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Graphite/TiO2 Nanoparticle-Based Flexible Sensor for Volatile Organic Compound Detection with Machine Learning-Assisted Classification

Khadija Javaid[1], Madeeha Nasir[2], Saeed Rasheed[3]

[1] Department of Physics University of Agriculture Faisalabad, Pakistan
Email: khadijaalvi124@gmail.com
[2] Department of Physics University of Agriculture Faisalabad, Pakistan
Email: madeehanasir321@gmail.com
[3] Department of Computer Science University of Agriculture Faisalabad, Pakistan
Email: saeed.rasheed0211@gmail.com

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Abstract

Flexible and low-cost chemical sensors have attracted significant attention for environmental monitoring, industrial safety, and healthcare applications. In this work, a Graphite/TiO_2 nanoparticle-based flexible sensor was fabricated on a cellulose paper substrate using a simple pencil drawing technique followed by the deposition of titanium dioxide (TiO_2) nanoparticles through a drop-casting method. The fabricated sensor was characterized using UV–Visible spectroscopy to investigate its optical properties. The sensing performance of the device was evaluated for the detection of volatile organic compounds (VOCs), including ethanol, chloroform, and ethyl acetate. The sensor exhibited distinct resistance changes upon exposure to VOC vapors, demonstrating its capability for chemical sensing. Among the tested analytes, ethanol showed the highest sensitivity of 117.1 with a response time of 10.3 s and a recovery time of 31.1 s, while chloroform and ethyl acetate exhibited sensitivities of 47.9 and 43.2, respectively. The enhanced sensing performance is attributed to the combined effect of the conductive graphite network and the high surface activity of TiO_2 nanoparticles. Furthermore, a machine learning-assisted classification framework based on the K-Nearest Neighbors (KNN) algorithm is proposed for intelligent VOC identification using sensor parameters such as sensitivity, response time, recovery time, and resistance variation. The developed Graphite/TiO_2 flexible sensor demonstrates excellent potential for low-cost, portable, and intelligent VOC monitoring applications.

Keywords: Graphite Sensor, TiO2 Nanoparticles, Flexible Sensor, VOC Detection, Machine Learning, KNN, Electronic Nose

Introduction

The rapid advancement of sensing technologies has created a growing demand for flexible, lightweight, and low-cost sensors capable of operating in diverse environmental and industrial conditions. Flexible sensors have attracted considerable attention due to their potential applications in environmental monitoring, healthcare diagnostics, food quality assessment, industrial safety, wearable electronics, and smart sensing systems [1]. Unlike conventional rigid sensors, flexible sensors can be fabricated on lightweight substrates and can conform to curved surfaces while maintaining their sensing performance. These characteristics make flexible sensors highly suitable for next-generation portable and wearable electronic devices. Among various sensing materials, carbon-based materials have emerged as promising candidates because of their excellent electrical conductivity, mechanical flexibility, chemical stability, and cost-effectiveness. Graphite is one of the most widely available allotropes of carbon and consists of layers of carbon atoms arranged in a hexagonal crystal structure [2]. The weak van der Waals forces between adjacent layers allow graphite to be easily transferred onto different substrates through simple mechanical methods. Due to its high electrical conductivity and ease of deposition, graphite has been extensively utilized in electronic devices, electrodes, energy storage systems, and chemical sensing applications.

