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1.0 Introduction

The sense of smell is one of the essential senses of human being. The sense of smell arises from the stimulation of the receptors present in the human olfactory system by odorant molecules emitted from an object [1]. The identity and quality of many substances can be inferred simply by sensing the odour. In many industries the quality of product is maintained after sensing its odour like the industries of perfumes, colognes, wines, cuisine along with the personal care products. In fact a unique odour signifies the identity of individual brands. Most commonly followed procedure in an industry is, a group of people are appointed to fill out questionnaires on the odour associated with the products [2-4]. Brattoli et al. reported in [5] that according to Aristotle people with narrower nasal ducts have a keener sense of smell whereas Roman philosopher Lucretis related the shape of the odorant molecules with the quality of the odours.

The human nose possesses about 100 million aroma receptors that can identify approximately 10,000 different odours [6]. Odour is a mixture of light and small volatile molecules that exists in air, at a concentration which is able to stimulate an anatomical response. Human can detect the presence of different odours in the ambient air after inhaling the air. Human olfaction is often considered as a tool for assessing the quality in various fields, such as food and beverage [7-10] or clinical diagnosis [11-12]; chemical contaminant of both indoor and outdoor air [13-14] in automobile industries [15], military, space and mines etc.

Volatile form of organic compound may consists of number of components each of which may contribute unique characteristic to the quality of the volatile component. A change in the concentration of the components is easily detectable by human nose but changes in odourless components are often missed out by human nose. In fact human olfactory performance is not consistent as it may get
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affected by mental and physical health and fatigue. Therefore efforts were made to develop an instrument based on the similar principle as the human nose works to carry out in real-time assessment of the odour in a reproducible and stable way. Diverse gas sensors when arranged in an array, individually they may provide a unique representation of the odour just like Biological olfactory receptor neurons (ORNs) used to do.

Odours can be characterized by four parameters: intensity, threshold, quality and hedonic assessment [2]. Intensity is the strength of sensation and it increases as the concentration of odour components increases. Threshold value is determined by the lowest concentration of the odour components up to which human olfactory organ can sense. Quality of the odour is expressed by associating the odour to odour quality of some known substrate. Hedonic assessment is the final assessment associated with the pleasantness or unpleasantness of the odour [16].

This research is intended to develop a portable odour detection system with improve computation and classification performance. This chapter discusses the various gas sensing technologies, concept of the odour detection system, feature extraction procedures, features optimisation and pattern recognition techniques usually applied to artificial odour detection system. The chapter also presents the literature survey, objective and outline of the thesis.

1.1 Artificial odour detection system

The design idea of an artificial odour detection system comes from the capability of the mammalian olfactory organ. With the progress in the sensor technology, electronic devices as well in different computational algorithms, the different basic units of the mammalian olfactory organ can be designed artificially. The following section discusses the human olfactory system.
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1.1.1 Human olfactory system

The human olfactory system consists of three parts – the olfactory epithelium, olfactory bulb, olfactory tract [16]. Olfactory epithelium present in the upper part of the human nasal cavity is the main area for olfactory sensitivity. The surface of the olfactory epithelium contains olfactory receptor neurons (ORN) which gives rise to long hair like extensions known as cilia, immersed in mucus. The epithelium consists of about 100 million ORNs. Each ORN consists of a distinctive protein chain that traverses the cell membrane.

![The Olfactory System](image)

**Figure 1.1 The Olfactory System [17]**

The odorant molecules bind to the olfactory receptor on the external surface of cilia, it activates a particular G protein (Guanosine nucleotide binding proteins) which once activates triggers a cascade of biochemical events resulting in an electrical signal. G protein activates adenylate cyclase, and produces Cyclic
adenosine monophosphate (CAMP). CAMP then binds and opens a cyclic nucleotide – gated ion channel in the cell membrane increasing the flow of positive ions into the cell. The depolarisation into the cell produces action potentials. The axons arising from the ORN make their first synapses with the second order neurons in the structure called olfactory bulb. In the olfactory bulb reception, re-organization and re-transmission of received impulses are handled. The structure that bundle the axon-dendrite in olfactory bulb is known as Glomeruli cells. Each glomerulus receives axon input from those ORNs which contain identical olfactory receptor and receptor G-protein. The Glomerulus synapse with mitral and tufted cells of the olfactory bulb and excites glutamate as the primary neurotransmitter to act on the N-methyl-D-aspartate (NMDA) receptors of the mitral and tufted cell dendrites. The neural outputs from mitral and tufted cells are then projected to higher olfactory centers in the brain. The prepyriform cortex and the amygdale is the brain structure that processes memory, emotions and the olfactory signals. Brain collects all the features from individual receptor cell and uses them to represent the odour. The characteristic information of different odours is stored in the brain. When an odour is sensed, brain starts to access memories, compare with the stored features and identify it if already stored in memory [7],[17-18]

Each odorant has a defined molecular structure and set of physicochemical properties that encode the sensation perceived by the human observer [19-20]. But sensitivity to these volatile components varies from person to person depending on their age, physiological moment and health [6]. For these reasons gas chromatography and mass spectrometry have been started to use to access the quality of products through odour evaluation and identification and also to obtain more consistent results. But these procedures are found to be slow and expensive as well as the device used are not portable [2],[4]. Consequently there is enormous demand to develop an alternative system that can mimic the human sense of smell. In this regard gas sensing materials led to the development of
odour sensors. The odorant molecule produces changes in the physical and chemical properties of the gas sensing materials which can be recognized as an analog signal. Although the sensitivity, selectivity and stability of these sensor materials are the main issues yet these are considered as the most popularly used sensing devices in the present era [21]. Several types of sensors are available in the market, which exhibit physical and chemical interactions with the chemical molecules when they are in contact.

