Chapter 1

Introduction and Literature Survey

1.1 The Historical Background

1.1.1 The Etymology of Word 'Gas'

The term "gas" was coined by Jan Baptist Van Helmont (1580-1644) in the early 17th century [1]. He is also credited for identifying carbon dioxide as the first gas (see Fig. 1.1 [2]) except for air. From the 17th century to the early 19th century, scientific research aimed to explore the physical properties of gases. This study area was also intended to know how gases relate to chemical reactions. Identifying gas composition was an important goal [3].

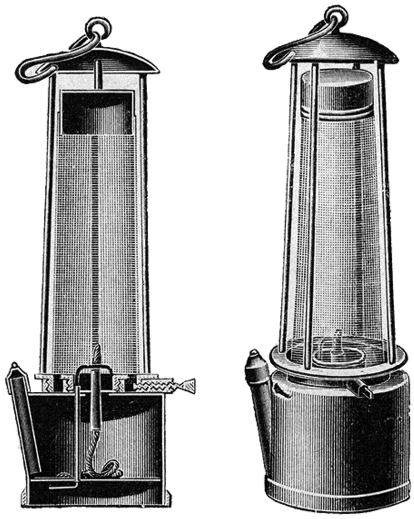
FIGURE 1.1: Jean-Baptiste Van Helmont: The Etymologist of Word "Gas" (Source: CurioKids - Jean-Baptiste Van Helmont)

1.1.2 The Evolution of Gas Detectors

Empirically, the detection of gases is led by the olfactory sense. Humans own five senses, including the olfactory one. However, the human olfactory system cannot sense odorless gases. Also, toxic gas in the ambiance could be fatal to humans since it is impossible to escape from olfactory functions due to its direct connection with breathing. This constraint paves the way for the requirement of gas detectors.

Gas detectors could be understood as a means of the safety system. These are important because many gases exist that can harm human beings. On observing the impact of harmful gases on human health, the need for gas detectors became a concern. Before the invention of sensors, from the 19th century to the early 20th century, coal miners used canary birds (see Fig. 1.2a [4]) as an early warning or alarming system to hazardous/fatal gases, viz., carbon dioxide, carbon monoxide, and methane [4]. As an instrumental means for gas detection, the safety lamp or Davy's lamp (see Fig. 1.2b [5]) has the oldest known history in coal mines [6]. Early warning gas detection systems relied on less accurate gas detectors in this age of gas detection.

(a) Canary Bird with Coal Miner



(b) Davy's Lamp

FIGURE 1.2: Early Means for Gas Detection in Coal Mines (Credits: Wikipedia)

1.1.3 Gas Chromatography-Mass Spectrometry (GC-MS)

Except for hazardous gas detection, in another aspect, the detection of other volatile chemicals or odors was also needed for human well-being. Humans have used their noses (natural olfactory system) to assess food based on the fragrance, what they should eat and what they should not eat. The pleasant odor of any food helps to guess it to be edible and delicious. With this tradition, humans use their noses analytically to measure the quality of edible things and cosmetics (see Fig. 1.3). A common practice of using sensory panels is found in the food and cosmetic industries, where a group of people aims to assess the corresponding items using their olfactory senses [7]. This approach fails if the people do not have sound health because the olfactory function is related to the health conditions. For illustration, humans can feel the fade up of olfactory systems while having cough & cold. Because of this constraint, for accurate assessment, a technology, "gas chromatography-mass spectrometry (GC-MS)," has started being used with the assessors in human sensory panels [8].

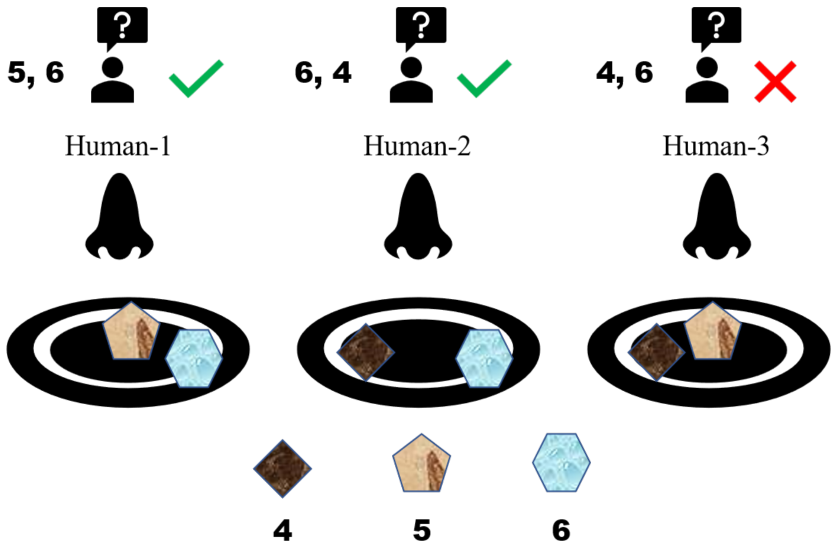


FIGURE 1.3: Human Sensory Panels for Olfactory Assessment

GC-MS technology combines two chemical identification approaches: gas chromatography (GC) and mass spectrometry (MS). GC separates the mixture into its constituents. On the other hand, MS separates and determines the ions available in the gaseous state (see Fig. 1.4). However, even being a better technology than its predecessors for chemical detection, it also encounters some issues, viz., it is not portable, costly, and has relatively slow performance. Human assessors assisted with the GC-MS could not meet all expectations for making sensory evaluation technology quick-responsive, and cheaper. This need paves the way to discover new technology that should be robust, portable, inexpensive, and quick performing. Consequently, the invention of gas sensors led to an innovative technology "model nose" that uses an array of gas sensors and is also titled as "electronic nose (e-Nose)."

1.2 Introduction

The e-Nose technology takes around the gas sensing system mimicking human olfactory systems. It employs an array of gas sensors to detect the gases and represents

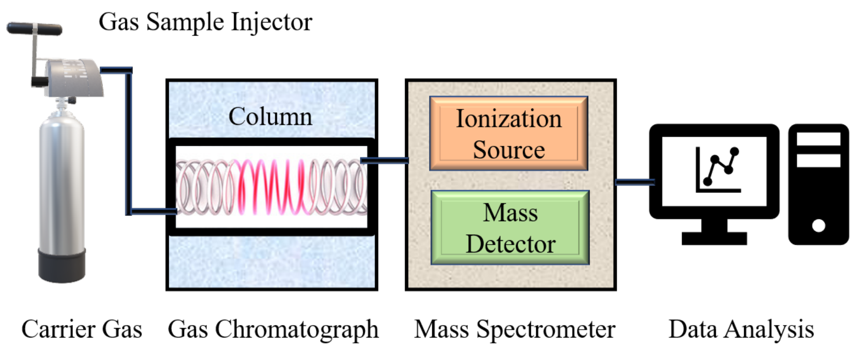


FIGURE 1.4: Schematic Blocks of GC–MS Instrument

the hardware aspect of the system. The signals observed in detecting gases are conditioned and processed for final assessment; it depicts the software aspect of the system. Proceeding in a particular sequence, it would be a point of importance to shed light on gas sensors, gas sensor arrays, e-Noses, and their applications.

