Artificial Neural Networks for the Concentration Estimation of Volatile Organic Gases

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Abstract

The cascade and parallel artificial neural networks (ANN) structure were used to estimation the concentration of volatile organic compounds An array of piezoelectric quartz crystals were used to detect volatile organic gases. Steady-state frequency shifts have been used as the input patterns for ANN structures. The network structures and network performances were discussed.

1 Introduction

Toluene and other volatile organic vapours in ambient air are known to be reactive photochemically, and can have harmful effects upon long-term exposure at moderate levels. These type organic compounds are widely used as a solvent in a large number chemical industry and in printing plants [1].

Developing and designing sensors for the specific detection of hazardous components in the mixture of many others is important [2].

In recent years a variety of selective coating (adsorbates) has been investigated for chemical sensors. The molecules to be detected (analytes) interact with these adsorbates. They may be identified quantitatively by changes of physical or chemical parameters of adsorbate / analyte system such as the refractor index, capacitance, conductivity, or total mass. The last can be monitored by quartz crystal microbalance (QCM) sensors, which are widely used as thickness monitors [3,4].

However, the complete selectivity cannot be realised. Therefore, a variety of different methods have been developed to overcome this problem by using an array of different sensors and evaluating the data in a subsequent data processing step similar to the olfactory system of humans with a few receptors and subsequent data evaluation in the brain.

Artificial neural network (ANN) models or simply "neural nets" go by many names such as connectionist models, parallel distributed processing models, and neuromorphic systems. Whatever the name, all these models attempt to achieve good performance via dense interconnection of simple computational elements. In this respect, artificial neural net structure is based on our present understanding of biological nervous systems [5,6].

For complex ternary mixtures and long-term measurements the artificial neural network offers advantages in predictability [7].

2. Artificial Neural Net (ANN) Models

Instead of performing a program of instructions sequentially, neural net models explore many competing hypotheses simultaneously using massively parallel nets composed of many computational elements connected by links with variable weights .

Computational elements ore nodes used in neural net models are nonlinear, are typically analogue, and may be slow compared to modern digital circuitry .

The net topology, node characteristics, and training or learning rules specifies neural net models. These rules specify an initial set of weights and indicate how weights should be adapted during use to improve performance. Both design procedures and training rules are the topic of much current research [5,6].

The potential benefits of neural nets expend beyond the high computation rates provided by massive parallelism. Neural nets typically provide a greater degree of robustness or fault tolerance than sequential computations because there are many more processing nodes, each with primarily local connections. Damage to a few nodes or links thus need not impair overall performance significantly. Most neural net algorithms also adapt connection weights in time to improve performance based on current result [5,6]

The artificial neuron was designed to imitate the first order characteristics of the real biological neuron. Essentially a set of inputs is applied, each representing the output of another neuron. Each input is multiplied by a corresponding weight analogous to a synaptic strength, and all the weighted inputs are then summed to determine the activation level of the neuron [7] Figure 1 depicts a model that implements the above functional description.

Ynet=W1 X1+W2 X2 +........+Wn Xn

Activation function used in this study is f(x) = 1/(1+exp(-x)). Thus

Yout=1/(1+exp(-Ynet))

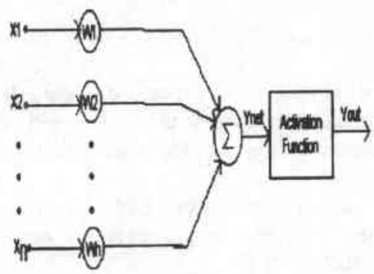

Figure1. Artificial neuron model

A multi-layer perceptron (MLP) neural networks trained with the back propagation supervised learning method was used to train and test the data obtained both from the simulation and the real time system performances. Back propagation learning involves using an iterative gradient-descent algorithm to minimise the mean square error between the actual outputs of the network and the desired outputs in response to given inputs [8].

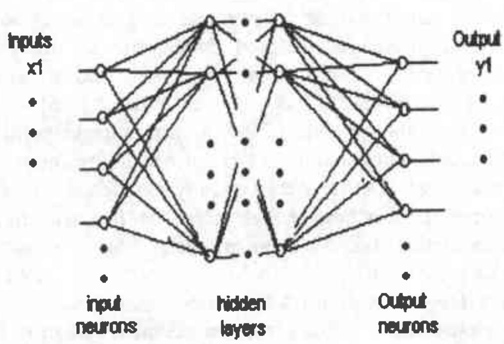

Figure2. A MLP Artificial neural network

The following steps are involved in constructing and training an MLP network [8] :

1) Defining the structure of the network (the number of layers and neurons in each layer)
2) Selecting the learning parameters (learning rate and momentum coefficient)
3) Initialising the connection weights
4) Selecting an input-output pair from the training examples set and presenting it to the network
5) Calculating the output values of the neurons in the hidden and output layers
6) Comparing the output values of network with the desired output values and calculating the output errors
7) Adjusting the connection weights of the network with the decrease the output errors
8) Repeating step 4 to 7 until the error is acceptable or a predefined number of iterations are completed.

