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Development of WT-ANN Model in thick film SnO2 Gas Sensor for Precise Detection of Volatile Organic Compounds in Exhaled Breath

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Abstract: Breath analysis for early-stage detection and monitoring of chronic illnesses, aiming to reduce medical costs and improve patient quality of life. Electronic sensors, functioning as diagnostic tools, can analyze body odors and detect pathological gases. This study focuses on tin oxide (SnO2) thick film gas sensors for detecting VOCs exhaled in breath, including acetone, ethanol, and benzene, which are indicators of diseases like diabetes, lung cancer, and fatty liver disease. A custom gas chamber equipped with a sensor array was constructed, and the sensors' responses to different gas concentrations were recorded. Using artificial neural networks (ANNs), specifically the Wavelet-Transformed ANN (WT-ANN) model, and the study demonstrated the precise detection of VOC concentrations. The WT-ANN employs B-spline wavelet transfer functions for enhanced nonlinearity, allowing for accurate correlation of complex data. Initial results showed that the system could closely estimate acetone concentrations, with minimal error. The findings suggest that the WT-ANN model, combined with semiconductor-based gas sensors, might assist as a non-invasive instrument for diagnosis diseases like diabetes, lung cancer, and fatty liver disease by identifying specific VOC patterns in exhaled breath. The study underscores the potential of ANN-based breath analysis systems in medical diagnostics and highlights the need for continued research to refine this innovative approach.

***Keywords*:** *Gas sensor, Artificial Neural Network (ANN), Wavelet transform, Volatile Organic Compounds (VOC), Tin oxide, Concentration*

1. Introduction

Gas sensors are widely used for the detection of hazardous, flammable, and explosive gases in commercial manufacturing environments. The safety of manufacture is directly impacted by the quality of these sensors [1]. Furthermore, gas sensors are essential for everyday tasks like air quality monitoring, environmental monitoring, and medical diagnosis [2]. The past few years have seen a great deal of research focused on various nanoscale gas sensors [3]. Based on how effectively it detect the environment, gas sensors are divided into different kinds, including electrochemical, semiconductor, and combustion catalytic sensors [4]. Because of their affordability, portability, ease of manufacturing, and high sensitivity, metal oxide semiconductors (MOS) like zinc oxide (ZnO), Indium oxide (In2O3), tin oxide (SnO2), tungsten oxide (WO3), and nickel oxide (NiO) are thought to be among the best constituents for creating resistive gas sensors [5].

In recent years, scientists have been working to develop robust and dependable MOS gas sensors. They have been focusing on enhancing the sensor's reaction quality aspect, temperature of operation, selectivity, stability over time, and response/recovery speed [6]. It has been demonstrated that modifying MOS with other MOS and noble metal is a successful way to boost the sensitivity and selectivity of the sensor. In order to identify H2 among other gases, A Pd functionalized SnO2 sensing film on a microscale was developed by Toan et al. that demonstrated ultra sensitivity and selectivity [7]. Nevertheless, it is still unable to resolve the issue of gas detection at ambient temperature, much like the majority of conventional MOS. High operating temperatures have been noted to limit the device's usefulness in many real-world applications and necessitate greater power and integration complexity [8]. Additionally, high temperatures make it inappropriate for the detection of explosive gases. Finally, humidity will have an impact on primarily MOS-based sensors' resistance and response [9]. Designing a dependable gas sensor that is not affected by humidity is vital because there are situations in which high humidity is present, such as identifying the exhaled ethanol gas of an intoxicated driver or the gas marker of exhaled acetone in a patient with diabetes [10]. Thus, the construction and design of synthetic MOS gas sensors at minimal temperatures of operation continues to be an intriguing and difficult research topic, particularly at room temperature [11].

