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Principal Component Analysis as an exploration tool for kinetic modeling of food quality: A case study of a dried apple cluster snack

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ABSTRACT

A Multivariate Accelerated shelf-life Testing (MALST) study of a dried apple cereal-like snack (commercially known as cluster) stored at 18 °C, 25 °C or 35 °C for 17.5 months was conducted. The measured attributes were water activity (Aw), color DE, moisture and sensory properties (aroma, taste, texture and color). The data were deployed to adjust the multivariate kinetics (including the interactions of the attributes) using Principal Component Analysis (PCA), and the results were compared to those obtained using a univariate kinetic model. The predicted shelf-life for the reference storage condition obtained using the multivariate model was 18.3 months, whereas a predicted shelf-life of 15.6 months was obtained using the univariate model. Thus, although the results of both methods are similar, the multivariate kinetic model revealed all of the product shelf-life attributes and their interactions. Finally, the multivariate model reflected the variability of the biochemical phenomena underlying product degradation.

1. Introduction

The shelf-life of food is a key consideration for foodstuffs developed on an industrial scale. The shelf-life is the period in which a product has acceptable functionality in terms of its sensory and nutritional qualities (Hough and Wittig, 2005; Man and Jones, 1999). This parameter is also important to ensure the safety of food (Holley and Patel, 2005) and optimize the food supply chain (Casp and Abril, 2003).

Shelf-life determination is usually conducted by measuring quality attributes to construct a model of the kinetics of deterioration under ambient conditions or, alternatively, under extreme conditions using accelerated aging methods (Hough et al., 2006), which is also known as accelerated shelf-life testing (ALST); these methods were proposed by Labuza (1982).

The empirical models that are commonly used for industrial purposes are Q_{10} (a measurement of sensitivity to an increase of 10 °C) and the Weibull survival analysis method (Linnemann et al., 2006; Palazón et al., 2009). Although a suitable estimation of shelf-life can be achieved with these models, they do not always represent the nature of the food aging process (Cardelli and Labuza, 2001). Furthermore, the relationships among the variables involved in food deterioration are not taken into account simultaneously. Thus, shelf-life determination becomes complex when there are multiple attributes that each affect the expiration date. Because the natural phenomena are multivariate (Martens and Martens, 2001), as is the case of food deterioration), chemometrics tools could be useful to determine the shelf-life of food. In this regard, Principal Component Analysis (PCA) is one of the most popular multivariate techniques because it reduces the dimensionality, compresses the noise and correlates measurements in a simple informational sub-space of the data set (Brereton, 2009). Thus, by merging multivariate statistics and ALST, a new methodology called Multivariate Accelerated shelf-life Testing (MALST) and the concept of multivariate kinetics were conceived (Pedro and Ferreira, 2006). The MALST method of shelf-life determination has been applied in relatively few practical situations. In this study, we applied MALST to the deterioration kinetics of a new product on the market, a dried apple cereal-like snack that is commercially known as Cluster, to elucidate the complex behavior of its attributes during storage.

Abbreviations: MALST, multivariate accelerated shelf life testing; PCA, Principal Component Analysis; PC, principal component; DE, color DE.

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2. Theoretical considerations

2.1. PCA and multivariate kinetic modeling

Algebraically, principal components (PC) are linear combinations of p-random variables (x1, x2,…,xp) that allow the PCA to condense information in two ways: first, by identifying the relationships between different observations that comprise the scores matrix, and second, by determining the relationships between different variables of the data set, known as the loadings matrix (Saavedra and Córdova, 2011). The axes derived from this analysis represent the maximum variance directions, wherein the first principal component (PC1) is located along the direction of maximum variance of the data set, and the second component (PC2) is disposed along the direction of the second greatest variance, and so on. All of the PCs are simultaneously orthogonal to each other, and there is no co-variance among them. In addition, the line projected by each PC is the best fit to all points simultaneously, through least squares optimization (Eriksson et al., 2006).

With this method, the quality attribute data obtained over time under each storage condition are arranged in matrices ($\boldsymbol{X}_{\Theta,\mathrm{T}}$) for a subsequent PCA. The assumption of the MALST technique is that the variations in the quality attributes are the main sources of variability under the different storage conditions. Thus, PCA is driven by time-related phenomena. The first set of time-related PCs describes the major factors of deterioration, while the next describes the noise or the processes not related to degradation. By relating the first PCs over time, multivariate kinetics can be adjusted using the following parameters: $\boldsymbol{k^m}$, the temperature-dependent multivariate reaction rate constant, which is derived from the linear combination of each observation and is provided by the score matrix, and $\boldsymbol{Ea^m}$, the multivariate activation energy (kJ/mol), which is obtained using an Arrhenius model. In a manner analogous to the calculation of the Q_{10} coefficient, the multivariate acceleration factor ($\alpha^m_{\mathrm{T}+\delta\mathrm{T},\mathrm{T}}$) is obtained according to the reference storage condition (18 °C) (Pedro and Ferreira, 2006).

