

# Neural Network Supported Chemiresistor Array System for Detection of NO<sub>2</sub> Gas Pollution in Smart Cities (NN-CAS)

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**Abstract**—Neural Networks supported Chemiresistor array system is designed and laboratory tested for the detection of emissive gasses from vehicles and other sources of pollution. The designed and tested system is based on an integrated PbPc array of chemiresistors that sends signals corresponding to emitted NO<sub>2</sub> gas to Signal Processing Unit. The process comprises using relative conductivity values of Edge sensors to Central sensor for detected gas as an indicator of response characteristics and profiling for NO<sub>2</sub> gas pollution level. The process continues up to the limit where Edge Sensor values for relative conductivity equates, then the relative conductivity for the Edge Sensors is used as a control value to shut down the sampling system and send a warning message of excessive pollution. Pollution could be due to a number of factors besides vehicles, such as gas leaks. Optimization of array elements response is carried out using Neural Networks (Back Propagation Algorithm). The proposed system is promising and could further be developed to become a vital and integrated part of Intelligent Transportation Systems (ITS) in order to monitor emission of hazardous gases, and could be integrated with Road Side Units (RSUs) of urban areas in smart cities.

**Keywords**—Gases; chemiresistors; neural networks; sensor array; correlation; road side unit; intelligent transportation systems; smart cities

## I. INTRODUCTION

Emissions of NO<sub>x</sub> and NO<sub>2</sub> from vehicles are critical to quality of air particularly in urban areas, and could very well affects air quality at regional and global levels.

Recently, two important factors are considered that contributes to pollution and concentration of NO<sub>2</sub>: NO<sub>x</sub> in urban areas:

- 1) The ratio of NO<sub>x</sub> that is NO<sub>2</sub> coming out of vehicles exhausts.
- 2) Diesel engines emissions of NO<sub>x</sub>

Congested cities and their residents exposed to levels of NO<sub>2</sub> gas that often exceed the acceptable air quality standards. Due mainly to diesel cars. The level of contribution of NO<sub>x</sub> by the diesel car is determined as per area and number of vehicles and congestion levels. However, it is found that large number of NO<sub>2</sub> parts in the NO<sub>x</sub> emissions of diesel engines is mainly a function of intense road traffic usually on artery roads.

NO<sub>x</sub> contains NO and NO<sub>2</sub>, where NO<sub>2</sub> is critical as it has an adverse health effects in urban areas. Diesel engines are not fitted with efficient systems for removing NO<sub>x</sub> emissions similar to petrol engines, thus, resulting in higher ambient concentration of NO<sub>2</sub> in urban and major cities.

The primary health effects attributable to NO<sub>2</sub> are related to respiratory conditions. Inhalation of NO<sub>2</sub> causes inflammation in the lungs, affecting immunity to lung infections and resulting in loss of breath, wheezing, coughing and bronchitis with possibility of developing asthma. NO<sub>2</sub> can cause has both acute and chronic health effects.

Studies showed that Lead Phthalocyanine (PbPc) is very sensitive complex to Dioxide gases; specifically NO<sub>2</sub>, where its conductivity affected more by the adsorption of gases as a charge-transfer complex is formed between the Phthalocyanine donor and the gas acceptor.

## II. RELATED WORK

Urbanization adds pressure to the resources such as energy, water, sanitation, and public services. Thus, socio-economic and environmental issues have become closely related. Cities contribute to environmental change on local, regional, and global scales. Studies showed that cities accounts for large amount of global greenhouse gas emissions as a function of energy consumption. City planners and researchers worldwide are investigating ways to control traffic in order to improve air quality, and provide enhanced living conditions [1-4].

The solution is in making cities “smarter” through different approaches to resources management and infrastructure, and by concentrating on greener environment, and smart governance, which will result in a better quality of living for citizens. This can be enabled by utilization of Information and Communication Technologies (ICTs) tools, which can provide eco-friendly solutions for cities. Such work lead to the concept of Smart Cities, whereby the vision is to include the basic services in the city, such as clean water, clean environment, energy and infrastructure, for all citizens, which can be achieved by creating smart environment that covers:

- 1) Environmental Sustainability
- 2) Energy Consumption Control

This can be accomplished by focusing on smart transportation that connects different modes of transportation into an integrated system, thus, giving city planners the ability to better control the flow of traffic.

