Integrated Gas Sensing and Biomarker Detection

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Sensor Technology and Machine Learning Applications

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INTRODUCTION

Sensor technology and development have received considerable attention from researchers in the fields of chemistry, physics, electronics and computer science. They have also grown considerably over the last few decades, due to the increasing demand for reliable, real-time and non-invasive diagnostic and monitoring solutions across a wide range of industries. The increase in environmental pollution, ranging from healthcare to environmental monitoring and industrial safety, makes sensors indispensable tools for detecting a wide variety of chemicals, gases and biomarkers.

The discovery of advanced materials, improved manufacturing techniques and powerful data analysis tools has expanded the capabilities of sensors, particularly in the fields of gas detection and environmental monitoring. Miniaturization also makes it possible to integrate sensors into portable systems. Various research projects have been published on the development of sensors in different fields which are complementary to each other in order to have an intelligent detection system.

Several research projects have been published on the development of sensors in different fields that complement each other to obtain an intelligent detection system. These areas of research include chemistry, physics, computing and instrumentation, with specific test benches depending on the technology used for the sensor (e.g. resistive, electrochemical, capacitive, acoustic …) to test and validate the detection systems.

This book is a revolutionary resource that provides an in-depth view on the sensing system and the pathway for researchers to improve their work on sensing systems, also it bridges the gap between advanced gas sensing technology and the transformative potential of machine learning.

Unlike many traditional texts that focus only on the types of sensors and techniques used for sensor improvement or the theoretical aspects of gas sensing, this book focuses on the critical role that machine learning can play in improving the accuracy, efficiency and functionality of gas sensors in real-world applications. It offers a unique and practical approach either on the technical part and manufacturing approaches to improve gas sensors or on the part of analyzing sensor data with ML & AI, addressing challenges such as sensor drift, environmental interferences and the need for real-time predictive models.

What sets this book apart is its specialized focus on the intersection of machine learning and gas sensing systems. While existing literature may touch on either gas sensors or machine learning separately, this book brings them together in a way that is not only technically insightful but also highly relevant to industries such as environmental monitoring, industrial safety, healthcare, automotive, and smart cities.

This book is a perfect overview for early career researchers, engineers and PhD students for research in the field of sensor improvement on the different parts going through all stages of manufacturing development and modification needed to improve performance as well as on the processing part through machine learning, to optimize sensor networks or to implement smart solutions in various sectors.

In this book the tools and knowledge needed to push the boundaries of what is possible are presented in detail. It is a mix of theoretical ideas and practical application-oriented content, it offers readers an overview and a complete roadmap to integrate advanced data science in the world of gas detection and biomarkers.

One of the most significant challenges in gas sensor technology is achieving high selectivity in environments where multiple gases are present. The ability to detect specific gases in complex mixtures is essential for applications ranging from industrial leak detection to environmental monitoring and even medical diagnostics. In this book, we explore various approaches to improve the selectivity and sensitivity of gas sensors, including chemical surface modifications and temperature modulation. These techniques have been shown to enhance sensor response by increasing the interaction between the sensor surface and target gases, as well as by optimizing the sensor's performance in fluctuating environmental conditions.

In addition, the chapters highlight the transformative role of machine learning (ML) and artificial intelligence (AI) in gas sensor systems. ML and AI have revolutionized many industries, and their application to sensor technology is no exception. The book explores how advanced signal processing techniques, coupled with powerful machine learning algorithms, are helping to interpret complex sensor data, improve sensor calibration, and enable real-time detection and quantification of gases with unprecedented accuracy. By leveraging these techniques, gas sensors can adapt to a wider range of environmental conditions, detect multiple gases simultaneously, and provide more accurate readings over time, even in the presence of interfering substances.

Biosensors, which are designed to detect biological markers such as proteins, hormones, and other biomarkers, are another major area of focus in this book. These sensors are particularly important in healthcare, where they can provide quick, non-invasive diagnostics. One of the most exciting advancements in the field of biosensing is the development of electrochemical immunosensors for detecting specific biomarkers such as tumor necrosis factor-alpha (TNF-α) in saliva. By utilizing gold-based electrodes and advanced detection techniques, these biosensors can detect low concentrations of biomarkers, offering an accessible and affordable alternative to more traditional diagnostic methods. The book delves into the detailed electrochemical characterization of such biosensors and discusses how various detection methods, such as chronoamperometry and impedance spectroscopy, can be employed to enhance the sensitivity and specificity of these devices.

The chapters also cover the critical aspects of data acquisition and sensor characterization, highlighting the various electrical & Optical measurement techniques used to assess the performance of gas and biosensor systems. These techniques are crucial for understanding how sensors behave under different environmental conditions and for ensuring their long-term stability and reliability.