Another assumption of the MALST is that a PCA can accommodate non-linear patterns in the scores of the time-related PCs (Naes et al., 2004), which means that multivariate kinetics can describe deteriorative phenomena independently of whether they follow 0-order kinetics.

Finally, the shelf-life is estimated by calculating the cut-off criteria (t_c) corresponding to the matrix product of the specification vector (i.e., the values of all of the quality attributes at 18 °C) and the loadings matrix of each time-related PC.

2.2. Univariate kinetic modeling

The kinetics of food quality loss can be represented by the following equation:

$$-\frac{dA}{dt} = kA^n \tag{1}$$

where A indicates the measured quality, t is time, k is the reaction rate time constant and n represents the reaction order.

The temperature sensitivity of the rate constant can be analyzed using the Arrhenius equation:

$$\ln k = \ln k_{\mathrm{ref}} - \left(\frac{Ea}{R}\right)\left(\frac{1}{T} - \frac{1}{T_{\mathrm{ref}}}\right) \tag{2}$$

where k_{ref} is the rate constant at the reference temperature (T_{ref}), E_{a} is the activation energy of the studied reaction and R is the universal gas constant.

An acceleration factor related to the reference storage condition (18 °C) can be written as $\alpha_{\mathrm{T}+\alpha\mathrm{T},\mathrm{T}}$ for all the quality attributes.

3. Materials and methods

Samples of the new product, a dried apple snack called Cluster, which was developed by an exporting agribusiness in Maule, Chile, and recently came on the market, were used in this MALST study. The snacks are made from a mixture of small cubes of apples and natural fruit sugars with a low amount of sulfites added as preservatives (the product formulation is not shown because it is intellectual property). The mixture of apple pieces and fruit sugars is dried using hot air and then subjected to a puffing process to shape the snack. The resulting product (bulk density of 0.18 g/cm^3 ± 0.05) is then packed in high barrier metalized bags (HYC Packaging Inc., Chile, water permeability <0.3 g/m^2 × day at 25 °C and <0.8 g/m^2 × day at 35 °C).

3.1. Sample storage

For the ALST, the samples were stored under the reference storage condition and at higher temperatures. Quintero et al. (2012) used this methodology to evaluate the quality of apple leather (a dehydrated snack) during storage at 20–30 °C. Furthermore, because the temperature cannot exceed 45 °C without the risk of inducing deteriorative reactions that are unrepresentative of what may occur under truly representative circumstances (Robertson, 2010), the samples were incubated at 18 °C, 25 °C and 35 °C without exposure to light. The humidity in the temperature controlled-chambers was maintained at 75% RH ± 5% (Precision Scientific, Jouan Inc., Winchester, USA) with air circulation. The sampling consisted of randomly removing three samples for analytical determination (in triplicate) and six samples for use in a sensory panel. All of the quality attributes were measured during 17.5 months of incubation.

3.2. Analysis of quality attributes

The following attributes were quantified using analytical methods: water activity (Aw), moisture content, sulfite content (SO_2) and color CIE-L^*a^*b (DE). The Aw measurements were conducted using an Aqua LAB instrument (Decagon Devices Inc., Washington, USA) at 20 °C ± 0.3 °C (Aw ± 0.003). The moisture content (g/100 g product) was determined using the AOAC analytical method 2000-934 (AOAC, 2000a). The sulfite content (SO_2, mg/kg on a dry basis) was quantified using the optimized Monier-Williams analytical method according to AOAC 2000-990 (AOAC, 2000b). The CIE-$L^*a^*b^*$(DE) color value were determined using a Chromameter CR-200b instrument (Minolta, Japan).

Complementary sensory analyses of taste (flavor), color, aroma and texture (crispness) were conducted to validate the quality of the product. For this purpose, 6 samples were distributed among 8–10 semi-trained panelists (depending on their availability) who were personnel of the agroindustry associated with this research. The sensory parameters were rated from 0 to 6, where 0 was the total absence of the parameter and 6 was the highest score for the sample. According to the technical specification of the product, the sensory attributes must receive a minimum score of 3 to meet the cutoff criteria for acceptability. These analyses were conducted in the Research and Development Department Laboratory of this enterprise between February 2010 and July 2011.

3.3. Multivariate exploration of product stability

To study the overall product stability, the data for all of the quality attributes at every sampling time point were arranged in a matrix according to each storage condition ($\boldsymbol{X}_{\mathbf{T}}$ matrix: 28 observations and 8 variables), where each observation is the average