Recently, graphite-on-paper technology has gained significant attention as a simple and environmentally friendly approach for fabricating flexible electronic devices. In this technique, graphite is directly deposited onto a cellulose paper substrate using a conventional pencil drawing method [3]. The cellulose paper acts as a flexible, biodegradable, lightweight, and low-cost substrate, while the deposited graphite serves as a conductive sensing layer. Compared with conventional fabrication techniques such as chemical vapor deposition, lithography, and sputtering, the graphite-on-paper method offers several advantages, including simplicity, rapid fabrication, low manufacturing cost, and minimal equipment requirements. Consequently, paper-based graphite sensors have been investigated for strain sensing, humidity sensing, pressure sensing, and chemical sensing applications. Despite the advantages of graphite-based sensors, their sensing performance can be further enhanced through the incorporation of nanomaterials. Nanomaterials possess a large surface-to-volume ratio, providing a greater number of active sites for molecular adsorption and interaction [2]. Titanium dioxide (TiO_2) nanoparticles are among the most widely studied nanomaterials for sensing applications because of their remarkable physical and chemical properties. TiO_2 nanoparticles exhibit high chemical stability, non-toxicity, corrosion resistance, hydrophilicity, biocompatibility, and strong photo catalytic activity. Furthermore, their large surface area facilitates efficient adsorption of gas and vapor molecules, making them highly suitable for chemical sensing applications [4]. The combination of graphite and TiO_2 nanoparticles provides a synergistic effect that can significantly improve sensor performance. The graphite layer offers a conductive pathway for charge transport, while TiO_2 nanoparticles enhance the interaction between target molecules and the sensing surface. When volatile organic compound molecules are adsorbed onto the Graphite/TiO_2 sensing layer, charge transfer processes occur, leading to measurable changes in electrical resistance. These resistance variations can be utilized for the detection and quantification of different chemical species. Volatile Organic Compounds (VOCs) represent a large class of carbon-containing compounds that readily evaporate at room temperature. VOCs are extensively used in industrial, pharmaceutical, agricultural, and laboratory applications [5]. Common VOCs include ethanol, methanol, acetone, benzene, chloroform, toluene, and ethyl acetate. Although these compounds are important in numerous industrial processes, excessive exposure to VOCs can pose significant risks to both human health and the environment. Prolonged exposure may lead to respiratory problems, headaches, dizziness, neurological disorders, and other adverse health effects [3]. Therefore, the development of sensitive, reliable, and portable VOC sensing systems is essential for environmental monitoring, workplace safety, and public health protection. Traditional VOC detection techniques such as gas chromatography, mass spectrometry, and spectroscopic methods provide excellent analytical performance but often require expensive instrumentation, trained personnel, and laboratory-based operation. In contrast, flexible chemical sensors offer a low-cost and portable alternative for real-time VOC monitoring [1]. Therefore, considerable research efforts have been directed toward the development of novel sensing materials capable of achieving high sensitivity, rapid response, fast recovery, and long-term stability [6].

In recent years, artificial intelligence (AI) and machine learning (ML) have emerged as powerful tools for enhancing the performance of chemical sensing systems. Machine learning algorithms can analyze complex sensor response patterns and extract meaningful information from multidimensional datasets [7]. These algorithms enable automatic classification, pattern recognition, anomaly detection, and concentration estimation of target analytes. The integration of machine learning with chemical sensors has led to the development of intelligent sensing platforms commonly referred to as electronic noses (E-noses) [8]. Among various machine learning techniques, the K-Nearest Neighbors (KNN) algorithm is widely employed due to its simplicity, robustness, and effectiveness. KNN is a supervised learning algorithm that classifies unknown samples based on the similarity of neighboring data points within the feature space. Sensor parameters such as sensitivity, response time, recovery time, and relative resistance change can be utilized as input features for KNN-based classification [9]. Consequently, the combination of Graphite/TiO_2 flexible sensors with machine learning algorithms can significantly improve VOC identification and sensor selectivity. Although numerous studies have reported graphite-based sensors, paper-based flexible sensors, and TiO_2 nanoparticle-enhanced sensing devices, limited research has focused on the development of Graphite/TiO_2 nanoparticle-based flexible sensors for VOC detection [7]. Furthermore, the application of machine learning techniques for intelligent classification of VOCs using such sensing platforms remains relatively unexplored. Therefore, there is a need to investigate low-cost sensing systems capable of detecting VOCs while providing the foundation for future AI-assisted chemical recognition [10]. The present work aims to fabricate a Graphite/TiO_2 nanoparticle-based flexible sensor on a cellulose paper substrate using a simple and cost-effective pencil drawing technique. The fabricated sensor is characterized using UV–Visible spectroscopy, and its sensing performance is evaluated toward ethanol, chloroform, and ethyl acetate vapors. Furthermore, a machine learning-assisted framework based on the K-Nearest Neighbors (KNN) algorithm is proposed for future intelligent VOC classification. The developed sensing platform is expected to contribute toward the advancement of low-cost, portable, flexible, and intelligent chemical sensing technologies [11].

