Abstract—In this work, neural networks methods MLP type were applied to a database from an array of six sensors for the detection of three toxic gases. The choice of the number of hidden layers and the weight values are influential on the convergence of the learning algorithm. We proposed, in this article, a mathematical formula to determine the optimal number of hidden layers and good weight values based on the method of back propagation of errors. The results of this modeling have improved discrimination of these gases and optimized the computation time. The model presented here has proven to be an effective application for the fast identification of toxic gases.

Keywords—Back-propagation, Computing time, Fast identification, MLP neural network, Number of neurons in the hidden layer.

I. INTRODUCTION

THE control of the air quality becomes an essential priority for researchers from different backgrounds, particularly when it comes to the pollutant gases emitted by the production units [1]-[10]. These gases have a direct and fatal impact on human health [11]-[13]. It is necessary to have a continuous monitoring system in order to measure air security in factories and units of production involving toxic gases. Recent developments of intelligent sensors have provided a rapid progression in the detection of toxic gases due to their broad spectrum of sensitivity [14]-[21]. The detection of these gases has resulted in a different set of descriptors (the electrical signals from the sensors) as demonstrated in the ANN models. These models have been frequently used for modeling air pollutant concentrations [22]. The ANNs in this sense can be successfully used for modeling complex nonlinear systems and for forecasting signals in a wide range of engineering applications [23]-[29].

The number of hidden layers, the neuron numbers in each layer and the activation functions are parameters which influence the performance of neural networks in different learning algorithms [30]-[34]. F or this we proposed a mathematical formula to determine these optimal parameters of MLP model.

The main objective of this work is to apply our model to identify three toxic gases namely: nitrogen dioxide (NO2), hydrogen sulfide (H2S) and their mixture in low concentration. To achieve this objective, we used a database obtained from a gas sensor array which consists of six chemical sensors of type TGS (called electronic noses) based on metal oxide [35], [36]. Each sensor emits an electrical signal characterized by four variables: the initial conductance (G0), the dynamic slope of the conductance (dG/dt), the conductance curve (A) and the steady-state conductance (Gs) [5], [35]-[37].

In this study, we evaluated the performance of MLP with one hidden layer using sigmoid activation function through back propagation algorithm. First, we developed our model of such multilayer perceptron (MLP) to supervise the learning on-line for the optimization of the neuron numbers in one hidden layer and computation time. Second, we compared this type of learning responses to the challenges of the gases identification with the values of mean square error in minimum iterations [38]. Finally, we compared the results to some previous research.

The remaining of the paper is organized as follows: Section II deals with the methodology which refers to the materials and methods. Section III presents the results and the discussion. Finally, Section IV concludes the paper.

II. MATERIALS AND METHODS

A. Feature Extraction

The features obtained were extracted from the temporal responses of the sensor array for the detection of the toxic gases H2S, NO2 and their mixture (H2S-NO2) realized by [35], [36]. The sensor array comprised six TGS-xx (with xx = 800, 813, 822, 825, 832 and 2105), Taguchi Gas Sensor obtained from Figaro Engineering, Incorporation [37]. We are concerned with information obtained from this experiment. For this, we deal with first three basic representative features (G0, dG/dt, Gs) from the response signal extracted with the ignorance of the fourth feature (A).

1) G0: the initial conductance of a sensor calculated as the average value of its conductance during the first minute of a measurement.

2) Gs: the steady-state conductance calculated as the average value of its conductance during the latest minute of a measurement.
3) dG/dt: the dynamic slope of the conductance calculated between 2 and 30 to 50 minutes of a measurement.
4) A: the area conductance curve in a time interval between 2 minutes and d G/dt time of measurement. This area was calculated by the trapeze method.

These first three features were extracted from the response of each sensor. Given the fact that there were 6 sensors within the array, each measurement was described by 18 features.