1.1.2 Gas Sensors

The last two decades have seen significant research effort being directed towards the development of gas sensors. The precise operating principle of a gas sensor depends upon the selection of the sensing material (e.g. metal oxide, catalyst, polymer, optical etc.) and the associated transduction principle [22-24]. The ideal sensors should possess high sensitivity towards chemical compounds...
and low sensitivity towards humidity and temperature. It should have medium selectivity so that it may respond to a range of different compounds. Besides the gas sensors should exhibit a steady and reproducible signal for a period of time. A few factors affecting the gas sensor’s instability are design errors, structural changes, chemical reactions leading to poisoning, changes in the surrounding environment etc. To avoid such instability, the material selected for sensing purpose should possess high thermal and chemical stability, using optimum grain size of the sensing material etc. As reported in literature, gas sensing technologies can be divided into two groups: methods that are based on variation of electrical properties and other properties [25-32] as shown in the Figure 1.2.

1.1.2.1 Metal Oxide semiconductor sensors

Metal oxide semiconductor (MOS) sensors were first used commercially in the 1960 in Japan under the names of Taguchi (the inventor) or Figaro (the company) as a gas alarm [31]. These sensors output are based on changes of conductivity induced by the adsorption of gases and subsequent surface reaction. Commercially available MOS sensors consist of a metal oxide semiconductor (either of p-type or n-type) film presenting a high surface to bulk ratio deployed on a ceramic insulated substrate between two ohmic contacts to measure the change in resistance/conductance [27-28].

Normally MOS gas sensors have an optimum working temperature of 250-350°C. When the MOS sensor is heated at about 100-200°C, O₂ molecules present in the ambient are adsorbed on the surface of metal oxides. Due to high electron affinity they would extract electrons from the conduction band Ec and trap the electrons at the surface and form an O²⁻ ion molecules as shown in the equation 1.1. This will lead to a bending of the conduction band and forms an electron-depleted region resulting in surface resistance increase.

\[ O_2 \text{ (adsorbed)} + e^- = O_2^- \]  

1.1
At higher temperature the oxygen ion molecules dissociates into oxygen ion atoms with one and two negative charges by attracting one and two electrons from the conduction band of the semiconductor material as shown in the equation 1.2 and equation 1.3.

\[
\frac{1}{2} O_2 + e^- \xrightarrow{K_{oxy}} O_{ads}^- \tag{1.2}
\]

\[
\frac{1}{2} O_2 + 2e^- \xrightarrow{K_{oxy}} O_2^- \tag{1.3}
\]

Where \( K_{oxy} \) is the reaction rate constant [33].

When the oxygen ions on the semiconductor surface come in contact with the target gas molecules, they give up the electrons back to the surface [32]. The chemical reaction between gas molecule and oxygen ions is shown in Equation 1.4

\[
X + O_{ads}^{b-} \xrightarrow{K_{gas}} X' + b e^- \tag{1.4}
\]

where \( X \) is the target gas and \( X' \) is the resultant gas, respectively. The \( b \) value is the number of electron and \( K_{gas} \) is the reaction rate constant of the gas reaction.

As the electron goes back to the conduction band of the semiconductor material, the conductivity of the material increases. The change in resistance again depends on the type of the semiconductor. In case of an \( n \)-type semiconductor, the resistance increases in presence of oxygen, as the electrons are removed by the oxygen. However in presence of the reducing gases oxygen reacts with the gas leaving the electron into the semiconductor. This leads to the decrease in sensor resistance. For a \( p \)-type semiconductor under oxygen ambient,
the oxygen atoms are adsorbed on to the surface and exciting electrons from the valence band raising the number of charge carriers. This leads to the decrease of the sensor resistance. In presence of the target gas, oxygen reacts with the gas leaving the electron back to the valence band and recombine with holes. This leads to an increase of the sensor resistance. The process is shown in the Figure 1.3. In presence of an oxidising gas the process will be just opposite [32].

The sensitivity and selectivity of MOS sensors can be modified by doping the semiconductor with noble metal catalysts (e.g. Pt, Pd, Al, Au), by modulating the operational temperature (e.g. 200–500°C) or by introducing thermal gradients/cycles. Doped sensors show greater sensitivity to oxygenated volatile organic compounds (e.g. alcohols, ketones etc.) than to aliphatic, aromatic or chlorinated compounds. Doping with Pt and Pd increases the sensitivity of SnO₂ sensors to gases such as benzene and toluene [27-28]. In 1962 Mr. Naoyoshi Taguchi developed the first semiconductor device to detect low concentrations of
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combustible and reducing gases. Later the devices are known as Taguchi Gas Sensors (TGS) [33]. These gas sensors have been widely used in the development of artificial olfaction systems.

1.1.2.2 Conducting Polymer gas sensors

Conducting organic polymer like polypyrrole, polyaniline, polythiophene are used as a gas sensors since 1980. They are highly sensitive and respond very quickly to the tested gas at room temperature. Conducting polymers can be easily synthesized through chemical or electrochemical processes and possess good mechanical properties, for facile fabrication of sensors [34-35].

![Configuration of a conducting polymer gas sensor](image)

**Figure 1.4** Configuration of a conducting polymer gas sensor

When vapours of an analyte come in contact with the oxidised polymer, the conducting polymer reacts with the analyte, causing a rapid change in the conductivity. Although mainly sensitive to polar volatile compounds, their selectivity and sensitivity can be modified by the use of different functional groups, polymer structure and doping ions [36-37]. Composite polymer with thermoplastic binders or glass fibres (e.g. polypyrrole with polyimide, polypyrrole with SnO₂, or with copper and palladium inclusions) shows large responses to non-polar volatiles. In addition, biomaterials such as enzymes, antibodies, and cells may readily be incorporated into polymer structures. A
variant of this type of sensors is based on electrically insulating polymers loaded with carbon black as electrically conducting filler.