Moreover, the book emphasizes the importance of portability and real-time capabilities in modern sensor systems. With the increasing demand for mobile and user-friendly diagnostic tools, the integration of these sophisticated sensors into portable, low-power devices is essential. Advances in miniaturization, coupled with improved signal processing and energy-efficient designs, have enabled the development of compact sensors capable of providing accurate, on-site measurements without sacrificing performance. This has significant implications for environmental monitoring, healthcare diagnostics, and industrial applications, where immediate feedback is often crucial.

Finally, the book explores the future direction of gas and biosensor technologies, highlighting the potential for further integration of machine learning and AI into sensor systems. As we move towards more complex and dynamic sensing environments, the use of AI-driven algorithms to optimize sensor calibration, predict sensor drift, and provide real-time adjustments will be key to unlocking the full potential of these technologies. The combination of highly sensitive materials, advanced data analysis techniques, and innovative sensor designs promises to usher in a new era of smart, adaptive sensors that can meet the demands of a wide range of applications.

In summary, this book aims to provide a comprehensive overview of the latest advancements in gas and biosensor technologies, offering valuable insights into the challenges and opportunities that lie ahead. The integration of multiple disciplines—materials science, electronics, machine learning, and artificial intelligence—has already made a significant impact on the development of next-generation sensors. By providing a detailed exploration of these cutting-edge technologies, we hope to inspire further research and innovation in this rapidly evolving field. Through collaboration and interdisciplinary efforts, the potential for creating highly efficient, reliable, and versatile sensors for gas detection and biomedical applications is immense, with far-reaching implications for health, safety, and the environment.

CHAPTER 1

ENHANCING GAS SENSOR SELECTIVITY AND PERFORMANCE: CHEMICAL SURFACE MODIFICATION, TEMPERATURE MODULATION, AND MACHINE LEARNING APPROACHES

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Abstract

Gas sensor technology has significantly progressed to respond to the growing requirement for selective, reliable and accurate gas detection in a diverse range of industries. This chapter explores the fundamental concepts and recent developments in gas detection, with a focus on strategies designed to improve sensor performance and selectivity. It begins with an overview of gas sensor technology, followed by an examination of techniques for enhancing selectivity, a critical challenge in multi-gas environments. Methods such as chemical surface modification and Temperature Modulation are discussed as key approaches to improving sensor sensitivity for specific gases. The chapter then delves into the role of signal processing and machine learning, highlighting how advanced algorithms improve the interpretation of complex sensor data, enhance selectivity, and enable precise gas identification and quantification. The chapter concludes by exploring the applications of machine learning in gas detection, demonstrating its impact on improving the accuracy, adaptability, and intelligence of gas sensing systems. This discussion underscores the integration of chemistry, engineering, and artificial

intelligence as a pathway to developing next-generation gas sensors that can meet evolving sensing demands.

1 Introduction

In industry, environmental surveillance, personal safety and portable devices, the use of gas sensors is vital. They are critical for the advance detection of dangerous gases, which helps to protect the environment and people's health, and to avoid accidents.

Despite their importance, gas sensors face significant challenges and opportunities. A primary challenge is to enhance both sensitivity and selectivity, enabling the detection of low gas concentrations while minimizing false alarms and interference from other substances. Recent advancements in materials and sensing technologies are paving the way for innovative solutions to these issues. Additionally, detecting gas mixtures and complex compositions complicates sensor selectivity and accuracy.

Miniaturization and integration represent another vital challenge in the evolution of gas sensors (Gomez Palacios & Bracamonte, 2022). The demand for compact, portable & smart devices necessitates smaller and lighter sensors that can be integrated into smartphones, wearables, and other technologies for personal environmental monitoring (Agrawal et al., 2021). This trend not only facilitates mobile gas detection but also enables large-scale monitoring efforts (Zong et al., 2025). Furthermore, the integration of gas sensors with advanced data analytics techniques, such as machine learning (ML) and artificial intelligence (AI), offers exciting opportunities for improved detection and analysis(Nasri et al., 2023). These technologies can enhance sensor performance, enable predictive maintenance, and extract valuable insights from the data collected.

The advent of the Internet of Things (IoT) also presents significant prospects for gas sensors. Connected sensors facilitate real-time monitoring, large-scale data collection, and advanced analytics, enabling proactive gas management, rapid emergency response, and resource optimization (Ali et al., 2025). Additionally, the durability and autonomy of gas sensors are critical considerations. Sensors must be robust enough to operate effectively in challenging environments with varying temperature and humidity levels. Improving energy autonomy—either through alternative energy sources or by reducing power consumption—is also essential (Liu et al., 2014; Tai et al., 2020) . Ongoing research and development efforts aim to create manufacturing techniques that lower production costs while maintaining sensor performance and quality .