Analysis and modelling of urban air quality was most of the time based on the assumption that vehicles on the road perform similarly to the way they do under development environments, this can lead to inaccurate prediction of the vehicles effect and contribution to air pollution and harmful emissions. The application of PbPc sensor array chemiresistors to the detection and subsequent analysis of gases emitted round urban areas and congested cities such as NO<sub>2</sub>, should provide reliable metric that can also be used in both real life and in development environments and can help in narrowing the gap between the development sites and real life applications in real time [5-9].

As Smart Cities are associated with a higher quality of life, technology makes it possible to compile massive amounts of real-time data to optimize the urban infrastructure, thereby improving the efficiency of public and transport services.

A chemiresistor array system (CAS) is generally recognized as a system that encompasses array of chemical sensors with selective detection capabilities and pattern recognition capability, able to specify individual vapor components or combination of vapors. The CAS recognizes the presence of a chemical through fingerprinting of its chemical elements using an array of sensors backed by intelligent software for pattern recognition [10-15].

There are two major components forming the CAS:

- 1) Chemiresistor Sensing Array (CSA).
- 2) Intelligent Part employing Artificial Neural Networks (ANN).

Such a combination makes CAS a promising tool for detection of chemicals and hazardous gases. Each chemical produces a unique characteristic of its own, once exposed to the chemiresistor sensing array. The experimental data is used to train an intelligent classification system, such as Neural Networks in order to optimize the CAS characteristics and to provide an ability to predict future values based on chemical level changes [16-20].

CAS detects chemicals by interacting with its CSA responsive materials, resulting in a change in the material characteristics and producing a unique response associated with a specific chemical or gas.

ANN is a learning and classification algorithm, and can also be used as an optimizing algorithm. ANN changes its input, hidden, and output neuron weights to interrelate and correlate complex relationships among input-output variables. Backpropagation (BP) algorithm, is an affective ANN technique, which is an iterative gradient algorithm aims at decreasing the root mean square error.

In this paper, a fresh approach to the use and application of Chemiresistor Arrays System is proposed which utilizes chemical sensing, in particular NO<sub>2</sub> together with Neural Networks optimization. Such approach will support environmental mobility of vehicles through big data collection

and analysis and vehicle to infrastructure interface (V2I). The system can be further developed to support traffic light control and green wave for certain vehicles such as diesel engines when integrated with Road Side Units (RSUs) and interfaced using wireless communication systems [21-22].

### III. MATERIALS AND METHODS

Chemiresistor array units are used for the tests. The NO<sub>2</sub> detection system employs a number of chemiresistors with vacuum sublimed PbPc films of uniform thickness on Sapphire ( $\alpha$ -Al<sub>2</sub>O<sub>3</sub>) substrates. Fig. 1 shows 4-electrodes, 3-chemiresistor array device used in the testing, while Fig. 2 shows a cross sectional view of each chemiresistor within the array. Testing of the devices response to donor gases, in particular NO<sub>2</sub> using two devices is carried out as shown in Fig. 3.

Back Propagation Algorithm (BP) is used to carry out training of the Neural Networks system in order to optimize the response characteristics of the used chemiresistor arrays shown in Fig. 4.

Back Propagation (BP) works by repeatedly modifies the weights of the connections in the network in order to minimize the difference between the actual output of the network and the desired output. The internal 'hidden' units which are not part of the input or output stores within their weights the important features of the learnt pattern(s), which are captured by the interactions of these units. The algorithm is used to efficiently train a neural network through a chain rule, where, after each forward pass through a network, backpropagation performs a backward pass while adjusting the network weights and biases.

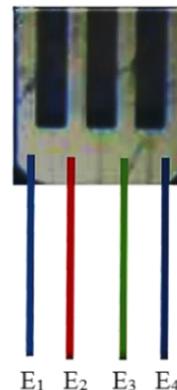


Fig. 1. 3-Chemiresistor Integrated Array Device.