Materials and Methods

Materials

The materials used in the fabrication of the flexible chemical sensor included cellulose paper, graphite pencils of different grades, titanium dioxide (TiO_2) nanoparticles, ethanol, chloroform, and ethyl acetate. The cellulose paper was used as a flexible substrate because of its low cost, lightweight nature, biodegradability, and mechanical flexibility. Graphite was deposited on the paper surface using commercially available graphite pencils to form the conductive sensing layer. Titanium dioxide (TiO_2) nanoparticles were employed to enhance the sensing performance due to their high surface area, chemical stability, and excellent adsorption characteristics. The VOC analytes selected for sensor testing were ethanol, chloroform, and ethyl acetate [12]. These compounds were chosen because they are commonly used in industrial, pharmaceutical, and laboratory applications and represent important volatile organic compounds requiring monitoring [13].

Sample Preparation

The conductive graphite layer was prepared using a direct pencil drawing technique on cellulose paper. A4-size cellulose paper was selected as the substrate because it provides mechanical flexibility and good adhesion for graphite particles. Initially, different grades of graphite pencils, including 2H, 4H, 6H, HB, 3B, 8B, and 9B, were investigated to determine the most suitable conductive material [11]. The resistance of each graphite trace was measured repeatedly to evaluate reproducibility and conductivity. The graphite layer was deposited by repeatedly drawing straight lines on the paper surface. Several drawing cycles were performed to ensure uniform graphite coverage and to obtain a continuous conductive path. During the deposition process, special attention was given to maintaining a uniform thickness of the graphite layer over the entire sensing area. The resistance of the deposited graphite layer was measured after each deposition cycle [14]. The pencil grade exhibiting the most stable and suitable electrical resistance was selected for device fabrication. The prepared paper substrate was then cut into the desired dimensions for sensor construction [10].

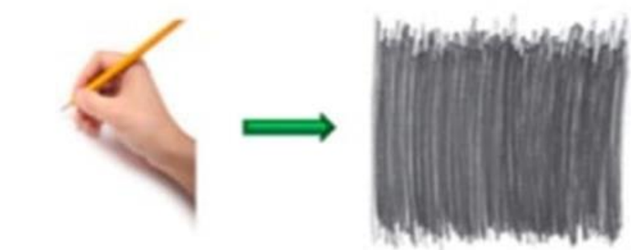

Figure1. Schematic illustration of graphite deposition on cellulose paper using the direct pencil drawing method.

Device Fabrication

The flexible chemical sensor was fabricated on a cellulose paper substrate using a simple and cost-effective fabrication procedure. First, the sensor pattern was designed and transferred onto the paper substrate [5]. A conductive graphite layer was then formed by applying graphite onto the designated sensing area through the pencil drawing technique. After obtaining a sufficiently conductive graphite film, titanium dioxide (TiO_2) nanoparticles were deposited onto the graphite-coated region using a drop-casting method. The nanoparticle suspension was carefully dropped onto the sensing area to achieve a uniform coating. Due to the porous and absorbent nature of the paper substrate, the TiO_2 nanoparticles adhered effectively without requiring additional adhesive materials [15]. The deposited TiO_2 layer was allowed to dry at room temperature to form a homogeneous sensing film. The presence of TiO_2 nanoparticles increased the active surface area available for adsorption of VOC molecules, thereby improving sensor sensitivity. Electrical contacts were established by attaching conductive wires to the graphite-coated regions using insulating tape. The fabricated sensor was then connected to the measurement system for electrical characterization and VOC sensing experiments [16].

