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AI-enabled rapid method for complex quality assessment of edible oils

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Summary: The research aimed to replace a set of standard methods for edible oil quality control by developing an AI-enabled rapid headspace analysis procedure. The use of a ceramic sensor array confirmed the feasibility of assessment of oil oxidation under static conditions, however, it was unable accurately predicting individual quality parameters. Due to the impracticality of applying selective enhancement approaches to ceramic sensors, an array of commercially available microsensors were used in combination with different temperature modulation modes.

Keywords: SMOX-based sensors, temperature modulations; quality assessment; edible oils; AI.

Introduction. The applications of chemical sensors for monitoring the quality/safety of food products, including edible oils, have not found sufficient implementation to date in the industry. If the control of technological processes is mainly monitored by physical sensors, monitoring a complex food matrix has been limited due to constraints in sensor characteristics and the lack of progress in data science. However, advancements in today's chemical sensor development, such as the miniaturized Sensirion Gas Platform (SGP) multi-pixel gas sensor [1], as well as deep machine learning algorithms incorporating elements of artificial intelligence (AI), offer the potential to enhance the sensitivity and selectivity of novel alternative methods and to provide necessary multidimensional information about the sample's state and the physicochemical reactions occurring within it.

Needs of industry. Quality control of vegetable oils ready for distribution is mandatory requirements regulated by both international and local authorities [2, 3] through a set of physico-chemical methods [4, 5]. Such methods are characterized by significant disadvantages, such as the necessity to use a large amount of suitable solvent mixtures for sample dissolution before titration (peroxide and acid values (PV and AV, respectively)), long measurement times, poor repeatability (moisture and volatile matter content, MVC), lengthy and multi-stage sample preparation for the analysis of the anisidine value (p-AV), and the need to measure a set of parameters together to account for possible various types of spoilage determined by the different compositions of oils. The current speeds and production volumes ask for a critical examination of traditional analytical chemistry approaches for food analysis to ensure effective monitoring of their quality and safety.

Experiment and results. Samples of various cold-pressed and refined vegetable oils were taken from production for quality analysis during the oxidation process: sunflower, rapeseed, and olive oils of different geographical origins. The oils were exposed to autoxidation to facilitate the transfer of the obtained models to real-life conditions, because the mixtures of formed oxidized compounds and their concentrations vary in the nature and composition of oils, as well as in the conditions and extent of oxidation.

The reference parameters, required to enable a comprehensive monitoring of oil quality, were used, regardless of the possible product spoilage mechanism. We monitored: MVC and AV as indicators of lipolysis; PV and p-AV values, which together can provide information about primary and secondary products of oxidation.

At the initial stage, sensors TGS 2600, TGS 2620, and FIS SB-AQ1-06 were investigated (Figaro, USA; Nissha FIS, Japan). Extracted parameters at the beginning and end of the transient response to oil vapors under constant sensor heating were used as input data for principal component analysis (PCA).

PCA was used for exploratory analysis and discovering informativeness and hidden dependencies in the data. Its essence lies in assuming linearity of data relationships and their projection onto a subspace of orthogonal vectors where the variance is maximized. These vectors, called principal components (PC), determine the directions of greatest variability (informativeness) of the data. In other words, it's a linear projection that minimizes the mean squared distance between the original points and their projections. The data matrix was autoscaled. PCA was performed based on the singular value decomposition algorithm and cross validated. PC1 corresponds to the direction of maximum variation in the data. In the Fig.1, we observe the clear trend of changes in the quality of oil samples along PC1 (86% of explained variance), as well as the separation of two types of oils along PC2 (13%).

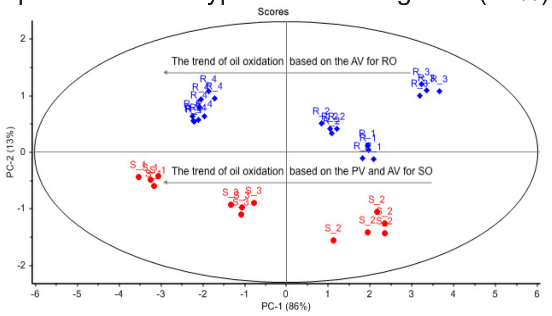

Fig. 1. PCA scores plot based on the responses of three sensors to various qualities of sunflower (SO) and rapeseed (RO) refined oils from six different manufactures.

For the differentiation among individual quality parameters and for a more precise prediction of the PV, AV, p-AV, MVC, it is necessary to increase the dimensionality and orthogonality of the sensor arrays. The sensors used in the first set of experiments also show strong multicollinearity (correlation of more than 0,96 between the TGS 2600 and TGS 2620) in prediction the PV and AV parameters.

A possible approach to selectivity enhancement is the operation of the sensors in different heating profiles; besides that, such practice is not recommended by manufacturers, their relatively large mass makes fast modulation impossible, besides this they have a considerable power consumption and even influence on the composition of the gaseous samples they are exposed to. The alternative increase of the sensor array by increasing the sensor number is not considered feasible for this application. The SGP 40 sensor (Sensirion AG, Switzerland), in this context, presents itself as an optimal solution for a miniaturized device with the capability to enhance selectivity through individual temperature modulation of each of its four pixels (Fig. 2). Figure 2 shows one modulation of 19 temperature steps (1 ramp), which resulted in 76 responses (19 steps x 4 pixels) from the device for a 3-minute measurement.

The used sensor array consisted of three SGP40 sensors (3 x 4 pixels) with different temperature modulation modes for each, mounted in a sensor chamber that allows for direct measurement of the oil headspace.

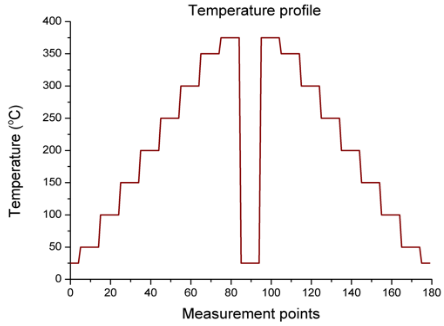

Fig. 2. One of the three temperature modulation modes, applied for the SGP40 sensors.

As the sensors measure the total VOC content simultaneously present in the oil headspace, our approach ensures the high sensitivity and broadband-sensing capabilities towards various classes of VOCs and individual target gases. The same procedure was performed for ambient air to take into consideration the baseline change, humidity compensation and the sensor signal normalisation.

In parallel the composition of oil VOCs during oxidation was investigated using GC-MS. Groups of markers that most correlate with quality parameters (PV, AV, MVC, p-AV) were selected. Based on this data, specific gas mixtures were prepeared for investigating the sensor characteristics of the array using gas mixing system, as well as proposing conversion factors from signals to the correlating physicochemical parameters.

Recurrent neural network (LSTM) with long-term memory was used to analyze time-series data sets of the oil oxidation process and operating states of sensors. For classification different gas markers to 4 groups related to different quality parameters was used convolutional network.

The research is at control-defining stage, as well as the drawing of final conclusions.

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