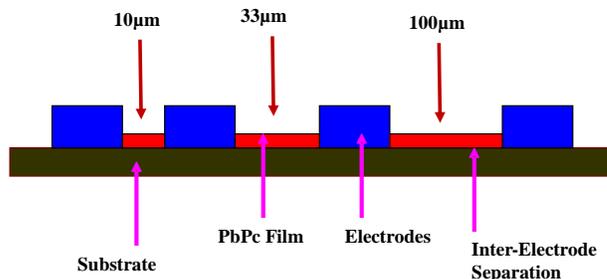


Fig. 2. Cross Section of the used PbPc Chemiresistor Array.

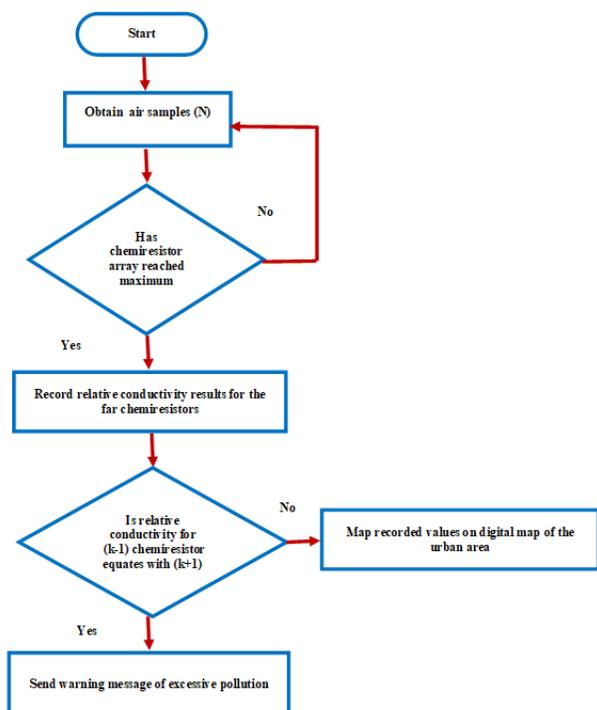


Fig. 3. PbPc Array Algorithm for NO<sub>2</sub> Detection.

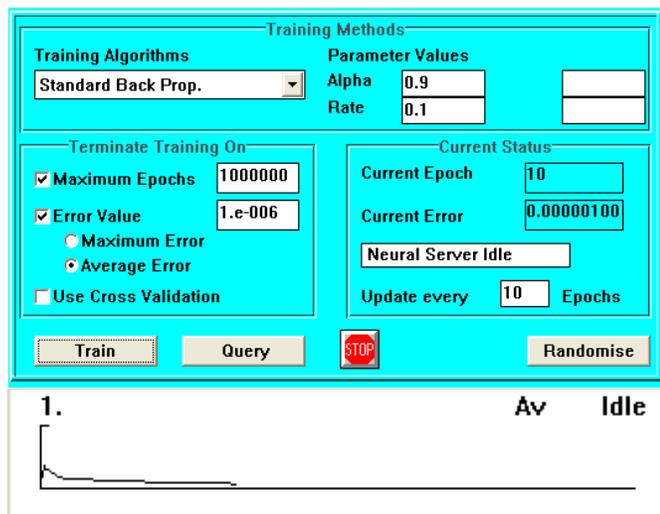


Fig. 4. Neural Networks (BP) Training System with Training Curve.

Optimization of the CAS response using BP is carried out by reducing the error function through minimization of the error function (cost function) described by equation (1).

$$E(t) = \frac{1}{2} (d_{L(i+1)}(t) - a_{L(i+1)}(t))^2 \quad (1)$$

Where;

$d_i(t)$  : The desired response

$a_i(t)$  : The actual response

To carry out error minimization using BP, a gradient descent rule is used to update weights between output and hidden layers and hidden and input layers as shown in equation (2).

$$W_{L(i+1), L(i)}(t + \Delta t) = W_{L(i+1), L(i)}(t) - \text{Alpha} \left( \frac{\partial E(t)}{\partial W_{L(i+1), L(i)}} \right) \quad (2)$$

Where;

$\text{Alpha}$  : Learning Rate.

