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Multivariate analysis of hyper/multi-spectra for determining volatile compounds and visualizing cooking degree during low-temperature baking of tubers

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A B S T R A C T

This study was conducted to assess the potential feasibility of using hyperspectral imaging (900–1700 nm) for rapid determination of the volatility of tuber compositions (VTC) and prediction of the tuber cooking degree (TCD) in low temperature baking (LTB). Tuber samples of six categories from different origins were imaged and calibrated. The partial least squares regression (PLSR) and three-layer back propagation artificial neural network (TBPANN) models were established to predict VTC and TCD using the entire spectral range and the feature wavelengths. The optimal combination of characteristic wavelengths (991, 1031, 1071, 1138, 1252, 1403, 1460 and 1641 nm) were selected by first derivative and mean centering iteration algorithm (FMCIA) rather than other conventional methods. Based on the qualified eight wavelengths, the FMCIA-TBPANN approach yielded greater overall performance for predicting both VTC and TCD. Furthermore, the distribution maps of VTC and TCD were generated using a resulting function to visualize each pixel of spectral image. This demonstrated the capability of spectral imaging technique for rapid and accurate evaluation of VTC and TCD during LTB.

1. Introduction

Unlike perishable fruit and vegetables that require preservation techniques such as drying (Cui et al., 2008; Sun and Woods, 1994), cooling (Mc Donald and Sun, 2001; Sun, 1997; Wang and Sun, 2004; Zheng and Sun, 2004) and freezing (Kiani et al., 2011) to maintain their quality and can normally be consumed without cooking, the tuber crops including potato (*Solanum* spp.) and sweet potato (*Ipomoea batatas* L.), which are the third major staple foods after cereal and legume, together with which accounting for approximately 90% of the world's food calories intake and providing human with valuable starch, protein, oils, minerals and vitamins (Bender and Smith, 1997; Aina et al., 2012), are always cooked by baking, frying or boiling before consumption (Mujumdar and Law, 2010; Tarmizi and Niranjan, 2013). Along with driving off the surplus moisture inside, the main principle of baking is to get the inside of the product properly cooked before the outside dries out and becomes tough, unpleasantly dark or even burned. Moreover, the potential harmful bacteria is typically killed (above 68 °C) during cooking with multifarious flavor substances enhanced. A total of 228 compounds have been identified in aroma volatiles isolated from baked potatoes alone (Coleman et al., 1981), and the variation of most of the volatiles of the baked potato was caused by the effects of cultivar and site (Oruna-Concha et al., 2001; Thybo et al., 2006). These volatiles were found to derive from the basic nutrients such as carbohydrates, proteins, fats, free amino acids, as well as minerals and vitamins (Dresow and Böhm, 2009). The volatiles such as moisture clusters are inserted in a sizeable H-bond network forming a stretched pattern, and the reactivity of each constituent within baked products is influenced by its affinity among water molecules (Infantes et al., 2003). Therefore, it is necessary to monitor the volatile parameters that may affect the tuber cooking degree (TCD) during baking. Although food can be sufficiently cooked in a short time period at high temperature, the nutrition destroyed may result in generating harmful substances (Goldberg et al., 2004; Przybylski and Aladedunye, 2012). Besides, when carbohydrates and proteins are mixed together in food such as potato and sweet potato, the levels of acrylamide ($CH_2{=}CH{-}CO{-}NH_2$; melting point of 84.5 ± 0.3 °C) increase during baking (Pedreschi et al., 2010; Keramat et al., 2011a, 2011b; Gökmen and Palazoğlu, 2008). This kinetic process is in accordance with a function of temperature, baking time,

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moisture content and matrix of product (Keramat et al., 2011a; Tumuluru et al., 2013; Romano et al., 2008; Uribe et al., 2011).

Low temperature baking (LTB) was emerged as the times require using temperatures of 65–90 °C for a prolonged time to preserve food nutrients (Vaudagna et al., 2002). Using this process, the sensory quality of food can be effectively preserved since the loss of volatile compounds are reduced. The volatility of tuber compositions (VTC) is an important cooking feature that indicates the release speed of volatile matter of the baking tuber samples. However, most of the volatile compounds only exist in trace amounts and their chemical signatures are different and complicated, which makes them more difficult to analyze (Adahchour et al., 2003). Some sophisticated approaches have been developed in an attempt to facilitate the precise measurement, but these methods are laborious and high-cost generally (De Lacy Costello et al., 2001; Oruna-Concha et al., 2002). The TCD is another critical index for industrial production with respect to its quality and safety, especially for delicatessen that can be consumed without further thermal treatment. Nowadays, most measurements of TCD during processing are time consuming. Not only are a few products checked, but also a very tiny volume of the chosen products is actually inspected. As a result of these limitations, many foods are over-cooked to make sure that all parts have completely been cooked. This might lower the final product quality and also requires using up excessive energy. As there is a need for non-invasive and real-time detection of TCD for improved monitor of the cooking process, the ideal control system in the food industry should be able to record the TCD during the whole production volume.

