Food Research International 78 (2015) 410–423

Contents lists available at ScienceDirect

Food Research International

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

Quality changes of pasteurised mango juice during storage. Part II: Kinetic modelling of the shelf-life markers

Scheling Wibowo, Tara Grauwet, Getnet Belete Gedefa, Marc Hendrickx, Ann Van Loey *

Laboratory of Food Technology, Leuven Food Science and Nutrition Research Center (LFoRCe), Department of Microbial and Molecular Systems (M^2S), Katholieke Universiteit Leuven, Kasteelpark Arenberg 22 box 2457, 3001 Heverlee, Belgium

ARTICLE INFO

Article history:
Received 30 July 2015
Received in revised form 2 September 2015
Accepted 5 September 2015
Available online 10 September 2015

Keywords:
Mango juice
Kinetics
Fingerprinting
Shelf-life
Targeted quality parameters
Volatiles

ABSTRACT

The present work shows the potential of the integrated fingerprinting-kinetics approach in evaluating shelf-life changes of pasteurised mango juice (cv. 'Totapuri'). Seven mango juice formulations (i.e. control (mango puree and water), ascorbic acid-enriched (AA_{250} and AA_{500}), citric acid-enriched (CA, CA + AA_{250} and CA + AA_{500}) and sugar-enriched (S) samples) were pasteurised and stored at 42 °C for 8 weeks. In this part, the kinetics of the shelf-life markers selected from the multivariate fingerprinting approach was modelled. Changes in selected targeted parameters could be best described by a zero-order (colour values, °Brix, furfural, HMF), a first-order (ascorbic acid), a fractional conversion (fructose, glucose, oxygen) and a second-order model (sucrose). Differences in the rate constant were observed, with faster ascorbic acid degradation and furfural formation in AA-enriched samples and faster hydrolysis of sugars and HMF formation in CA-enriched samples compared to control samples. To describe changes in selected volatiles (terpenes, sulphur compounds, acids, ketones and esters), different kinetic models were selected. Two trends were observed: changes as affected by different mango juice formulations (e.g., faster reaction in CA-enriched samples or in a lower pH condition) and changes irrespective of the formulations. Referring to the literature, in general, acid-catalysed reactions, ascorbic acid degradation and oxidation reactions are the main reactions responsible for the observed quality changes in stored mango juice.

1. Introduction

As perishable food products, fruits are commonly preserved by applying thermal treatment to extend their shelf life. Targeting not only to reduce microbial population but also to inactivate endogenous enzymes, industrial heat processing techniques such as pasteurisation are often applied for high acid foods (pH < 4.6). In this way, a high quality and an ambient temperature shelf-stable product can be achieved (Barrett & Lloyd, 2012; Silva & Gibbs, 2004). However, it is well-known that the quality of most foods decreases with time. During storage, fruit-based products including fruit juices can undergo important quality-related chemical changes such as colour changes (e.g., browning), flavour degradation and nutrient losses. Consequently, these changes can affect the degree of acceptability by the consumers. Few studies have reported significant quality losses in thermally-treated fruit juices during shelf-life (Falade, Babalola, Akinyemi, & Ogunlade, 2004; Oliveira, Ramos, Minim, & Chaves, 2012; Berlinet, Ducruet, Brillouet, Reynes, & Brat, 2005; Kaanane, Kane, & Labuza, 1988).

Shelf-life can be defined as a finite length of time after manufacturing and packaging during which the food product retains a required level of quality acceptable for consumption (Nicoli, 2012). Furthermore, shelf-life can be influenced by intrinsic (e.g., product characteristics) and extrinsic (e.g., environment) factors (Robertson, 1999). Since studying shelf-life changes at ambient storage temperature can be time- and resource-consuming, conducting an accelerated shelf-life testing (ASLT) is often done by the food industries. According to Robertson (1999), ASLT works on the basic assumption that the principles of chemical kinetics can be applied to quantify the effects of extrinsic parameters (e.g., temperature, humidity and light) on the rate of deteriorative chemical reactions. Generally, ASLT involves the use of higher testing temperatures, in this way, changes can be observed in a shorter time. Assuming that quality degradation reactions are temperature dependent, results from the higher temperatures can be converted to the lower storage temperatures, with the use of e.g., Arrhenius equation, thus, allowing predicting the shelf-life of a product.