At room temperature (RT), carbon materials can detect molecules at the trace level due to their larger surface area. However, they become fewer selective and exhibit a lower

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recovery rate due to their high binding energy with the gas molecules [12]. However, with a comparatively quicker recovery rate, when it comes to detecting different gas molecules at higher concentration levels, metal oxides (MOx) are good possibilities. However, in order to produce advantageous (O_2^-,O^- and O^{2-}) oxygen adsorbents on sensing substrates; higher operating temperatures (OT) are necessary for them.

Selectivity and drift issues can be effectively addressed by smart device developers with the help of machine learning (ML). One of the main elements influencing the performance of a sensor is selectivity, which applies to environmental and medical monitoring applications alike [14]. To find a specific VOC trace in human breath among thousands of others, for example, medical professionals use breath analyzers in order to accurately diagnose diseases [15]. For a correct diagnosis, it is therefore highly recommended that a breathalyzer be able to identify the traces of a particular VOC concentrations with superior selectivity [16]. Even though detection at the trace level could fail necessary for environment monitoring, a gas sensor's excellent selectivity is still a crucial component of its overall efficiency [17].

In order to address drift compensation and selectivity issues, ML has been heavily utilized in electronic noses and smart gas sensors over the past few decades. Drift errors have been studied using various kinds of techniques, including ML, multivariate analysis, and univariate analysis [18]. ML is currently being applied to selectivity and drift compensation. Through data processing, reliable feature information that are able to identify those particular gas's "fingerprint" is extracted from the dynamic sensor response [19]. There have been reports on a several different techniques for signal and processing of data, such as frequency domain, transient, and steady-state models. Systems with maximum output accuracy are those built using techniques for extraction of features and data processing in the frequency and transient domains [20]. One method for reducing redundant information in high-dimensional data that has been processed is dimensionality reduction. Principal component analysis (PCA), an unsupervised technique, is used to identify one main component with the most important data can be extracted from a signal that contains hundreds of features [21]. In order to assess the prediction accuracy of raw data, this creates distinct signatures against particular gases, which are subsequently trained and tested on [22]. Both linear classifiers based on statistical theory and nonlinear classifiers based on neural networks are used in the development of pattern recognition algorithms. k-nearest neighbours (KNN), classification and regression trees (CART), Gaussian naïve Bayes (NB), support vector machines (SVM), random forest (RF), and artificial neural networks (ANN) are examples of common classifiers [23]. Diverse well-known works have addressed the issue of distinguishing between different gases with a single sensor. However, because of the small sample size used in the testing, they have either shown limited accuracy or cannot be confidently generalized. Hence there is a novel network to recognize the patterns in the gas sensing array for medical field.

The main contribution of the work is enumerated as

- The development and application of a Wavelet-Transformed ANN (WT-ANN) model combined with semiconductor-based gas sensors that can accurately identify VOCs in exhaled breath and identify conditions like fatty liver disease, diabetes, and lung cancer.
- By employing B-spline wavelet transfer functions, the WT-ANN enhances nonlinearity, enabling accurate correlation of complex data and reliable gas concentration estimation.
- This study demonstrates the potential of non-invasive breath analysis as a diagnostic tool, with promising initial results and a pathway for further refinement and development.

The remainder of the article is organized as follows: Section 1 illustrates the introduction; Section 2 summarizes previous research; Section 3 interprets the suggested approach; Section 4 presents the suggested method's results; and Section 5 summarizes the paper.

2. Literature Survey

Chu et.al [24] detected 11 various combinations of carbon monoxide (CO) and nitrogen dioxide (NO2), with concentrations that vary from 0 to 50 ppm, a sensor array made up of four sensors has been used. Average resistance over time was introduced to guarantee high recognition accuracy while mitigating the impact of sensor noise. Then, from each sample, 12 features were extracted, that includes recovery time, response time, and response value. Following that, different gases were identified with accuracy in classification of 94.55% and 100%, respectively, C-means clustering and back propagation neural network (BPNN) are utilized. Additionally, the genetic algorithm (GA) was used to enhance the performance of BPNN. Additionally, the input sample feature that has the biggest impact on the BPNN model has been investigated using a random variable substitution technique. Dynamic curves have been converted into grey images via grey processing, and a 100% identification accuracy has been achieved by automatically extracting high-level features using a convolutional neural network (CNN) from these images. However, the system requires a long training time to converge and cannot achieve quantitative identification.