Generally polymers readily absorb water vapour and as a result, the concentration of available binding sites for other volatiles decreases drastically reducing the sensitivity of conducting polymer gas sensors at high humidity levels. As some authors have suggested, the implementation of “filters” may retain undesirable compounds such as ethanol or water prior to analysis. Another drawback of this technology is the poor reproducibility in manufacturing polymer sensors. However, conducting polymer (CP) based sensors show linear responses and higher selectivity as well as faster response and base line recovery compared to MOS sensors [38], [7].

1.1.2.3 Carbon Nanotubes

Metal oxide semiconductors possesses the problem of poor sensitivity at room temperature, while carbon nanotubes (CNTs) are proved to be a high sensitive gas sensors. Discovered in 1991, by Iijima, Carbon nanotubes are long needle like tubes comprises of coaxial tubes of graphitic sheets, ranging in number from 2 upto about 50 [1].

![Figure 1.5 Configuration of carbon nano tube gas sensor](image-url)
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The tubes may be one atom thick layer of graphite rolled up into cylindrical form (single walled carbon nano tubes) or multiple layer of graphite wrapped up together to form tubular shape (Multi walled carbon nano tubes). Due to the c-c bond, Carbon nano tubes are considered as the strongest and stiffest fibre [38]. The one dimensional structure of the carbon nanotubes leads the electronic transport over long length without scattering. It enables to conduct current without any change in resistance. However the electronic conduction gets effected by the gas adsorption and collision with the tube wall [39]. In [40], Bushmaker et al. reported that single gaseous ion adsorption on CNTs, resulted in discrete, quantised resistance increase of over two orders of magnitude.

Kong et al. [41] demonstrated that when carbon nanotubes (SWNTs) were exposed to gaseous molecules such as NO$_2$ or NH$_3$, the electrical resistance of it increases or decreases. The sensors are also found to have very fast response time with very high sensitivity at room temperature compared to other solid state sensors. The high sensitivity eliminates the need of other supporting technologies like pre-concentration, as required to increase the sensitivity in other solid gas sensors. It also has the advantages of low cost, low weight and simple configuration with high adsorptive capability, large surface-area-to-volume ratio and quick response time, resulting in significant changes in capacitance and resistance [11]-[12].

1.1.2.4 Moisture absorbing materials

Moisture absorbing materials are used to detect the water vapour concentration. The water content present in the atmosphere may change the dielectric constant of the material. If moisture absorbing material is used as a substrate of the Radio frequency identification (RFID) tags antenna, then the RFID reader could detect easily the ohmic loss, changing the resonance frequency. Low cost of the material makes it suitable for mass production of the
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Sensor, although much report on the sensor is not available in the literature [42], [2].

1.1.2.5 Optical gas sensor

An optical sensor in detection system consists of four different components: a light source, suitable optics, sensing materials and a photo detector. The light source is used to excite the volatile components, producing a signal that can be measured in terms of resulting absorbance, fluorescence, polarization, refractive index, interference, scattering and reflectance [1].

![Figure 1.6 Structure of optical gas sensor](image)

Many chemical molecules are found to exhibit adsorption in the ultra violet (UV)/ visible or mid infrared regions of the spectrum. Thus using an IR source, the adsorption spectra in different spectral region can be observed after application of the tested gas. The adsorption spectra represent the characteristic fingerprint of the tested chemical molecules [2].

Response of the optical gas sensors can be obtained in real time as the sensor produces output in a very minimal time with minimal drift and high gas specificity with zero cross response to other gases [2]. As the incident light intensity can be determined, the measurements taken at the detector end are
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reliable. Gas sensing by optical method is easy and could achieve higher sensitivity, selectivity, and stability than non optical methods. More over their performance will not deteriorated by the changing environment. However their applications are restricted because of its high cost and due to miniaturization.

1.1.2.6 Gas Chromatography

It is a quantitative analytical method that can give excellent separation performance, high sensitivity and selectivity in case of the different components present in a sample. However the cost of the technology is high and also it is not useful for portable application [1].

In gas chromatography, the sample is injected continuously with an inert mobile gas through a column. While passing through the column, based on the concentration ratio, the components get separated between the mobile phase gas and the liquid stationary phase and the solid phase. As a result the rate of adsorption would be different for each phase of components and also causes different rate of movement inside the column. Thus the substances are identified based on the order in which they reached the outlet and also from the time the analyte stays in the column.

Figure 1.7 Gas chromatography
1.1.2.7 Acoustic wave gas sensors

The acoustic wave gas sensors are made up of piezoelectric material with electrodes that used to excite surface wave oscillations applying voltage. The acoustic wave deformed the crystal surface. For gas sensors the surface acoustic wave devices with dual delay line structure, the adsorbant membrane is used to coat one arm of the delay line and the other line is used as a reference. The change in frequency after adsorption of the vapour is given by,

\[ \Delta f_v = \Delta f_p C_v K_p / \rho_p \]  

Where \( \Delta f_v \) the change in the frequency is, \( \Delta f_p \) is the change in frequency caused by the membrane, \( C_v \) is the vapour concentration, \( K_p \) is the partition coefficient and \( \rho_p \) is the density of the polymer membrane used.