1.2.1 Gas Sensors

In 1953, two scientists (W. H. Brattain & J. Bardeen) studied the surface properties of elemental semiconductor germanium [9]. They found that semiconductor material modifies their electrical property (resistance) being in contact with the gaseous ambiance. This change in resistance indicated the utilization of semiconductor materials for gas detection. Based on this phenomenon, the foundation of gas sensors prevailed by observing the successful implementation of gas detection using a sensing layer made of zinc oxide [10]. Notably, in 1971, the first metal-oxide-semiconductor gas sensor that used tin oxide as a sensing material was patented [11]. The tin oxide was preferred over other metal oxides due to its thermal stability, higher sensitivity, and low operating temperature requirement.

Literally, gas sensors represent chemical detectors having some transducing functionality capable of detecting chemical signals and converting them into measurable information. These are categorized based on the phenomena used for gas sensing. For illustration, catalytic gas sensors (see Fig. 1.5) are used to detect combustible gases and are so-called due to their working principle, which depends on catalytic combustion. In this phenomenon, the ignition temperature of flammable gases is curtailed by using the catalytic property of metal oxides and their compounds. These gas sensors detect combustible gases and vapors before reaching lower explosive limit (LEL) or the concentrations to the explosive range [12, 13].

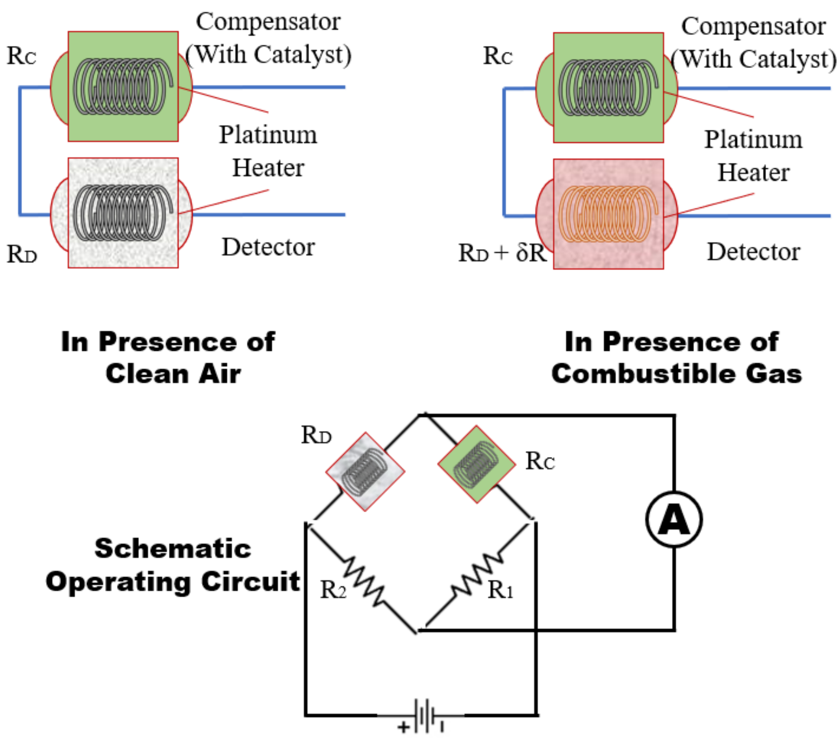


FIGURE 1.5: Schematic Circuit for Catalytic Gas Sensor

Further, electrochemical gas sensors result in gas sensing due to chemical reactions between gas molecules and oxygen in the sensing material (see Fig. 1.6). A current is caused by this reaction in proportion to the concentration of gases. It is measured as transduced information on the two electrodes where the chemical reaction occurs, resulting in the gas sensing process [14].

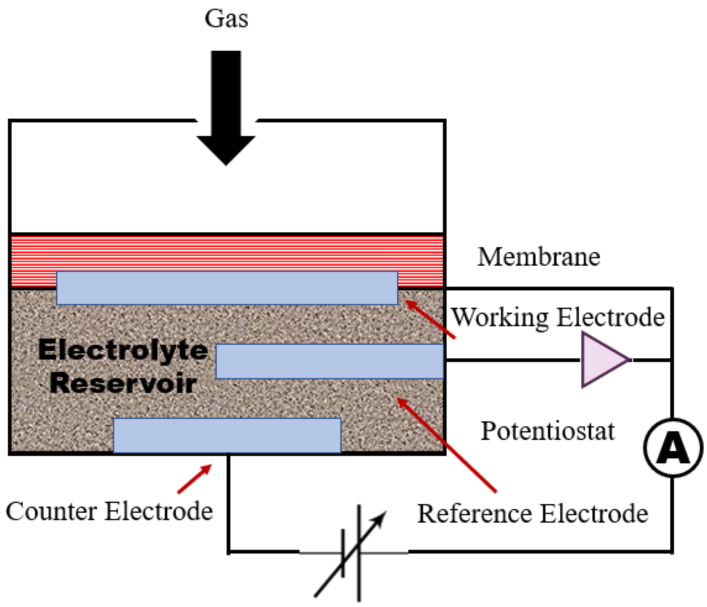


FIGURE 1.6: Circuitry of Electrochemical Gas Sensor

On the other hand, optical gas sensors are made of materials that change their optical properties being in contact with the gases. This change led to the means of gas detection (see Fig. 1.7). For example, some sensor employs partially palladium-coated optical fibers, called optodes/optrodes. On the interaction of the palladium with the gas, optical fiber is stretched in both directions resulting in the change of its effective optical path length. This change is measured by interferometry, causing gas detection [15].

Another category of gas sensors is made of materials sensitive to mass, viz., Surface Acoustic Wave (SAW) and Quartz Crystal Microbalance (QCM) gas sensors (see Fig. 1.8). These sensors exhibit the gas sensing process using vibration frequency without any intervention of chemical or physical reactions. Here, frequency materials are covered with a thin layer of mass-sensitive material capable

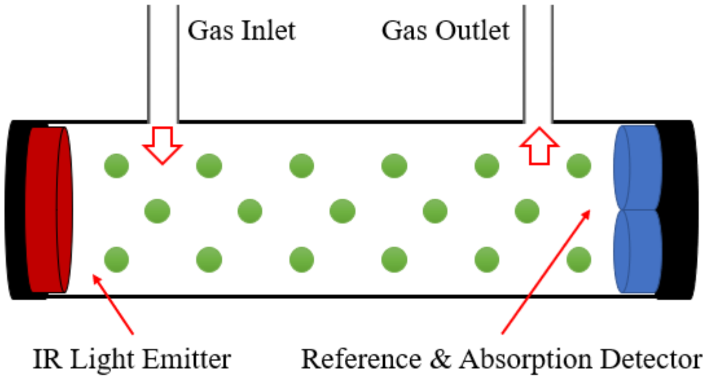


FIGURE 1.7: Schematic of NDIR (Non-Dispersive Infrared) Gas Sensor

of adsorbing gas molecules. Then, gas detection occurs by analyzing the material frequency and studying adsorbed material's characteristics [16, 17].