Ma et.al [25] suggested to use a novel technique in conjunction with a deep learning model (DLM) and dynamic response map to increase the sensor array module's capacity to identify various substances. The findings showed that the sensor array's multidimensional dynamic response signals could be thought of as an image form. Consequently, ten various types of VOCs and their mixtures were identified using image recognition processing and recognition techniques. To distinguish between various VOCs, Utilizing support vector machine (SVM) learners, the error-correcting output codes (ECOC) model was applied. The test findings demonstrated that the sensor array data-based model was able to classify the VOCs more precisely than the model with a single sensor. Additionally, a straightforward VOC classification was trained into the DLM network with a 92% accuracy rate. However, the training procedure for the basic DLM model appeared to be overfitting. As a result, the pre-trained VGG-19 model from transfer learning was further modified to enhance the DLM's generalization property, achieving 90% accuracy for test cases. In order to increase the variation across sensors, all sensor responses at a given time were normalized before the model was constructed. Nonetheless, there are still issues with identifying the constituents of a mixture.

Iwata et.al [26] used a neural network-based regression and a ML algorithm to examine the gas through incorporated gas sensors of the TiO_2 nanotube (NT) type. It was created an integrated TiO_2-NT gas sensor featuring multiple sensing components, each of which had a distinct response characteristic. Next, each sensing element's output signals after being exposed to a gas mixture were measured. The gas mixture mostly contained nitrogen and oxygen with a small amount of carbon monoxide. It was used the ML technique to analyze the sensor elements' output signals and forecast the TiO_2-NT sensors for gases were sensitive to concentrations of CO and O_2. To collect sensor output data, seven sets of mixed gas concentrations with different concentrations of each component gas were examined. Four or five of the seven datasets were used as ML training data for the neural network technique, and the concentrations of CO and O_2 in the final three or two datasets were predicted. As a result, it was verified that a larger gas concentration prediction accuracy was significantly improved by the quantity of sensor elements. For a carbon monoxide concentration of 0.02%, using the output signals from ten sensor elements, the gas concentration could be predicted with less than 0.001% accuracy. However, its accuracy may decrease with gas mixtures outside of the training range and is more complex and expensive due to the requirement for a large number of sensor elements and a large amount of training data.

Li eta.al [27] suggested a cooperative approach based on ML algorithms and sensor integration to achieve accurate NO_2 and NH_3 gas detections in actual mining settings. A wearable sensing array based on the composite of graphene and polyaniline is established with the aim of achieving significant improvements in sensitivity and selectivity in mixed gas environments. With the introduction of partial least squares (PLS) and backpropagation neural network (BP-NN) algorithms, it is possible to achieve NH_3 and NO_2 concentrations showed over 99% theoretical prediction level across a broad range of relative humidity, suggesting significant potential for real-world mining identification. Additionally, these algorithms can settle the inference of moisture and increase the precision of concentration forecasting and gas identification. An experimental wearable bracelet is designed to provide wireless real-time alerts in the event of potentially dangerous gas leaks in mines with different relative humidity. It incorporates sensing arrays and ML algorithms. Interfering gases rarely have an impact on the target gas's concentration prediction in hazardous environments due to the sensing materials' exceptionally high selectivity.