Acoustic wave while propagating through a medium interacts with the medium and induces sensor responses which includes many linear and non-linear property of the medium related to mass density, elasticity, electric and magnetic properties in case of the piezoelectric materials. As the acoustic wave propagates through the surface of the medium, any perturbation of the surface of the medium affects the wave. The surface elastic waves are found to be dependent on the temperature, pressure, force, gas, viscosity etc. All these factors affect the surface of the medium physically or chemically, changing the elasticity of the surface. This deformation when superimposed with the particle vibration due to acoustic wave propagation causes changes in velocity or amplitude of the propagating acoustic wave [1]. The changes in the velocity can be monitored by measuring the frequency or phase characteristics of the acoustic wave [2]. An acoustic gas sensor contains a receptor that is sensitive to an analyte and a transducer to convert the received signal into electrical one. The design of an acoustic wave
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Figure 1.8 The Acoustic wave gas sensor

The Acoustic wave gas sensor consists of a surface acoustic wave (SAW) delay line which is covered by a membrane which can adsorb a particular gas. Any change in the physical property of the membrane due to the adsorption of the gas results in the change in characteristics of the acoustic wave [1].

1.2 Artificial olfactory system: The Electronic Nose System

The sense of smell in mammals is stimulated only by gaseous molecules that come in the air. The odorant molecules stimulate the sensory nerve cells activating the protein molecules attached with it and produces the enzyme adenylate cyclase. This enzyme triggers the generation of action potential. The axons from all the receptor cells transmit the action potential to the brain as features. Brain collects all the features from individual receptor cell and stores then in the memory as odour. Upon receiving new features, brain starts to access memories, compare with the stored features and identify it if already there in memory. In 1961, RW Moncrieff presented the idea of development of an instrument based on the adsorption of odorant molecules on various films, simulating the natural olfactory process along with the additive features of detecting, estimating and classifying odours [2]. Wilkens et al. in [6] devised an electrochemical device which was later refined to use as a detector for
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measurement of volatile flavours and odours. They measured the respond current after the interaction of the volatile molecules with the polarised microelectrodes for qualitative and quantitative responses to volatiles. They demonstrated the responses of several odorants at a number of electrodes is similar to that occur in human olfactory receptor cells. It can be considered as the first step in the development of E-nose. In [16], Persaud et al. reported that the device made up of semiconductor transducers can discriminate between a wide variety of odours without the use of highly specific receptors. In [20], Sankaran et al. provided the recent development of an olfactory sensors that utilizes the model of the mammalian olfactory system. Gardener in [21] described the Electronic nose using the following definition- “An Electronic nose is an instrument, which comprises an array of electronic chemical sensors and an appropriate pattern-recognition system, capable of recognizing simple or complex odours”. In the artificial olfactory system, receptor cells are replaced by an array of chemical sensors. The sensors generate analog electrical signals when the odour molecules react with the sensor surface. The olfactory neurons are represented by a data processing unit, whereas the brain is represented by pattern recognition system.

Figure 1.9  Comparison of mammalian olfactory system and artificial olfactory system [43]
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Thus the odour sensing systems mainly consist of three components [21].

- Sensorial detection system
- Signal Preparation and
- Pattern recognition system.

![Diagram of Components of an E-nose system](image)

**Figure 1.10 Components of an E-nose system**

1.2.1 Sensor array

Chemical sensors for artificial olfaction should be responsive to molecules in the gas phase. Commercially available sensors for the design of an artificial olfactory system popularly known as E-nose are of various types [2],[5] including conductive sensors (metal-oxide semiconductor, conductive polymer), piezoelectric sensors (quartz crystal microbalance, surface acoustic wave), MOS field-effect transistor (MOSFET) sensors, optical sensors and spectroscopy-based sensors (mass spectrum, ion mobility spectroscopy).

Chemical sensors are found to be consists of chemically sensitive material interfaced with a transducer that can convert the change in the material to electrical signal. The output electrical signal is properly conditioned, processed and then analysed. Based on the chemical sensitivity, semiconducting metal oxides gas sensors, have been widely used to make sensor arrays for odour analysis. A good sensor should have highest sensitivity to the target group of odours with a threshold of detection similar to that of the human nose i.e. about
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To use it in diverse applications the sensors should have low selectivity so that it is sensitive to wide range of chemical vapors. It should have low operating costs and must have short recording and analysis times for real time systems with high sensor array stability. The whole system must be portable and small with built-in recording and analysis capabilities [23].

The sensor array is one of the main components in an E-nose system. The sensor array is constructed by using several cross selective sensors. MOS gas sensors are most popular for the development of E-nose due to its wide availability and low cost. When the sensor array is exposed to a target gas, each of the sensors in the array responds differently. This produces a pattern of responses for a target gas, which can be considered as a fingerprint of the target gas. This pattern of responses is compared by a pattern recognition engine for recognition of an unknown gas.

1.2.2 Signal Pre-processing

The individual sensors within the electronic nose produces a time dependent 1\textsuperscript{st} order electrical signal in response to odours [24]. The amplitude, rise and fall of the signal depends on the following parameters-

- The flow delivery system and the carrier that carries the target odour.
- The nature of the odour, i.e. type and concentration.
- The reaction kinetic of the target odour with sensor material surface.
- The diffusion of the odour within the active material
- The nature of the sensing material
- The nature of the substrate supporting the active material.
- The ambient conditions i.e. the temperature of the sensing material, humidity, pressure etc.

The signal response have to be pre-processed to compensate noise, drift etc. to improve the subsequent processing stage. The inputs to the data pre-processing
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module are in the form of voltage representing the transient response or the static response of the sensor array. Different data pre-processing techniques are responsible for shifting, compressing, and normalizing the raw data into a format that improves the performance of the subsequent steps for recognition [24].

The electronic nose produces huge amount of data based on the number of sensor present in the sensor array and the sampling frequency at which sensor data is collected [26-27]. Pre-processing is always required to remove the redundant data but retaining the original information as much as possible. There are three main signal pre-processing steps: baseline manipulation, data compression and normalization. All these steps focuses mainly on compensation of the drift, extracting informative parameters as features from the sensor array and then preparing the feature vector for further analysis.

