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Detection algorithms for the Nano nose

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DETECTION ALGORITHMS FOR THE NANO NOSE

by

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ABSTRACT

Detection Algorithms for the Nano Nose

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The Nano nose is an instrument with an array of nano sized optical sensors that produces digital patterns when exposed to radiation passing through a gaseous mixture. The digital patterns correspond to the amount of photocurrent registered on each of the sensors. The problem is to find the gas constituents in the gaseous mixture and estimate their concentrations. This thesis outlines an algorithm using a combination of a mixed gas detector and a gas concentration predictor. The mixed gas detector is an array of neural networks corresponding to the number of gases. There are two techniques outlined for the implementation of the gas concentration predictor which are the partial least squares regression (PLS) and the Kalman filter. The output of the developed algorithm would not only show the detection of the individual constituents in the gaseous mixture but also provide the prediction of their concentrations. The algorithm designed is entirely re-configurable providing greater amount of flexibility and has detected the constituents along with the prediction of their concentrations of a mixture of three gases.

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CHAPTER 1

INTRODUCTION

1.1 The Gas detector

The gas detector is an instrument that provides information about the presence of toxic gases [1]. Gas detectors have wide applications ranging from the domestic smoke detector to atmosphere monitoring. The rise of computational intelligence has brought about a revolution in the field of gas sensing. Recent technological developments have paved the way to achieve the objective of creating an instrument called the electronic nose that would mimic exactly the mechanism of human olfaction [2]. The electronic nose typically uses resistance based sensors and quartz crystal based sensors [3]. However recent developments in the field of Nanotechnology [4] have paved way to the creation of nano sized gas sensors which are far more efficient and overcome many of the shortfalls faced by use of traditional sensors used in the electronic nose.

This thesis is an attempt to develop an algorithm for a gas sensing instrument known as the Nano Nose that uses nano sized optical sensors for the simultaneous detection of constituent gases and the prediction of their concentrations in a gaseous mixture.

1.2 The Electronic nose

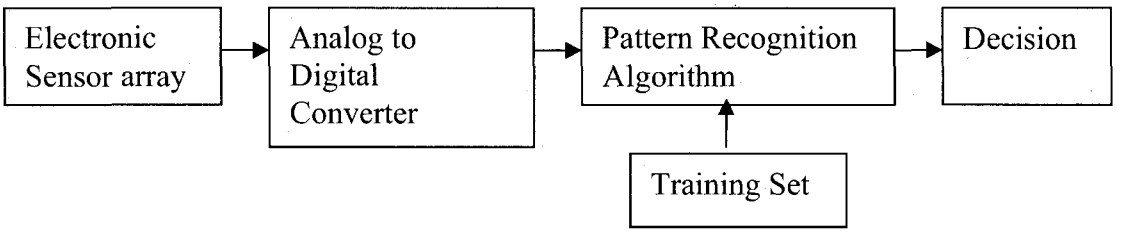

Figure.1.1 The mechanism of gas sensing in the electronic nose

An electronic nose [2] is a chemical constituent detection instrument that comprises an array of electronic sensors coupled with a suitable pattern recognition system. The electronic nose has been inspired by the mechanism of the human olfaction. The components of the electronic nose are as shown in Figure [1.1]. The electronic sensor array is an array of gas detection sensors. The function of the sensors is to basically convert the odor signal in to electrical signals. The sensors used mostly in the electronic nose are resistor based sensors and quartz crystal based sensors [3] which utilize semi-conducting oxide as the sensing material. These electrical signals in the analog form are digitized by the Analog to Digital convertor (A/D converter) and then the resulting digital signal pattern is fed to a pattern recognition algorithm that would identify the odor signal with the help of a knowledge base and the chemical constituent would be detected.

1.3 The Nano Nose

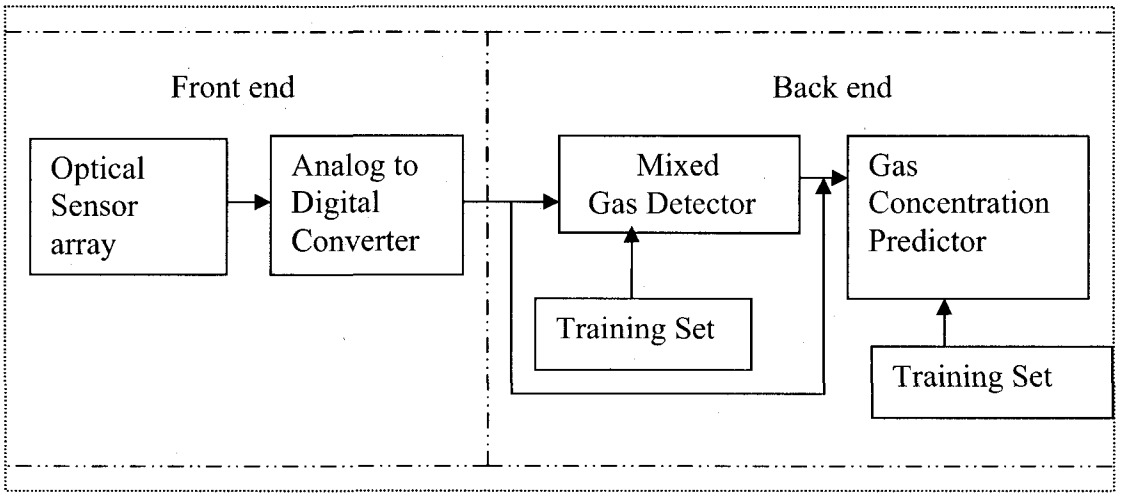

Figure.1. Block diagram of the Nano Nose

The nano nose takes its name from its predecessor, the Electronic nose. The sensors used in the Nano Nose are optical nano sensors. This optical sensor array generates an analog signal pattern and relays it to the Analog to Digital converter (A/D). The combination of the optical sensor array and the A/D coverter is known as the Front end of the Nano Nose. The output of the A/D converter is a digitized signal. This digitized signal is given as input simultaneously to the mixed gas detector and the gas concentration predictor. The output of the mixed gas detector is the data of the gas constituents present in the sample mixture and the output of the gas concentration predictor is the concentration data of the chemical constituents present in the sample mixture. This Thesis is an attempt to develop an algorithm to suit the requirements of an array of these optical nano sensors to eventually detect specific gases and also predict their constituent concentrations. The focus of this thesis is primarily on the back end of the Nano Nose.

Chapter 2 gives a detailed description of the Nano Nose. The description of the detector is provided in Chapter 3. The details of the concentration prediction algorithms along with their corresponding theoretical explanation are provided in Chapter 4. The results of the experiments conducted are summarized in Chapter 5.