In fact, the VTC and TCD vary not only in different tuber categories, even imparity distribution at different locations of the same sample due to heterogeneity. However, the efficient evaluation of chemical heterogeneity is one of the main premises that impel the development of hyperspectral imaging (Liu et al., 2014b; Lorente et al., 2012; Menesatti et al., 2009; Shahin et al., 2014; Singh et al., 2010; Wu et al., 2013). This is due to that the information of both image provided by the computer vision technique (Wu and Sun, 2013c; Wang and Sun, 2002; Jackman et al., 2009) and spectrum provided by the spectroscopic technique is integrated into one syncretic system for visualizing both the geometrical features and the physicochemical properties of miscellaneous food ingredients (Gómez-Sanchis et al., 2014; Lorente et al., 2013; Pu et al., 2015; Wu and Sun, 2013a) and various quality and safety attributes (ElMasry et al., 2012a,b; Barbin et al., 2012, 2013; Wu and Sun, 2013a,b; Kamruzzaman et al., 2012, 2013; Feng and Sun, 2012, 2013; Liu et al., 2014b; Feng et al., 2013). The spectra of any point in the food sample can be used for calculating concentrations of chemical compositions, because each pixel has its corresponding spectrum (Liu and Ngadi, 2013; Su and Sun, 2016b; Sun, 2010; Yu et al., 2014). The concentration gradients of chemical compositions are usually more interesting than average concentrations. During recent years, hyperspectral imaging has been utilized as a competent detection instrument that thoroughly changed and promoted the prospect of assessment of food quality in multifarious analytical processes (Cen et al., 2014; Cheng and Sun, 2015; Cheng et al., 2014a; Kamruzzaman et al., 2015; Mahesh et al., 2015; Su et al., 2015; Su and Sun, 2016a; Tao and Peng, 2015; Wei et al., 2014; Zhu et al., 2013). The changes of chemical compositions in food can be mapped and visualized using hyperspectral imaging and developed models (ElMasry and Wold, 2008; Sun, 2016; Zhu et al., 2014). Even so, because of the difficulty to rapidly determine the property of all kinds of the complicated volatiles generated during cooking, the analysis of food volatile was straitness and generally focused on monitoring specific volatile component (Duckham et al., 2001). For instance, the volatile basic nitrogen content in grass carp and prawn were successively determined and visualized based on hyperspectral imaging in tandem with multivariate analysis and image processing (Cheng et al., 2014b; Dai et al., 2016). However, it was noticed that there were just one conventional wavelength selection method and one category of grass carp or prawn being used in their researches. As far as we know, no research has yet been published to evaluate of the changes of tuber volatiles and their relationships with cooking degrees based on hyperspectral imaging, not to mention using both new and traditional wavelength selection methods to detect different categories of both potatoes and sweet potatoes, and comparing effects of various methods to different sample categories.

Therefore, a further objective of this study was to investigate the potential capability of hyperspectral imaging for rapid determination and visual prediction of the VTC and TCD during LTB. The detailed procedures of this study were as follow: (1) Studying partial least squares regression (PLSR) and three-layer back propagation artificial neural network (TBPANN) calibration models for determination of VTC and TCD using hyperspectral imaging, (2) Developing a creative algorithm to hunt characteristic wavelengths of the most efficient combination for building multivariate PLSR and BPANN models, (3) Comparing the validity of the innovative algorithm to conventional wavelength selection methods for establishing the most robust multispectral imaging system, (4) Using image processing algorithms to visualize the spatial distribution and gradation of VTC and TCD on prediction maps.

2. Material and methods

2.1. Determination of tuber quality attributes and collection of hyperspectral image

Tuber samples of six cultivars (12 samples for each cultivar) in terms of white potato (WP) (variety: Cultra, origin: Ireland), golden wonder potato (GWP) (origin: Ireland), rooster potato (RP) (origin: Ireland), organic potato (variety: Melody, origin: UK), sweet potato 1 (SP1) (variety: Covington, origin: USA) and sweet potato 2 (SP2) (variety: Evangeline, origin: Egypt) were respectively collected and used in this current study. All these fresh and fine samples were transported to laboratories of Food Refrigeration & Computerized Food Technology (FRCFT), University College Dublin (UCD), Ireland,

Table 1
Reference values of VTC at different baking times.

Time (min)	WP		GWP		RP		OP		SP1		SP2	
	Max	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max	Min
40	0.314	0.214	0.294	0.174	0.270	0.173	0.220	0.135	0.423	0.260	0.328	0.222
80	0.276	0.222	0.271	0.201	0.249	0.174	0.223	0.151	0.340	0.226	0.322	0.254
120	0.247	0.211	0.240	0.187	0.234	0.176	0.212	0.148	0.290	0.197	0.285	0.236
190	0.217	0.197	0.213	0.179	0.201	0.170	0.203	0.150	0.234	0.169	0.244	0.214
260	0.128	0.120	0.124	0.111	0.116	0.104	0.124	0.098	0.131	0.100	0.141	0.129

WP: White potato, GWP: Golden wonder potato, RP: Rooster potato, OP: Organic potato, SP1: Covington sweet potato, SP2: Evangeline sweet potato, Min: Minimum value, Max: Maximum value.