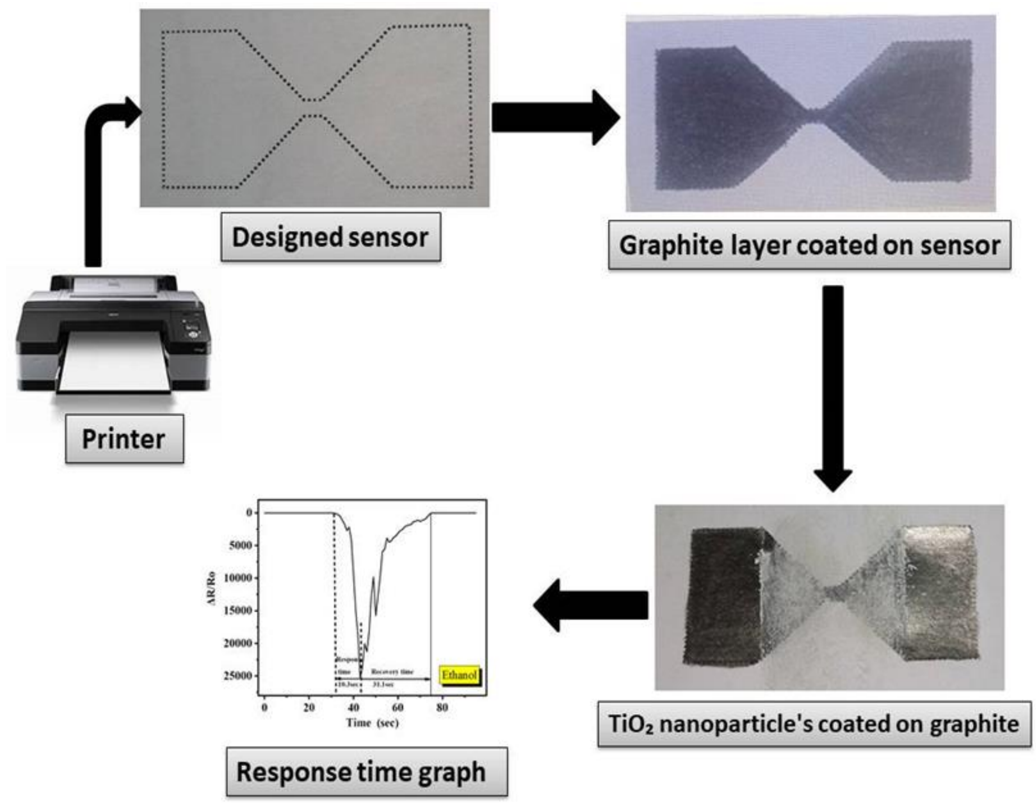

Figure 2. Fabrication process of the Graphite/TiO_2 nanoparticle-based flexible sensor.

UV–Visible Spectroscopy Characterization: The optical properties of the fabricated sensing material were investigated using UV–Visible spectroscopy. UV–Visible spectroscopy is a widely used analytical technique that measures the absorption of ultraviolet and visible radiation by a material as a function of wavelength. The absorption spectrum provides valuable information regarding electronic transitions occurring within the sensing material [15]. When electromagnetic radiation interacts with the material, electrons absorb energy and move from lower energy states to higher energy states. These transitions can be observed through absorption peaks in the UV–Visible spectrum. The UV–Visible characterization was performed over an appropriate wavelength range to evaluate the optical behavior of the Graphite/TiO_2 sensing layer. The obtained spectrum was used to analyze the absorption characteristics and confirm the interaction of TiO_2 nanoparticles with the graphite film [17].

Electrical Measurements and VOC Sensing

The electrical performance of the fabricated sensor was evaluated using a Keithley Source Meter. The instrument was used to measure changes in electrical resistance during exposure to different volatile organic compounds [18]. The sensor was exposed separately to ethanol, chloroform, and ethyl acetate vapors under controlled conditions. Upon exposure to VOC molecules, adsorption occurred on the Graphite/TiO_2 sensing layer, resulting in charge transfer interactions and measurable changes in resistance. The sensor response was recorded continuously as a function of time. The following sensing parameters were determined:

Sensor Response: The sensor response was calculated from the change in resistance before and after VOC exposure.

Response Time: Response time was defined as the time required for the sensor to reach approximately 90% of its maximum response after exposure to the target analyte.

Recovery Time: Recovery time was defined as the time required for the sensor to return to approximately 90% of its original resistance value after removal of the analyte.

Sensitivity: Sensitivity was determined from the relative change in electrical resistance resulting from VOC adsorption on the sensing surface [19].
The sensing performance of the fabricated Graphite/TiO_2 sensor was evaluated by comparing the response characteristics obtained for ethanol, chloroform, and ethyl acetate vapors.

Results and Discussion

UV–Visible Analysis:

The optical properties of the fabricated Graphite/TiO_2 sensing layer were investigated using UV–Visible spectroscopy. The obtained absorption spectrum provides valuable information regarding the electronic transitions occurring within the sensing material. The absorption behavior confirms the interaction between the graphite layer and TiO_2 nanoparticles and provides insight into their optical characteristics. The UV–Visible spectrum exhibited significant absorption in the ultraviolet region, indicating the presence of strong electronic transitions. The observed absorption can be attributed to the excitation of electrons from lower energy states to higher energy states within the sensing material. The incorporation of TiO_2 nanoparticles contributes to enhanced optical absorption due to their semiconductor nature and high surface activity. The strong absorption characteristics suggest that the Graphite/TiO_2 composite possesses favorable electronic properties that can facilitate charge transfer processes during VOC adsorption. These charge transfer interactions play an important role in the sensing mechanism by producing measurable changes in electrical resistance [14].