CHAPTER 2

DESCRIPTION OF THE NANO NOSE

2.1. Introduction

The Nano Nose is divided in to two sections, the front end and the back end. The front end of the nano nose comprises of the components which are a bank of light emitting diodes (LED), the optical sensor array and an A/D convertor and may also contain a memory unit to serve as a buffer. The back end comprises of an array of neural networks and a concentration prediction algorithm. The section of the front end of the Nano Nose focuses on the procedure of the generation of digital signal patterns when the optical sensor array is exposed to a variety of gaseous mixtures in a controlled environment. The section of the back end of the Nano Nose focuses primarily on the utilization of the signal patterns generated by the front end of the Nano Nose to detect the individual gas constituents by means of a mixed gas detector, composed of an array of neural networks and the estimation of their concentrations is achieved by means of a concentration prediction algorithm. This algorithm is implemented by means of a regression technique, the partial least squares (PLS) or by the usage of an estimator, the Kalman filter. The subsequent sections give a brief introduction to the Beer's law and further give a detailed description of the construction of the front end and the back end of the Nano Nose.

2.2 Beer's law

The Beer's absorption law for monochromatic radiation [5] shows the decrease of the intensity of light passed through a chemical species is a function of the absorption coefficient. ρ As shown in the equation (1.1)

$$P_{\lambda z} = P_{0\lambda z} e^{-\rho z q_{\lambda z}} \quad (2.1)$$

In the equation (2.1), z is the Length of the absorption path; ρ is the Density of the absorbing gas; $P_{\lambda z}$ is the spectral intensity at wavelength λ_a as seen by the detector. $P_{0\lambda z}$ Is the spectral intensity at wavelength λ_a emitted by the source; $q_{\lambda z}$ is the Absorption coefficient at wavelength λ_a of the gas to be measured.

2.2. Transmittance (T)

It is defined [6] as the ratio of the received light intensity P, to the incident light intensity P_0 as shown in the equation (2.2).

$$T = P / P_0 \quad (1.2)$$

Equation (2.2) can be written in the form of equation (2.3) by substitution from equation (2.1)

$$T = P_{\lambda z} / P_0 = e^{-\rho q_{\lambda z} z} \quad (1.3)$$

The transmittance values can be obtained directly from the individual spectra of the gas species. There exists a finite relationship between the transmittance values recorded at each wavelength and the photocurrent produced by each of the optical sensors. This relationship is assumed in the Nano Nose to be linear.

2.3 Front end of the Nano Nose

The front end of the Nano nose comprises of an array of LEDs (light emitting diodes) operating in the visible region to the IR region (0.6um to 4 um) range placed at one end of a rectangular gas chamber and optical gas sensors placed at the other end as shown in the Figure1.2.

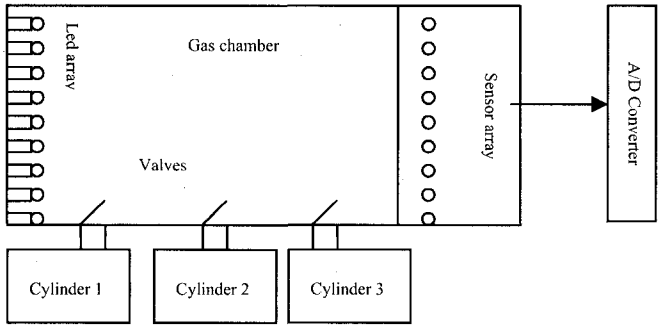

Figure 2.1 Front end of the Nano-nose

Radiation from the light emitting diode (LED) array in the spectral range extending from the visible region to the IR region (0.6um to 4um) passes through the gas chamber and falls on the sensors producing a pattern of photocurrents that are digitized at a later stage. Each sensor produces a response only when radiation of a particular wavelength that it corresponds to, is intent on it. The response is measured in terms of photocurrent (uA). Analog signals are generated from the sensor array based on the relationship between the Intensity of radiation from the LED array and absorption by the sensor as a function of wavelength based on the Beer's law explained in Section 2.1. The analog signal is given as the input to the analog to digital converter (A/D). The output of the A/D converter stage is a digital signal pattern .The digital signal pattern is a one dimensional matrix vector consisting of elements of eight to twelve bits wide each corresponding to the

photocurrent of the corresponding sensors. In the calibration phase of the front end of the Nano Nose, the valve of cylinder1 is opened periodically increasing the concentration of the first gas in the gas chamber in discrete time steps where the release of the valve corresponds to a known concentration of gas entering the chamber. At each step, the signal pattern from the sensor array is digitized and stored in a memory module. The process is repeated with the second and the third gases contained in the cylinder2 and cylinder3. Then the process is repeated with all possible combinations of mixtures among the three gases. The signal patterns thus obtained form the knowledge base or the training set which would be used by the back end of the nano nose to make a prediction of the concentrations of constituents when the sensor array is exposed to an unknown gaseous mixture comprising of these three gases.

2.4 Back end of the Nano Nose

The back end of the Nano Nose comprises of a mixed gas detector and a gas concentration predictor. The objective of the back end is the utilization of the digitized signal pattern corresponding to an unknown gaseous mixture, generated by the front end of the nano nose to achieve the detection of its respective constituents and the prediction of their concentrations. In order to accomplish this task, the mixed gas detector is configured as an array of neural networks. There are two techniques presented in this thesis for the implementation of the gas concentration predictor algorithm. They are the Partial least squares (PLS) based on the concept of regression analysis and the Kalman filter based on the concept of state estimators. The subsequent sections provide details of the mixed gas detector and the gas concentration predictor.

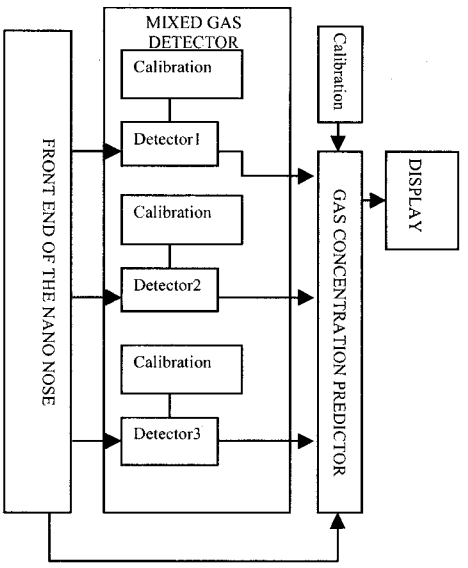

Figure2.2. Back end of the Nano Nose

2.4.1 Mixed gas Detector

The input signal to the mixed gas detector block is the digital signal pattern generated by the front end of the Nano Nose. The mixed gas detector is composed of an array of neural networks. Each neural network is trained by means of a calibration block to detect a specific gas. The calibration block contains the digital signal patterns corresponding to the known constituent concentrations obtained in the calibration phase of the front end. The output of each neural network is a value corresponding to the interval of (0, 1) showing the presence of each gas. The algorithm is configured to quantize this output to a binary '1' showing a presence of the gas if its value is greater than zero. The reason for choosing neural networks for the detection of specific gases is due to the widely reported usage of them in the recognition of odors [8] [9]. The usage of neural networks is found to be superior to that of the traditional chemo metric methods because of their capability

to handle even nonlinear signals that are mostly encountered in real time from the sensor array [2]. The most popular artificial neural network (ANN) is the feed forward multi layer perceptron (MLP) trained using the back propagation algorithm [20].

