Postharvest Biology and Technology 133 (2017) 104–112

Contents lists available at ScienceDirect

Postharvest Biology and Technology

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

A primary study on forecasting the days before decay of peach fruit using near-infrared spectroscopy and electronic nose techniques

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ARTICLE INFO

Keywords:
Peach fruit
Near-infrared spectroscopy
Electronic nose
Decay
Chemometrics

ABSTRACT

Forecasting the number of days until peach fruit decay is important not only for consumers to determine when to eat the fruit, but also for sellers to determine their sale strategies. However, traditional visual observation, chemical and anatomy-digital caliper methods are applicable only when the decay has already begun. In this work, the possibility of forecasting the days before decay (DBD) of peach fruit was explored by means of near-infrared (NIR) spectroscopy and an electronic nose (e-nose). Partial least squares regression, least-squares support vector machines, and multiple Gaussian fitting regressions were used for model calibration. Successive projections algorithm, uninformation variable elimination, and competitive adaptive reweighted sampling were used for variable selection. The best DBD prediction model had a correct answer rate of 82.26%. The results show that the combination of NIR spectroscopy and e-nose data holds promise as a reliable and rapid alternative to forecasting the DBD of peach fruit. This study reveals the attractive prospect of non-destructively estimating how long peach fruit can be edible before decaying, which is important for improving both the daily lives of people and management efficiency in the peach industry.

1. Introduction

Peach (*Prunuspersica* L. Batsch) is among the most appreciated fruit by consumers not only because of its tender texture and pleasant flavor, but also because its nutrients, including polyphenols, soluble sugar, organic acids, vitamins, minerals, and dietary fiber, are vital for the healthy functioning of the body, (Chang et al., 2006; Gil et al., 2002; Pla et al., 2012). Peach fruit is inherently perishable and it is highly prone to infection by pathogens and further decay during the postharvest period. Like other fruit, decayed peach fruit lose their market value. Therefore, it is important for both consumers and sellers to know how many days remain for peach fruit before the fruit decay − in other words, to estimate how long peach fruit can be edible before decay − because the information can help consumers determine when to eat the fruit and sellers determine their sale strategies.

The decay process of fruit includes three major steps: cell damage, enzymatic oxidation and browning (Li and Thomas, 2014). In general, people evaluate whether the fruit is decayed or not through the appearance of the fruit based on their empirical observation or sometimes based on fruit texture by touch. However, both visual and touch-based examinations have several disadvantages, such as being subjective, laborious, tedious and inconsistent. On the other hand, based on destructive sampling by cutting the fruit, decayed tissues inside the fruit can be identified by observing any discoloration and indentation (Pang et al., 1996) or by measuring either the contents of phenolic substances or the activities of polyphenol oxidase and peroxidase in the tissues (Billaud et al., 2004). However, chemical methods have high costs and require lengthy sample preparation, and both chemical and anatomy-digital caliper methods are selective examinations and cannot be used to handle a large number of fruit, as they are destructive and time consuming. Moreover, the above methods are all specialized in detecting fruit that already have begun to decay. The eye of inexperienced or general consumers cannot visually forecast when the fruit will decay. People must wait until the fruit begins to rot so the damage becomes visible on the fruit surface (Van Zeebroeck et al., 2007). Regarding shelf-life prediction, predictive models between quality, time and temperature have been established for fruit such as kiwifruit(Terasaki et al., 2013), tomatoes (Dermesonlouoglou et al., 2007), and melons (Amodio et al., 2013). However, these models were established based on bulk batches of fruit and therefore are applicable for forecasting days

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http://dx.doi.org/10.1016/j.postharvbio.2017.07.014
Received 4 May 2017; Received in revised form 15 July 2017; Accepted 31 July 2017
0925-5214/

before decay for a general group of fruit rather than every single fruit. To the best of our knowledge, there are few reports on forecasting the days left before decay for a single peach fruit. In addition, it should be noted that the forecast process should avoid destroying the samples; regarding the perspectives of both consumers and sellers in practice, after the forecast process, the fruit usually is not eaten immediately but is stored.

During postharvest periods, the physiological and quality of peach fruit, including internal components (Sandín-España et al., 2016; Xi et al., 2014) and volatile substances (Evrendilek, 2016; Zhang et al., 2010), change. Consequently, based on these changes, there might be potential for forecasting the days before decay for a single peach fruit. In recent years, near-infrared (NIR) spectroscopy and electronic nose (e-nose) systems have been researched as potential tools for the non-destructive analysis and assessment of fruit quality and safety(Baietto and Wilson, 2015; Giovenzana et al., 2015). NIR spectroscopy measures various fundamental molecular vibrations, including C—H, O—H, N—H, and C═O functional groups, which are the basics chemical constituents critical for the quality prediction of fruit. Many studies have been reported on using NIR spectroscopy to detect soluble solid contents, firmness and other quality attributes of peaches (Nascimento et al., 2016), apples (Khatiwada et al., 2016), and pears (Sun et al., 2016). However, despite many successful applications for the evaluation of fruit quality, Vis-NIR spectroscopy is not good at measuring volatile substances, which constitute another important quality attribute of fruit. An e-nose is a bionic instrument with an array of sensors to mimic human olfaction with no separate mechanism. The e-nose is based on the sensor arrays and pattern recognition systems to detect and recognize odors and flavors. With the advantages of relatively fast assessment of headspace, ease of operation, and cost effectiveness, the e-nose has been used in considerable numbers of applications to determine quality of fruit, including peaches (Rizzolo et al., 2013; Zhang et al., 2012), pears (Zhang et al., 2008), and mandarins (Hernández et al., 2007). In addition, both Vis-NIR spectroscopy and the e-nose are chemical-free assessment methods that can perform non-invasive measurement and require minimal sample preparation. Therefore, it is of our interest to investigate the feasibility of using NIR spectra to measure the components and e-nose signals to measure the volatile substances to forecast the days before decay (DBD) of peach fruit.