Kwon et.al [28] Discussed for the purpose of swiftly and accurately identifying hazardous gases, Spiking neural networks (SNNs) and gas sensors modelled after field-effect transistors (FETs) are the foundation of a novel artificial olfactory system proposed. A FET-type gas sensor with a micro-heater was built using an In_2O_3 film as the material that senses to detect the gases NO_2 and H_2S. After the sensor was analyzed with the micro-heater bias, pre-bias, and gas concentration, 4.8 s of measured transient currents were used to generate an efficient data set for training a neural network. The backpropagation algorithm, the most popular pattern recognition algorithm, was then applied to the data set to train an ANN. In the hardware-based SNN, Conversion of the weights acquired by ANNs into synaptic device conductance. With just 12 sensors, the SNN predicts NO_2 and H_2S concentrations with a low error rate of roughly 3%. Furthermore, Due to its neuron's ability to directly convert sensor current into voltage spike rate, the SNN is able to predict gas concentration in real-time (within 5 seconds). Unfortunately, obtaining multiple accurate readings of the sensor currents necessitates the use of an extra circuit to provide a mean current and a high-precision AD converter, which increases the system's power consumption.

As a result measuring as a non-invasive and non-contact method of determining the concentration of gases in exhaled breath, offering potential benefits over traditional diagnostic methods for conditions like diabetes and asthma, which are costly, time-consuming, and complex. However, the proposed system faces challenges such as long training times, difficulty in achieving quantitative identification, and decreased accuracy with gas mixtures outside the training range. Moreover, the complexity and expense of the system are exacerbated by the need for a large number of sensor elements and extensive training data. Despite the high selectivity of the sensing materials, which minimizes the impact of interfering gases in hazardous environments, challenges remain in obtaining accurate readings of sensor currents, requiring additional circuitry and increasing power consumption. Overall, while the proposed method presents a promising alternative for diagnosing asthma and diabetes, it still requires further refinement to address its limitations and optimize its performance.

3. Proposed Methodology

Technological developments in the fields of electronics, biochemistry, artificial intelligence, and aroma-sensors have enabled the development of devices that are able to measure and characterize volatile aromas released from a wide range of sources. Such devices are referred to as electronic sensors. A multisensory array is the standard component of an electronic sensor system. The sensors that make up the cross-reactive sensor array are progressively different and have been selected to react to a broad range of chemical classes and distinguish between various mixtures of potential analytes.

Biomedical applications of aroma sensor technology include the diagnosis of various diseases, including asthma, diabetes (blood sugar), tuberculosis, lung cancer, breast cancer, and others, using a sensor array. Inhaling oxygen and exhaling carbon dioxide is part of being human. Fewer than fifty VOCs, out of the hundreds present in human breath at low concentrations, are found in most healthy individuals under normal physiological conditions. On the other hand, patients with diseases typically have much fewer aberrant VOCs. As a result, the identification of particular volatile metabolites released from patients' expired breath not only offers markers of specific diseases but also reflects the overall physiological state as a useful index of disease and an indication of general health. Early indicators of disease of physiological disorders are thus provided by these volatile markers of disease, which are frequently released several hours to several days prior to the appearance of physically noticeable symptoms of disease. Novel molecular markers for distinct diseases—both infectious and non-infectious—that serve as indicators. Three distinct kinds of volatile species were used in this instance, each at varying concentrations. These three are benzoene, ethanol, and acetone. The samples that make up the data set for these volatile species are matched to the gas and auxiliary sensor outputs. An array of gas sensors that responds with an odour pattern is called an electronic sensor. The sensor array must be coupled with a variety of sensors that have varying selectivity patterns in order for a single sensor in the array to respond to a wide range of compounds rather than being extremely specific. The system is made up of six different kinds of FIGARO USA Inc. TGS class gas sensors that are all supplied with the same heater voltages. A semiconductor layer of tin dioxide (SnO2) serves as the sensing element. The following are TGS 2610, TGS 2611, TGS 2620, TGS 822, TGS 825, and TGS 816. Because of their high sensitivity, metal oxide sensors are among the most widely used technological options for sensor arrays. Their lack of selectivity is their primary drawback. Based on the change in conductivity of these sensors in the presence of reducing and oxidizing gases, their functioning is comprehended. The type of metal oxide and its concentration, as well as the gas's nature, determine how much of a reaction occurs. Figure 1 shows the flow chart of the work is given below.

