



Temperature modulation of electronic nose combined with multi-class support vector machine classification for identifying export caraway cultivars

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ABSTRACT

Caraway is one of the most consumed medicinal spice around the world. Different cultivars of caraway represent differences in the aromatic profiles which mark the difference in their selling prices in the international market. The present study provides a non-destructive methodology based on metal oxide semiconductor (MOS) based electronic nose (e-nose) and chemometrics for rapid classification of five different caraway cultivars (Zarand, Jupar, Kerman, Khabarbaft and Kohbanan) from Iran. To acquire enhanced aromatic profiles the study utilises temperature modulation technique in a MOS based electronic nose. The temperature modulations were performed with two voltage functions i.e. rectangular and sinusoid, and the best voltage function for classification was evaluated and reported. Measurements were performed in three phases and recorded transient responses of eight MOS sensors were considered for data analysis. To visualise the MOS sensor array data principal component analysis (PCA) was used. For classification purpose, linear discriminant analysis (LDA) and multi-class support vector machine (SVM) were performed on the PCA transformed data. Results showed that data visualisation with PCA clearly identify separate clusters over the PC transformed space. A maximum classification accuracy of $97.92 \pm 3.82\%$ was obtained for the SVM classification model on the rectangular voltage function. The performance of LDA modelling was similar to the SVM results in the case of rectangular voltage function, but in the case of the sinusoid form, the SVM results showed better accuracy to classify the caraway cultivars. As a consequence, it can be concluded that MOS based e-nose and chemometrics could support the rapid and non-destructive classification of caraway cultivars. Furthermore, the temperature modulation with rectangular voltage function can provide higher classification accuracy.

1. Introduction

Cumin is a plant from Apiaceae family (*Umbelliferae*) and one of the most important and consumed medicinal herbs and spices around the world (Bharti et al., 2018). The difference in the percentage of aromatic compounds in cumin types like caraway obtained from different areas has led to the differentiation of some cultivars of caraway compared to other cultivars, which causes the adulterations in purchase or exportation for this product (Tahri et al., 2016). Due to the fact that the percentage of the constituent compounds affects the quality of the odour, this attribute can be used to detect different cumin cultivars.

Today, various analytical techniques are being used to recognise the cumin cultivars but most of them are expensive, and the necessity of using non-expensive, fast and reliable innovative tools such as electronic noses is emphasised in the literature (Tahri et al., 2016). An

electronic nose is a device designed to detect and distinguish complex odours using an array of sensors. Metal oxide semiconductor (MOS) sensors are the most popular in electronic nose studies due to the low price and high sensitivity for biological materials such as agricultural and food products. However, some problems and challenges exist in the use of MOS sensors. Some of the challenges include high power consumption, low selectivity, slow recovery time and long response time (Monroy et al., 2012). Slow recovery time is a critical limitation where the sensors should be exposed to rapid detection of gases. One of the approaches to overcome the latter problems is the temperature modulation (Herrero-Carrón et al., 2015). In this technique, the working temperature of the sensors varies as a function of the voltage applied to the heater installed on the sensor array. In fact, this technique utilises modulation in heating temperature to improve the sensors discrimination ability by exploiting different physicochemical properties at

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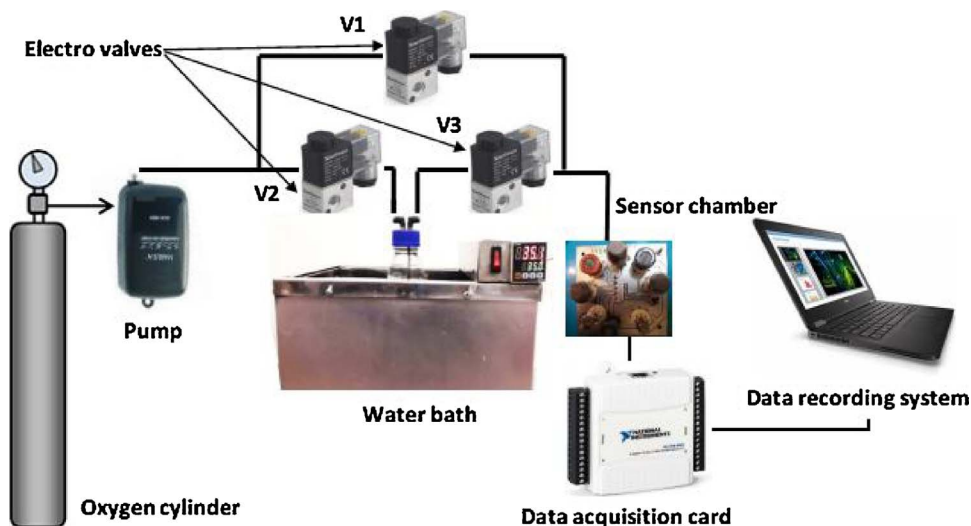


Fig. 1. Schematic view of the experimental set-up.

different temperatures. For instance, many researchers showed that temperature modulation of MOS improves selectivity (Fort et al., 2002, Gramm, 2003, Ngo et al., 2007). Besides, the transient response of the sensor is considered for gas detection rather than steady-state response (Hossein-Babaei and Amini, 2012). Thus, due to considering the transient state of the signal, the time of the measurement reduces significantly leading to lower power consumption.