The learning Rate is increased from 0.1 to 0.9 and decreased from 0.9 to 0.1 as shown in Fig. 4, in order to compute weight updates using equations (3) and (4).

$$\text{Alpha}_{\text{increasing}} = \text{Alpha}_{\text{min}} + (\text{Alpha}_{\text{max}} - \text{Alpha}_{\text{min}}) \left( \frac{\text{Max Epochs} - \text{Current Epoch}}{\text{Max Epochs}} \right) \quad (3)$$

$$\text{Alpha}_{\text{decreasing}} = \text{Alpha}_{\text{max}} - (\text{Alpha}_{\text{max}} - \text{Alpha}_{\text{min}}) \left( \frac{\text{Max Epochs} - \text{Current Epoch}}{\text{Max Epochs}} \right) \quad (4)$$

## Results

Tables I and II show data for two PbPc sensor arrays used in validating the designed system, while Fig. 5 shows the Neural Network model used for training with distributed weights.

TABLE. I. SENSOR ARRAY 1

Real Test	Normalized conductivity in relation to Inter-Electrode Separation		
	Chemi1,2 10:33	Chemi1,3 10:100	Chemi2,3 33:100
NO <sub>2</sub> Levels ppm			
0	0	0	0
1	0.66	0.34	0.51
3	0.69	0.44	0.64
5	0.71	0.47	0.66
7	0.72	0.48	0.67
9	0.73	0.49	0.73

TABLE. II. SENSOR ARRAY 2

Real Test	Normalized conductivity in relation to Inter-Electrode Separation		
	Chemi1,2 10:33	Chemi1,3 10:100	Chemi2,3 33:100
NO <sub>2</sub> Levels ppm			
0	0	0	0
1	0.64	0.34	0.54
3	0.67	0.44	0.65
5	0.68	0.46	0.68

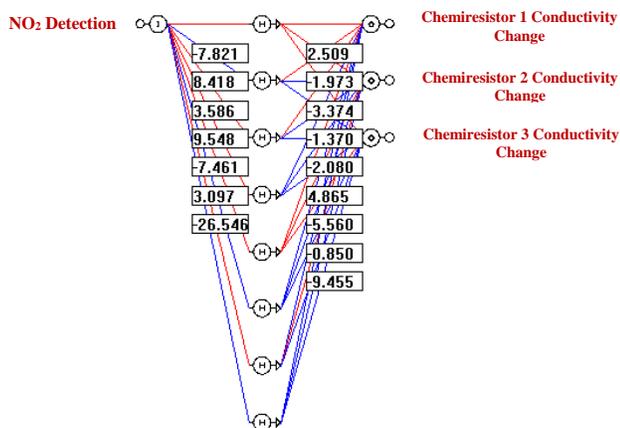


Fig. 5. Neural Networks Model used for Training, Optimization, and Prediction.

#### IV. DISCUSSION AND CONCLUSIONS

Tables III and IV show the predicted results using Neural Networks (BP) System, while Fig. 6 and 7 show the optimized response curves for the PbPc arrays, with Fig. 8 and 9 showing the convergence factor in relation to the relative conductivity change of the PbPc sensor array as a function of NO<sub>2</sub> gas concentration.

The relative conductivity of the Central Sensor can be approximated and related to the edge sensors, using the expression in equation (5). In addition, the actual convergence factor (*k*) for each gas concentration is also calculated using the expression in equations (5), together with Neural Networks predicted data, which should fulfill the criteria described by the expression in equation (6), while latching conditions for the system of array sensors is applied using the average convergence factor (*k<sub>Avg</sub>*) as shown in equation (7).

$$Convergence (Central Sensor) = \left[ \frac{\sum Relative\ Conductivity (Edge\ Sensors)}{Total\ Number\ of\ Array\ Sensors} \right] \quad (5)$$

$$Convergence (Array) = \left( \frac{Lim (Relative\ Conductivity\ Far\ Left\ Edge\ Sensor)}{Lim (Relative\ Conductivity\ Far\ Right\ Edge\ Sensor)} \right) = 1.. \quad (6)$$

$$Latching = \left[ \frac{\sum Relative\ Conductivity (Edge\ Sensors)}{Average\ Convergence\ Factor (k_{Avg})} \right].. \quad (7)$$

The results from the two PbPc sensor array devices showed different response sensitivities towards NO<sub>2</sub> gas, whereby array 1 (average convergence factor 3.05) latched at higher concentration levels compared with array 2 (average convergence factor 3.3). Both devices have comparable results up to 5 PPM of NO<sub>2</sub> concentration. This is a design issue, which necessitates the use of Neural Networks to predict data to enable design optimization and performance enhancement.

