Innovative Food Science and Emerging Technologies 42 (2017) 33–41

Contents lists available at ScienceDirect

Innovative Food Science and Emerging Technologies

journal homepage: www.elsevier.com/locate/ifset

Assessment of high pressure processed mandarin juice in the headspace by using electronic nose and chemometric analysis

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A R T I C L E I N F O

Keywords:
Locality preserving projections
Data reduction
Extreme learning machine
Chemometrics
Citrus juice

A B S T R A C T

High Pressure Processing (HPP) is a high efficient method for food preservation. As an innovative inspection method, electronic nose (E-nose) was applied to assess the HPP mandarin juices in the headspace. In this work, mandarin juices were processed by HPP at range of 0–500 MPa and diagnosed by E-nose. To improve the efficiency of E-nose, locality preserving projections (LPP) was introduced to extract information of E-nose data and compared with principal component analysis (PCA) and linear discriminant analysis (LDA). Three data extractions (stable value, max value and area value), three data reductions (PCA, LDA and LPP) and two classification algorithms (support vector machine and extreme learning machine) were applied to improve the diagnostic accuracy of E-nose. This study shows that the performance of E-nose can be enhanced by appropriate data extraction and data reduction and also gives a hint of E-nose inspection for HPP fruit juice.

Industrial relevance: HHP is a high efficient technology for food preservation, including volatile compounds and solid contents. E-nose, which detect the components changes in sample's headspace, has been widely applied for the food inspection as an innovative detection method. According to authors' best knowledge, researches about E-nose detection for HHP products are not very common. In this study, E-nose is applied to detect the HHP-processed mandarin juices in the headspace. Besides, three data extractions, three data reductions and two classification algorithms were applied to improve the accuracy of E-nose determination in two HHP-process cases. This paper describes the possible application of E-nose to discriminate HHP-processed juices at different pressures. E-nose combined with appropriate pattern recognition could be used as a rapid and high efficient method to discriminate HHP-processed fruit juices.

1. Introduction

In recent years, consumer's demand for fresher, safer and higher quality food has promoted researches on nonthermal methods of food preservation as an alternative to thermal processes (Raso & Barbosa-Cánovas, 2003). During nonthermal processing, the temperature of foods is held below the temperature normally used in thermal processing, therefore, a minimal degradation of food quality is expected (Butz & Tauscher, 2002). High Pressure Processing (HPP) has been known to be a promising preservation technique in the field of nonthermal processing. Food processed by HPP has been proved to keep its original color, freshness and flavor, and to prolong its stability and shelf life (Andrés, Mateo, Guillamón, Villanueva, & Tenorio, 2016; Hartyáni, Dalmadi, & Knorr, 2013; Laboissière et al., 2007; Liu et al., 2016).

For modern food industry, food inspection needs high-end analytical instrument, chemical analysis, and microbiological testing. High-end analytical instrument, such as high performance liquid chromatography (HPLC) (Briones-Labarca, Plaza-Morales, Giovagnoli-Vicuña, & Jamett, 2015) and gas chromatography with mass spectrometry (GC–MS) (Deng et al., 2013), might not be well suited to this field due to their high costs and time consumption for sample preparation. Traditional chemical analysis, which needs complex operations to get one or two quality parameters, could not provide a comprehensive profile of the assessed sample. Microbiological testing is a most straightforward way to inspect the effect of HPP on food product, however, the operation of microbiological testing is time-consuming and needing for skilled personnel (Berna, Lammertyn, Saevels, Natale, & Nicolaï, B. M., 2004).

In this sense, a strategy consisting of a non-selective sensor array and an appropriate pattern recognition (PARC) system is capable of recognizing simple or complex vapors in sample's headspace (Distante, Leo, Siciliano, & Persaud, 2002). Electronic nose (E-nose), a simulation of human nose, mainly consists of a sensor array and a PARC system and has been proven to be a good alternative for traditional techniques in food industry. A wide application of E-nose in food field has been explored, like shelf-life

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http://dx.doi.org/10.1016/j.ifset.2017.05.003
Received 13 April 2016; Received in revised form 20 April 2017; Accepted 13 May 2017
Available online 15 May 2017
1466-8564/

assessment (Chatterjee, Bhattacharjee, & Bhattacharyya, 2014; Giovenzana, Beghi, Buratti, Civelli, & Guidetti, 2014), quality prediction (Ghasemi-Varnamkhasti, Mohtasebi, Siadat, Ahmadi, & Razavi, 2015; Zhao et al., 2016), storage monitoring (Mirasoli et al., 2014; Rutolo, Iliescu, Clarkson, & Covington, 2016), microbial content prediction (Gobbi et al., 2015; Yang et al., 2016). But E-nose applications for HPP food are not very common.

There are few researches about E-nose application for HPP food, and the results in those researches are not satisfying. Hartyáni et al. (2011) applied E-nose to discriminate citrus juices treated by pulsed electric field and by HPP. The principles of the two methods applied leads to some different characteristic in sample's headspace, so E-nose could discriminate this kind of method difference but not related to samples with different pressure levels by same processing method. Hartyáni et al. (2013) applied E-nose to investigate the *Alicyclobacillus acidoterrestris* inoculated in HPP-processed apple and orange juice. In this work, no acceptable separation level were found via the pressure treatment. This result might be due to the efficiency of HPP for food preservation, which can keep the original color, freshness and flavor of food products effectively. So the changes in the samples headspace results almost negligible, and E-nose's sensors could hardly notice them with normal pattern recognition.