This chapter provides an overview of foundational and modern approaches to gas sensing, starting with traditional techniques and materials used in sensor construction. It explores strategies for enhancing sensor selectivity and reliability, including chemical surface modifications (Woo et al., 2016), temperature modulation (Zhao et al., 2020), and advanced signal processing methods (Nasri et al., 2023). Notably, the integration of machine learning (ML) and artificial intelligence (AI) has opened new pathways for sensor optimization, allowing for dynamic adaptation to environmental conditions and increased accuracy in complex settings.

2 Ameliorate Performance selectivity

In gas sensing technology, the performance of a sensor is critically evaluated based on its selectivity. This parameter defines the sensor's capability to accurately detect specific target gases in complex environments, often containing multiple gaseous species.

Selectivity is defined as the sensor's ability to preferentially detect a specific target gas while exhibiting minimal or no response to other non-target gases present in the environment. Achieving high selectivity is essential in applications such as environmental monitoring, industrial safety, and medical diagnostics, where accurate identification of a particular gas is necessary.

Several methods have been employed to enhance the selectivity of gas sensors like Chemical Surface Modification, Temperature Modulation, and Signal Processing Techniques using ML & AI**.** These methods are explained in the following subsections.

2.1 Chemical Surface Modification

To improve the selectivity using the Chemical Surface Modification, the **s**ensors can be coated with functional materials designed to selectively interact with the target gas. This functionalization can either enhance the sensor's affinity for the desired gas or block the interactions with interfering species.

Various structures can be employed in gas sensors to enhance their performance. One effective approach is the decoration of organic semiconductors with metal oxides, which can significantly boost both selectivity and sensitivity. The choice of oxide material is determined by the specific gas being targeted. Moreover, the dimensionality of the sensing material (whether 0D, 1D, 2D, or 3D) and the available surface area for gas adsorption also play a crucial role in improving sensor efficiency.

To enhanced H_2 sensing performance by decorating ZnO nanoparticles with Pd using UV irradiation. The fabricated transparent sensor demonstrated high sensitivity to H_2 gas, particularly at 250°C, and could detect H_2 in mixtures with benzene and toluene. The improved response was attributed to Pd's catalytic effect, the formation of Pd-ZnO heterojunctions, and PdHx, offering promising results for practical H_2 detection applications (Kim et al., 2024).

In addition , Han et al presents a method to enhance the sensitivity of a p-type metal oxide semiconductor gas sensor for NO_2 detection. The sensor was fabricated using CuO nanowires grown by thermal oxidation and decorated with ZnO nanoparticles via the sol-gel method. The CuO/ZnO heterojunction improved NO_2 sensitivity compared to the pristine CuO sensor by reducing the width of the hole accumulation layer (HAL) and increasing the initial resistance. The sensor's morphology, composition, and structure were characterized using FE-SEM, EDX, and X-ray diffraction techniques(Han et al., 2021).

Mankar et al. enhanced ammonia gas sensing in $SmFeO_3$ (SFO) thick films by modifying them with cobalt (Co) and palladium (Pd). Co-SFO films were fabricated and further dipped in palladium nitrate to improve sensitivity. The Pd-decorated films exhibited increased sensitivity to 50 ppm ammonia and reduced operating temperatures, with the 3-minute Pd treatment showing the best performance. The improved sensitivity was attributed to the chemical sensitization effect of palladium(Mankar & Kapse, 2024).

Moreover, Cai et al. focuses on improving acetone gas sensing by decorating SnO_2 nanowires (NWs) with Co_3O_4 nanoparticles (NPs) using a vapor-liquid-solid (VLS) and hydrothermal process. The strategy involved optimizing the size and uniform dispersion of Co_3O_4 NPs on SnO_2 NWs, resulting in a 17-fold increase in sensor responsiveness to 50 ppm acetone compared to sensors with pure SnO_2 NWs. The enhanced sensor also detected acetone at a low concentration of 0.1 ppm. The improvement is attributed to the creation of a p-n heterojunction from the well-distributed Co_3O_4 NPs, which significantly boosted the sensor's performance(Cai & Park, 2023).