Fig. 6 and 7 show relative conductivity response of both devices, which presents the power increase of relative conductivity of the Edge and Center elements of the array. They also show the convergence process between the two Edge elements as they equate to same value. This is also a design

issue as the electrode separation between each Edge element and the Center element is approximately a factor of 3.

Fig. 8 and 9 present a clearer view of the field interaction between array elements in the form of the convergence factor as it initially varies before it decreases and converges to the value of approximately 3. Thus, conforms to the electrode separation in the original design.

TABLE. III. NEURAL NETWORKS OPTIMIZATION FOR ARRAY 1

Prediction	Normalized conductivity in relation to Inter-Electrode Separation			Convergence Factor
	NO <sub>2</sub> Levels PPM	Chemi1,2 10:33	Chemi1,3 10:100	
0.000	0.000	0.000	0.000	0.0
0.004	0.002	0.001	0.001	3.0
0.008	0.004	0.002	0.003	3.5
0.010	0.005	0.002	0.004	4.5
0.040	0.022	0.010	0.016	3.8
0.080	0.050	0.022	0.034	3.8
0.100	0.065	0.030	0.044	3.6
0.400	0.375	0.157	0.240	3.9
0.800	0.618	0.300	0.453	3.6
1.000	0.660	0.340	0.510	3.4
1.400	0.690	0.383	0.570	3.3
1.800	0.696	0.404	0.600	3.2
2.000	0.695	0.412	0.608	3.2
2.400	0.692	0.425	0.623	3.1
2.800	0.690	0.435	0.635	3.0
3.000	0.690	0.440	0.640	3.0
3.400	0.691	0.449	0.648	3.0
3.800	0.695	0.456	0.654	2.9
4.000	0.697	0.459	0.656	2.9
4.400	0.703	0.463	0.660	2.9
4.800	0.710	0.470	0.660	2.9
5.000	0.710	0.470	0.660	2.9
5.400	0.714	0.473	0.660	2.9
5.800	0.716	0.475	0.661	2.9
6.000	0.717	0.476	0.661	2.9
6.400	0.719	0.477	0.663	2.9
6.800	0.720	0.479	0.667	2.9
7.000	0.720	0.480	0.670	2.9
7.400	0.721	0.482	0.677	2.9
7.800	0.722	0.483	0.687	2.9
8.000	0.723	0.484	0.697	2.9
8.400	0.725	0.486	0.703	2.9
8.800	0.728	0.489	0.722	3
9.000	0.730	0.490	0.730	3

TABLE. IV. NEURAL NETWORKS OPTIMIZATION FOR ARRAY 2

Prediction NO <sub>2</sub> Levels ppm	Normalized conductivity in relation to Inter-Electrode Separation			Convergence Factor k
	Chem1,2 10:33	Chem1,3 10:100	Chem2,3 33:100	
0.000	0.000	0.000	0.000	0
0.004	0.002	0.001	0.001	3
0.008	0.004	0.002	0.003	3.5
0.010	0.005	0.002	0.004	4.5
0.040	0.021	0.010	0.016	3.7
0.080	0.046	0.022	0.035	3.7
0.100	0.060	0.028	0.046	3.8
0.400	0.350	0.152	0.255	4
0.800	0.595	0.298	0.482	3.6
1.000	0.640	0.340	0.540	3.4
1.400	0.673	0.386	0.597	3.3
1.800	0.679	0.408	0.621	3.2
2.000	0.678	0.416	0.628	3.1
2.400	0.674	0.428	0.638	3.1
2.800	0.671	0.436	0.646	3
3.000	0.670	0.440	0.650	3
3.400	0.670	0.446	0.656	3
3.800	0.671	0.451	0.662	2.95
4.000	0.673	0.453	0.665	2.95
4.400	0.676	0.456	0.671	2.95
4.800	0.679	0.459	0.677	2.95
5.000	0.680	0.460	0.680	2.96