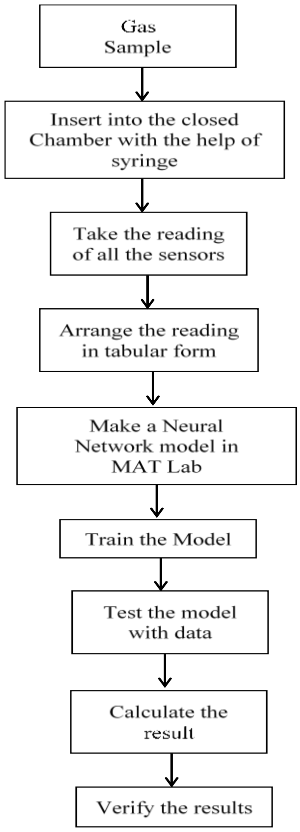

Figure 1: Flow chart of the proposed work

An ANN is the most widely used ML technique. It is built by connecting several processing nodes, also known as neurons or nodes, in successively linked neuronic layers. One popular form of ANN is the multi-layered perceptron (MLP), which typically consists of Hidden and output are the two feedforward neuronic layers. It is always known because there are a similar number of variables that depend and nodes for output. Alternatively, the trial-and-error method is typically used to find a sufficient number of concealed nodes. Mathematical processes that are both linear (L) and non-linear (NL) can be combined to create an artificial neuron. The node's entrance vector (X) multiplied by the weight coefficients (W) and bias (b) is combined in the linear portion (Eq. 1).

$$L = \sum WX + b \qquad (1)$$

The linear component result must be passed over a certain equation, the transfer function (g), by the non-linear part. Equation (2) describes the process by which the neuron's output (out) was attained.

$$out = g(LP) \quad (2)$$

In fact, the transfer function facilitates the simulation of non-linear problems by neurons and artificial neural networks. The primary constraint of the MLP model is its limited capacity to include just a limited number of pre-established transfer functions. Among the most widely used transfer functions, such as the radial basis, too little non-linearity in the logarithm, sigmoid, and tangent allows for the accurate correlation of highly non-linear issues.

To construct the WT-ANN model, researchers used the wavelet transformations included in the MLP body as a transfer function. Within the WT-ANN's hidden layer (g^{hid}), a function with configurable nonlinearity called the B-spline wavelet is frequently employed as a transfer function. The B-spline wavelet transfer function's (BSWTF) mathematical formula is displayed in equations (3) and (4).

$$g^{hid}(x) = \sqrt{a\phi}(ax/\gamma)^{\gamma} \exp(2\pi i\beta x) \quad (3)$$

$$\phi(k) = \begin{cases} 1 & k = 0 \\ \sin(\pi k)/\pi k & k \neq 0 \end{cases} \quad (4)$$

where α, β, and γ are the BSWTF's nonlinearity and shape-related parameters. Fig. 2 shows the wavelet transfer functions of the B-spline with various values of α, β, and γ. It is evident that even the most complicated occurrences may be correlated by this function due to its sufficient nonlinearity. Furthermore, by adjusting its characteristics linked to form, its shape may be engineered.

The WT-ANN was used to calculate the acetone-detecting capacity of the tin oxide sensor in relation to the acetone, Ethanol & Benzene concentration, operating temperature, and chemistry of the nanocomposite. The neuronic layers hidden and output, as well as an input layer, make up the built WT-ANN. All of these levels are feed forwardly linked. A B-spline wavelet transfer function is used by the hidden layer, while a linear transfer function is employed by the output layer.