In addition, the selectivity of gas sensors was improved by functionalizing tin oxide (SnO_2) films with size-controlled platinum (Pt) nanoparticles. Using magnetron-sputtering inert-gas condensation, Pt nanoparticles with a narrow size distribution (around 3 nm) were deposited on SnO_2 films. The research found that adjusting the deposition time of Pt nanoparticles allowed for fine-tuning of the sensor's selectivity between CO and volatile organic compounds (VOCs). Optimal deposition times were identified to enhance sensor sensitivity, while excessive coverage did not further improve sensitivity. The study highlights that precise control over nanoparticle size and coverage can significantly enhance the gas sensor's selectivity(Sosada-Ludwikowska et al., 2024).

The table.1 illustrates different approaches to enhance gas sensor selectivity through surface functionalization with various materials and nanostructures.

Table 1.1 Summary of Chemical Surface Modification Techniques for Enhancing Gas Sensor Selectivity

Study	Technique	Gas Analyzed	Outcome
ZnO nanoparticles with Pd (Kim et al., 2024)	Decoration of ZnO nanoparticles with Pd using UV irradiation	H_2	Enhanced sensitivity to H_2, especially at 250°C, due to Pd's catalytic effect and Pd-ZnO heterojunctions.
CuO/ZnO heterojunction (Han et al., 2021)	CuO nanowires decorated with ZnO nanoparticles via sol-gel method	NO_2	Improved NO_2 sensitivity by reducing HAL width and increasing initial resistance.
Co-Pd modified SFO (Mankar & Kapse, 2024)	$SmFeO_3$ thick films modified with cobalt and palladium	Ammonia (NH_3)	Increased sensitivity to 50 ppm ammonia at lower operating temperatures, attributed to Pd chemical sensitization.
SnO_2 nanowires with Co_3O_4 (Cai & Park, 2023)	SnO_2 nanowires decorated with Co_3O_4 nanoparticles	Acetone	17-fold increase in sensor response to 50 ppm acetone, with detection as low as 0.1 ppm.

SnO_2 films with Pt nanoparticles (Sosada-Ludwikowska et al., 2024)	Tin oxide (SnO_2) films functionalized with size-controlled platinum nanoparticles via magnetron sputtering	CO and VOCs	Fine-tuned selectivity between CO and VOCs by controlling Pt nanoparticle size and deposition time.

2.2 Temperature Modulation

Temperature modulation is a key technique for enhancing odorant discrimination. By altering the operating conditions, gases display unique responses across different temperature ranges. In the following section, we review various studies that have employed this approach to improve sensor selectivity.

Metal oxide (MOX) sensors have been used for resistive gas detection, but their broad-spectrum response at a constant temperature limits their selectivity. To improve this, a gas sensor featuring Pt-modified zinc oxide was developed using homogeneous precipitation and screen-printing techniques. The study introduces a novel approach that combines temperature and light modulation, producing distinct Resistance-Temperature (R-T) curves and parameters, along with photo-response and photo-relaxation characteristics. This method, when coupled with pattern recognition, successfully classified five gases—ethanol, methanol, acetone, formic acid, and ethyl ether—with a classification rate of 100%, compared to 95.55% achieved with temperature modulation alone. These results demonstrate that integrating temperature and light modulation significantly enhances the selectivity of gas sensors (Deng et al., 2017).

Additionally, Llobet et al. enhanced detection performance by employing dynamic sensor techniques, specifically through temperature modulation. This approach helps to optimize the sensor's response by altering the surface interactions between the sensor and the target gases. Although significant research has been conducted, selecting modulation frequencies has generally been an empirical and unsystematic process. A novel approach introduces the use of pseudo-random binary sequences (MLS) to modulate sensor temperatures across a broad range of frequencies. By applying circular cross-correlation between the MLS and sensor responses, the impulse response of the gas-sensor system can be determined. Analysis of this impulse response in the frequency domain allows for the identification of critical frequencies that carry important information for gas detection and quantification(Llobet et al., 2004).

Furthermore, Herrero-Carrón et al. developed a temperature modulation algorithm called "active and inverse." The term "active" refers to the fact that the modulation continuously adjusts based on the sensor's real-time response, while "inverse" indicates that the target sensor response is set first, and then the necessary modulation is calculated to reach that target. Their results show that this algorithm reliably classifies odorants. Additionally, they were able to classify odorants in sequence without the need for any cleaning process between different odorants(Herrero-Carrón et al., 2015).

Therefore, to improve sensor selectivity, Fan et al. employ temperature modulation to better capture the sensor's dynamic responses and extract more detailed features. They use two types of heating voltage signals: a low-frequency square wave for rapid temperature changes and a triangular wave for more gradual heating. These techniques enable the classification and concentration prediction of ethanol, methanol, methyl ethyl ketone (MEK), ethyl acetate, and their mixtures. Following feature extraction, a neural network is applied for gas classification and concentration prediction, achieving 100% accuracy with both heating methods(Fan et al., 2024).