The mixed gas detector in the Nano Nose is a multi layer perceptron trained using the back propagation algorithm. If the performance of the network is found to be satisfactory in the training phase, it is tested later to identify unknown gaseous mixtures [2]. A greater number of gases can be identified by adding entries to the training set and the design of the neural network can be changed if it does not conform to the required performance metrics such as convergence time and accuracy.

2.4.2 Gas concentration predictor

The input signals to the gas concentration predictor are the digital signal pattern generated by the front end of the Nano nose and the outputs of the neural networks of the mixed gas detector. The concentration predictor has its own calibration block which contains a similar training set to that of the mixed gas detector with digital signal patterns corresponding to known concentrations. The concentration predictor is a vital component of the Nano Nose. The algorithms used for the prediction of concentration are based on a modified form of Beer's law [10] that is explained in Chapter4. The two algorithms that are found to be compatible with the requirements of the Nano Nose are the Partial Least squares (PLS) regression technique and the Kalman filter estimator technique. The partial least squares technique is superior to other techniques such as Classical least squares (CLS) and the Principal components analysis. These techniques though widely in use for odor detection [2] have some limitations which are discussed in Chapter4. The usage of

the Partial least squares (PLS) in spectrographic analysis has been reported by Geladi [11]. The combination of the PLS algorithm and the mixed gas detector shows a modest increase in the prediction accuracy of the concentration predictor when a prediction accuracy of not less than 10ppm is required. The usage of the Kalman filter is found in applications as diverse as gyroscopes and image processing techniques [17] along with system control applications where the future state of the system is predicted and validated with successive measurements.

The Kalman filter has been reported to be applicable to concentration detection of chemical constituents by Arribbas [16] with an approximation of the measurement equation to the Beer's law. The Kalman filter used in the gas concentration predictor incorporates the reported technique however this thesis explains the improvement in the prediction accuracy when used with the mixed gas detector.

The Chapter 3 gives a detailed explanation of the implementation of the mixed gas detector while Chapter4 gives the details of the implementation of the concentration predictor with the Partial least squares(PLS) and the Kalman filter.

CHAPTER 3

MIXED GAS DETECTOR

3.1 Introduction

The mixed gas detector in the Nano Nose is an array of neural networks each designed to detect a single gas. The training set for each neural network is provided by the calibration of the front end of the Nano Nose where digital signal patterns are obtained by the bank of optical sensors with varying concentrations of individual gases in the chamber. These patterns are stored in a memory module made available to each neural network in the detector. The concept of using separate neural networks for individual gases stems from the need for the decrease in the convergence time of the system [21]. An introduction to the neural networks and the back propagation algorithm is given in the subsequent sections.

3.2 Structure of the neural network

Each neural network in the mixed gas detector consists of three layers, the input layer, the hidden layer and the output layer. The training set consists of the digital patterns obtained during the calibration phase of the front end which are vectors with the number of elements corresponding to the number of sensors in the sensor array and a scalar indicating the presence or absence of the gas with a binary one or zero. The number of nodes in the input layer corresponds to the number of sensors. The assumption of the optimum number of sensors in the mixed gas detector was found as nine. This is explained in Chapter5 where the results are described.

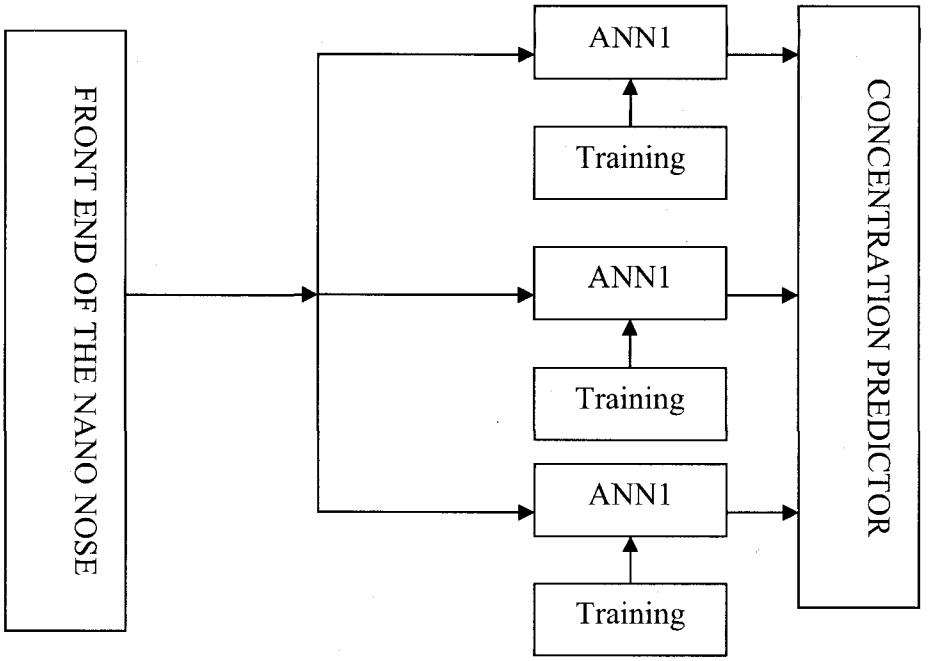

Figure.3.1 Block diagram of the mixed gas detector

Each neuron in the network is a node that receives inputs from many interconnections called *synapses* which are the outputs of other neurons [20]. Each interconnection carries a certain weight that is multiplied to the signal passing through it.

The resultant signal from the i^{th} neuron received at the input of the j^{th} neuron is represented by equation (4.1)

$$u_j = \sum_i x_i w_{ij} - \theta_j \quad (3.1)$$

In the equation (4.1), the function u_j is known as the activation function [2]. The result of the activation function is then passed as an input to the transfer function of the j^{th} neuron. The term θ_j represents a bias term. The transfer function mostly used is the sigmoid function as shown in equation (4.2).

$$S(u_j) = \frac{1}{\left(1 + e^{-u}\right)} \quad (3.2)$$

The most important property of the sigmoid function is that it accepts inputs over an infinite range and produces outputs in a finite range [20]. The structure of each neural network in the mixed gas detector is as shown in Figure [2].