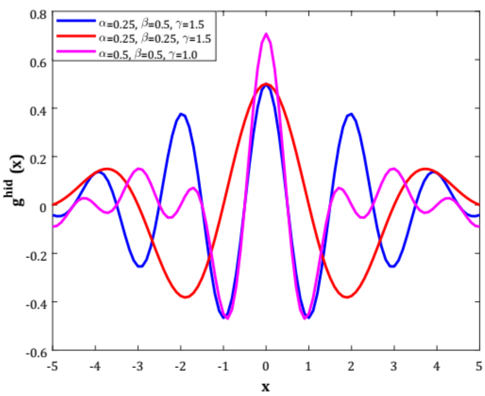

Figure 2: B-spline wavelet transfers functions with various values of α, β, and γ

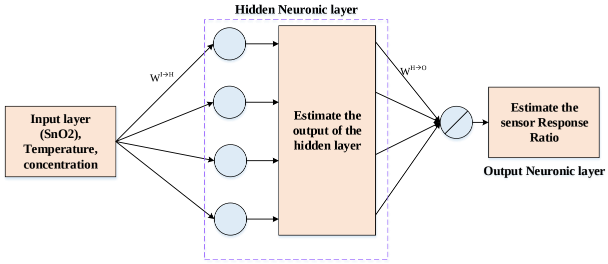

Figure 3: Architecture of the WT-ANN

In order to obtain the output vector (Out^{HL}), certain numerical operations based on Eq. (5) applied to X's input vector in the hidden layer. This figure 3 shows that by using weighted linkages ($W^{I\to H}$), the hidden layer's nodes are fully connected to the vector of independent variables (X).

$$Out^{HL} = g^{hid}\{(\sum W^{I\to H} \times X - b)/a\} \quad (5)$$

The movable coefficients between the input and hidden layers are a and b. A B-spline wavelet transfer function in the hidden layer of the WT-ANN is validated by Equation (5).

The anticipated sensor resistance ratio (SRR^{Pred}) may be obtained by the weighted connections between the output and hidden layers ($W^{H\to O}$) and the Out^{HL} are multiplied because the output layer of the WT-ANN has a linear transfer function is given as equation (6)

$$SRR^{Pred} = \sum W^{H\to O} \times Out^{HL} \quad (6)$$

The changeable coefficients among the output and hidden layers are displayed in the, as should be highlighted. During the cross-validation stage, all WT-ANN coefficients were adjusted using the proper optimization procedure.

4. Result and Discussion

A simulation model is developed using Neural Network toolbox of MATLAB® software. that there are 130 readings are taken, out of which 98 are used to trained the network and 25 are used for testing remaining are consider as a unknown samples.

In this work two programs are formed one for the verification of gas and other for specifications.

Maximum results shown at a time = 115

Maximum number of iterations = 2472

Maximum allowed mean square error = 0.0000017

Number of training inputs = 98;

Number of testing inputs = 25

The data which is given to input matrix. Out of 130 data only 98 samples are taken which are firstly scaled and then given to input matrix.

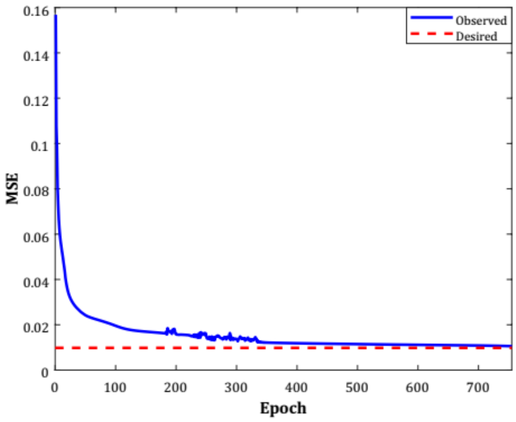

Figure 4: MSE through the WT-ANN's cross-validation learning algorithm.

Figure 4 depicts the MSE for WT-ANN's. Optimizing the model's parameters increases the predictive accuracy and reduces the Mean Squared Error (MSE) produced by the learning algorithm in the WT-ANN cross-validation stage. Through the process of minimizing the error between predicted and actual values during validation, the WT-ANN is guaranteed to generalize well to new data.