In complex gas mixtures where trace minor components can interfere with detection, Ji et al. propose a method to mitigate performance degradation. This method involves analyzing the microscopic characteristics of gas sensitivity and response curve errors across different time domains. The approach identifies specific time domains to optimize sensor performance. For example, cooling time domains are selected to enhance the detection of primary gases while minimizing interference from minor components. In contrast, high-temperature time domains are used to better tolerate errors induced by these trace gases. By integrating these time domains, the method establishes an anti-interference time domain that improves the sensor's ability to distinguish target gases and reduce the impact of minor components. The effectiveness of this approach is confirmed through a decision tree algorithm. In summary, Ji et al.'s method enhances sensor selectivity and diminishes the influence of trace gases, thereby making semiconductor sensors more effective in complex gas environments (Ji et al., 2023).

Table 1.2 Summary of Gas Sensor Techniques with Temperature Modulation and Their Outcomes

Study	Technique	Gas Analyzed	Outcome
Pt-modified ZnO sensor (Deng et al., 2017)	Temperature & light modulation with pattern recognition	Ethanol, methanol, acetone, formic acid, ethyl ether	Classification rate of 100%, higher than 95.55% with temperature modulation alone.
Llobet et al. (Llobet et al., 2004)	Dynamic sensor technique, temperature modulation, pseudo-random binary sequences (MLS)	Complex gas mixtures	Identified critical frequencies for gas detection and quantification using cross-correlation analysis.
Herrero-Carrón et al. (Herrero-Carrón et al., 2015)	"Active and inverse" temperature modulation algorithm	Odorants	Reliable classification of odorants without the need for cleaning between odorants.
Fan et al. (Fan et al., 2024)	Temperature modulation using square and triangular wave heating signals	Ethanol, methanol, MEK, ethyl acetate, and mixtures	Achieved 100% accuracy in gas classification and concentration prediction using neural networks.
Ji et al. (Ji et al., 2023)	Time-domain analysis, cooling and high-temperature domains to minimize interference from trace gas components	Complex gas mixtures	Improved sensor selectivity and reduced interference from minor components using a decision tree algorithm.

The table 2 outlines various strategies for improving sensor selectivity via temperature modulation, with certain methods leveraging signal processing and machine learning techniques. In the next subsection, we will delve into the use of advanced data processing methods.

2.3 Signal Processing & Machine Learning Techniques

Advanced data processing methods, including machine learning and pattern recognition algorithms, can enhance sensor selectivity. These techniques analyze the sensor's response patterns to differentiate between target and non-target gases, effectively filtering out noise and improving the accuracy of gas detection. By leveraging these algorithms, sensors can achieve better performance in distinguishing between various gases and minimizing interference from unwanted signals.

Despite efforts to optimize the structures and materials of specific gas sensors for targeted detection, these sensors often still respond to other gases. To address this issue and enhance sensor performance, researchers are increasingly adopting advanced data processing technologies. For instance, machine learning techniques can be employed to improve selectivity and stability while accounting for environmental factors such as humidity and temperature.

In a sensor network, each sensor has unique characteristics—such as differing sensing materials, electrodes, and designs—that provide varied measurement data for each gas. This diversity in data is leveraged in the learning process to enhance selectivity.

The e-nose system, as depicted in Figure 1, comprises two main components: the smart gas sensor network for data collection and the machine learning-based analysis and processing system. The data processing begins with extracting characteristic parameters from the sensor responses, a process known as feature selection. Subsequently, supervised and unsupervised machine learning algorithms are applied to these features to improve the selectivity of the sensor. This integrated approach is referred to as a smart sensor or electronic nose.

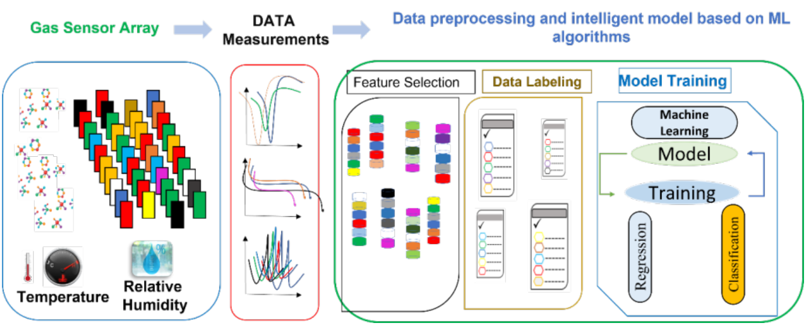

Fig. 1-1 Smart gas sensor system using machine learning(Nasri et al., 2023)

Advances in technology have led to the integration of machine learning (ML) algorithms into gas sensors, significantly enhancing their capabilities beyond traditional threshold limits. These smart sensor systems now offer more complex data analysis and decision-making processes, resulting in improved accuracy and versatility. The general architecture of such systems includes key stages involving data processing and ML-driven analysis.