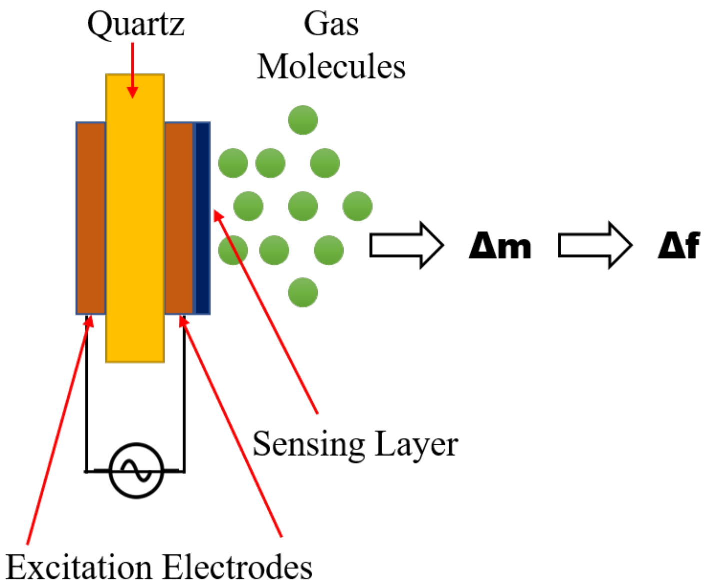


FIGURE 1.8: Mass Sensitive QCM Gas Sensor

Furthermore, plenty of metal oxides have semiconductor properties and are well-suited for detecting oxidizing, reducing, and flammable gases (see Fig. 1.9). These materials exhibit changes in conductivity being in contact with the gases. The inherent electronic structure of these materials determines their suitability for designing gas sensors [18]. Hence, metal-oxide-semiconductor gas sensors employ a change in conductivity (resistance) for gas detection.

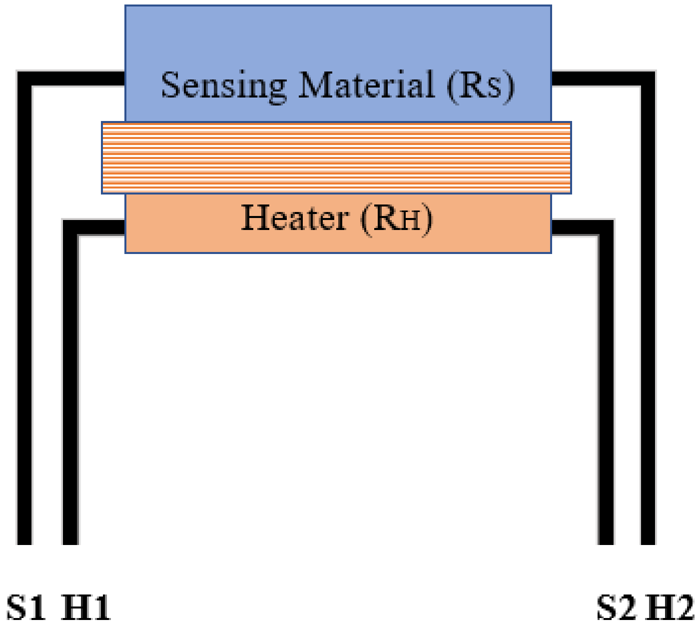


FIGURE 1.9: Schematic of Metal Oxide Semiconductor (MOX) Gas Sensor

1.2.2 Gas Sensor Array

Basically, gas sensors are designed to detect specific gases/odors. However, gases are found in the form of mixtures in natural ambiance; and, gas sensors are cross-sensitive for other gases as well. Hence, except for the gases aimed while designing the sensor, each gas sensor works as a non-selective gas sensor for rest of the gases. With this inference, a model nose [19] was proposed in the early 1980s that used an array of non-specific gas sensors (see Fig. 1.10). This work reported that non-selective sensors could simultaneously achieve high-performance discrimination among gases instead of particular gas sensors. This pioneering use of gas sensor array led to the breakthrough of the artificial olfaction system or e-Nose.

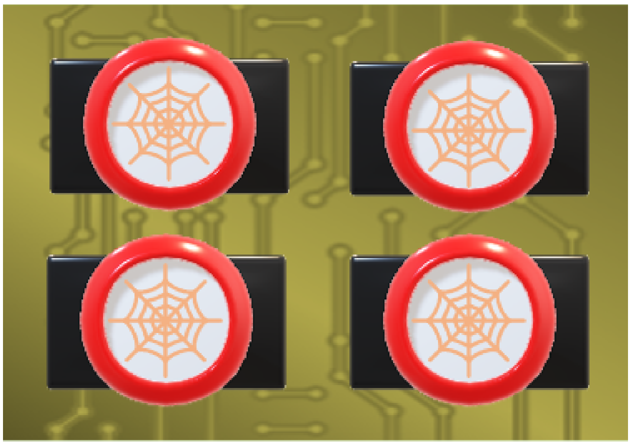


FIGURE 1.10: A Schematic Diagram of Gas Sensor Array

1.2.3 Electronic Noses (e-Noses)

An e-Nose is an instrumentation technology that mimics the human olfactory system [20]. The human olfactory functioning through a realistic nose fulfills numerous purposes: safety & security (see Fig. 1.11), healthcare & nutrition, the sensation of pleasure or inconvenience, and general well-being [21]. Researchers have been trying to implement the full-scale capability of the realistic nose, artificially incorporating gas sensors for decades. In this context, an e-Nose employs an array of gas sensors (non-selective) incorporated with signal conditioning/pre-processing and pattern recognition techniques.

1.2.4 Applications of e-Noses

The e-Noses are multilateral, as evidenced by their variety of applications. The corresponding list of applications that utilize e-Noses is not limited to:

Environment: air quality monitoring [22–24], and air pollution monitoring [25],

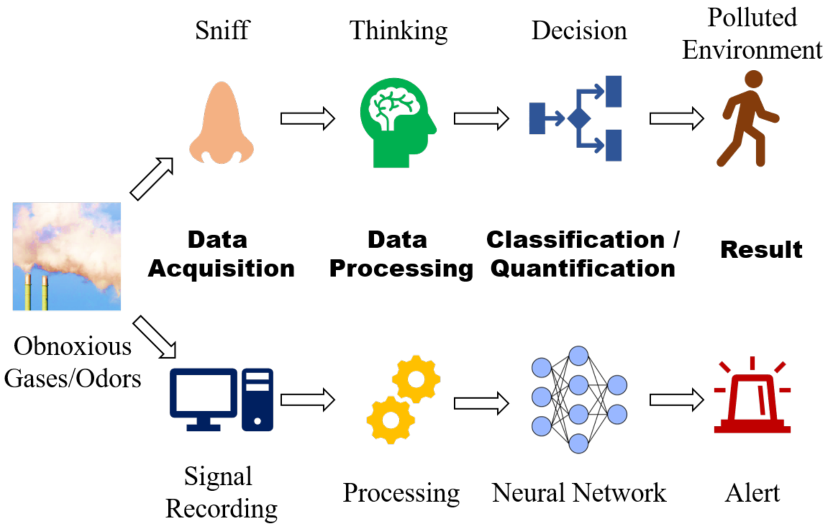


FIGURE 1.11: An Analogous Schematic Representation of Electronic Nose Principle

Healthcare: early screening of a variety of cancers [26–30], chagas disease [31], kidney disease [32], Covid-19 [33–35], lung disease [36], respiratory disease [37], tuberculosis (TB) [38], urine related diseases [39, 40],

