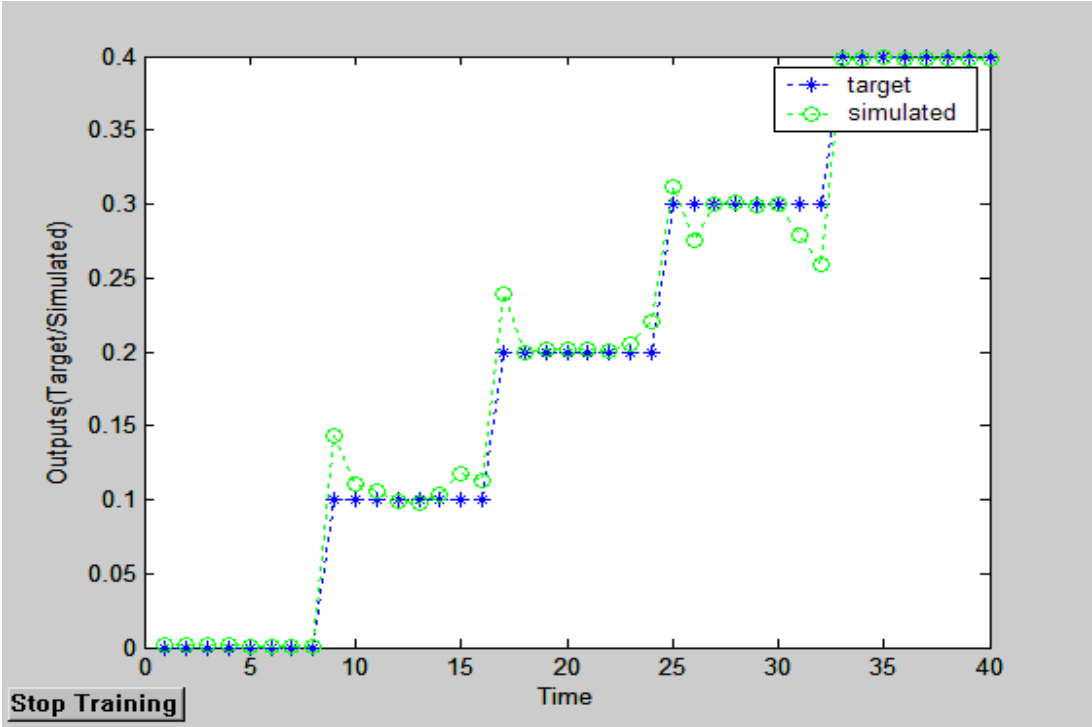

Figure 7: Relationship between the actual and predicted data for acetone