B. Database

The consideration of database is composed of 180 samples distributed in three classes (NO2, H2S, and NO2-H2S (mixture)). The data were divided into two parts: 80% are used for learning and 20% are used for testing.

The selection of samples used in learning and testing are done randomly and none randomly.

C. Artificial Neural Networks

The first concept of Artificial Neural Network was introduced in 1943 by [38], [39]. It is based on mathematical laws and structures. ANN is a set of processing elements (or nodes) loosely analogous to neurons in the brain. This model is fortified and developed by the introduction of the Back Propagation (BP) training algorithm feed forward in 1986 to overcome difficulties detected by [39]. In brief, ANNs architecture consists of neurons arranged in a layered topology containing an input layer, a hidden layers, and an output layer, which are all interconnected. Many theoretical and experimental works have shown that a single hidden layer is sufficient for ANNs to approximate any complex non-linear function [40]. For this reason, our paper focuses on ANN study of MLP type, this model is based on a feed-forward neural-network with a single hidden layer. The back propagation algorithm is used to train the network. Furthermore, the chosen activation functions are two sigmoid functions 

\[ \phi_1(x) \text{ and } \phi_2(x) \] functions in the hidden and output layers, respectively.

The rest is explained in the following notations:

- \( w_{ij} \): the weights connecting input with hidden layer and the weights connecting hidden layer with output respectively.
- \( x_i \): Input vectors.
- \( y_j \): Calculated output of the hidden layer.
- \( t_k \): Calculated output and desired output of neural network respectively.
- \( \eta \): Learning rate.
- \( N, P, K \): Numbers of units in input, hidden and output layers respectively.

The outputs of the hidden layer are also weighted by the weights \( w_{jk} \) and then transmitted to the output layer according to:

\[ c_j = \sum_{i=1}^{N} w_{ij}x_i + a_j \] (1)

\[ y_j = \phi_1(c_j) \] (2)

The outputs of the hidden layer are also weighted by the weight \( u_{jk} \) and then transmitted to the output layer according to the following equations:

\[ o_k = \sum_{j=1}^{P} u_{jk} y_j + b_k \] (3)

\[ t_k = \phi_2(o_k) \] (4)

The objective function of the proposed model is the error MSE between the calculated output and the desired output:

\[ \min(MSE) = \min \left\{ \frac{1}{2n} \sum_{i=1}^{n} \sum_{t=1}^{T} (t_{i,t} - z_{i,t})^2 \right\} < 10^{-4} \] (5)

with \( n \): Number of samples, \( n=1 \) “real time Learning”

The last constraints guarantee two conditions:
1) The existence of only one hidden layer.
2) Time of iterations (of samples) \( < (G_0/2) \) time, and excellent Identification Accuracy.

The neural architecture optimization problem can be formulated

\[ \left| \phi_2 \left( \sum_{j=1}^{P} \phi_1 \left( \sum_{i=1}^{N} w_{ij}x_i + a_j u_{jk} + b_j \right) - z_{k,t} \right) \right| \leq 10^{-4} \] (6)

\[ \text{with}\]
\[ \varphi_i(x) = \frac{1 - e^{-\gamma_i x}}{1 + e^{-\gamma_i x}}, \quad i = 1:2 \] (7)

and \( w, u, a, b \in [-1,1] \), and \( 0 \leq \eta \leq 1 \).

The determination of these key parameters \((w, u, a, b, \)and coefficients of activation functions\() present the solution of this problem.

For this reason, we used the gradient descent in order to minimize error functions. The rest algorithm comes after to adjust the weight connection iteratively [40].