3.3 Training of the mixed gas detector

Each neural network of the mixed gas detector is trained with the responses of the sensors in the calibration phase. The training set consists of 31 rows and 10 columns. The first nine elements of each vector correspond to the photocurrents generated by the sensors. The tenth element corresponds to a binary '1' or '0' stating the respective presence or absence of the gas. The training of each neural network is the mapping of a set of input photocurrent vectors to a set of output scalars [20] stating the presence or absence of the gas . In the beginning of the training a set of arbitrary weights are present on the synapses. The calculation of the output of the network is completed in the first iteration using these weight values and the output $y(t)$ is compared with that of the desired output, $d(t)$. The resulting error $d(t) - y(t)$ is fed back to the network. In the second iteration the weights are incremented and after calculation of the output ,the error is fed back to the network. Thus this procedure of the increment of the weights is repeated in a sequential manner until a tolerant value of the difference in the value of $d(t) - y(t)$ is found. This procedure is known as the delta rule [20] and is shown in the equation (4.4). The equation (4.3) shows the sequential increase of the i^{th} weight in each iteration.

$$\Delta w_i = w_i(t+1) - w_i(t) \quad (3.3)$$

$$\Delta w_i = \eta [d(t) - y(t)] x_i(t) \quad (3.4)$$

In the equation (4.4) ,the term η is the learning rate constant; the term $x_i(t)$ represents the input to the i^{th} neuron.

3.4 Levenberg-Marquardt training of the mixed gas detector

The neural networks used in the gas concentration predictor are feed forward multi layer perceptron(MLP) based networks. They are trained using the Levenberg-Marquardt algorithm known as the back propagation algorithm [18] that is a supervised form of learning similar to the delta rule as described in section 2.1. The least permissible error is always a tradeoff between accuracy of the system and the number of iterations. Each iteration is known as an epoch. The neurons in each layer are connected through synapses to each neuron in the previous layer as shown in figure 1.The state of the network is represented by a vector representing the set of weights in the network at any time instant. The neural network in the case of the gas detection converges very fast because of the reduced training set used as well as the lower number of neurons which are forty, used in the hidden layer. The back propagation algorithm uses a procedure called gradient descent where the algorithm moves from one state to another in the direction of minimum error. A low tolerance value of the error between the desired output and the network output usually requires a greater number of hidden layers, number of neurons in each layer and number of epochs. This tolerance value in the mixed gas detector was fixed as 0.01. The optimum values for all these parameters are a trade off between the accuracy of the prediction and the convergence time.

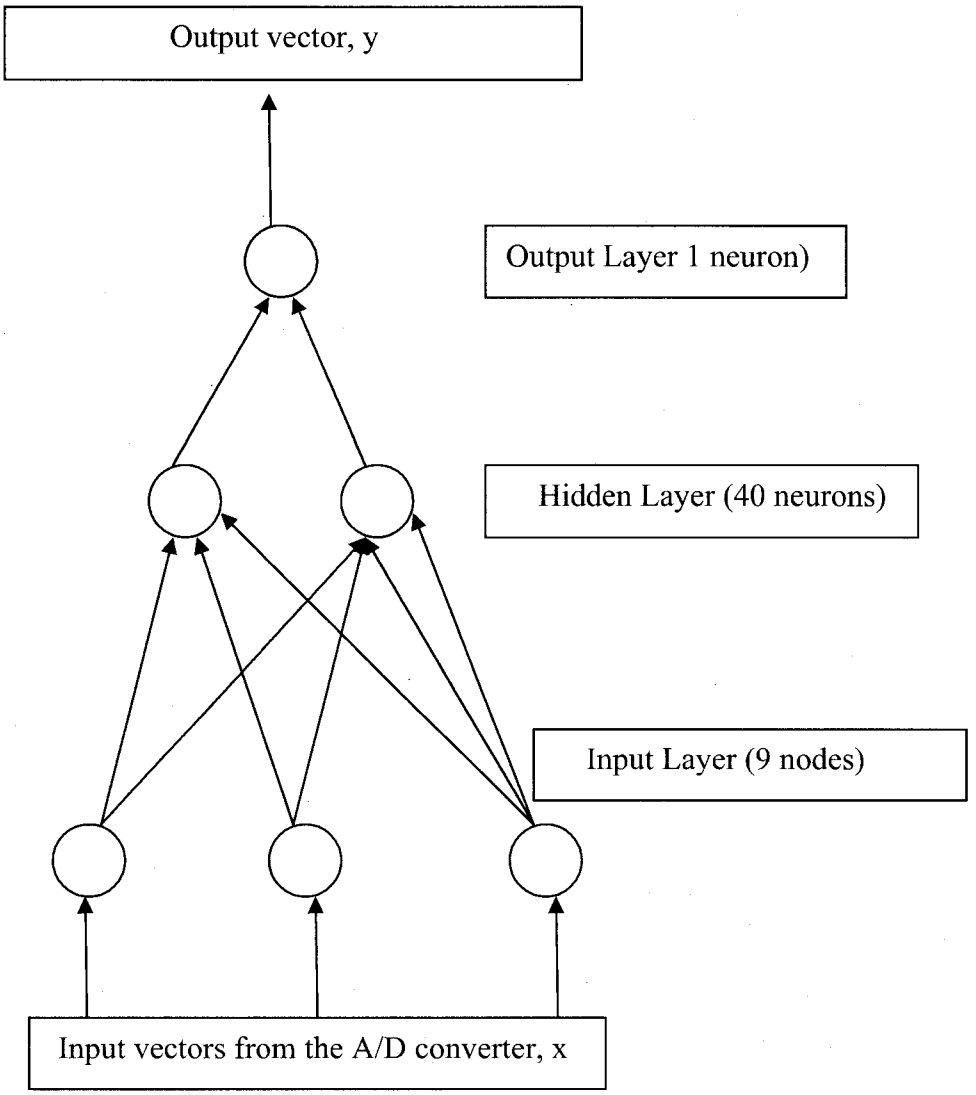

Figure3.2.The structure of the neural network in the mixed gas detector

The delta rule of the back propagation network is written in a slightly modified form as shown in the equation (3.5) the term z_k represents the desired output and the term y_k represents the output of the k^{th} neuron.

$$\Delta w_i = \eta[z_k - y_k]x_h \quad (3.5)$$

The back propagation algorithm is found to be very efficient and suited to the re-configurable requirement of the mixed gas detector as number of nodes in the input layer and the number of hidden layers as well as the number of neurons in each hidden layer is re-configurable. The usage of an array of neural networks in conjunction separately with the concentration prediction methods namely, the Kalman filter and the Partial least squares technique significantly decreased the number of training vectors used to make a prediction of the constituent concentrations. This decrease in the number of training vectors led to an increase in the accuracy of the prediction results as shown in Chapter5.