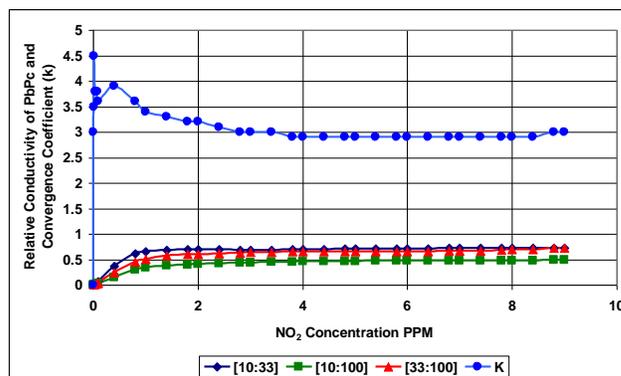


Fig. 8. Predicted Sensor Response and Convergence Coefficient for Array 1.

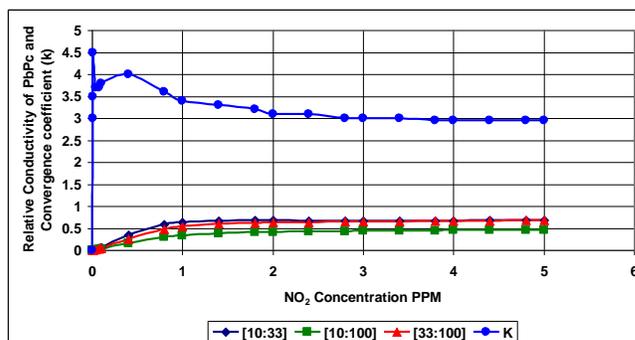


Fig. 9. Predicted Sensor Response and Convergence Coefficient for Array 2.

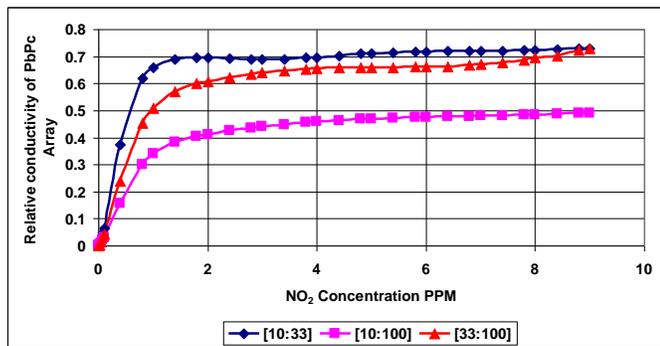


Fig. 6. Predicted and optimized sensor response for array 1

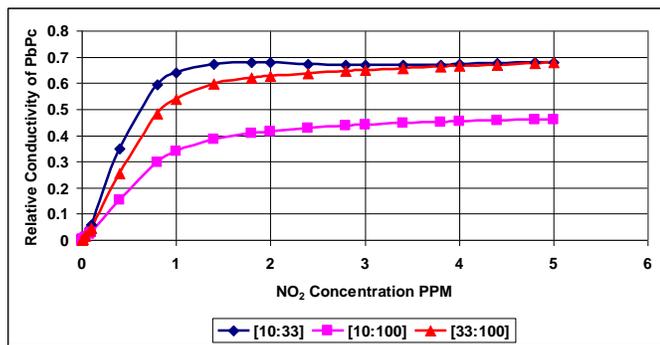


Fig. 7. Predicted and Optimized Sensor Response for Array 2.

Employing Neural Networks allowed for:

- 1) Acquiring results for other NO<sub>2</sub> concentration levels.
- 2) Design optimization based on prediction.
- 3) Detection of expected increase or decrease of NO<sub>2</sub> in an area as a function of current values correlated with traffic volume and other sources of NO<sub>2</sub> emission.

In conclusion, the design and testing of the PbPc sensor arrays was successful and more so with the incorporation of Neural Networks. Smart cities and smart transportation systems, aim to provide less polluted urban areas and such chemiresistor arrays can be very useful in this context. Developing A wireless Sensor Networks (WSN) version of the PbPc array will certainly advance its application and enhance the monitoring and reporting facilities through wireless data routing and collection to a sink with a cloud interface to control centers.

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