Adaptation of weights \( u_{jk} \):

\[ u_{jk}(t+1) = u_{jk}(t) + \eta(t_k - z_k)\varphi_{2}^{\prime} (\alpha_j) y_j \] (8)

Adaptation of weights \( w_{ij} \):

\[ w_{ij}(t+1) = w_{ij}(t) + \eta \sum_{k=1}^{K}(t_k - z_k)\varphi_{2}^{\prime}(\alpha_i)u_{jk}\varphi_{2}^{\prime}(c_i)(c_i) \] (9)

F. Other Performance Measures

The generalization performance of the classification model was accessed using the standard statistical measure accuracy.

\[
\text{Accuracy} = \frac{\text{Number of correctly classified data}}{\text{total number of data}} \times 100
\] (10)

III. RESULTS AND DISCUSSION

In the previous method, we attempted better key parameters of the neural model which includes the architecture of the network. To achieve this objective, we fixed only one hidden layer instead of other layers. In addition to that, we varied the neuron numbers, rate learning and coefficients of activation functions \((\gamma_1 << 1 \) and \( 0.6 < \gamma_2 < 1 \)). This simulation is based on certain performance criteria in terms of statistical data (MSEs, Discrimination and identification Accuracy) and time computation account. The latter must be less than the initial conductance of a sensor time.

Fig. 1 shows the training time influenced by the number of nodes in one hidden layer.

Fig. 2 contains the average errors of 150 errors to each structure started from 2 till \( N \) of neurons in one hidden layer. For this, we notice that the optimal number of nodes is \( n \) (matrix includes 16 nodes) in normal on-line training taking into consideration the stopping criterion \( G_0/6 \) time (=10 seconds). With the possibility of achieving fast training by relying on stopping criterion 3 seconds (using ordinary laptop), only with \( 2 \times 2 \) nodes, instead of 10 seconds, which gave similar performance Fig. 2. In addition, we observed that the average error increases when we augment the neuron number in a fixed minimal iteration. However, it decreases if we augment the iteration number in this case.

Figs. 3-5 explain the minimum MSEs during learning and testing in different subsets randomly and non-randomly.

Figs. 7 and 8 are added to verify the power of our model in terms of criterion MSEs when it augments the iteration number; this shows how our model is useful if the time of computation is ignored.

Figs. 4 and 7 indicate more aspects than error-testing. These encompass the number of gas classes and the number of samples in each group. In addition, this figure shows MSEs=7x10\(^{-06}\) which refers to the mixture of gases.
Fig. 5 Evolution of the minimums MSEs during learning with 100 iterations (randomly)

Fig. 6 Evolution of the minimums MSEs during testing (randomly)

Fig. 7 Evolution of the minimums MSEs during testing with 1300 iterations (nonrandomly)

Fig. 8 Evolution of the minimums MSEs during testing with 1300 iterations (randomly)

Fig. 9 (b) shows an excellent classification and identification accuracy 100%, it is visualized in Fig. 10. They include these classes. These results reflect the power of our model despite of the complex conditions which are: the concentration 1ppm, small data base and the stopping criteria 10 seconds, with training errors in 50 iterations as in Fig. 9 (a). We are concerned with different iterations to reflect the performance of our model in many situations shown.

Fig. 9 Classification and identification of three toxic gases over number of iterations 50

Fig. 10 Visualization of three toxic gases classified and identified

Compared to previous research that contains great architecture (hidden layers), learning batch (off-line) using the toolbox without taking into consideration computing time [35], [36], [41]. Also the discrimination of different concentration; however, our model is concerned only with one ppm (complex concentration) in real time by using complex learning on-line (real time) with fast identification in term of computation time plus high accuracy.

IV. CONCLUSION

In this research, we present an artificial neural network (ANN) model based on the multi-layer Perceptron (MLP) for classifying and identifying the three toxic gases in low concentration (one part per million). In order to prove the power of our model, it is applied to give useful results in the
accurate identification and classification with the possibility to make the training faster based only on 3 seconds instead of 10 seconds.

In addition, it can be an excellent application in engineering to monitor the identification of gases in real time when there is a danger that cannot be detected by human smell sense. It is a practical concept to install the computer models in a high industrial area for air security.

REFERENCES