1.2.2.1 Baseline manipulation

The sensor responses are manipulated with respect to the base line for the purpose of drift compensation, contrast enhancement and scaling [28-29]. Considering the dynamic response of the sensor the following techniques are normally used.

1. Differential: Here the baseline is removed from the sensor response so that any additive noise or drift present in the sensor signal gets removed. Thus baseline manipulated sensor response is [26].

\[ Y_S(t) = X_S(t) - X_S(0) \]  \hspace{1cm} 1.6

2. Relative: The Relative measurement can be obtained dividing the sensor response by the base line response. It removes the multiplicative drift and a dimensionless response is obtained.

\[ Y_S(t) = \frac{X_S(t)}{X_S(0)} \]  \hspace{1cm} 1.7
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3. Fractional: The baseline is subtracted and then divided from the sensor response. It is a per unit change with respect to the baseline, which compensates for sensors that have intrinsically large response levels.

\[ Y_S(t) = \frac{(X_S(t) - X_S(0))}{X_S(0)} \]  

4. Log parameter: This method is useful when the variation of the concentration is very large. The logarithmic change in conductance will linearize the sensor output and it will take the value zero in absence of odor input [30-31].

The choice of the baseline manipulation technique is based on the sensor technology used and the application. However researchers reported that out of all these the fractional change in conductance provides the best pattern recognition performance for MOS gas sensor [28].

1.2.2.2 Compression

The second stage of the pre processing of data is the compression where the huge sensor data has been reduced to a few feature descriptive vectors. The feature vectors are so selected such that they carry the most differential properties without removing the essential information. In most of the cases information is extracted from single parameter when the sensor response reached the steady state, simply neglecting its transient part. But the transient part may also carry information. It has been reported that transient part shows more repeatability than the steady state response. There are many algorithms that can be used for feature extraction from the time dependent sensor response.

Steady State: The steady state of the sensor response is considered as feature vector in most of the application [43]

\[ Y = R(T)_{\text{MAX}} \]
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The transient part of sensor response also carries useful information. Therefore researchers have applied different procedures to extract information from the transient part of the response. Three methods have been reported for extracting features from the transient part of the sensor response - the Sub-sampling method, the Parameter-extraction method and the System-identification method.

1. Sub-sampling method: In this method information is extracted from the dynamic part of the response by sampling the transient part at different time interval.

2. Parameter-extraction method: This method compresses the transient response by extracting features such as the slope, curve integral, rise time, maximum or minimum value [43].

3. System identification method: This method fit a theoretical model to the transient response and then the parameters of the model are taken as the features [43]. For example exponential curve fitting method which usually shows lossless compression but its computation takes time.

Sub-sampling and pattern extraction methods are normally used for compression purpose.

1.2.2.3 Normalization

Finally normalization methods are used to compensate the variation of responses due to variation of temperature, odour concentration etc. Here the values are scaled to readjust the sensor responses to an equal basis. The following methods are normally used

1. Vector normalization: Here example vector is divided by its Euclidean norm so that it lies in a hyper sphere of unit radius.

\[ Y = \frac{R}{(\Sigma R^2)^{1/2}} \]
2. Sensor scaling: Here the feature vectors are adjusted so that its coordinates have zero mean and unit variance.

\[ Y = (R - \bar{R})/\sigma_R \]  

where mean is \( \bar{R} \) and standard deviation is \( \sigma_R \) per sample.

3. Dimension auto scaling: Each dimension is normalized so that it has zero mean and unit variance.

\[ Y = (R - R')/\sigma_R, \]  

\( R' \) is the mean and \( \sigma_R \) is the standard deviation per dimension.

### 1.2.3 Pattern recognition

The pre-processed and feature extracted data is then introduced to a pattern recognition (PARC) engine for identification of the odour. The nature of the PARC engine can be classified into parametric or nonparametric and supervised or non-supervised engine. The parametric technique is based on the assumption that probability density function (PDF) can be used to describe the sensor response. While in non parametric technique, no function is used to describe the sensor signal. In a supervised PARC method, first a set of known odours are systematically introduced to the sensor array, and then they are classified according to their characteristics into different classes. When, in the next stage, an unknown odour is tested, the PARC method automatically compares the new one against the one already present in the database and predicts the class. The unsupervised PARC methods do not use a separate training stage, but predicts the different classes from the response characteristic vectors automatically [29]. The different PARC algorithms can be divided into two groups - classical statistical method and the Intelligent pattern analysis [31],[41],[44-46].
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1.2.3.1 Statistical pattern analysis

It is signal processing method in which each pattern is represented in terms of \( d \) number of features and is viewed as a point in \( d \) dimensional space. The effectiveness of the method depends on how well the patterns from different classes are separated [44]. Classifier can categorized based on certain features like supervised or unsupervised, model based or model free, quantitative or qualitative.

1.2.3.1.1 Linear calibration method

Linear calibration method uses linear algebra to process sensor array signal. In these methods it is assumed that the response of each odour sensor is proportional to the component concentration and the response of sensor array is the sum of the individual sensor response. The multiple regression method (MLR) is the one commonly used to analyze mixture of gases. MLR uses sensor response variables \( X_{ij} \) to predict the concentration \( C_j^s \) of a component using the following equation [26]

\[
C_j^s = b_{1j}X_{1j} + b_{2j}X_{2j} + b_{3j}X_{3j} + \ldots \ldots \ldots \ldots + b_{nj}X_{nj}
\]  

1.13

MLR is used to calculate the values of the regression coefficients \( b_{ij} \) for the sensors, minimizing the sum of squared deviation between the predicted component concentration values \( C_j^s \) and actual measured values.