Two approaches can be used in studying food quality changes, the targeted and the untargeted analytical or fingerprinting approach (Grauwet, Vervoort, Colle, Van Loey, & Hendrickx, 2014). The targeted approach is a more hypothesis-driven approach, which is commonly used to obtain insight into specific chemical reactions by selecting specific food characteristics to be studied at the start of the investigation. Nevertheless, focusing on a (set of) particular chemical reaction(s) or characteristic(s), this approach may fail to uncover unknown quality changes. In contrast to the targeted approach, the fingerprinting

* Corresponding author.
E-mail addresses: ann.vanloey@biw.kuleuven.be, https://www.biw.kuleuven.be/m2s/clmt/lmt/ (A. Van Loey).

http://dx.doi.org/10.1016/j.foodres.2015.09.001
0963-9969/

approach offers a more hypothesis-free approach. In this approach, the identity of the chemical compounds is unknown and all changes are taken into account. However, considering the expected diversity of the compounds studied, the identification of the compounds can still be a challenge. In our previous work, the potential of the untargeted fingerprinting and kinetics approach to obtain insight into different chemical reactions during shelf-life was demonstrated in fruit-based (orange juice) and vegetable-based (broccoli and carrot) products (Kebede et al., 2015a,b; Wibowo, Grauwet, Kebede, Hendrickx, & Van Loey, 2015b).

As previously mentioned, the intrinsic factors, such as the different food composition may influence the chemical reactions occurring during shelf-life or storage. Therefore, in the present work, in order to obtain insight into shelf-life quality changes in mango juice, different mango juice compositions were prepared by adding different potential precursors (ascorbic acid, citric acid and sugars) to the control juice (mango puree and water). These precursors are known to be involved in different quality-related chemical reactions (e.g., degradation of ascorbic acid, acid-catalysed degradation of sugars) (Wibowo, Grauwet, Santiago, et al., 2015c). Pasteurised samples were stored under accelerated shelf-life conditions of 42 °C and analysed for a wide range of quality attributes: (*i*) targeted (colour, acidity, sugars, oxygen, vitamin C, furfural, HMF and carotenoids) and (*ii*) untargeted (volatile fraction). In the first part of this study (Part I), a multivariate integrated targeted and untargeted approach was used, in which all obtained targeted and untargeted data were integrated into one multivariate data set. Subsequently, shelf-life markers (i.e. compounds significantly changing during shelf-life) were determined by means of Variable Identification (VID) coefficients (criterion VID > |0.90|).

To the best of our knowledge, no open literature can be found which monitors shelf-life changes of any juice during storage on such a wide range of quality attributes and relies on the potential of multivariate data analysis in order to select those attributes which are highly correlated with shelf-life. Besides answering the question on which attributes are highly correlated with shelf-life (Part I), the next question is how fast these changes actually occur and how different the reaction rate is for the different mango juice formulations. In order to do so, in this part of the work (Part II), the kinetics of the shelf-life markers were empirically modelled (no aim of mechanistic explanation of the reaction mechanism) and kinetic parameters were estimated for each individual formulation. Using this quantitative data analysis technique, significantly different reaction rates could be distinguished.

2. Materials and methods

2.1. Experimental set-up

The whole experimental set-up of this study is schematically presented in Fig. 1. Mango juice was produced as such (control) and at different formulations (Section 2.2). Juices were thermally pasteurised and stored at accelerated shelf-life conditions (42 °C) for a period of 8 weeks (Section 2.2). At particular selected time moments, mango juices were sampled. In Part I, mango juices were characterised for a range of targeted quality parameters as well as for a volatile fingerprint (untargeted). All obtained targeted and untargeted data were combined in one dataset and analysed with multivariate data analysis. Quality parameters clearly changing over shelf-life or shelf-life markers were selected using VID (Variable Identification) coefficients (criterion VID > |0.90|). In Part II, the kinetics of the selected shelf-life markers obtained from Part I, will be further zoomed into as influenced by the different mango juice formulations.