Automobile: vehicular-engine health monitoring through exhaust monitoring [41],

Agriculture: agricultural product quality inspection [42–45], detection of pesticides [46], condition monitoring of granaries [47], assessment of vegetable/edible oils [48], discrimination among rice species [49], and grain quality monitoring [50],

Foods & Beverages: foods analysis [51, 52], assessment of quality deterioration [53], monitoring beers' flavors [54], and alcohol characterization [55],

Cosmetics: fragrance analysis for cosmetic products [56],

Robotics: olfactory functioning in robots [57–59],

Safety & Security: smoke detection or classification [60, 61], fire detection [60, 62], estimation and discrimination of industrial gases [63, 64], and

Forensics: the scope of forensic science also endorses e-Nose applications [65].

Along with these notified applications, a few reviews [66–69] have also been referred to widen your information about e-Nose applications (also, see Fig. 1.12).

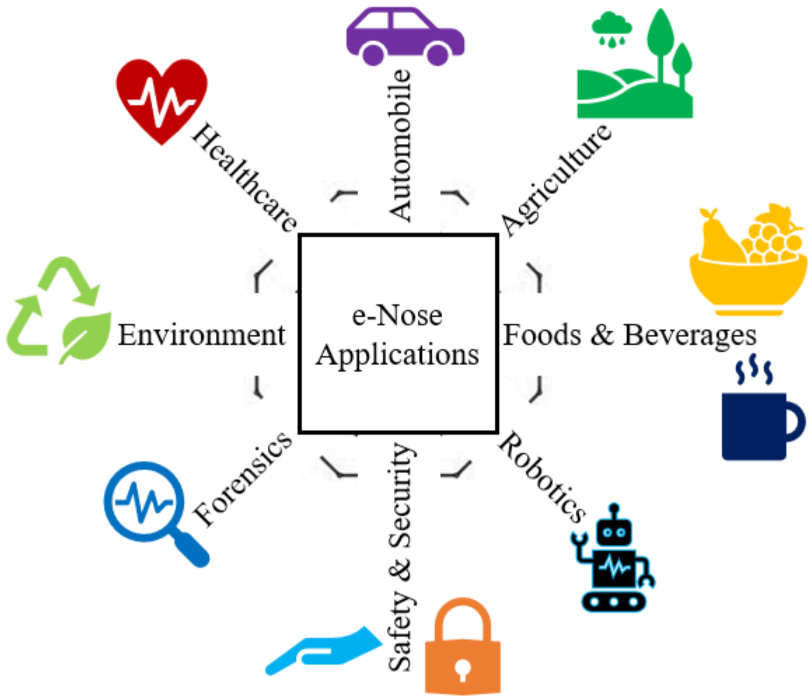


FIGURE 1.12: A Schematic Picture of Gas Sensing Applications

It is observed that industrial sites affect nearby living beings due to the leakage or emission of various obnoxious gases/odors that severely cause adverse health impacts. Thereby, e-Noses are required as preventive measures for early screening of pollution-borne diseases to curb severeness. A few industries have a history of causing calamity (such as the Bhopal Gas Tragedy) due to leakage of hazardous gases/odors. Moreover, mining industries (especially coal mines) are also prone to face dangerous gases/odors (carbon monoxide, carbon dioxide, methane, etc.) lethal to workers employed. Such hazardous scenes in domestic/industrial paradigms had developed interest among researchers to invent efficient instruments and methodologies for monitoring dangerous gases/odors. The aforesaid crucial need for precise gas sensing systems enforces state-of-the-art research in both industries and academia.

1.3 Literature Survey

A vast variety of published literature shows the evolution of advanced gas sensing materials (see Fig. 1.13) and technologies (see Fig. 1.14) to design efficient gas sensor elements [70–72], [17], [73–75]. Nevertheless, achieving high standard sensitivity and selectivity is still a challenge [76–78]. The low sensitivity of the gas sensor element shows inefficiency in detecting the lower concentrations. On the other hand, the gas sensor element's low selectivity shows inefficiency in detecting the particular gas/odor. Due to its non-selective nature, the gas sensor elements simultaneously respond to multiple gases/odors. Thus, low sensitivity and selectivity are challenges in fabricating gas sensor elements [79].

Subsequently, further challenges occur due to environmental conditions of working ambiance [80–83], [18]. The poisoning of the gas sensor elements is one of the significant issues caused by the contamination of sensing material due to the unwanted gases/odors available in the working ambiance. Hence, due to poisoning caused by environmental contaminants, the responses of gas sensors are started to deviate from their original form [84–88]. This deviation in the responses is popularly known as the drift in sensor characteristics [84], [86–88]. Also, it is an inevitable issue; however, its impact is suppressed at the signal processing stage. Another challenge is the mixture of gases available in the authentic ambiance consisting of the desired gas/odor and the unwanted gas/odor simultaneously. Hence, it is very tedious to detect the desired gas/odor. Also, only gas mixtures are available in

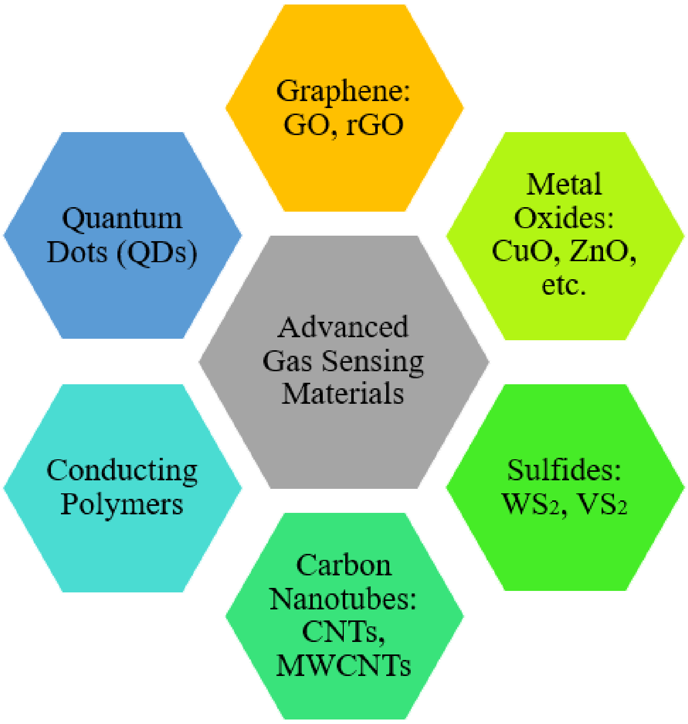


FIGURE 1.13: Advanced Gas Sensing Materials

the real-world scenarios [89–96]. However, the encountered gas mixtures may be simple (binary) or complex (ternary, quaternary, etc.). Researchers in academia and industries have proposed several methodologies to solve this issue [89–91], [93–96].