CHAPTER 4

GAS CONCENTRATION PREDICTOR

4.1 Introduction

The gas concentration predictor comprises an algorithm capable of the utilization of a training set and the output signals of the mixed gas detector to compute the probable concentrations of an unknown sample of gaseous mixture. The training set is the set of the digital vectors containing the sensor responses to known gas constituent concentrations obtained in the calibration phase of the front end of the nano nose. The output signals of the detector are invaluable to the gas concentration predictor as it utilizes them to assign a specific portion of the training set corresponding to the gas constituents present in the unknown sample. The advantage of the usage this mechanism is the decrease in the convergence time of the algorithm as well increased prediction accuracy. There are two alternatives to the choice of the algorithm to be used in this module which is the Partial least squares algorithm (PLS) and the Kalman filter algorithm. These algorithms are consistent with the Beer's law. The subsequent sections provide details of the modified form of the Beer's law on which the concentration prediction techniques are based Partial least squares (PLS) technique and the Kalman filter.

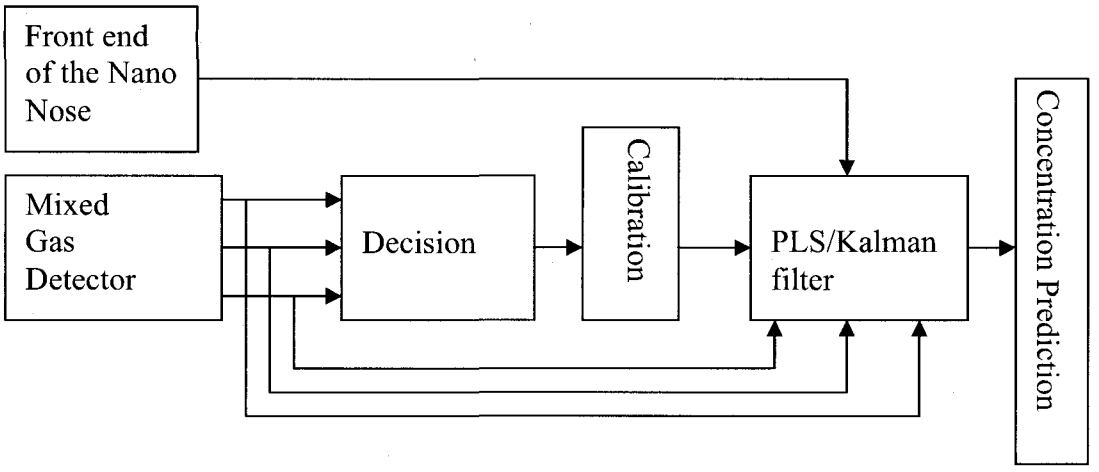

Figure 4.1 the block diagram of the gas concentration predictor

4.2 Modified form of Beer's law

The Beer's law states that at each wavelength there is a linear relation between the concentration (c) of the absorbing species and its spectral absorbance (A). In the case of a gaseous mixture the Beer's law can be written in the following form [10] as shown in equation (4.1)

$$A_i = \sum_{j=1}^{p} a_{ij} b c_j \quad (4.1)$$

In the equation (4.1), A_i is the absorbance of a multi component sample. a_{ij} Is the absorptive of component j at wavelength, i. b Is the path length , c_j is the concentration of the j^{th} component in a mixture containing p components. The product of $a_{ij}b$ could be written as k_{ij} as b is a constant as shown in the equation(4.2).

$$k_{ij} = a_{ij} b \quad (4.2)$$

The equation (4.1) could be written as shown in equation (4.3) with the substitution of the term, k_{ij} from the equation (4.2).

$$A_i = \sum_{j=1}^{p} k_{ij} c_j + e_i \quad (4.3)$$

The term e_i in the equation (4.3) is the residual term which has a normal distribution and its variance proportional to $T-2$ where T is the transmittance value of the spectrum at each wavelength.

A set of simultaneous equations can be used to describe equation (4.3) and it can be written in a matrix form as shown in equation (4.4).

$$A = CK + E \quad (4.4)$$

In the equation(4.4), A is the absorbance matrix of dimensions $m \times n$, where m is the number of mixtures and n is the number of considered wavelengths in the spectrum, p is the number of components in the mixture. C is the concentration matrix of dimensions $m \times p$, K is a matrix of dimensions $p \times n$ containing the information of the pure spectra of each component.

4.3 Introduction to Partial least squares regression (PLS)

The Beer's law shows a linear relationship between the absorbance of a gas measured at a particular wavelength and the concentration of the gas measured at the same wavelength [13]. The method of regression analysis is used to model this relationship between the absorbance variable deemed to be the response variable and concentration variable deemed to be the regressor variable.

There are various techniques of regression such as simple linear regression, Classical least squares and partial least squares regression. The reason for choosing partial least squares (PLS) as the algorithm for the concentration predictor is explained in this section. The simple linear regression technique, [19] is a least squares parameter estimation technique. It is used to model the relationship between regressor variable C and the response variable A. It finds a solution based on a linear relationship between the absorption variable of a gas constituent and its respective concentration based on the method of least squares. The limitation with this technique is that it cannot be utilized for the analysis of gaseous mixtures involving more than one constituent. The method of classical least squares [10] overcomes this limitation as it has two phases the calibration phase and the prediction phase. The objective of the calibration is to estimate the K matrix using the solution obtained by the application of the method of least squares [3] as shown in the equation (4.5).

$$K = (C^T C)^{-1} C^T A \quad (4.5)$$

Using the value of K obtained in the equation (4.5), a prediction can be made for an unknown sample as shown in equations (4.6),(4.7).

$$a = cK + e \quad (4.6)$$

In the equation (4.6) a denotes the absorption matrix for an unknown sample, a $1 \times n$ row vector, c denotes the unknown concentration of the p components to be found. e Is the $1 \times n$ row vector representing the residual. The value of c is obtained by the usage of the least squares method as shown in equation (3.37).

$$c = aK^T (KK^T)^{-1} \quad (4.7)$$

The limitation with this solution is that the matrix K has the possibility to be singular in which case the solution would be invalid.

The method of Principal component analysis [12] is a coordinate transformation method that forms the basis for the Partial least squares technique. The absorption matrix A of dimensions $m \times n$ matrix can be written as the products of two vectors, a score vector t_h and a loading vector, p'_h as shown in equation (4.8).

$$A = t_1 p'_1 + t_2 p'_2 + t_3 p'_3 + ... + t_n p'_n \quad (4.8)$$

$$A = TP' \quad (4.9)$$

The equation (4.8) can be written in the matrix form as shown in the equation (4.9). The solution to equation (4.10) is given by the NIPALS [12] (non linear iterative partial least squares) algorithm. The scores represent the nature of the relativity between the successive observations of the absorbance values and the loadings represent the projections of a unit vector on the principal component line. However the solution will not be complete [10] as scores and vectors for the absorption matrix would be calculated without any consideration of the C , concentration matrix as shown in equation(4.9).

$$A = TP^T + E \quad (4.9)$$

The Partial least squares method, explained in the subsequent section takes consideration of the A matrix as well as the C matrix for the calculation of the K matrix. Hence PCA and the NIPALS algorithm are considered to be the building blocks of the Partial least squares algorithm.