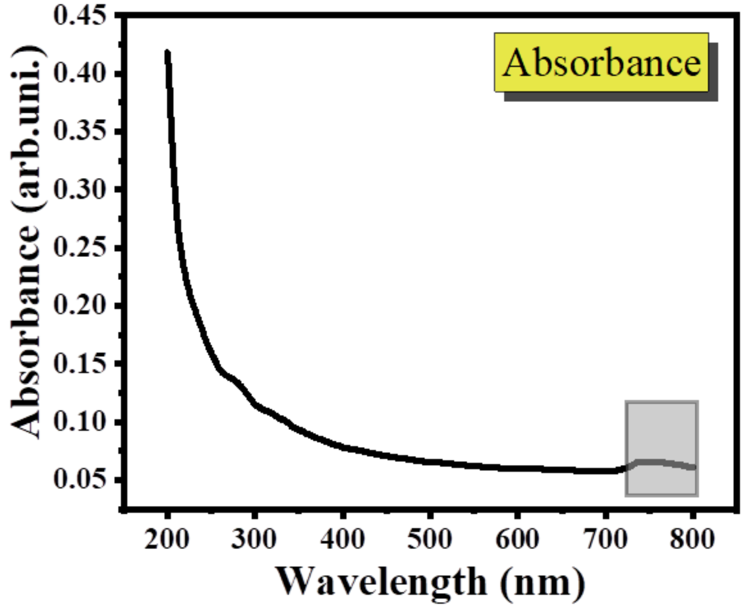

Figure 3. UV–Visible absorption spectrum of the fabricated Graphite/TiO_2 sensing layer.

VOC Sensing Performance

The sensing performance of the fabricated Graphite/TiO_2 flexible sensor was evaluated using three volatile organic compounds, namely ethanol, chloroform, and ethyl acetate [20]. The sensing response was monitored by measuring the resistance variation of the sensor during exposure and recovery cycles. The adsorption of VOC molecules on the Graphite/TiO_2 sensing surface results in charge transfer interactions that alter the electrical conductivity of the sensor. These conductivity changes were utilized to determine the response time, recovery time, and sensitivity of the fabricated device [21].

Ethanol Sensing Performance

Among the tested analytes, ethanol exhibited the strongest sensing response. Upon exposure to ethanol vapor, the sensor resistance changed rapidly due to the adsorption of ethanol molecules onto the Graphite/TiO_2 sensing layer. The fabricated sensor demonstrated a response time of 10.3 s and a recovery time of 31.1 s. The sensitivity toward ethanol was calculated to be 117.1, indicating excellent interaction between ethanol molecules and the sensing surface. The enhanced response can be attributed to the high adsorption affinity of ethanol molecules toward TiO_2 nanoparticles, which promotes efficient charge transfer and increases the conductivity variation of the sensing layer [20].