2.2. Mango juice formulation, processing and storage

Mango juice was prepared in seven different formulations; the first formulation was the control juice, which was prepared by mixing not from concentrate (NFC) mango puree cv. 'Totapuri' (16.7–17.6 °Brix) with water in 1:1 ratio (*v*/*v*). The other formulations were prepared by adding 230 mg L^{-1} and 460 mg L^{-1} ascorbic acid (AA_{250} and AA_{500}), 7.8 g L^{-1} citric acid (CA), combination of citric acid and ascorbic acid (CA + AA_{250} and CA + AA_{500}) and sugars (S) consisting 9.82 g L^{-1} of fructose, 20.39 g L^{-1} of glucose and 19.52 g L^{-1} of sucrose to the control juice. Conditions for addition of the reaction precursors (e.g., ascorbic acid, citric acid, sugars) were selected based on measured concentration of these precursors in orange juice (Wibowo, Grauwet, Santiago, et al., 2015c). Each formulation (C, AA_{250}, AA_{500}, CA, CA + AA_{250}, CA + AA_{500} and S) was pasteurised in a tubular heat exchanger at 92 °C for 30 s, followed by filling with headspace into 500 mL polyethylene terephthalate (PET) bottles. After cooling, mango juice was stored in temperature-controlled incubators (IPP500, Memmert, Schwabach, Germany) at 42 °C for 0, 1, 2, 4, 6 and 8 weeks protected from light. At each sampling time, all samples were transferred into smaller tubes (±30 mL), frozen in liquid nitrogen and stored at −80 °C. Prior to targeted and untargeted analyses, each sample tube was thawed in a circulating water bath at 25 °C.

2.3. Analysis of targeted quality parameters

2.3.1. Colour measurement

Colour of the mango juice samples was evaluated on the basis of the CIELAB colour values by using a HunterlabColorQuest 45/0 spectrophotometer (Hunterlab, Reston, Virginia, USA).

The instrument (45°/0° geometry, Illuminant D65, 10° observer) was standardised with a black and white ceramic tile (X = 78.66, Y = 83.31, Z = 88.40) before each measurement. 3 mL of sample was poured in the glass cell and covered with a white plate. Colour measurements were carried out in triplicate with five readings for each sample. The recorded XYZ tristimulus values were then converted to CIE L^*, a^* and b^* colour values. The L^* value (measure of lightness, ranges from 0 (black) to 100 (white)), the a^* value (measure of redness (+) or greenness (−)), and the b* value (measure of yellowness (+) or blueness (−)). The

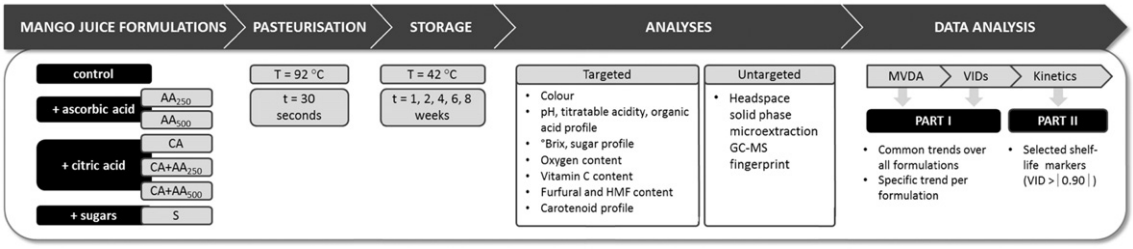

Fig. 1. Schematic overview of the mango juice experimental set-up, consisting of formulations, pasteurisation and storage conditions, list of quality parameters analysed and consecutive data analysis approach. In part I, all obtained targeted and untargeted data were analysed by multivariate data analysis (MVDA). By the use of variable identification coefficients (VIDs), targeted quality parameters and volatiles (untargeted) clearly changing during shelf-life could be selected. In part II, the shelf-life changes of selected markers are further zoomed into, in specific kinetic studies.