The data generated by the MOS sensor array usually consist of recording the sensor responses along the time. For an array consisting of the single sensor, the analysis of data is pretty simple, however, when the number of the sensor increases the complexity of data increases. The increase in complexity results in the multivariate data which require advanced pattern recognition tools to extract the meaningful information from the data-set. One such important method to develop a first understanding of collected data is the principal component analysis (PCA) (Wold et al., 1987). The PCA supports the visualisation of multivariate data by identifying orthogonal latent spaces to represent the maximum amount of variation. Later, the multivariate data is transformed with the help of latent spaces and visualised in 2D or 3D plots. Many applications of PCA can be found related to visualising the data generated through MOS sensor arrays (Aleixandre et al., 2008, Yu et al., 2009, Singh et al., 2014). Once, the data has been visualised and transformed with PCA; the data can be further used to perform the modelling as needed. In the present work, the aim was to perform the classification of five different varieties of caraway. Therefore, the PCA transformed data was used to perform the classification analysis. There are different methods to perform the classification available in the domain of chemometrics (Marini, 2010). However, in present work, we limited to two methods, i.e. linear discriminant analysis (LDA) and multi-class support vector machines (SMV). The LDA is popular pattern recognition method which aims to find the linear combination of features to perform the classification. The SVM utilises the concept of hyperplanes to make the data linearly separable by projecting it to high spaces. The choice of two methods was based on their popularity in the chemometric domain as well their successful application in processing the data generated from MOS gas sensor array. Some application of LDA and SVM for successful classification analysis with MOS gas sensor array data can be found in the literature (Hotel et al., 2018; Qiu and Wang, 2017; Gorji-Chakespari et al., 2017).

Present study was aimed at the temperature modulation of the electronic nose which has been developed recently in (Ghasemi-Varnamkhasti et al., 2018). This temperature modulation approach was used to classify five export caraway cultivars called Jupar, Khabarbaft, Zarand, Kerman and Kohbanan originating from Iran. All the five caraway cultivars used were valuable cultivars for export aims to Iran and

a reliable and fast recognition of the cultivar types was of particular interest to the cumin packaging industry. The MOS e-nose based sensor approach was used due to the similar appearance of different cultivars for which visual inspection based distinction is not possible. The data generated with different MOS based sensors was accessed with chemometrics. Firstly, PCA was utilised to transform the data into a few latent variables to perform data visualisation and support the classification. Furthermore, the performance of rectangular and sinusoidal temperature modulation to classify different caraway cultivars was accessed with LDA and multi-class SVM.

2. Materials and methods

2.1. Sample preparation

The samples used in the study i.e. the Caraway cultivars (Zarand, Jupar, Kerman, Khabarbaft, and Kohbanan) were sourced from the locations in Kerman province, Iran. These cultivars are considered for the export to the world.

2.2. Experimental set-up

The experimental set-up employed consisted of a customised e-nose (Tohidi et al., 2018). The system includes a sensory array, sampling and sensory chamber, data recording unit, water bath, pump, tubes, pneumatic valves and appropriate data analysis method and pattern recognition algorithm. The experimental set-up is shown in Fig. 1.

The sensor array consists of eight individual MOS. Four sensors such as TGS2602, TGS2620, TGS813 and TGS822 were purchased from Figaro Engineering, Inc. (Glenview, USA), three sensors including MQ3, MQ8 and MQ136 were supplied from HANWEI Electronics Co. (Hanwei, China) and one obtained from FIS Inc (Osaka, Japan) that were placed in a Teflon cylindrical chamber. The sensor names and their specifications are presented in Table 1.

In addition, a single chip Sensirion SHT75 sensor was used to record simultaneously temperature and humidity inside the sensory chamber. All the sensors were placed in a Teflon-based sensory chamber attached to sample inlet and outlet path (1/8" push-fit, Pneu-store). The sample inlet path in the sensor chamber was connected to the sampling chamber. By passing through oxygen as a carrier gas around the sample, a mixture of air and volatile organic compounds (VOCs) from the sample was fed to the sensors' chamber. As reported earlier in our paper (Ghasemi-Varnamkhasti et al., 2018), the measurement process includes three different stages: (1) concentration, (2) measurement and (3) purge.

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