The research on semiconductor gas sensors rapidly had been increased in the 1980s. Since then, continuous efforts have been made to achieve high-performance gas sensors. High selectivity and sensitivity, quick responsiveness, and reliable operation at the expense of low power are expected salient characteristics. Except for excellent selectivity, oxide semiconductor-based chemo-resistive gas sensors are suitable according to the rest parameters [97]. Due to straightforward circuitry (see Fig. 1.15) and inexpensive, oxide-based solid-state semiconductor gas sensors have widespread applicability [97], [17].

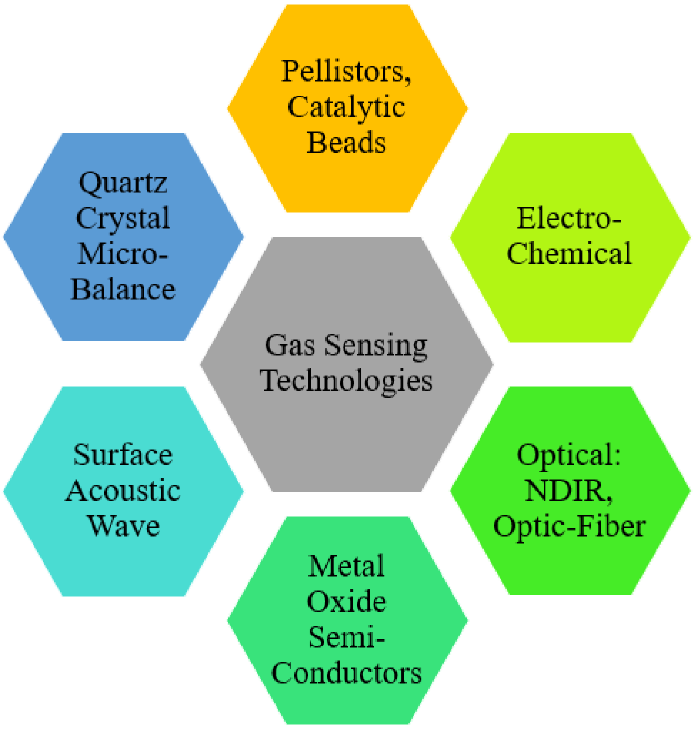


FIGURE 1.14: Gas Sensor Technologies

While experimenting on e-Nose, Taguchi Gas Sensors (TGS) were the first choice due to their suitability and commercial availability [98, 99]. The monopoly of TGS devices for designing low-cost GSS is sustained even today [100–107]. However, their sensitivity to humidity results in extensive drift [98].

With this introduction from the gas sensor to e-Nose, it is evident that the research in the area of gas sensing broadly encompasses two significant paradigms: 1. Fabrication of Gas Sensors: Includes advanced research for sensing materials and fabrication technologies. 2. Instrumentation of Gas Sensors: Includes application of gas sensor arrays to e-Noses and machine olfaction systems.

Researchers continuously try new and innovative approaches to fabricate the gas sensors in the first paradigm, exhibiting improved sensitivity and selectivity. In

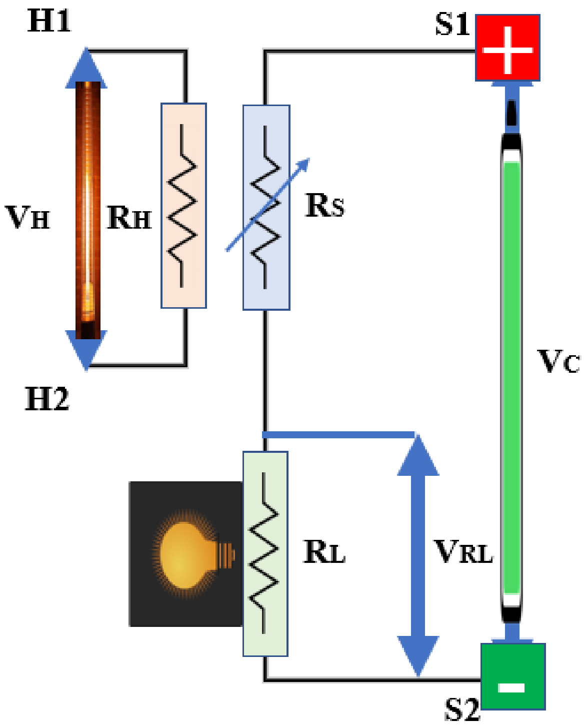


FIGURE 1.15: MOX Gas Sensor Circuit

the second paradigm, researchers use an array of gas sensors and pattern recognition techniques (statistical, probabilistic, neural networks, etc.) to achieve high-performance gas sensing systems, even using gas sensors exhibiting low sensitivity and selectivity. The core research in this paradigm tends to design efficient algorithms for sensor data processing using artificial intelligence, machine learning, deep learning, etc.

With the work reported in [19], to discriminate among gases/odors, the issue of sensor selectivity was solved using an array of some non-selective gas sensor elements. GSS consisting of a gas sensor array, hold the capability to deliver good results compared to a single sensor element. In this connection, the researchers developed a system called the e-Nose using the synergy of gas sensor array responses and pattern recognition techniques. Thus, any GSS has two broad paradigms to explore for performance enhancement: the fabrication and sensor data processing levels. The early methodologies before sensors for gas/odor detection could work only signaling/alarming due to their poor performance. With the advent of gas sensors, the area of gas sensing is setting record achievements day by day. Researchers have been studying GSS for decades with the synergy of electronic gas sensors and pattern recognition techniques to benefit each domain of science and engineering.

The systems employing electronic gas sensors (e.g., e-Noses, GSS) show the potential of the model nose to mimic artificial olfaction technology. Before going into a comprehensive discussion on e-Nose, a schematic block diagram of an e-Nose has been presented for better understanding. It is a system that broadly consists of three building blocks, viz., gas sensor array (data acquisition module), signal conditioning (sensor data pre-processing module), and pattern recognition (discrimination module) [108–110]. A schematic block diagram representing these building blocks is shown in Fig. 1.16.

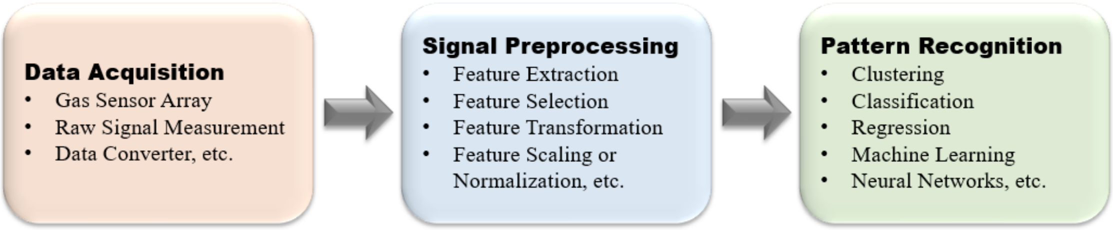


FIGURE 1.16: Three Basic Building Blocks of e-Nose

The first building block includes the content discussed so far till the innovation of the gas sensor array. In this continuation, the signal conditioning or pre-processing techniques for gas sensor array responses are being reviewed, inherently held under the second building block of an e-Nose.