In this work, three data extractions (stable value, max value and area value), three data reductions (principal component analysis (PCA), linear discriminant analysis (LDA) and locality preserving projections (LPP)) and two classification algorithms (support vector machine (SVM) and extreme learning machine (ELM)) were applied to improve the diagnostic accuracy of E-nose. The main objectives of this research are: (1) to characterize the HPP processed satsuma mandarin juices by E-nose; (2) to compare extraction data, and reduction data methods to extract useful information and avoiding redundant ones; (3) to apply classification models to evaluate the effectiveness of the applied extraction and reduction methods.

2. Materials and methods

2.1. Preparation of citrus juices

Two cultivars of satsuma mandarin (*Citrus unshiu Marc.*, Miyagawa wase and Ueno wase) were analyzed. Ueno wase (UW) and Miyagawa wase (MW) were hand harvested from a local orchard located in the southwest of Hangzhou, China. On November 15 in 2013, 10 trees were selected on the basis of their healthy, and 12 UW fruits with uniform size, weight and color were picked from each tree. On December 13 in 2014, 18 trees were selected, and 9 MW fruits were picked from each tree.

Once arrived in the laboratory, all fruits were peeled and crushed into juice (JYL-C051, Joyoung, China) together. To remove solid particles, the juice was filtered through cotton cloth. For UW, the concentration of juice was diluted to one-tenth of original liquid before HPP treatment. For MW, the original juice was processed by HPP without any dilution. The environment temperature for sample preparation and later sample assessment was at 20 °C ± 0.5 °C.

2.2. High hydrostatic pressure process

The HPP system is composed of a data logger (34970A, Agilent Technologies GMBH, Germany), a high pressure unit (Baotou Kefa High Pressure Technology Co., Ltd., China) with a maximum capacity of 5 l and a potential maximum pressure of 500 MPa, and a thermostat jacket connected to a water bath (SC-25, Safe, China). Four K-type thermocouples (OMEGA Engineering, Stamford, CT, USA) were installed in the container for temperature recording, and were attached to a data logger (34970A, Agilent Technologies GMBH, Germany) through the connection board and connectors that installed in the plug. Before sample processing, the pressure vessel was maintained at room temperature (20 °C ± 1 °C) by the thermostat jacket. In this study, distilled water was used as pressure transmitting medium. 300 ml juice was vacuum packed using polyethylene bag, then the bag with juice was heat sealed and vacuum packed (filled with 100 ml distilled water) again using polyethylene bag. Samples were placed into the high pressure vessel and subjected to pressure treatments for 10 min at room temperature. The pressure holding times mentioned did not include the pressure come-up time. The rate of pressure increase was maintained approximately at 120 MPa/min and the pressure release time was kept < 5 s. The medium temperature increase due to adiabatic heating during HPP treatments was about 2 °C per 100 MPa on an average.

For UW juice, the samples were treated at 100, 200, 300 or 400 MPa for 10 min at 20 °C ± 1 °C respectively, and untreated juice samples held at 20 °C ± 1 °C for the duration of the pressure treatment was used as a control. Thus 5 groups were designed (4 levels of HPP pressure and a control), 24 samples were reserved, and 120 samples (24 samples × 5 groups) were prepared for E-nose assessment.

For MW juice, the samples were processed at 100, 200, 300, 400 and 500 MPa respectively, and a control group were also prepared. The holding time for pressure treatment was 10 min, and the temperature was 20 °C ± 1 °C. 6 groups (5 levels of HPP pressure and a control) were designed. To get more samples, 27 samples were reserved for each group, thus 162 samples (27 samples × 6 groups) were prepared for E-nose assessment.

2.3. Electronic nose analysis

The E-nose sensors used for the assessment of the sample headspace are based on thin films of metal oxide semiconductor (MOS) materials and deposited into a small chamber (V = 1.8 ml) (PEN II, Airsense Corporation, Germany). The sensor array was composed of 10 different MOS sensors as given in Table 1. Each sensor has a certain degree of affinity towards specific chemical or volatile compounds.

10 ml of the citrus juice was placed in a 500 ml beaker sealed by plastic wrap, and for headspace gas generation, the sample was remained still for 30 min. Headspace gas in the beaker was extracted at

Table 1
MOS sensors used and their main applications (PEN2, Airsense Analytics, Germany).

Number	Sensor name	General description	Reference (threshold)
S1	W1C	Aromatic compounds	Toluene, 0.1 g/l
S2	W5S	Very sensitive, broad range sensitivity, react on nitrogen oxides, very sensitive with negative signal	NO_2, 1×10^{-3} g/l
S3	W3C	Ammonia, used as sensor for aromatic compounds	Benzene, 1×10^{-2} g/l
S4	W6S	Mainly hydrogen, selectively, (breath gases)	H_2, 0.1 g/l
S5	W5C	Alkanes, aromatic compounds, less polar compounds	Propane, 1×10^{-3} g/l
S6	W1S	Sensitive to methane (environment) ca. 1×10^{-2} g/l. Broad range, similar to S8	CH_3, 0.1 g/l
S7	W1W	Reacts on sulfur compounds, H_2S 1×10^{-4} g/l. Otherwise sensitive to many terpenes and sulfur organic compounds, which are important for smell, limonene, pyrazine	H_2S, 1×10^{-3} g/l
S8	W2S	Detects alcohol's, partially aromatic compounds, broad range	CO, 0.1 g/l
S9	W2W	Aromatics compounds, sulfur organic compounds	H_2S, 1×10^{-3} g/l
S10	W3S	Reacts on high concentrations > 0.1 g/l, sometime very selective (methane)	CH_3, 10 CH_3, 0.1 g/l