4.4 Partial least squares regression (PLS) for concentration prediction

The Partial least squares regression is a technique that is utilized in the concentration prediction part of the Nano Nose. The Partial least squares could be regarded as an extension of the NIPALS algorithm. The training set utilized for this algorithm is different to that of the training set utilized in the mixed gas detector. The training set consists of 1660 rows and 12 columns. The first nine elements of each row correspond to the calibrated digital signal pattern from the front end and the last three columns correspond to the known gas concentrations. The reason as to why this particular configuration with regard to the training set has been selected is the assumption of nine sensors in the sensor array and the assumption of the number of gas constituents to be therein the mixture. The Beer's law for multi component samples [10] is given by the following equation as mentioned in the equation (4.10).

$$A = CK + E \quad (4.10)$$

Calibration:

In the calibration step, the absorption matrix A and the concentration matrix C could be decomposed in terms of their respective score vectors T, U and loading vectors P, Q as shown in equation(4.11),(4.12).The absorption matrix A and the concentration matrix C are mean centered in the Step1. The procedure of mean centering improves the centering of the data [12].

$$A = TP' + E \quad (4.11)$$

$$C = UQ' + F \quad (4.12)$$

The following algorithm [12] gives the description of the calculation of the score and the loading vectors.

Step1: Mean center the matrices A and C as shown.

$$A = A - amean \quad (4,13)$$

$$C = C - cmean \quad (4.14)$$

In equations (4.13), (4.14), $amean$, $cmean$ are the vectors containing the mean of matrices A, C respectively.

Step2: Initialize $u_j = C_j$, any column of the concentration matrix, C and $tr_j = A_j$, any column of the absorption matrix, A and $j = 1$.

The steps 3 through step19 involve the calculation of the matrices W, T, P, Q, U and B from the variables w, t, p, q, u, b as shown in equations (4.15) through ((3.67).

Step3: $w_j = A'u_j$ (4.15)

Step4: $w_j = w_j / \| w_j \|$ (4.16)

Step5: $t_j = tr_j$ (4.17)

Step6: $t_j = Aw_j$ (4.18)

Step7: $q_j = C't_j$ (4.19)

Step8: $q_j = q_j / \|q_j\|$ (4.20)

Step9: $u_j = Cq_j$ (4.21)

If $t_j = tr_j$ continue with Step 12 else re-iterate from Step 3.

Step12: $t_j = tr_j$ (4.22)

Step13: $p_j = A't_j / t'_j t_j$ (4.23)

Step14: $p_n = p_j / \|p_j\|$ (4.24)

Step15: $t_j = t_j p_n$ (4.25)

Step16: $w_j = w_j p_n$ (4.26)

Step17: $b_j = t_j / t'_j t_j$ (4.27)

Step18: $A = A - t_j p'_j$ (4.28)

Step19: $C = C - b_j t_j q'_j$ (4.29)

Stop if $j = r$ (where r is number of rows of the absorption matrix, H) else $j = j + 1$ and re-iterate from Step2. The values of w, t, p, q, u, b are saved for each iteration and make up the matrices W,T,P,Q,U and B respectively.

Prediction:

The prediction of the unknown concentration of the constituents [21] from the test vector, V which denotes the unknown mixture, is made from following equations (4.30) and (4.31).

Step1: $R = W(B'W)^{-1} PQ'$ (4.30)

Step2: $c_p = cmean + (V - amean)R$ (4.31)

c_p Is the unknown concentration to be estimated, *cmean* is the mean of the C block previously calculated. V Is the $1 \times n$ sample vector for which concentration is to be determined.

4.5 Introduction to the Kalman filter

The Kalman filter is a technique for the estimation of the instantaneous state $x_k \in R$ of a linear dynamic system perturbed by white noise by using measurements linearly related to the state [14]. The Kalman filter has been reported to be much superior to the classical least squares technique [16] and is an alternative procedure

to the Partial least squares regression (PLS) which can be used in the gas concentration predictor. The most important advantage of the usage of the Kalman filter in gas concentration prediction is the non necessity of the calculation of the inverse of a matrix in the course of computation. The equation (4.32) represents the measurement equation [15] used to determine the state x_k of a linear dynamic system.

$$z_k = H_k x_k + v_k \quad (4.32)$$

In the equation (5.2), the term H_k represents a $m \times n$ matrix that relates the state to the measurement z_k. The term v_k is the measurement noise also assumed to be a zero mean Gaussian process, $v_k \approx N(0, R_k)$.

The objective of the Kalman filter algorithm [15] is to find an estimate of the state vector x_k represented by $\hat{x}_k$, a linear function of the measurements $z_{1,\ldots..} z_k$ which would minimize the mean square error as shown in equation (4.33).

$$P_k = E[x_k - \hat{x}_k]^T E[x_k - \hat{x}_k] \quad (4.33)$$

In the equation (5.3) the term P_k represents the error covariance.

4.6 The Kalman filter in the concentration predictor

The measurement equation as shown in the equation (4.34) is comparable to Beer's law [16]. The equation (4.35) shows the similarity of the two equations.

$$z_k = H_k x_k + v_k \quad (4.35)$$

$$a_k = K_k c_k + e_k \quad (4.36)$$

The measurement vector z_k is the system absorbance a at the k^{th} wavelength; the state of the system x_k is the concentration vector c . The H_k is the functional relationship between the absorption and concentration, K_k .The equation (4.36) is the matrix expression of the Beer's law only for a single gas constituent. This can be seen in the equation (5.17).

$$\begin{bmatrix} A_1 \\ A_2 \\ . \\ . \\ A_k \end{bmatrix} = \begin{bmatrix} K_{11} & . & . & K_{1n} \\ K_{21} & . & . & . \\ . & . & . & . \\ K_{k1} & K_{k2} & . & K_{kn} \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \\ . \\ . \\ C_k \end{bmatrix} + \begin{bmatrix} e_1 \\ e_2 \\ . \\ . \\ e_k \end{bmatrix} \quad (4.37)$$

The A_i is the measured absorbance at the i^{th} wavelength, each row of the matrix C is the concentration of the i^{th} component, K_{ij} the proportional constant, and e_i is the measurement noise at each wavelength.

The elements of the K matrix can be calculated by the measurement of the spectra of individual components. When mixtures of standards are used the equation (4.37) is modified as the equation (4.38).

$$\begin{bmatrix} A_{11} & A_{12} & . & A_{1k} \\ A_{21} & . & . & A_{2k} \\ . & . & . & . \\ A_{m1} & A_{m2} & . & A_{mk} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & . & C_{1n} \\ C_{21} & . & . & C_{2n} \\ . & . & . & . \\ C_{m1} & C_{m2} & . & C_{mn} \end{bmatrix} \begin{bmatrix} K_{11} & . & . & K_{1n} \\ K_{21} & . & . & . \\ . & . & . & . \\ K_{k1} & K_{k2} & . & K_{kn} \end{bmatrix} \quad (4.38)$$

In the equation (5.18) the matrix C in the equation (5.18) is the matrix of m standard mixtures of n components each. In the matrix A each row represents the absorbance spectrum from each mixture for k selected wavelengths. The matrix K is the transpose of the K matrix in the equation(5.17).