As reported in [111], up to 1994, no work utilized transient responses of the gas sensor array for the corresponding signal processing. In the meantime, e-Noses used only steady-state responses for signal conditioning using various manipulations, viz., differences, relative, logarithm, and normalizations. These signal conditioning methods help reduce the impact of influencing factors, e.g., sensitivity to temperature and non-linearity due to concentration. By making the data scaled and normalized, signal conditioning also helps in reducing errors during the computation process. Furthermore, signal conditioning or data pre-processing includes dimensionality reduction and feature extraction to enhance data viability and apply appropriate pattern recognition to pre-processed data. With these aspects, pre-processing information strengthens the data-driven performance of GSS. A review of these [94, 112, 113] outstanding works makes a comprehensive list of pre-processing techniques, as shown in Table 1.1.

In contrast to the practical benefits of pre-processing data, while classifying the gases/odors, processed data do not work well during quantification. It happens due to modifications in the data by applying pre-processing techniques. The quantification of gases/odors is asserted by the data variations caused by the corresponding gas/odor concentration. These variations are suppressed while applying

Table 1.1: Pre-processing Functions on Sensor Data.

Function	Expression	Gas Sensors	Ref.
Difference	$x_{ij} = (V_{ij}^{max} - V_{ij}^{min})$	MOX	112
Relative	$x_{ij} = (V_{ij}^{max} / V_{ij}^{min})$	MOX	113
Fractional Difference	$x_{ij} = (V_{ij}^{max} - V_{ij}^{min}) / V_{ij}^{min}$	MOX	113
Logarithm	$x_{ij} = log(V_{ij}^{max} - V_{ij}^{min})$	MOX	94
Sensor Normalization	$x'_{ij} = x_{ij} / (x_{ij}^{max_j} - x_{ij}^{min_j})$	MOX	94
Array Normalization	$x'_{ij} = x_{ij} / \sum_i x_{ij}^2$	MOX	113

transformations based on differences, relative, logarithm, and normalization expressions.

Hence, the quantification cannot determine concentration measurements accurately using pre-processed data. A robust pattern recognition technique is required to deliver accurate concentration measurements using raw or original data to overcome this constraint.

As mentioned earlier, pattern recognition is the third and last module in an e-Nose. It employs the multivariate analysis of signals resulting from the gas sensor array of discrete/integrated non-selective and cross-sensitive gas sensor elements [114]. It would be worth mentioning that the conventional pattern recognition techniques include approaches based on neural theory, and statistics. These pattern recognition techniques are utilized for both purposes, viz., classification, and quantification of gases/odors. On the one hand, the membership of the pattern is estimated while classifying the gases/odors. On the other hand, the concentration of gases/odors is estimated during quantification. For better visualization, refer to Fig 1.

In the context of e-Nose, the published works to date have significantly considered principal component analysis (PCA), discriminant function analysis (DFA), and clustering algorithms (CA) under statistical techniques of pattern recognition. The second paradigm of pattern recognition techniques includes multilayer perceptron-based artificial neural networks. Statistical pattern recognition techniques are widely applied to the steady-state-based sensor responses captured for different gases/odors [115]. Up to two decades of evolution of gas sensor array, dynamic responses of sensors had not been utilized significantly [111, 115]. Although, analysis of dynamic responses of the gas sensor array is the signature field in the current scenario. However, the dynamic analysis of responses encounters various challenges, viz., computational complexity, feature selection, and dimensionality reduction. An exhaustive list of pattern recognition techniques includes multiple data processing techniques to process the static as well as dynamic responses of the gas sensor array.

Irrespective of the types of gas sensors used in the gas sensor array, the final results obtained using an e-Nose rely on pattern recognition techniques for classifying and quantifying gases/odors.

1.4 Pattern Recognition Techniques Used in e-Nose Systems

Although almost every category of pattern recognition techniques has been squeezed to classify/quantify the gases/odors. But neural networks are still dominant since the beginning of gas sensor array responses to implement the classification or quantification of gases/odors. Also, the central theme of this thesis demonstrates the application of one of the best architectures of neural networks, popularly known as convolutional neural networks, to classify/quantify the gases/odors. Before discussing neural network applications in detail, we shed light on reviewing other pattern recognition techniques in gas sensing.

1.4.1 Principal Component Analysis

The principal component analysis (PCA) is an unsupervised pattern recognition technique. PCA transforms the high-dimensional data analysis space into lower-dimensional data analysis space by squeezing salient information from the data.

With this notion, PCA reduces the dimensionality of the data and the computational complexity used in further analysis. Aishima has utilized PCA to discriminate various liquors using their aromas [116]. Using the association of fabricated gas sensor array and PCA, Di Natale et al. (1995) successfully implemented the system to identify the different vintage years of wine belonging to the same category [117]. In conjunction with a pattern recognition technique, Lee et al. (2000) have utilized PCA to classify and quantify the explosive gases/odors such as methane, propane, and butane [118]. They have used a gas sensor array that integrates nine gas sensor elements for the purpose mentioned above. Further, a nanomaterial-based gas sensor array was used in [119] to identify five Chinese liquors. Authors have used the synergy of PCA and discriminant analysis (PCA-DA) and achieved 76.8 percent recognition accuracy. Lu et al. (2006) used a carbon nanotube-based gas sensor array to discriminate six gases (nitrogen dioxide, hydrogen cyanide, hydrogen chloride, chlorine, acetone, and benzene) recorded through the concentration exposure in parts per million (PPM) levels [120].

1.4.2 Probability-Based Techniques

These pattern recognition techniques use the posterior probability of membership or the Bayesian approach. Brahim-Belhouari et al. (2005) used Gaussian mixture models (GMM) to identify gases/odors and their mixture [121]. Authors have applied GMM to the responses of an integrated gas sensor array which has been fabricated to the recognition of combustible gases. With this approach, the authors achieved 96 percent recognition accuracy.

1.4.3 Cluster Analysis-Based Techniques

The first notion about cluster analysis-based pattern recognition techniques is that they are unsupervised. Aishima has used hierarchical cluster analysis (HCA) to discriminate among various liquor aromas [116]. It is used to sort the relationships using tree-based inference based on the distances or similarities.

1.4.4 Discriminant Analysis-Based Techniques

The discriminant analysis-based techniques are parametric pattern recognition techniques. Here, the mathematical objective combines linearly discriminating parameters for discriminant analysis. The combined clusters of discriminating parameters are compelled to be as much as possible statistically distinct. In such approaches, the coefficient's weight of the linear discriminant functions is obtained by maximizing the ratio of inter-cluster and intra-cluster variances. A multiple discriminant analysis (MDA) has been used to differentiate or classify the wines in [122]. Moreover, Aishima has used linear discriminant analysis (LDA) to discriminate various liquors using their aromas [116].