Partial least squares (PLS) and the principal component regression are the other two linear calibration methods. In this model the concentration vector is related to the response matrix \( R \) by \( c = Rm + e \), where \( m \) is the regression vector containing all the model parameters and \( e \) is an error vector containing the concentration residuals of the other gases. The regression vectors are estimated in PLS and PCR by finding the pseudo-inverse response matrix in terms of orthonormal and diagonal matrices. PLS is often applied to gas mixture analysis.
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because it accepts collinear data, separate out the noise and make meaningful linear combinations of different concentrations. The difference between PCR and PLS is that the PCR does not includes any information related to the concentration.

These techniques are useful only in case of small and low concentration range. In order to handle non linear data the sensor response against concentration have to be linearized using pre processing techniques first or using non linear MLR model. Instead of predicting the chemical concentrations, it is more important to classify the component.

1.2.3.1.2 Linear Discriminant Analysis (LDA)

In Discriminant Feature Analysis (DFA), the data are assumed to be multinormal distributes and then the discriminant function $Z_p$ is calculated ,

$$Z_p = a_{1p}X_{1j} + a_{2p}X_{2j} + \ldots \ldots + a_{np}X_{nj}$$  \hspace{1cm} 1.14

Where $X_{ij}$ are the sensor response and the $a_{ip}$ is the coefficients to be determined based on the analysis of maximum F-ratio (between and within variation). Once the regression coefficients $a_{ip}$ is determined for a known data, following supervised learning, they can be used to form classification functions, which can predict the class of unknown response data. The commonly used approach for performing DFA is LDA. In this approach a straight line hyperplane is used to pass through the data assuming some criterion. In \textit{Mahalanobis} linear discriminate analysis (MLDA), \textit{Mahalanobis} distance metric is trained by computing a mean vector for each class and the pooled covariance matrix is used to define the class boundaries. Where as in \textit{Bayes} linear discriminant analysis (BLDA), the training is performed using mean vector for each class, and the pooled covariance matrix is used to position a linear separating surface [31].
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1.2.3.1.3 Principal Component Analysis (PCA)

It is a linear unsupervised technique used to display the response of sensors to simple or complex odours. The method is based on expressing the response vector in terms of linear combinations of orthogonal vectors along a new set of coordinate axes. Along the new axes the variance of sensor response becomes maximum and uncorrelated. Each orthogonal vector known as principal component represents certain amount of variance represented by the corresponding eigen values. The eigen vector associated with the largest eigen value corresponds to the first principal component [45]. PCA is often used as a visualizing tool to represent the multidimensional feature in 2-3 dimensional space.

1.2.3.2 Intelligent Pattern Analysis Techniques

It is often desirable for a PARC method which can handle non linear data and has the capability of self learning and self organizing as well as high noise tolerance. The new developments in PARC methods are artificial neural network (ANN) inspired by the pattern identification done by the human brain. ANN consists of parallel interconnected and adaptive elements in a way the neurons are connected in the brain.

1.2.3.2.1 Artificial Neural Network (ANN)

ANN consists of parallel interconnected, and adaptive, processing elements which can mimic the neurons networks of human brain [47]. Recently many ANN algorithms have been widely used in odour recognition task. In multilayer network the processing elements are organized in three layers: input layer, hidden layer and the output layers of neurons. The number of input nodes are determined by the number of odour sensors present in the array and numbers of features. The numbers of neurons in the hidden layers is determined experimentally and the number of neurons in the output layer is based on the number of odours to be
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recognised. The interconnection between the neurons in the different layers and the learning rules determines the performance of the neural network.

The three layered back propagation is the most popular ANN used for network training. Through iterations and modifications the average squared errors of the test data are used to determine the optimal weights and biases [47]. To train the network, it is provided with a number of sample inputs with their corresponding outputs (supervised learning). Each neuron adds its weighted inputs and nonlinear transformation usually sigmoid function is performed on the sum to obtain the neurons output. The calculation is carried out for each neurons, each layer passes it to the output layer. In the learning phase, the weights are adjusted to minimize the error i.e. the difference between the actual output and the required output. In the learning phase the weights are updated during each presentation of the training samples on each iteration. Thus the weights are modified to minimize the mapping error and when stabilized the network is said to be trained. The total sum squared error can be used to represent the performance of the network. Once the network is trained, it is ready to predict the class of any unknown odour. The success of the network depends on the architecture as well as the weights which are obtained from learning.

As an alternative method, genetic algorithm can be used which can determine automatically a suitable network architecture. This search algorithm based on the mechanics of natural selection is proposed by Holland in 1975. The structure and initial parameters of the neural network i.e. learning rate, initial weights, number of layers, number of neurons in each layer and connectivity etc. are coded using binary strings, which are concatenated to form chromosomes. Random interactions of bit information are carried out, for generating off spring superior to parents. The continuous repetition of the procedure generates optimal species with the strongest adaptability [48]
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The probabilistic neural network (PNN) operates defining a probability density function (PDF) for each data class based on training data set and an optimized kernel width. The PDF defines the boundaries of each data class and the kernel width determines the interpolation between two adjacent classes. Here the input layer of neurons used to pass the new patterns to the hidden layer. Here the product of the new pattern and the training pattern set is computed. The summation layer consists of one neuron for each data class and sums the outputs from all hidden neurons of each respective data class. It is forwarded to the output layer where the probability of the new one to belong to that class is calculated.

1.2.3.2.2 Fuzzy Based Pattern Analysis

Fuzzy set theory (FST), is defined for the data set whose boundaries are not sharp. It provides the output in terms of linguistic variables and imprecise language as defined by human (like hot, cold, slow etc). Fuzzy clustering deals with splitting a set of patterns into number of classes, with respect to similarities between the patterns belonging to the same class. It can be precisely used as a optimisation tool for class centers and spreads. The fuzzy c–means algorithm provides an iterative approach for this optimisation. In a type of fuzzy neural network (FNN), the initial weights are determined using membership class restrictions imposed on a variable defining the range of values. Use of FNN leads to signal conditions that translate many overlapping parameters of the sensor array response into one that can be better handed by the classifier [45].