3. A Coated QCM Sensor Array

Chemical and biochemical sensors have a wide spectrum of applications in the field of environmental sensing. Since totally selective sensors based upon key-lock interactions do not exist for the detection of volatile organic vapours, the cross-sensitivities of carefully chosen sensor elements can be exploited in a sensor array by applying different algorithms of multi-component analysis and pattern recognition. The criteria for the choice of these sensor elements are a certain selectivity, sufficient sensitivity and long-term stability, which ensure reproducible results over a period of months [9].

In order to meet these requirements we developed an array of 4 QCM sensor devices with tetrakis alkaly thin substituted metalphtalocyaninnes as a sensitive layers.

The transducers employed were QCM with fundamental frequency of 10 MHz. The setup consisted of two QCM for each sensor, one of them as reference QCM. Each QCM was powered by an oscillator circuit. A mixer circuit was used for measuring the frequency shift of coated QCM

The frequency shift of a quartz crystal, Δf, due to deposition of some material (analyte molecules) on or its removal from the crystal surface is [3,4].

$\Delta f = - C\Delta m$

where C is a constant determined by the vibrational frequency, frequency constant of the crystal, density of quartz, and effective area of vibrating plate. Δm is correlated with the gas-phase concentration of the analyte and therefore the frequency shift as well. The relative frequency shift data were used to perform the multi-component analysis.

Frequency shift (Hz) vs. concentration (ppm) characteristics were measured for toluene, benzene, hexane, and acetone.

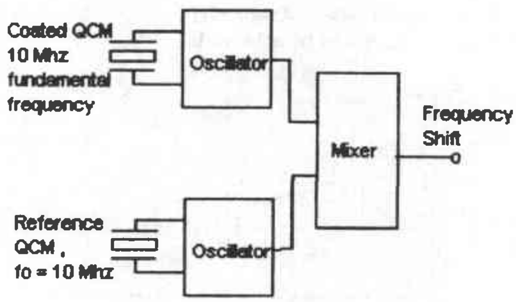

Figure 3. Block diagram of frequency shift measurement circuit

The test vapours were generated from cooled bubblers using synthetic air as carrier gas and then diluted to known concentrations by computer – driven mass flow controllers. The humidity content was adjusted in the same manner. All vapours were mixed and temperature stabilised before entering the chamber. All sensor responses were measured simultaneously in the same gas atmosphere.

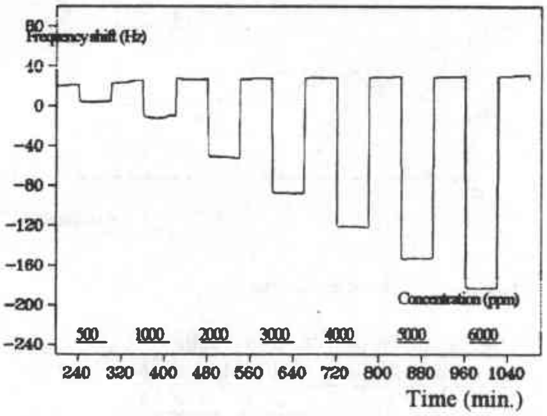

Figure 4.0 An example frequency shift (Hz) vs. concentration (ppm) at room temperature for our measurements

4. Method

In the first step we used three layer ANN. Figure 5. shows the structure of this ANN. For hidden layer we used 10, 13 and 15 hidden neuron to see the effect of hidden neuron number. In the second step we used cascade and parallel ANN structures.

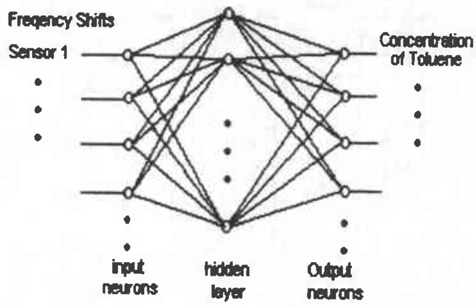

Figure 5. Neural architecture used to relate the sensor signal to the analyte concentrations

In the cascade ANN structure, the outputs of the first ANN are learning inputs of second ANN. Figure 6. shows the cascade ANN structure.