1.4.5 Nearest Neighbor-Based Techniques

The nearest neighbor-based techniques are the non-parametric pattern recognition techniques. It involves the determination of Euclidean Distance in the multidimensional analysis space depending on the data dimensionality. The outcomes of such processes depend on the taken number of neighbors (say k). Moret et al. (1984) have utilized 1, 3, and 5 neighbors to classify the wines using the nearest neighbor pattern recognition technique [122]. Also, Abe et al. (1988) have used kNN to classify various odorants, including alcohols and ketones, where k represents the neighbors [123]. Guney et al. (2012) have used kNN to classify the different concentrations of n-butanol. Also, they achieved 93 percent classification accuracy using kNN in their use case [124].

1.4.6 Genetic Algorithms

It is an optimization technique based on the evolutionary process that occurred in the genetics of living beings to lead to an optimal solution. Xiao-bo et al. (2002) have used a genetic algorithm (GA) to process the signals captured through a gas sensor array [125]. The authors have extracted optimal feature parameters using GA from the salient data to recognize two different categories of vinegar. Liu et al. (2018) have used GA and fuzzy SVM to classify the target odors [126].

1.4.7 Decision Tree-Based Techniques

The decision tree is a hierarchical process of binary decision-making steps. It is one of the popular classifiers used in gas sensing. An advanced decision tree structure has been used to classify the odor captured through an e-Nose [127]. Authors have classified 11 different odors with an accuracy of 97.18 percent, where the decision tree represents the knowledge about chemical compounds. Hassan et al. (2014) have also used a decision tree approach to classify the gases/odors [128]. In [129], the decision tree approach has not been used only for classification but also for dimensionality reduction for data of an e-Nose. Li et al. (2011) have used a binary decision tree classifier to facilitate low-power hardware implementation [130].

1.4.8 Support Vector Machine (SVM)

It has been a popular supervised pattern recognition technique since its inception. Both the classification and regression have been achieved using SVM. The geometric separation among classes is the central concept behind its mathematics. It is so-called due to support vectors representing the closest data points among different targets. Li et al. (2009) have used a gas sensor array incorporating SVM as a pattern recognition technique to detect sour skin disease for onions [131]. Authors have demonstrated a binary classification problem to classify between healthy and sour skin onions. In contrast to binary classification, Guney et al. (2012) have used multiclass SVM to classify various concentrations of n-butanol using the responses of a gas sensor array consisting of 12 gas sensor elements [124].

1.4.9 Ensemble Techniques

The ensemble algorithm of learning is executed by running the classifier multiple times to obtain the outcomes for the hypothesis. These outcomes are used to vote for the final result. For example, Vergara et al. (2012) have used consequences of SVM trained at different instances of time for a weighted combination of results that lead to the outcome [86]. The authors compensate the drift for classifying the considered gases/odors with this approach. Moreover, Sun et al. (2017) have demonstrated multiple classifiers ensemble using SVM, KNN, and LDA as base learners to identify the ginseng using e-Nose technology [132].

1.4.10 Artificial Neural Networks (ANNs)

With the pioneering work of a model nose using a gas sensor array consisting of non-specific gas sensor elements, Persuad et al. (1982) have utilized a neural approach based on the mammalian olfactory system to discriminate the complex odorant mixtures [19]. The proposal of the model nose revolutionizes the research in gas sensing. Moreover, Ema et al. (1989) have successfully implemented the discrimination among the aroma of liquors using a gas sensor array consisting of six quartz-resonators [133]. The authors used neural-network for pattern recognition in their corresponding task. Later, Gardner et al. (1990) have applied ANNs to an electronic olfactory system [134]. The authors reported the adaptability of their proposed technique for hardware implementation, showing the use case for alcohol. In [135], Stetter et al. (1993) have used neural network simulation incorporating the gas sensor array for quality classification of wheat samples. While Albrecht et al. (1994) have used Kohonen feature map-based neural network to identify airborne hazardous compounds with the help of an intelligent gas sensor system [136].

Gardner et al. (1996) have implemented a multilayer perceptron (MLP) neural network to detect vapors/odors by applying a self-organizing adaptive resonance technique [137]. In [138], Yang et al. (1997) have applied ANN to quantify hydrogen sulfide and nitrogen dioxide using a metal-oxide-semiconductor gas sensor array. Kermani et al. (1999) have used the combination of GA and ANN to classify fragrances, hog farm air, and soft beverages [139]. A portable e-Nose system has been designed in [140] using a gas sensor array incorporating ANN as pattern recognition. A thick-film gas sensor array incorporation with ANN has been used in [141] to recognize explosive gases/odors. A time-delay neural network was used in [142] to classify the vintages of wine. Xiaobo et al. (2003) have recorded a 98 percent success rate in classifying the vinegar by applying ANN to extracted or selected features from the data captured through a metal-oxide gas sensor array [143]. Furthermore, the dynamic responses captured using a gas sensor array have been used for hydrogen detection with the help of neural networks [144].

1.5 Observed Research Gaps from Literature Survey

Although, modern gas sensors can provide satisfactory performances in their application paradigms by sensing the corresponding gases/odors or Volatile Organic Compounds (VOCs). But selectivity, sensitivity, and drift are still the primary issues that affect their performance. The selectivity of gas sensors depicts their ability to detect only the targeted gas/odor. At the same time, the sensitivity of gas sensors defines the lowest detectable amount of concentration of gases/odors. The drift in gas sensor responses is the deviation exerted due to long-term use of the gas sensors and poisoning of gas sensors by contamination. The drift in responses also indicates the instability of gas sensors; a gas sensor cannot reproduce the same response at different times. The issues mentioned above affect the performance of gas sensors severely while detecting a single gas/odor.

Subsequently, a gas sensor array performs well with the synergy of pattern recognition techniques to classify/quantify the multiple gases/odors. This combination outperforms bypassing the issue of selectivity since a gas sensor array merely uses non-selective gas sensor elements. The pioneering concept of gas sensors array led to the development of electronic nose (e-Nose) systems. The better classification of gases/odors using conventional pattern recognition techniques requires data pre-processing. This requirement of data pre-processing techniques needs more computational power to be executed. With this fact, traditional methods are not well suited for real-time gas classification and resource-constrained environments. On the other hand, gas sensing systems are popular Cyber-Physical Systems (CPS) or Internet of Things (IoT) ecosystems applicable in various social paradigms such as environmental monitoring, healthcare, etc. With the evolution of 6G wireless communication technology, IoT ecosystems are being proliferated from macro to micro-level systems. Undoubtedly, microsystems always face resource-constrained scenarios.

Therefore, gas sensing systems should also be robust to 6G-IoT resource-constrained paradigms. After reviewing the literature, we observed two research gaps associated with the area of gas sensing. First is the accurate classification/quantification of gases/odors using convolutional neural networks capable of automatically extracting salient features without any additional data pre-processing. The second is the drift that requires the additional statistical algorithm to remove it before applying pattern recognition techniques. Here, a robust end-to-end classifier is needed to encounter the drift effect without using the additional algorithm.