An odour may consist of thousands of different compounds so use of specific sensors is an impractical idea. Instead of that use of a powerful PARC system for classification might be a good solution. The objective of all the above pattern recognition systems is to first train the network to classify the different odours in
such a way that the system can identify automatically an unknown class of data. Therefore PARC is an important unit for a successful odour detection system.

1.3 Sensor and Feature Optimization

Electronic-nose system consists of an array of gas sensors for odour sensing. The performance of E-nose can be enhanced and complexity can be reduced by using an optimized set of gas sensors in the array. Optimization of gas sensors may result in reduction of the number of gas sensors without reducing the classification performance. If the number of sensors is not optimized then it increases the system and PARC complexity and may result in poor performance of classification. Likewise the feature set extracted from the sensors may have redundant features. These redundant features may further reduce the classification accuracy. Therefore to enhance the classification performance of the E-nose system, it is necessary to optimize the sensor set and feature set. There are different optimization approaches investigated by researchers for sensor and feature optimization.

1.3.1 Exhaustive search method

Sensor and feature selection can be viewed as a problem of optimization. Different subset of sensors and features may be analysed in terms of best value of an objective function. The most straightforward method is to search for all possible combination for the best objective function. This is the exhaustive search method and produces the optimal results. This method however is computational intensive and if the number of possible subset is high then this method may not be practically viable.

1.3.2 Sequential Search

Sequential search is the easiest and frequently used optimization method. However it is most inefficient and produces suboptimal results. This method is
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also called linear search method and it is computationally efficient. There are two basis schemes of linear search method- sequential forward search (SFS) and sequential backward search (SBS). These methods have been widely used for feature selection. In SFS, the algorithm sequentially searches for best value of an objective function. It starts with an empty set of features and sequentially adds to it an unselected feature depending on the value of the objective function. In this way a subset of features is created and when the subset meets the goal the algorithm is halted. SBS approach starts with the complete set of features. As the algorithm progress it goes on rejecting one feature at a time depending on the value of the objective function until additional deletion causes the degradation of the objective function value.

1.3.3 Particle Swarm Optimization (PSO)

Particle swarm optimization is a population based computational method that is used for optimization of a problem through an iterative process. The algorithm initiates with random solutions of the population called particles. These random solutions are updated at each iteration during the search for optima. During the search for optimal solution one of the particle has optimal solution and other particles follow the particle. Every particle has a position (which represent its solution) and a velocity component which directs it to move in the search space. The solution of a particle is evaluated by a fitness function. The PSO algorithm keeps tracks of the best fitness value and its solution obtained by each particle and the global best fitness value and position obtained by any of the particle. The algorithm directs the particles to search in the direction of global best solution and finally after iterative process the PSO algorithm determines the optimal solution. This algorithm determines an optimal solution faster and efficiently than the exhaustive search method.
1.4 Portable odour monitoring system

An portable odour monitoring system can provide real time information about the presence, movement or disappearance of the odour continuously using gas sensors. In [49] Kim et al. reported the active industrialization of odour detection system in countries like Japan, Canada, Korea. However these products suffer from problems like high consumer price, difficulties in maintenance and repair. They presented the design of an odour monitoring system using pattern recognition algorithm for identification of malodorous substances in air. They used Genetic algorithm for extracting the patterns of harmful gases and ANN for testing purpose. In [52] Tang et al. presented the prototype of a portable electronic nose (E-Nose) consisting of eight sensor array, a data acquisition interface PCB, and a microprocessor and used to identify the fragrance of three fruits, namely lemon, banana and litchi. For classification they used KNN classifier and achieved in excess of 95% accuracy. In [53], Pan et al. reported a new portable intelligent E-Nose system for monitoring and analyzing livestock and poultry farm odours. They used 14 gas sensors along with “Odour Expert” system and concluded higher consistency in the field experimental results.

1.5 Electronic-Nose Applications

Electronic-nose systems have been designed specifically to be used for numerous applications in many different industrial production processes. A wide variety of industries based on specific product types and categories, such as the automobile, food, packaging, cosmetic, drug, analytical chemistry and biomedical industries utilize E-noses for a broad and diverse range of applications including quality control of raw and manufactured products, process design, freshness and maturity (ripeness) monitoring, shelf-life investigations, authenticity assessments of premium products, classification of scents and perfumes, microbial pathogen detection and environmental assessment studies. Researchers around the glove has employed E-nose for various end applications. In [50], Pinheiro et al.
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employed the commercially available (A32S Aroma Scan) E-Nose for aroma monitoring during wine fermentation. In [51], Brezmes et al. developed an E-nose consisting of 8 MOS gas sensors for non-destructive monitoring process of fruit ripening. In [54], Dutta et al. developed an E-nose consisting of four MOS gas sensors for the purpose of quality and flavor detection of tea samples.