The equation (5.19) shows the equivalent matrix equation.

$$A_c = C_c K^T \quad (4.39)$$

In the equation (5.19) the subscript term c denotes calibration.

Calibration:

The measurement equations shown in the previous section are modified as shown in equation (5.17), (5.18), (5.19) and (5.20). Each vector k_k can be calculated by means of the Kalman filter [13] as described by the following three equations.

Step1: Initialization $k(0) = 0, P(0) = 100I, R = 1X10^{-5}$ (4.40)

Step2: $g(i+1) = P(i)C_c^T(i+1)/[R + C_c(i+1)P(i)C_c^T(i+1)]$ (4.41)

Step3: $P(i+1) = [I - g(i+1)k^T(i+1)]P(i)[I - g(i+1)k^T(i+1)]^T + g(i+1)Rg^T(i+1)$ (4.42)

Step4: $k(i+1) = k(i) + g(i+1)[a_c(i+1) - c_c(i+1)k(i)$ (4.43)

Step 2 through Step 4 is iterated from $i = 1$ through $i = m$ where m is the number of mixtures. The objective of the calibration step is the calculation of k matrix which is the pure component spectra.

The term $k(i)$ is a $n \times 1$ matrix containing the proportionality constant estimates at each iteration , $P(i)$ is the $n \times n$ variance-covariance matrix, $c(i)$ is a $1 \times n$ matrix of the concentrations of the n standards in the mixture i ; I is the $n \times n$ identity matrix. R Is a scalar representing the predicted variance of white noise.

Prediction

The unknown concentration vector c can be calculated by equations (5.21) through (5.24) utilizing the value of k calculated in the calibration step.

Step1: Initialization $c(0) = 0, P(0) = 100\ I, R = 1 \times 10^{-5}$ (4.44)

Step2: $g(i+1) = P(i)k(i+1)/[R + k^T(i+1)P(i)k(i+1)$ (4.45)

Step3: $P(i+1) = [I - g(i+1)k^T(i+1)]P(i)[I - g(i+1)k^T(i+1)]^T + g(i+1)Rg^T(i+1)$ (4.46)

Step4: $c(i+1) = c(1) + g(i+1)[a(i+1) - c(i)k^T(i+1)]$ (4.47)

Step2 through Step4 are iterated for $i = 1$ through $i = n$ where n is the considered number of wavelengths in the gas spectrum.

The results of the Kalman filter as a gas concentration predictor are presented in Chapter 5. Though the number of training vectors is 1660 for the Kalman filter due to the utilization of the mixed gas detector this number is decreased to 400 or less. This decrease in the training vectors has significantly improved the prediction accuracy.

CHAPTER 5

EXPERIMENTAL RESULTS AND ANALYSIS

5.1 Introduction

The mixed gas detector and the concentration predictor were implemented using Matlab. The algorithms were tested using spectrographic data of a mixture of three gases. The three gases are Oxygen, Carbon-Dioxide and Ammonia. Mixed in the following conditions; Pressure =1013.23 bar, Temperature =296K.

5.2 Sensor array assumptions

The optical sensor array described in Chapters 1 and 2 is still in research with only a few of its transfer characteristics of each sensor available which leads to the assumption of the approximate transfer characteristics of each sensor for the implementation of the compatible algorithm for implementation of the mixed gas detector and the gas concentration predictor. After the precise transfer characteristics are established the algorithm would be fine tuned to suit the requirements of the sensors. The details of the assumed sensors and their corresponding wavelengths are given in Table.1. The assumption of the wavelengths was based on the analysis of individual spectra [6] of the three gases, Oxygen, Carbon dioxide and Ammonia. One of the objectives of the research was to find an optimum number of sensors in the sensor array as the manufacture of each optical sensor are time consuming. This number was found to be nine.

Table 5.1.Assumed sensors along with the corresponding wavelengths

Sensor Number	Wavelength(um)
1	0.68
2	0.76
3	0.86
4	1
5	1.6
6	2.1
7	2.8
8	3.4
9	4

5.3 Variation of the photocurrent and transmittance

The Table 2 shows the assumption of the variation of the photo current with the mean transmittance. These have also been obtained from the spectra of the three gases under consideration [6]. The test pattern is generated by the simulator that is currently in place of the sensor array. The pattern as shown in Table.2 shows the twenty values of photo currents, corresponding to the transmittance (T) values. Each sensor produces a photo-current in the range of 0uA to 10uA depending on the transmittance (T) value. The detectors were trained using training sets of 31rows each and 9 columns. The training set for the concentration predictor contained 1660 rows and 9 columns. There exists a finite relationship between the transmittance values recorded at each wavelength and the photocurrent produced by each of the optical sensors. This relationship is assumed in the Nano Nose to be linear.

Table 5.2.Assumption of the variation of transmittance (T) with Photocurrent (uA)

Transmittance(T)	Photocurrent (uA)
0.1	1
0.15	1.5
0.2	2
0.25	2.5
0.3	3
0.35	3.5
0.4	4
0.45	4.5
0.5	5
0.55	5.5
0.6	6
0.65	6.5
0.7	7
0.75	7.5
0.8	8
0.85	8.5
0.9	9
0.95	9.5
1	10

Noise is added to the test pattern to show the resilience of the detector-predictor algorithm. The characteristics of the noise are as given in the equation (5.1).

$$z = 0.08t \quad 0 \leq t \leq 8 \quad (5.1)$$

Table.5.3.Test patterns applied to the back end of the Nano Nose

Sensor Number	Test Vector1	Test Vector2
1	3.07	1.5
2	3.01	1.5
3	3.04	1.5
4	10.03	3.02
5	7.07	1.53
6	7.06	10.04
7	7.03	10.04
8	0	10.05
9	7.06	10.06

5.4 Details of the applied test patterns and results

The test vector 1 and test vector2 are shown in Table.3. c_{ox} Is the concentration of oxygen; c_{cn} is the concentration of carbon dioxide; c_{am} is the concentration of ammonia. The presence of a gas is indicated by an equal response of the sensors (generation of photo current) in a distinct wavelength range. Ammonia is active from 2um though 4um (Sensor No 6 through 9), while carbon dioxide is active from 1um though 4um exception being that is inactive at 3.4um (Sensor No 5 through 9 inactive at No 8) and oxygen is active from 0.68um through 1um (Sensor No 1 through 4).