1.6 Problem Statements

After reviewing the literature and taking insights into the current and future developments of gas sensing systems, some salient aspects are noted to pay attention. One of them is to use a widespread convolutional neural network for the classification/quantification of gases/odors. Another one is to make gas sensing systems suitable for 6G-IoT resource-constrained paradigms without significant degradation in the performance of the gas sensor node. Another is to design an end-to-end CNN architecture to suppress the impacts of drift without using an additional drift correction algorithm while classifying the gases/odors. These research gaps have been articulated under the following problem statements: It is observed that CNNs can be applied to transient responses for gas/odor classification. Besides this scope, if only steady-state responses are available to classify the gases/odors, no published work has been found to date to enable CNN in this case. Thereby, some approach is needed to generalize the applicability of CNNs to both steady-state and transient responses. There is no thumb rule to use fix number of sensors in the gas sensor array. Hence, the gas sensor array's increased number of sensor elements consumes significant power. It is also against the philosophy of miniaturization of a gas sensor node. With the development of 6G wireless communication connectivity, micro IoT systems (e.g., microrobots) are prone to resource-constrained applications requiring limited resources but without compromising performance. Therefore, an approach is needed to optimize gas sensor nodes to make gas sensing systems efficient for 6G-IoT resource-constrained paradigms. Although selectivity and sensitivity of gas sensors are being improved day by day using advanced gas sensing materials and fabrication technologies. But drift is still a severe concern for gas sensing applications. The impacts of drift on the classification of gases/odors are curtailed by using some drift correction algorithms on drift-affected data. In this case, pattern recognition techniques are applied to drift-corrected data. Thus, the gas classification task is accomplished in two stages: first drift correction and second pattern recognition. It makes the job prone to use extra computational power. Therefore, an end-to-end architecture is needed for gas/odor classification capable of suppressing drift impacts without using any additional drift correction algorithm.

1.7 Outline of the Thesis

The applications of gas sensor array-based gas sensing systems or e-Nose systems are not limited to areas of environment, healthcare, automobiles, agriculture, foods & beverages, cosmetics, robotics, safety & security, and forensics. However, these systems are used as compact gas sensing devices. In contrast, a gas sensor array also works as a discrete module of various cyber-physical systems in an open environment. As discussed in multiple chapters of this thesis, different novel data analytics approaches have been proposed to design computationally efficient intelligent gas sensing systems suitable for resource-constrained environments. The whole work of this thesis is primarily intended to apply CNN learning insight independent of the modality of gas sensor array responses (static or dynamic). The CNNs with our proposed approaches provide high-performance classification or quantification of gases/odors, significantly reduces power consumption, and are used as computationally-efficient architectures. The work presented in this thesis deal with various aspects, viz., CNNs applicability to both steady-state and transient responses, to suppress the drift effects without using additional statistical algorithms, and sensor node optimization to reduce effective power consumption.

In **Chapter 1**, the historical background of gas sensing systems with their state-of-the-art development is presented comprehensively. In a nutshell, the hardware aspect of gas sensing systems has been discussed to understand the area of research. In contrast, the software aspect of these systems has been discussed thoroughly to understand the application of Artificial Intelligence (AI) to make gas sensing systems intelligent and universal. The literature review has also been presented to find or describe the pinpointed problem statements. Novel solutions made by us have quenched the found research gaps.

The discussion of used materials and methods has been presented in **Chapter 2**, along with the technical background. This chapter clarifies how the researchers have found advanced neural networks better than conventional ANNs for gas sensing. Also, the illustrated working of MOX gas sensors has been presented.

In **Chapter 3**, an end-to-end hybrid CNN architecture has been proposed to overcome the drift problem. The proposed architecture involves multidimensional multiconvolution-based extracted features capable of suppressing the effects of drift. The operating principle of the proposed architecture depends on the consecutive 1D, 2D, and 3D features representing the temporal, spatial, and spatio-temporal significance of the features. Furthermore, our proposed algorithm is straightforward in contrast to the other published methods that use some additional signal processing and complex computations. Also, our proposed work outperformed other state-of-the-art methods.

Further in **Chapter 4**, we have proposed a novel solution to classify/quantify the gases/odors applicable to the steady-state and dynamic gas sensor array responses. In addition, our proposed approach is so efficient that it can provide higher performance even by using only the steady parts instead of using the whole range of responses that exert high computational cost. On the other hand, we have proposed the novel principal component-based padding making a convolutional-based classifier applicable to steady-state responses. The proposed principal component-based padding outperforms conventional zero-padding.

In **Chapter 5**, we have proposed an optimization approach for gas sensor nodes suitable for resource-constrained 6G-IoT scenarios. With the evolution of 6G communication technology, IoT systems can be used universally in micro to macro IoT-enabled ecosystems. However, the inevitable need for miniaturization of microsystems tends to be resource-constrained. For illustration, we have demonstrated our proposed approach to a gas sensor array consisting of four gas sensor elements. We can efficiently reduce the power consumption by 50 percent without significant degradation in the node's performance. This power reduction has been achieved by removing the redundant gas sensor elements from the used gas sensor array. Finally, after removing redundant sensor elements of the gas sensor node, the performance is sustained using a convolutional-based classifier model.

Chapter 6 discusses the work done in the preceding chapters to complete the thesis. It also depicts the main findings to provide the contributions of the dissertation. The generalizations of our work have been discussed to highlight the future scope.

1.8 Conclusion

The current chapter outlines the historical background of gas sensing up to its evolution and advancement with time. This chapter discusses the development in gas sensing from the inception of gas detection to artificial olfaction systems. It includes chronologically: the etymology of the word 'Gas,' the evolution of gas detectors, the development of various gas sensors, the proposal of the first gas sensor array, the growth of electronic nose (e-Nose) systems, and the use of Artificial Intelligence (AI) to make these gas sensing systems highly accurate for ubiquitous applicability. A comprehensive list of gas sensing applications has been given that includes a variety of research paradigms, viz., Environment, Healthcare, Automobile, Agriculture, Foods and Beverages, Cosmetics, Robotics, Safety and Security, and Forensics. The literature survey shows the significance of gas sensing applications in current scenarios. The hardware and software theories related to gas sensing systems have been highlighted with challenges in their scope. Advanced gas sensing materials and technologies have also been cited.

Furthermore, citing three significant blocks of e-Nose systems, we have illustrated a comprehensive list of possible pattern recognition techniques used in the third block dedicated to decision-making based on data analytics. This list is not limited to Principal Component Analysis, Probability, Cluster Analysis, Discriminant Analysis, K Nearest Neighbors, and Decision Tree-based Techniques. Also, the introductions have been given to Genetic Algorithms, Support Vector Machines, Ensemble Techniques, and Neural Networks. However, the operational insight of ANN has been shown in the forthcoming chapter. The problem statements were designed to fill the noticed research gaps in this discussion. With our proposed novel approaches, state-of-the-art developments in gas sensing can incorporate artificial intelligence. That makes them highly efficient cyber-physical systems (CPS), internet of things (IoT) systems, decision support systems, early warning systems, and screening systems that are evidently beneficial even for resource-constrained paradigms.