The first stage involves preparing raw sensor data through pre-processing techniques. This step includes methods such as noise reduction, normalization, and feature extraction. These processes are crucial for improving the quality of the data and ensuring that the most relevant features are highlighted for further analysis.

Once pre-processing is complete, the refined data is fed into a trained ML model. The model is specifically selected based on the application's requirements and is responsible for performing advanced analysis, predictions, or classifications. By employing sophisticated algorithms, the smart sensor system can handle various types of sensor data, enabling more informed decision-making.

Smart sensor, showed in Figure 2, models generally fall into two categories, each addressing different analytical needs. Regression-based models focus on predicting continuous outcomes, using ML algorithms to establish relationships between sensor data and future values. These models are ideal for applications where quantitative predictions are required, such as forecasting concentrations of gases over time. Classification-based models, on the other hand, specialize in categorizing sensor data into distinct classes or labels. These models are used when the task involves identifying different types of gases or concentrations, offering a more qualitative analysis.

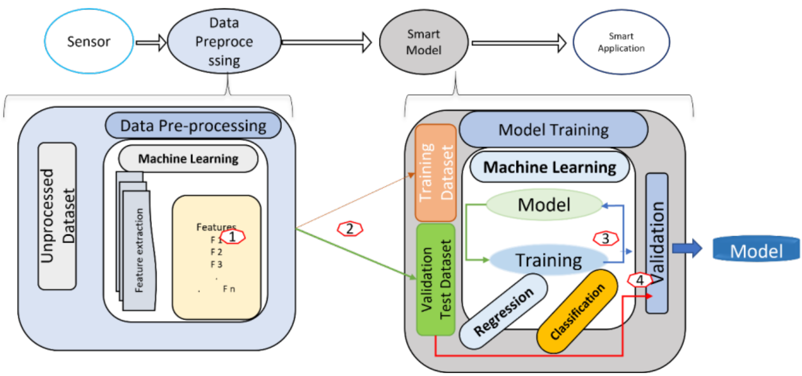

Fig. 1-2 Block diagram of a smart sensor system(Nasri et al., 2023)

The learning phase is essential for constructing an accurate predictive model. During this phase, the system utilizes two sets of variables: independent variables, which are external factors not directly influenced by the sensor's response, and dependent variables, which represent the sensor's output. The ML model learns the relationship between these variables, enabling it to identify patterns and make accurate predictions or classifications when new data is introduced.

This intelligent approach to gas sensing significantly enhances the sensor's overall performance. The ability to recognize patterns and relationships in the data allows the sensor to operate with greater precision, adapting to various applications such as environmental monitoring, industrial safety, and medical diagnostics. The integration of ML into gas sensors marks a significant step forward, paving the way for more responsive and adaptive sensing technologies across multiple fields.

Table 1-3 Overview of Advanced Data Processing Methods for Enhancing Gas Sensor Selectivity Using Machine Learning

Stage	Description	Techniques Used	Outcome
1. Data Collection	Sensors with varied materials, electrodes, and designs collect diverse measurement data for each gas	Smart sensor network (e-nose system)	Diverse sensor characteristics are leveraged to improve gas detection selectivity.
2. Pre-processing	Prepares raw sensor data by removing noise and normalizing data for further analysis	Noise reduction, normalization, feature extraction	Improves data quality and highlights relevant features for analysis.
3. Feature Selection	Extracts characteristic parameters from sensor responses	Feature selection methods	Identifies key features that are crucial for distinguishing between target and non-target gases.
4. Machine Learning Model Training	Trains models on pre-processed and selected features to predict or classify gases	Supervised and unsupervised ML algorithms	Enhances selectivity, stability, and accounts for environmental factors like humidity and temperature.

Prediction/Classification	Applies trained ML models to make informed predictions or classifications of gases	Decision-making algorithms	Improves the accuracy of gas detection, minimizing interference from non-target gases.

3 Machine learning in gas sensor

3.1 ML & IA algorithms

Machine learning (ML) in gas sensors is revolutionizing the way sensors detect and classify gases. Traditionally, gas sensors rely on physical or chemical reactions to detect the presence of specific gases, but these systems can be limited by issues such as poor selectivity, drift, and noise. ML offers solutions by leveraging complex data patterns that traditional models can't easily detect. Here's how ML is applied to gas sensors, as shown in the table. This table provides a concise overview of the major machine learning applications in gas sensing.