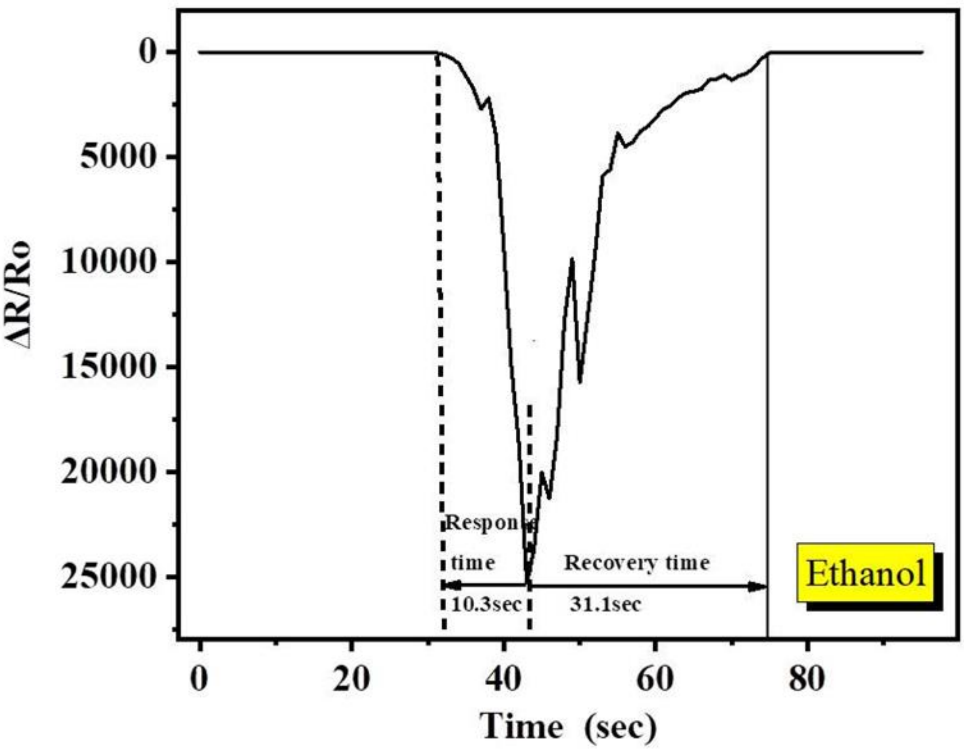

Figure 4. Dynamic sensing response of the Graphite/TiO_2 flexible sensor toward ethanol vapor.

Chloroform Sensing Performance

The sensing characteristics of the fabricated sensor were also evaluated for chloroform vapor. Upon exposure to chloroform, the sensor exhibited a noticeable resistance variation, confirming its capability to detect this VOC. The response time and recovery time were determined to be 16.3 s and 23.0 s, respectively. The calculated sensitivity was 47.9, which was lower than that observed for ethanol. The comparatively lower sensitivity may be associated with weaker adsorption interactions between chloroform molecules and the active sensing surface. Nevertheless, the sensor demonstrated reliable and repeatable detection behavior [18].

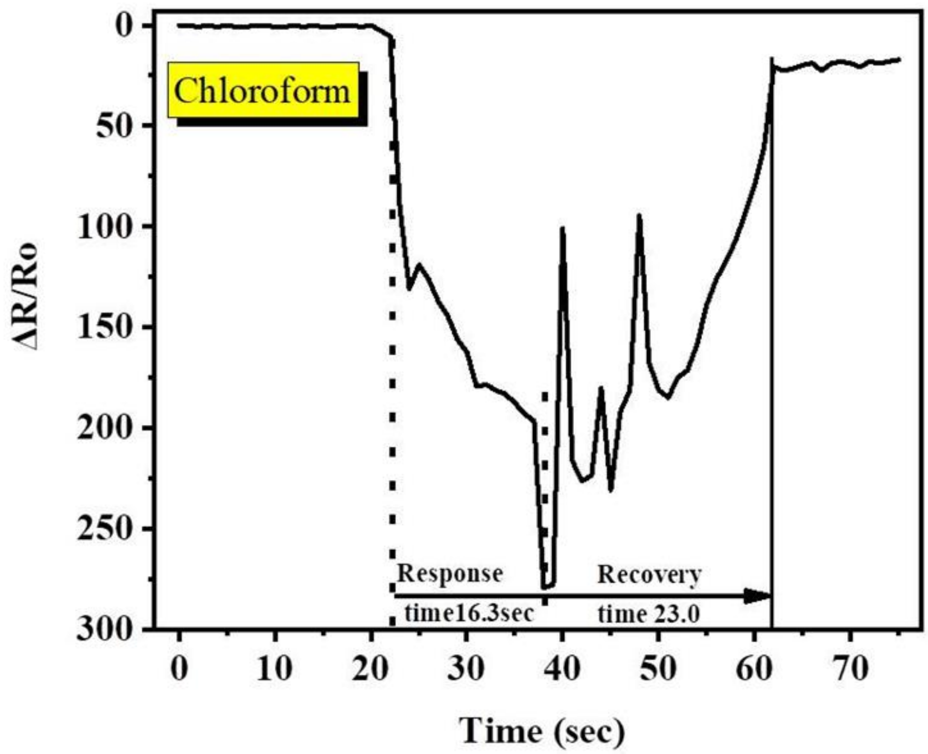

Figure 5. Dynamic sensing response of the Graphite/TiO_2 flexible sensor toward chloroform vapor.

Ethyl Acetate Sensing Performance

The fabricated sensor was further tested using ethyl acetate vapor. Similar to ethanol and chloroform, exposure to ethyl acetate produced measurable resistance changes, confirming the capability of the sensor to detect multiple VOC species. The response time and recovery time were recorded as 23.8 s and 45.8 s, respectively. The calculated sensitivity was 43.2. The longer response and recovery times indicate slower adsorption and desorption processes compared with ethanol and chloroform. However, the sensor maintained stable sensing behavior throughout the measurement cycle [21].