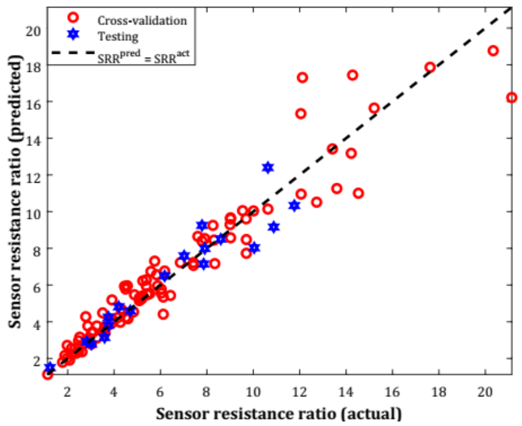

Figure 5: Relationship between the optimum WT-ANN's predicted SRRs and the corresponding real measurements.

Figure 5 shows Relationship between WT-ANN's predicted SRRs and the corresponding real measurements. A high degree of accuracy and dependability in the model's predictive abilities is indicated by the correlation between the optimal WT-ANN model's predicted Signal-to-Reference Ratios (SRRs) and their actual measurements. This illustrates the model's ability to accurately simulate real-world data.

Table 1: The Output of unknown's data

Sensors → Samples ↓	**TGS 2611 (inv)**	**TGS 2620 (inv)**	**TGS 822 (inv)**	**TGS 2610 (inv)**	**TGS 816 (inv)**	**TGS 825 (inv)**	**Result TGS 2611 TGS 2611**		**% Error**
							Name of gas	**Conc. (ml)**	
Sample 1 (Acetone, 3ml.)	4.4900	4.6050	3.3410	0.1020	0.1010	3.3370	**Acetone**	2.652	**+11%**
Sample 2 (Ethanol, 1ml.)	0.4120	0.4379	0.3186	0.0232	0.0185	0.3488	Ethanol	1.002	**-0.2%**
Sample 3 (Ethanol, 1ml.)	0.4242	0.4749	0.3426	0.0098	0.0096	0.3478	Ethanol	0.984	+1.6%
Sample 4 (Ethanol, 1ml.)	0.4086	0.4530	0.3393	0.0193	0.0134	0.3454	Ethanol	2.992	+0.2%
Sample 5 (Benzene, 2ml.)	0.2850	0.4592	0.2326	0.0096	0.0093	0.2708	Benzene	2.002	-0.2%

Table 1 indicates that the first sample of unknown gas is 3 millilitres of acetone. The data set is tested, and the results show that the concentration of acetone is 2.652 millilitres, which is close to the 3 millilitres. The nearby value is also displayed in all other data.

Therefore, it is possible to detect VOC traces using the existing experimental setup and an ANN tool. When such a compound is found in cases of diabetes, lung cancer, or asthma, it indicates the existence of a disease. Considering that there is no chance to test on humans. It is expected that the system will function satisfactorily for non-invasively detecting such diseases.

5. Conclusion

In conclusion, the use of the WT-ANN model, which incorporates wavelet transformations as transfer functions within a multi-layered perceptron, demonstrates a significant advancement in detecting volatile organic compounds (VOCs) such as acetone with high precision. By employing the B-spline wavelet transfer function in the hidden layer, the WT-ANN model enhances the nonlinearity necessary for accurately correlating complex occurrences, surpassing the limitations of traditional MLP models with standard transfer functions. This innovative approach was effectively utilized to measure the acetone-detecting capacity of a tin oxide sensor, showing promising results with concentrations closely matching the actual values. The successful application of the WT-ANN model to detect acetone suggests its potential for broader applications, including the non-invasive detection of diseases such as diabetes, lung cancer, and asthma. Although direct testing on human subjects was not conducted in this study, the encouraging results obtained indicate that the system could reliably identify VOCs related to these conditions. Consequently, the WT-ANN model holds promise for future development in medical diagnostics, offering a novel tool for early and accurate disease detection through non-invasive methods.

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