Because the spectral and e-nose data generally contain a large data matrix, multivariate analysis is required to break down the multiple variables of spectral and e-nose data into useful information, which was then used to establish quantitative models for the DBD. Specifically, the NIR spectra and e-nose features of the measured peach fruit were considered separately or combined together as independent variables, and the dependent variable was the DBD (days). On the other hand, both NIR spectral and e-nose data provide abundant information related to samples. In this study, there were 728 NIR wavelength variables and 44 e-nose features. Selecting several important variables is a key step for model calibration, which is helpful for predigesting calibration modeling and improving the results in terms of accuracy and robustness; the selection is also especially important for developing simpler and cheaper NIR spectroscopy and e-nose systems based on only the selected NIR wavelengths and e-nose sensors.

The main goals of this study were as follows: (1) acquire NIR spectral and e-nose profiles of intact peach fruit during the postharvest period; (2) build multivariate calibration models between the values of DBD of peach fruit and their spectra and e-nose fingerprints based on different calibration algorithms; (3) identify several optimal NIR wavelengths and e-nose sensors for DBD prediction; and (4) compare the performances of NIR spectroscopy and the e-nose system and evaluate if their combination could improve the accuracy of prediction.

2. Materials and methods

2.1. Sample preparation

Peach (*Prunuspersica* L. Batsch cv. Hujingmilu) fruit were harvested from a commercial orchard in Jiaxing, Zhejiang Province, China in 2015. On the day of harvest, fruit of uniform commercial maturity with no disease or mechanical wounding were selected and transported to the laboratory. A total of 96 peach fruit were obtained. During the postharvest period, fruit were stored at 20 °C, and their NIR spectral and e-nose data were acquired daily until the fruit were artificially evaluated as decayed. In detail, when the visible rot zone outside the wounded area on fruit was more than 1 mm wide, it was considered as decay fruit (Yang et al., 2011; Yu et al., 2012). Each fruit measured daily was regarded as one sample. In the end, 710 samples were obtained. Among them, 473 samples were randomly selected for calibration and the remaining 237 samples for prediction. The DBD of samples for calibration were in the range of 1 d to 16 d with a mean of 5.12 d and a standard deviation of 3.25 d, and the DBD range for prediction was also from 1 d to 16 d with a mean of 4.93 d and a standard deviation of 3.07 d. In this study, broad ranges of DBD were obtained, showing that the samples were representative for establishing robust spectral and e-nose calibration models.

2.2. NIR spectroscopic system

A NIR 256-2.5 spectrometer (Ocean Optics, Inc., Dunedin, FL, USA) was used to acquire the NIR spectra of peach fruit with wavelength range 900 to 2500 nm. The spectrometer was equipped with an LS-1 tungsten halogen light source, and SubMiniature version A(SMA)-terminated optical fibers, which were used for connecting both the light source and detector to the probe. Before the process of spectral measurement, a white diffusive standard measured using a WS-1 White standard with > 99% diffuse reflectivity and a dark standard obtained when the light source was turned off were used to calibrate the system. Spectra of 30 successive scans from four points 90° from each other in the equatorial region of the peach fruit were measured and averaged into one spectrum, which was set as the characteristic spectrum of the sample.

2.3. E-nose system

The e-nose system used was a Fox 4000 (ALPHA MOS, Toulouse, France), which consisted of a sampler, array sensors and pattern recognition software. The system has three metal oxide sensor chambers (A, B, CL) equipped with 18 sensors. Details of these sensors can be found in the literature (Huang et al., 2015). In the process of e-nose signal measurement, each fruit was placed in a tight container (1.5 l) for 600 s at 20 °C, after which 2 ml of headspace gas in the container was extracted with a syringe and injected into the Fox system. For accuracy of the results, the headspace gas was pumped into the sensor chamber at a constant rate of 2.5 ml s^{-1}. Each sample was tested for 120 s, and the cleaning phase was 240 s. In this work, four kinds of e-nose features, namely, the maximum response value, mean-differential coefficient value (MDCV) (Zhao et al., 2007), stable value (SV) (Hui et al., 2015) and response area value (RAV) (Wei et al., 2013) of each sensor were extracted and used for further data analysis.

2.4. Multivariate calibration

Two classic multivariate calibration methods of partial least squares regression (PLSR) and least squares support vector machine (LS-SVM) and a novel calibration method of multiple fitting regression based on Gaussian fitting function (MFRG) were considered. The performances of these three calibration algorithms were compared to select the best calibration strategy. PLSR is a classic linear calibration algorithm. It