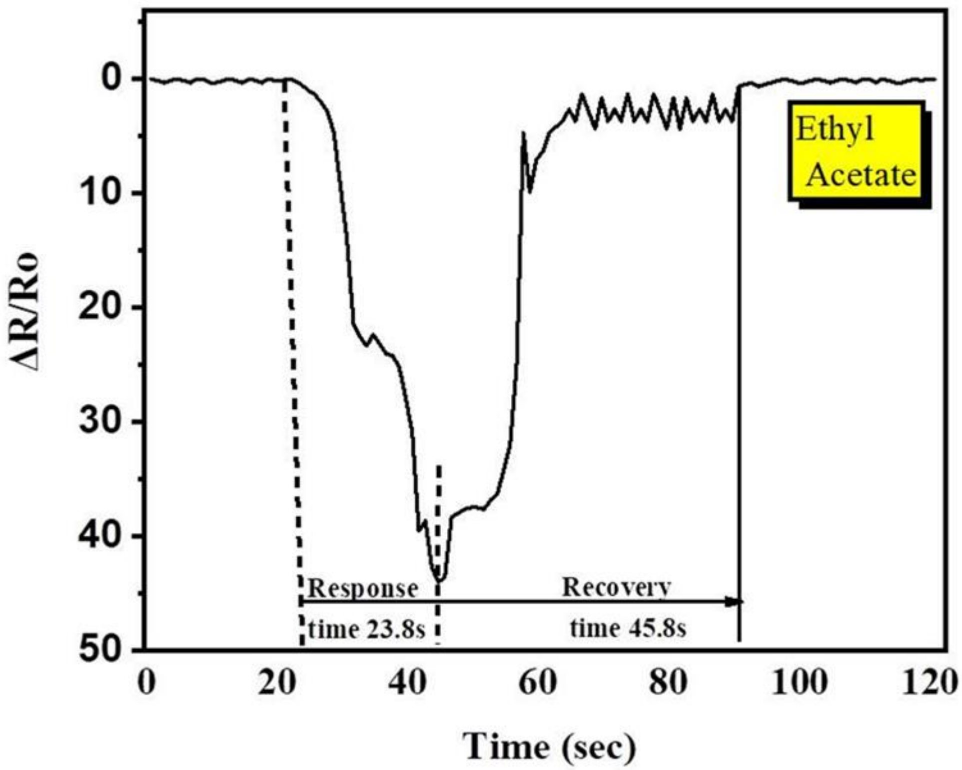

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Figure 6. Dynamic sensing response of the Graphite/TiO_2 flexible sensor towards ethyl acetate vapor.

Comparative VOC Analysis

A comparative analysis of the sensing performance was performed using the response time, recovery time, and sensitivity values obtained for each analyte.

Table 1. Comparative VOC sensing performance of the fabricated Graphite/ TiO_2 sensor.

VOC	Response Time (s)	Recove
Ethanol	10.3	31.1
Chloroform	16.3	23.0
Ethyl Acetate	23.8	45.8

The results clearly indicate that ethanol produced the highest sensitivity and fastest response among the tested VOCs. This behavior demonstrates the superior interaction of ethanol molecules with the Graphite/TiO_2 sensing layer

VOC Sensing Mechanism

The sensing mechanism of the Graphite/TiO_2 flexible sensor is based on the adsorption of VOC molecules onto the active sensing layer. When VOC molecules come into contact with the sensor surface, they interact with TiO_2 nanoparticles and the conductive graphite network. These interactions result in charge transfer processes that modify the carrier concentration within the sensing layer, leading to measurable resistance changes. The magnitude of resistance variation depends on the molecular properties of the target analyte, including polarity, molecular size, and adsorption affinity. TiO_2 nanoparticles provide a large number of active adsorption sites, while the graphite layer facilitates efficient charge transport. The synergistic combination of these materials enhances sensor sensitivity and improves detection performance.