1.6 Objective of the proposed work

Research in various aspects of the Electronic Nose has been performed by various researchers. MOS gas sensors are commonly used in odour detection systems. Researchers have operated MOS gas sensors in static operation mode and dynamic operation mode to extract relevant features. In dynamic operation mode the temperature of the sensor is dynamically varied by a heating waveform resulting in a characteristic response waveform from the sensor. The dynamic response of the gas sensors are found to produce a huge set of features that helps for better classification. Dynamic operation mode has been investigated by various researchers with diverse shapes of the heating waveform. In [55], Nakata et al. used a sinusoidal heating waveform for MOS gas sensor and extracted characteristic features using fast Fourier transform (FFT). The FFT features were used for gas discrimination. In [56], Ngo et al. interrogated an array of six MOS gas sensors with a triangular waveform of 25mHz to identify environmental and industrial gases. In [57], Bukowiecki et al. interrogated an array of four MOS gas sensors with various heating waveforms like sawtooth, triangular etc. in the design of a gas alarm system. They concluded that a gas could be identified from the resulting characteristic waveform of temperature modulation. In [58], Huang et al. also interrogated the MOS gas sensors with various heating waveforms such as rectangular, pulse, sawtooth, triangular, sinusoidal etc. and used five chemicals as odour source. They concluded that more discriminatory features are obtained when the sensors are modulated with a low frequency and a small number of sensors could be used for gas discrimination. In [59], Osuna et al. modulated the temperature of MOS gas sensors with sinusoidal waveforms of various
frequencies to enhance the selectivity of sensors. They concluded that low frequency modulating waveform provides more characteristic waveform of the target gas. Although the use of various heating waveform have been reported by various researchers, the optimization of best waveform for modulation in a particular application is not reported.

Sensor optimization enhances the performance of E-nose. Hence for a particular application the subset of sensors have to be optimized for enhanced classification performance and reduced system complexity. Sensor optimization in E-nose has been reported by various researchers. In [60], Pardo et al. optimized their sensor of E-Nose system which consisted of 20 sensors. They have used the exhaustive search approach to determine the best 5 sensor configuration suitable for their task. The objective function used was the classification performance of a classifier based on MLP and LDA. In [61], Phaisangittisagul et al. optimized sensor subset using a genetic algorithm based approach. The objective function used was the classification performance of a \(k\)-nearest neighbour (k-NN) based classifier. They have performed various experiments with different datasets. In the dataset of coffee, they presented results where their algorithm was able to optimize a sensor subset of 4 sensors from a set of 15 sensors.

Dynamic operation of MOS gas sensors results in huge amount of features for odour recognition and may contain redundant and less important features. Those redundant and less important features need to be eliminated or else it will lead to increasing complexity of PARC and degrade the classification performance. Feature selection has been reported by various researchers. In [62], Boilot et al. reported a feature selection method based on genetic algorithm. They were able to obtain a reduced feature subset containing 20 to 30 features from a total of 72 features in their E-nose system. The optimized feature subset enhanced the classification accuracy to 94.3% from 75.2% with the original dataset. In [63], Lin et al. reported a feature selection algorithm by combining support vector
machine (SVM) and particle swarm optimization (PSO). In the algorithm the classification accuracy of a SVM based classifier was used as the objective function. An enhanced classification accuracy of 81.62% to 100% was obtained among different datasets using the algorithm. It is very much necessary to optimize the features as well the number of gas sensors. For this a proper feature selection algorithm is also required so that the PARC unit can successfully detect an unknown odour.

On the basis of the literature review the present research work towards the development of a portable and embedded system for real time identification of odour is carried out with the following objectives.

1) Development of a prototype portable system for real time data acquisition and odour detection of different odours.

2) Optimization of sensor in the portable E-nose system based on exhaustive search method combined with Euclidean inter-intra class distance ratio.

3) Evaluation of best waveform for temperature modulation in the portable E-nose for generation of most informative features.

4) Optimization of features for performance enhancement and complexity reduction of the portable odour detection system by suitable feature selection method.

1.7 Contributions

The key contribution of this research work are summarized below-

1) An odour detection system with nine MOS gas was designed and developed to carry out further research. The system consisted of a microcontroller based heating waveform generation and driving circuit to modulate the temperature of MOS gas sensors. A real time microcontroller data acquisition system was developed along with LabView based software for computer based data acquisition.
2) The optimized subset of sensors of four sensors from among the array of nine sensors of the E-nose system designed for 16 different target gases has been found. The optimization was performed using exhaustive search method using Euclidean inter-intra class distance ratio as the objective functions. All the 511 possible combinations of nine sensor were considered and the Euclidean inter-intra class distance ratio was calculated. Based on the distance ratio the optimized subset of gas sensors has been established.

3) The best waveform for temperature modulation of MOS gas sensors in the portable E-nose system for detection of 16 different gases was evaluated. A total of nine different modulating waveforms were considered and the best waveform which resulted in best class separation of the target gas was determined using Euclidean inter-intra class distance ratio as a class separation measure.

4) The optimized feature subset with 14 features from among 40 features of four optimized sensors has been found. Two different feature selection algorithm were considered – sequential forward search and particle swarm intelligence using Euclidean inter-intra class distance ratio as the objective function. The particle swarm intelligence resulted better subset of features than the sequential forward search algorithm.

5) An odour classification algorithm based on artificial neural network was trained in Matlab software using the 14 optimized feature subset. The weights obtained from training were used to implement the artificial neural network recall phase on the microcontroller for embedded gas detection system.
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1.8 Thesis Organisation

The organization of this thesis is as follows:

Chapter 2: Experimental Setup: The Data Acquisition System – This chapter describes the experimental setup for odour data acquisition developed to carry out the research. The detail description of different components of the prototype system is described in the chapter.

Chapter 3: Optimization of Gas Sensor Array - In this chapter a literature review is presented on the different methods for sensor optimization. A method to optimize the sensor array in the portable E-nose system is described and results presented.

Chapter 4: Best Waveform for Temperature Modulation - In this chapter a literature review on the different temperature modulating waveform that are used for enhancing the features in MOS gas sensor array is presented. A method to determine the best waveform for temperature modulation is discussed and results are presented here.

Chapter 5: Feature Selection and Embedded Odour Detection System - This chapter presents a review of literature on different methods for feature selection. The chapter discusses and presents the results of various feature selection methods investigated during the research. The detail design step of PARC for the embedded odour detection system is discussed in this chapter.

Chapter 6: Conclusion and Future Scope - This chapter summarizes the thesis and presents the future scope of this research work.
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References


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