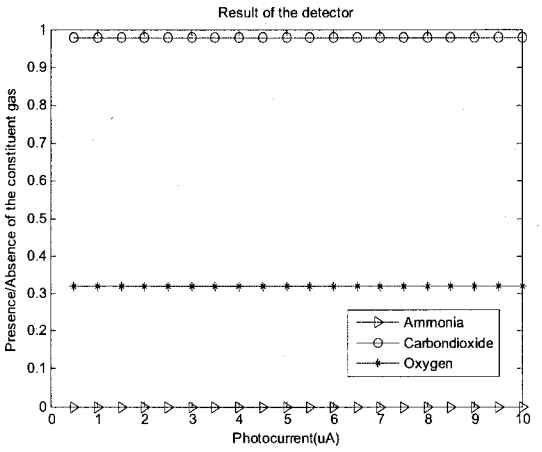

Figure 5.1 Result of the detector for Test Vector 1

Table 5.4.Predicted constituent concentration for Test Vector 1

Concentration (in ppm)	c_{ox}	c_{cx}	c_{am}
Measured	30	70	0
PLS	30.08	70.46	0
Kalman filter	33.9	76.8	0

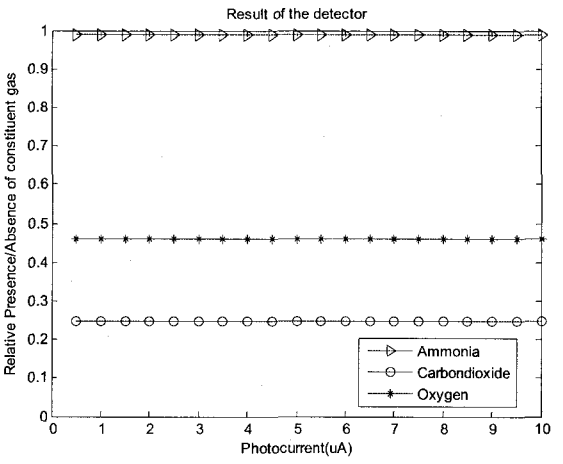

Figure 5.2 Result of the detector for Test Vector 2

Table 5.5 Predicted constituent concentration for Test Vector 2

Concentration (in ppm)	c_{ox}	c_{cx}	c_{am}
Measured	15	15	100
PLS	15.14	15.14	100.5
Kalman filter	14.22	14.22	106

5.5 Performance of the Kalman filter and the PLS algorithm

The performance of the Kalman filter and the PLS algorithm is measured in terms of the mean square error of the concentration prediction. Fig.5.3 and Fig.5.4 show the variation of the mean square error in prediction, given by equation (6.1), of the Kalman filter and the PLS algorithms when operated over different size of training sets. It is very much evident that mean square error, increases with increasing sizes of the training sets.

$$MSE = \sqrt{(AC)^2 - (PC)^2} \quad (6.1)$$

MSE Is the mean square error in the gas concentration prediction.

AC Is the actual value of the concentration.

PC Is the predicted value of the concentration.

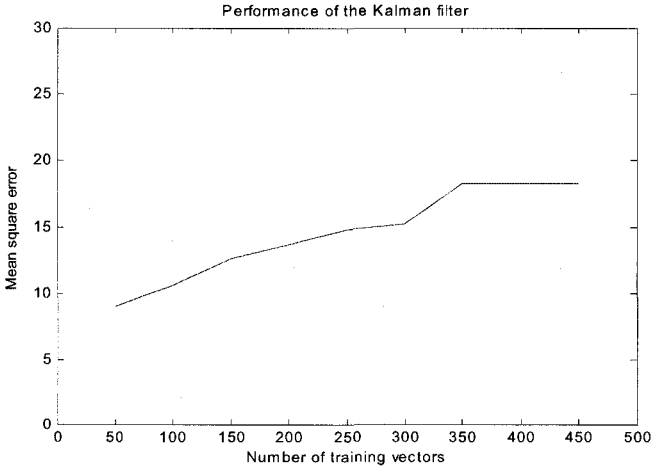

Figure 5.3 Performance of the Kalman filter

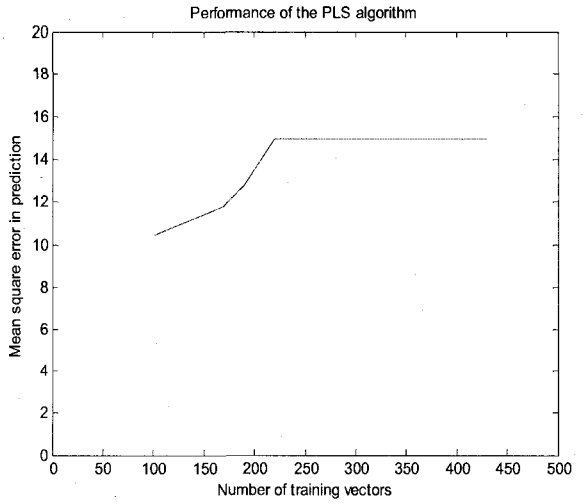

Figure 5.4 Performance of the PLS algorithm

CHAPTER 6

CONCLUSION

This thesis focuses on the development of a reconfigurable algorithm, compatible with the specifications of the transfer characteristics of an optical sensor array to achieve gas constituent detection and gas concentration prediction. The mixed gas detector has been implemented by an array of neural networks, each of which is trained to detect specific constituents. The advantage with using individual neural network for gas constituent detection is the decrease in the convergence time however the limitation with this model is that in the VLSI implementation an architecture supporting a greater number of neural networks would have to be developed.

There are two approaches presented for the implementation of the concentration predictor which are the, Partial least squares regression and the Kalman filter. The Partial least squares regression has been found to be more resilient to the Kalman filter in terms of prediction accuracy. However the Partial least squares regression method depending on the quality of the data has a tendency to generate nearly singular matrices in course of calculation, a tendency absent in the Kalman filter. The two combinations which are the neural-network, Partial least squares algorithm and the neural-network and the Kalman filter in this particular application is found to improve the concentration prediction accuracy in this particular application. The re-configurability of the algorithm can be seen in the variable number of nodes which can be used in the input layer of the neural

network corresponding to the number of sensors in the sensor array and similarly the variable size of the input vector given as input to the concentration predictor.

This thesis is a proposal of a solution to the problem of the selection of a suitable algorithm to fulfill the needs of a relatively new strategy to simultaneously detect and predict gas constituents under scoring the method of designing ahead in time.

6.1 Future Work

The long term objective of this thesis is to develop a hardware implementation using VHDL for each of the blocks described in the mixed gas detector and the gas concentration predictor. This would help in the development of a commercially viable battery powered gas detector-gas concentrator predictor or a hand held spectrometer. A variant of the mixed gas detector and the concentration predictor could pave way for them to be extended to serve a variety of electronic recognition applications particularly in the fields of signal and image processing.

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