VOC Molecules
(Ethanol / Chloroform / Ethyl Acetate)
↓
TiO_2 Nanoparticles
↓
Graphite Layer
↓
Paper Substrate
↓
Charge Transfer Process
↓
Resistance Change
↓
Sensor Response

Insert Figure 8. Proposed sensing mechanism of the graphite / TiO_2 flexible sensor during VOC adsorption and desorption

Machine Learning Assisted VOC Classification

Conventional gas and VOC sensors are capable of detecting changes in electrical resistance upon exposure to target analytes. However, when multiple VOCs produce similar sensor responses, distinguishing between different analytes becomes challenging. Machine learning techniques provide an effective solution by analyzing multiple sensor parameters simultaneously identifying unique response patterns associated with different VOCs. Recent advances in artificial intelligence have enabled the development of intelligent sensing systems capable of automatic recognition, classification, and prediction of chemical species. The integration of machine learning algorithms with flexible chemical sensors has led to the emergence of electronic nose systems that can perform real-time environmental monitoring with improved accuracy and reliability. In the present work, a machine learning-assisted framework based on the K-Nearest Neighbors (KNN) algorithm is proposed for future classification of VOCs detected by the fabricated Graphite/TiO_2 flexible sensor.

Feature Extraction

Machine learning algorithms require numerical input features that represent the behavior of the sensing device. The experimental parameters obtained from VOC sensing measurements can be used as feature vectors for classification.

The following sensor parameters were selected as input features:

- Sensitivity
- Response Time
- Recovery Time
- Relative Resistance Change ($\Delta R/R_0$)

These parameters provide sufficient information to differentiate between ethanol, chloroform, and ethyl acetate because each analyte exhibits a unique sensing signature.

Table 2. Proposed Features for KNN Classification

Feature	Description
Sensitivity	Relative sensor response
Response Time	Time required to reach 90% response
Recovery Time	Time required to recover 90% baseline
$\Delta R/R_0$	Relative resistance variation

K-Nearest Neighbors (KNN) Algorithm

K-Nearest Neighbors (KNN) is a supervised machine learning algorithm used for classification and pattern recognition tasks. The algorithm classifies unknown samples based on the characteristics of neighboring data points within the feature space. In KNN classification, the Euclidean distance between the unknown sample and all training samples is calculated. The sample is then assigned to the class that is most common among its K nearest neighbors.

The Euclidean distance is given by:

$d=\sqrt{\sum_{i=0}^{n}(xi-yi)}$

Where:

d = Euclidean distance

Xi = feature value of the unknown sample

Yi = feature value of the training sample

n = total number of features

The simplicity, robustness, and low computational complexity of KNN make it particularly suitable for small sensor datasets.

Proposed KNN-Based VOC Classification Framework

The proposed workflow for intelligent VOC recognition is illustrated below:

Graphite/TiO_2 Sensor
↓
Data Acquisition
↓
Feature Extraction
↓
Feature Matrix
↓
KNN Training
↓
VOC Classification

Output Classes

The classifier is designed to identify:

Ethanol, Chloroform, Ethyl Acetate, Each VOC possesses a unique combination of sensitivity, response time, and recovery time, allowing the KNN model to distinguish between analytes.

Potential Electronic Nose Applications

The integration of Graphite/TiO_2 flexible sensors with machine learning algorithms can facilitate the development of portable electronic nose systems. Such systems can automatically recognize different VOCs and provide real-time monitoring in various environments.

- Potential applications include:
- Environmental monitoring
- Industrial safety
- Air quality assessment
- Chemical leak detection
- Food quality monitoring
- Healthcare diagnostics

The combination of low-cost sensor fabrication and machine learning-assisted analysis offers a promising route toward intelligent sensing technologies.

Conclusion

A Graphite/TiO_2 nanoparticle-based flexible sensor was successfully fabricated on cellulose paper using a simple and cost-effective pencil drawing technique. The fabricated sensor exhibited excellent sensing performance toward ethanol, chloroform, and ethyl acetate vapors. Among the tested analytes, ethanol showed the highest sensitivity of 117.1 and the fastest response time of 10.3 s. The integration of TiO_2 nanoparticles enhanced the sensing performance through increased surface interaction with VOC molecules. Furthermore, the obtained sensing parameters demonstrate the feasibility of integrating machine learning algorithms such as KNN for intelligent VOC recognition and future electronic nose applications.

Future Work

Experimental implementation of the KNN classification. Comparison of KNN with other algorithms such as the Support Vector Machine (SVM) and Random Forest (RF). Detection of additional VOCs and gas mixtures. Integration with wireless and IoT-based monitoring systems. In development of portable electronic nose devices. Investigation of long-term stability and repeatability under practical operating conditions.

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