Preface

In the modern era, design and development of solid state gas sensing devices and the associated data processing techniques for detection and quantification of gases/odors and volatile organic compounds (VOCs) are increasing day by day. Electronic-nose (e-nose) is the desired system for present day requirements which is comprised of gas sensing devices (generally in the form of sensor arrays) and associated signal processing block. The signal processing block generally utilizes pattern recognition (PARC) techniques. Most of the gases/odors are very complex in terms of molecular structure which makes it difficult to identify them by their traditional methods such as molecular weight methods etc. Moreover, these traditional methods are rather slower which may not be appropriate for the present day requirements.

The e-nose, which mimics the human olfactory system, acts as a machine olfaction system. The responses of sensor array used in the e-nose are collection of electrical signals generated by each sensor element in the array and they collectively make a unique signature pattern for a particular gas/odor. This response of sensor array is generally used in the modern e-nose systems to detect a particular odorant in either single or mixture form. The obtained signature patterns are utilized by suitable pattern recognition technique for gases/odors identification and/or quantification.

Data preprocessing also plays an important role in the identification and quantification of gases/odors in precise way. The sensor array responses (raw data) generally may not be suitable for processing with the subsequent pattern recognition technique as it may be susceptible to noise or some missing values. Moreover, the raw data sometimes may not provide some hidden pattern of the dataset. Thus, choosing an appropriate data preprocessing technique plays an important role in the gas/odor identification/quantification task.

Sometimes, the raw data with high dimensionality may contain some redundant information. It is always helpful in reducing the dimensionality of the raw dataset without losing the useful information. This reduction of dimensionality helps to decrease the data processing time of the PARC technique which in turn enhances the response of e-nose system. Principal component analysis (PCA) and linear discriminant analysis (LDA) are the two popular techniques used in the pattern recognition tasks for data preprocessing and dimensionality reduction of the input raw data. PCA is unsupervised in nature while LDA is a supervised method of feature extraction since it takes class information into account. The PCA preprocessed data have shown appreciable improvements both in terms of classification and quantification results. PCA has less computational complexity and the results are found to be comparable with the supervised method like LDA.

After the raw data is preprocessed, next target is to choose an appropriate pattern recognition technique. Pattern recognition techniques can be divided into supervised, unsupervised and semi-supervised techniques depending on the class information of the training data are available or not. In the supervised PARC techniques, the class labels are available for the training data. Unsupervised methods do not need training data to have class labels. Semi-supervised methods, on the other hand, handles partially labeled training data. In supervised methods, artificial neural network (ANN) and support vector machines (SVMs) have shown their strength in various PARC problems. In the present work, both of these techniques have been used to classify as well as to quantify different gases/odors.

The present work is oriented towards the analysis and development of some soft-computational techniques to assess the gases/odors qualitatively as well as quantitatively. For qualitative and quantitative assessment of gases/odors using published dynamic response, a simple but effective technique called average slope multiplication (ASM) have been proposed. For binary mixture analysis using steady state responses, a thick film array was fabricated by the author to generate the steady state responses for gases/odors in both, individual as well as in mixture forms. The class and concentration estimation analysis of binary mixture of volatile organic compounds (VOCs) have been performed using support vector machines (SVMs) and multioutput support vector regression (*M*-SVR) methods.

The chapter wise outlines of the present thesis work are as follows:

Chapter-1 presents a brief introduction to the mammalian olfaction system and introduces the need of machine olfaction system. This chapter also introduces the tin oxide based sensor array devices and various soft computational techniques used in PARC systems suitable for classification/quantification of gases/odors. Subsequently, a relevant literature survey has been presented based on the previously reported works in this area. Finally, the scope and specific aspects of the present thesis work has been discussed.

Chapter-2 discusses the electronic properties of SnO_2 viz. bulk and surface properties and the gas sensing mechanism in brief. It explains the design, fabrication and characterization of tin oxide based thick film gas sensor array. The steps followed for the fabrication of thick film gas sensor array have been discussed in detail. Data acquisition system has been explained briefly. The validation of sensor array responses have been done with the proposed tin oxide based thick film sensor array model. The fabricated sensor array has been used for generating the responses of gases/odors in individual as well as mixture form in subsequent chapters (Chapter-3 and Chapter-5).

Chapter-3 presents a comparative study of the preprocessing tool such as principal component analysis (PCA) and linear discriminant analysis (LDA) in classification of gases/odors using two types of datasets. First dataset is published steady state responses of thick film sensor array taken by [Mishra and Agarwal (1998)]. Second dataset is the steady state responses generated from the thick film sensor array fabricated by the author. A simple multilayer feed-forward neural network with back propagation algorithm was designed as a classifier in the subsequent classification stage. The results of experiment performed for gases/odors classification shows that PCA can be preferred as compared to LDA for data preprocessing and dimensionality reduction due to its unsupervised nature and the promising results obtained.

Chapter-4 proposes a new method called average slope multiplication (ASM) for classification and quantification of gases/odors using published dynamic responses of thick film gas sensor array. The instantaneous values of the dynamic response/recovery plots were extracted for various test gases viz., LPG, CCl_4, CO, and C_3H_7OH and correlated to its neighboring response plots by the use of proposed ASM technique. It has been demonstrated that the proposed method offers excellent results for classification and simultaneous quantification of individual gases/odors using the dynamic responses of thick film gas sensor array with BPNN as a classifier. Principal component analysis (PCA) has been further used for data preprocessing and dimensionality reduction and for performance comparison purpose.

Chapter-5 presents the study on single as well as binary mixture of two volatile organic compounds (VOCs) viz. Acetone and 2-propanol in their gaseous form. A sensor array consisting of four sensor elements was fabricated by the author in the lab using thick film fabrication technology. The steady state responses of the sensor array were collected for the mentioned VOCs in their individual as well as mixture form. A hierarchical system consisting of gating network and three quantification networks was designed to first classify and then quantify the individual and mixture of VOCs. The classification results of gating network have been ensured using back-propagation neural network (BPNN) and support vector machine (SVM). For quantification, multioutput support vector regression (M-SVR) method was used in quantification networks for individual as well as binary mixture data.

Chapter-6 finally summarizes the entire work done in this thesis and concludes the major achievements of the present work. Scope of the future work has also been discussed to carry out future research work for the development of portable e-nose systems.