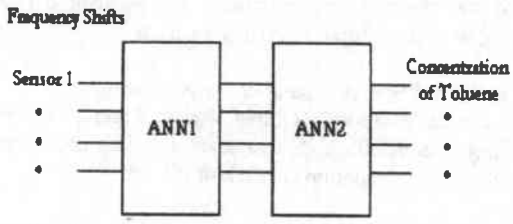

Figure 6. Cascade ANN structure

In the parallel ANN structure, range of measurement is divided into three parts, as an example, we used the following ranges:

ANN1 for 0 < , < 10000 ppm
ANN2 for 1000 ≤ , < 5000 ppm
ANN3 for 0 < , < 1000 ppm

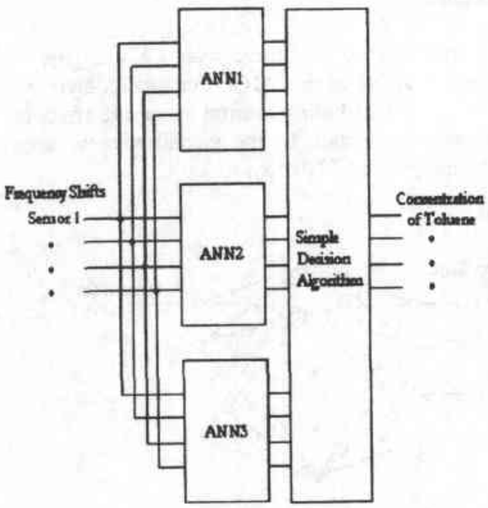

Figure 7. Parallel ANN structure

For the output we used a simple decision algorithm to outputs of ANN1;
- If the detected concentrations are between 5000-10000 ppm, then take output as ANN1's output
- If the detected concentrations are between 1000-5000 ppm, then take output as ANN2's output
- If the detected concentrations are between 0-1000 ppm, then take output as ANN3's output

In the cascade and parallel ANN structures, ANN's have three layers with 4 input, 4 output and 15 hidden neurons. In the all ANN structures, learning coefficient is 0.25 and momentum coefficient is 0.75.

For the performance measurement, we use the mean relative absolute error E(RAE) and the corresponding maximum error max(RAE) [6] ;

$$E(RAE) = \frac{1}{n_{test}} \sum_{tetset} \left(\frac{\left(P_{prdicted} - P_{true}\right)}{P_{true}} \right) \quad \forall P_{true} \neq 0$$

$$\max(RAE) = \max_{testset} \left(\frac{\left(P_{predicted} - P_{true}\right)}{P_{true}} \right) \quad \forall P_{true} \neq 0$$

5. Results and Discussions

The ability of ANN structures to estimation of the concentrations was observed.

Once the ANN structures are trained successfully and weights are determined, only forward propagation is performed and consequently very simple and fast discrimination can be achieved.

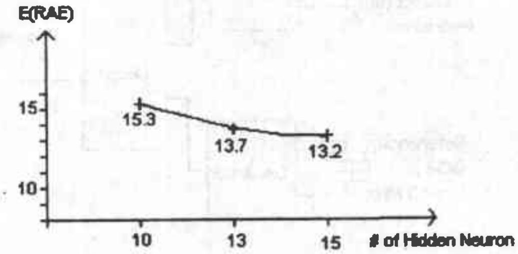

Figure 8. Error graphics of ANN with respect to # of hidden neurones

As seen in the figure 8, E(RAE) decreased with increasing hidden neuron number. So, for optimal solutions, in the parallel and cascade structure we used 15 neuron in the hidden layer.

It is shown that numbers of iteration in training improves the learning (figure 9).

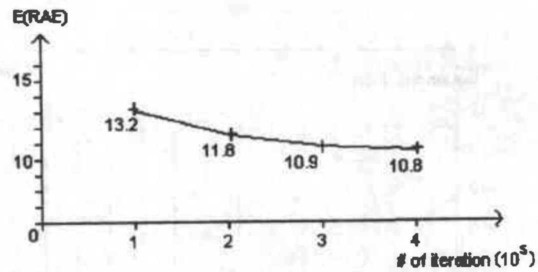

Figure 9. Effects of iterations

Table 1. Comparison of ANN results

	E(RAE)	MAX(RAE)
ANN	10.8	43
Cascade ANN's	5.8	38
Parallel ANN's	6.23	33

Table 1 showed that, all results have a good performance for detection of gas concentrations and Cascade and parallel ANN's reduce the E(RAE) and MAX(EAR). The performance of ANN's is improved by Cascade and Parallel structures.

In the cascade ANN structure second ANN behaves as a decision maker so improves the estimation results.

The parallel ANN structure takes advantage of the fact that a neural-network group decision is more accurate than decision of network [10}.

6. Conclusions

In this paper tree tape of neural network architecture were discussed.

It has been found that this ANN structures are capable both of discriminating reliably between various sorts of the volatile organic compounds and to estimate concentration of these compounds.

As a result, we can easily say that, ANN structures are suitable for difficult quantification problems and can be used efficiently for detection of unknown gas concentrations if training of networks is done well.

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