The table 4 summarizing the machine learning algorithms commonly used for enhancing sensor selectivity in electronic nose systems.

Table 1-4 Machine learning algorithms commonly used for enhancing sensor selectivity in electronic nose systems.

Algorithm	Description	Application in Sensor Systems	References
Linear Discriminant Analysis (LDA)	A linear classification algorithm that finds the linear combinations of features that best separate classes	Used for classifying gases by maximizing the separation between different gas categories.	(Boujnah et al., 2022a)
Principal Component Analysis (PCA)	A dimensionality reduction technique that transforms data into a set of linearly uncorrelated variables (principal components)	Helps in reducing the complexity of sensor data while retaining essential information for classification.	(Zeng et al., 2024)

Support Vector Machine (SVM)	A supervised learning algorithm that finds the optimal hyper-plane to separate data points in different classes	Provides accurate gas classification by identifying the best boundaries between target and non-target gases.	(Hadroug et al., 2024)
Random Forest (RF)	An ensemble learning method using multiple decision trees to make robust predictions	Enhances gas detection selectivity by combining predictions from various trees to improve accuracy.	(Tan et al., 2024)
Multilayer Perceptron (MLP)	A type of artificial neural network that consists of multiple layers to model complex patterns in data	Used for gas classification and concentration prediction by capturing complex relationships in sensor data.	(Lee et al., 2024)

Here's a detailed breakdown of key ML applications in gas sensing, including descriptions and examples of specific techniques:

Table 1-5

ML Application	Description	ML Techniques	References
Feature Extraction	Extracting meaningful patterns from sensor signals, especially in dynamic or modulated systems.	PCA, Feature Engineering	(R.M. et al., 2020) (Zeng et al., 2024)
Gas Classification	Identifying and distinguishing different gases based on sensor responses.	ANN, SVM, Random Forests, KNN	(Boateng et al., 2020; Thanh Noi & Kappas, 2017)
Concentration Estimation	Predicting gas concentration levels by mapping sensor responses to known concentrations.	ANN, Regression Models	(Ahmad et al., 2019; Shams et al., 2021)

Drift Compensation	Adjusting for sensor drift over time to maintain accuracy.	Time-series Models, ANN, Adaptive Algorithms	(Ren et al., 2024)
Data Fusion	Combining data from multiple sensors to improve detection accuracy and robustness.	Ensemble Learning, ANN, Data Fusion Algorithms	(Meng et al., 2020)
Anomaly Detection	Identifying abnormal patterns in sensor data to detect issues like malfunctions or unexpected gases.	Autoencoders, Anomaly Detection Algorithms (Isolation Forest)	(Mendes et al., 2022)

3.2 Example of ML & AI in gas sensor application

The integration of multiple non-selective sensors with advanced multivariate data processing methods is a leading approach to enhancing the selectivity of gas sensors, thereby improving the performance of electronic noses. The primary goal of machine learning (ML) algorithms in this context is to identify patterns in sensor data that can effectively differentiate between various gases or mixtures of gases (Men et al., 2014). It is advisable to experiment with several algorithms to determine the most effective one for accurate classification. Below, various machine learning algorithms and their application to different sensor networks are summarized as show in the table 6.

For example, Habib et al. utilized a dataset from a network of six gas sensors and applied decision trees and artificial neural networks (ANNs) for classification, achieving accuracy rates of 91.2% and 85.3%, respectively (Habib et al., 2019) .

In military applications, ML algorithms have been employed to classify Chemical Warfare Agents (CWA). Wiederoder et al. used a 12-unit sensor array with IDE electrodes and graphene nanoplatelet-polymer material. They applied Principal Component Analysis (PCA) to the data and then used four different ML algorithms to assess classification performance. This system demonstrated high discrimination capability for various analytes, including CWA simulants and common background interferents (Wiederoder et al., 2017).

Table 1-6 Table of Machine Learning Algorithm Performance Across Various Gas Sensor Networks

Sensor Network	Algorithms Used	Target Gases	Results/Accuracy	Reference
Network of 6 gas sensors	Decision Trees, ANN	General gas detection	Decision Trees: 91.2% accuracy, ANN: 85.3% accuracy	**Habib et al.** (Habib et al., 2019)
12-unit IDE sensor array with graphene-polymer	PCA, SVM, LDA, k-NN	5 CWA simulants, 8 background interferents	High discrimination capability for CWA simulants using different ML algorithms	**Wiederoder et al.** (Wiederoder et al., 2017)
Sensor array for mixed gases	Decision Trees, SVM, Naive Bayes, k-NN	Mixed gases	Optimized SVM and Naive Bayes achieved 100% accuracy	**Khan et al.** (Khan et al., 2020)
E-tongue with 7 detector units (IDE electrodes)	MLP, RF, XGBoost	Endocrine Disruptors (estrone, estradiol, bisphenol A)	XGBoost outperformed MLP and RF with RMSE values: 0.19 to 3.37 for individual EDCs and mixtures	**Christinelli et al.** (Christinelli et al., 2021)
MEMS gas sensor array	DBN-DNN, BPNN	Mixed gases	DBN-DNN model performed better than BPNN for gas identification and quantification	**Tang et al.** (Tang et al., 2020)
Gas sensor data	GasNet (DCNN), SVM, MLP	General gas classification	GasNet achieved higher accuracy than SVM and MLP, but with longer computation time	**Peng et al.** (Peng et al., 2018)
24 conductometric gas sensors	PCA, LDA, k-NN	Acetone, ethanol, water	LDA: 100% accuracy, PCA: 93.53%, k-NN: 73.14%	**Boujnah et al.** (Boujnah et al., 2022b)
12 different SAW sensors	k-NN, SVM	DCP, DBS, DMMP	Classification accuracy between 80% and 100%	**Sunil et al.** (Sunil et al., 2015)

Khan et al. tested decision trees, SVM, Naive Bayes (NB), and k-Nearest Neighbors (k-NN) algorithms to optimize the classification of target gases in both single and mixed conditions. By tuning parameters such as tree depth for decision trees and kernel types for SVM, they achieved up to 100% accuracy with the optimized models (Khan et al., 2020).

Christinelli et al. used an electronic tongue with seven IDE electrodes to detect endocrine disruptors (EDCs) like estrone and bisphenol A. They compared the performance of Multi-Layer Perceptron (MLP), Random Forest (RF), and Extreme Gradient Boosting (XGBoost) models, finding that XGBoost provided the best results with root mean square errors (RMSE) ranging from 0.19 to 3.37 for individual contaminants and mixtures (Christinelli et al., 2021).

A Shear Horizontal Surface Acoustic Wave (SH-SAW) sensor array was employed by Cruz et al. to identify NO_2 among other toxic chemicals. The SH-SAW sensors, fabricated with carbon-based materials, were analyzed using PCA, LDA, and k-NN. The study showed that while PCA provided statistical discrimination, LDA and k-NN were more effective in classifying mixed gases with high accuracy (Cruz et al., 2022).

Machine learning can also reduce the cost of e-nose sensors by optimizing sensor arrays. Sunil et al. used ML algorithms to select the best set of SAW sensors from twelve different ones, achieving classification accuracies between 80% and 100% with k-NN and SVM (Sunil et al., 2015).

Moreover, Tang et al. developed a Deep Belief Network – Deep Neural Network (DBN-DNN) for a MEMS gas sensor array. This model, built using MATLAB, outperformed the Back Propagation Neural Network (BPNN) by effectively addressing local extremum issues through unsupervised pre-training with Restricted Boltzmann Machines (RBMs). The DBN-DNN model's performance improved with more RBM layers, achieving up to 96.01% accuracy respectively (Tang et al., 2020).

Peng et al. introduced the GasNet model, a Deep Convolutional Neural Network (DCNN) for gas classification, which outperformed traditional methods like SVM and MLP in classification accuracy. However, it required significantly more computation time for training (Peng et al., 2018)

In addition, Boujnah et al. employed PCA, LDA, and k-NN to analyze data from 24 conductometric gas sensors for detecting acetone, ethanol, and water. They found that LDA provided the highest accuracy of 100%, with PCA and k-NN offering 93.53% and 73.14% accuracy, respectively (Boujnah et al., 2022b).

Conclusion

In conclusion, gas sensor advances have evolved considerably, going beyond traditional methods to address fundamental challenges such as limited selectivity, noise and drift. This chapter has explored the main methods for improving sensor performance, including chemical surface modifications, temperature modulation and advanced signal processing. The application of machine learning (ML) and artificial intelligence (AI) has proven to be a powerful approach, enabling gas sensors to achieve greater accuracy, better selectivity and reliable drift compensation.

Using artificial intelligence and machine learning tools such as PCA, SVM, Random Forests and Neural Networks, sensors can not only successfully identify gases, but can also provide concentration level estimates and identify gas anomalies. Thanks to these powerful algorithms, they have a robust data analysis ability that conventional sensors alone are powerless to reach, allowing gas detection systems to be more responsive, more accurate and also more stable. The integration of sensor technology, ML and AI is a promising approach to the future development of highly intelligent and responsive gas detection systems, adapted to a wide range of possible applications.

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