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The use of active PET to package rosé wine: Changes of aromatic profile by chemical evolution and by transfers

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ABSTRACT

Active Polyethylene Terephthalate (PET) bottles containing 1 or 3% of oxygen scavenger (named 1osPET and 3osPET) were used to pack rosé wine. Changes in the aromatic profiles were monitored during 12 months and compared to those of a wine packed in glass bottles. Wine in 1osPET bottles was differentiated from wine in glass or 3osPET bottles by ten aging markers such as cis-dioxane, ethyl pyruvate or furfural. Only trans-1,3-dioxolane allowed to discriminate wine in glass and in 3osPET bottles. Methionol, an oxygen sensitive aroma compound, was preserved in glass and 3osPET bottles but was slightly degraded (15%) in 1osPET bottles. Chemical reactions were the main cause of the aroma compound degradation. Indeed, the total amount of compounds sorbed only reached 160 μg considering the bottles and the joint of cap after 12 months of storage. The use of PET with 3% of oxygen scavenger is adapted to pack wine for at least 12 months.

1. Introduction

Maintaining the quality of foodstuffs is the main function of packaging. New trends are focusing on the development of active packaging, which can interact with the product or its environment and then improve food conservation. Control of oxygen ingress is one of the major challenges to preserve the quality of products. Indeed, the presence of oxygen facilitates microbial growth, increases oxidative reactions and induces the development of off-flavour and colour changes (Brody, Bugusu, Han, Sand, & McHugh, 2008). The consequences are more risk of contamination, losses of nutritional value, and organoleptic quality but also economic losses due to the eventual removal of goods and rejection by consumers. The shelf life of a product can be extended by limiting the exposure to oxygen by controlling the oxygen availability during processing, using modified atmosphere packaging as well as packaging which provides a functional barrier against oxygen (glass or packages that contain aluminium). Active packaging is another way to control oxygen ingress into the packaged foodstuff. Specific scavengers are used to react with oxygen and thereby consume dissolved oxygen of food and hinder the oxygen permeation to the packed food (Di Felice, Cazzola, Cobror, & Oriani, 2008; Galdi, Nicolais, Di Maio, & Incarnato, 2008). Scavengers can be introduced in sachets enclosed in package, in labels or directly incorporated into the package material matrix such as bottles or closures. The most commonly used reaction for oxygen scavengers is the oxidation of ferrous oxides (Charles, Sanchez, & Gontard, 2006; Vermeiren, Devlieghere, van Beest, de Kruijf, & Debevere, 1999). Other systems are based on the oxidation of ascorbic acid, sulphites, catechol, photosensitive dyes, unsaturated hydrocarbons and glucose oxidase, but also on nylons (Brody et al., 2008). Before being used as an oxygen scavenger in packages for foods and beverages the active substances are evaluated by the EFSA Commission Regulation (EC) No 450/2009 and are included in a positive Community list if the active substances do not raise a safety concern for the consumer at room temperature or below.

In the case of PET packaging, oxygen scavengers can be incorporated directly into the matrix or included in the internal layer of multilayer packages. Active PET packaging has already been tested for storing sensitive liquid foods such as orange juice (Berlinet, Brat, Brillouet, & Ducruet, 2006). Few studies were related to the use of PET bottles to pack white, rosé or red wine. Ough worked on white, rosé and red wines packed in glass and standard PET bottles and showed that the free SO_2 content reached zero in PET bottles compared to 8 mg/L in glass bottles after 12 months of storage causing an important flavour modification (Ough, 1987). The aromatic profile was similarly preserved in both types of bottles and sensory analysis revealed that red and rosé wines packed in PET bottles could be stored up to eight or nine months. Recently, Dombre et al. observed for a rosé wine that after 12 months of storage at 20 °C, methionol, which reacts with oxygen to form methional, an off-flavour in wine, was present in higher

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amounts in glass than in standard PET bottles (Dombre, Marais, Chappey, Lixon-Buquet, & Chalier, 2014; Dombre, Rigou, Wirth, & Chalier, 2015). Methionol, like other compounds, allows differentiating wine stored in glass or standard PET bottles. Giovanelli et al. showed that the phenolic compound of a red wine was more stable after 6 months of storage at 20–30 °C in the presence of an oxygen scavenger enclosed in a monolayer PET matrix (Giovanelli & Brenna, 2006). Mentana et al. monitored changes in the quality parameter (colour, sensory and aroma profile) of red and white wine stored during 7 months at 15–18 °C in monolayer PET bottles containing oxygen scavengers (Mentana, Pati, La Notte, & del Nobile, 2009). Although losses of some aroma compounds were evidenced in comparison to wine packed in glass bottles, the sensorial evaluation of the wine stored in PET bottles was still acceptable after 7 months of storage. However, sensorial evaluation of the wine showed significant differences between standard PET and active PET bottles, the organoleptic quality of the latter being slightly better than the other in terms of taste, colour and flavour. Ghidossi et al. studied the increase of aroma compounds such as sotolon, methional and phenylacetaldehyde that are associated with the oxidation of wine, in a wine stored during 18 months at 20 °C in different packages such as Bag-In-Box®, glass, monolayer and multilayer PET bottles (the multilayer containing an oxygen scavenger) (Ghidossi et al., 2012). The most oxidized wines were those stored in monolayer PET bottles and BIB® and the least oxidized wines were those contained in multilayer PET bottles and glass bottles.

All these studies highlight the fact that oxygen ingress in bottles caused by PET permeability has an impact on the wine quality and that the incorporation of an oxygen scavenger is an effective way to improve the performances of PET. Our objective was to propose a sustainable and just right solution to package rosé wine using monolayer PET including low oxygen scavenger amount with both good recyclability compared to multilayer packaging and sufficient oxygen barrier properties to preserve the wine during one year. This study was focused to the impact of the presence of an oxygen scavenger on the changes of aroma profile of a rosé wine bottled in a monolayer PET bottle. The performance of PET bottles with two different levels (1 and 3%) of an incorporated oxygen scavenger with respect to rosé quality parameters was compared to the performance of glass. In addition, the percentage of aroma compounds lost by sorption in the active PET bottle and cap was studied.

2. Materials and methods

2.1. Chemicals

Isoamyl acetate (molar mass 130 g/mol; vapour pressure 747 Pa; log P 1.36), isoamyl alcohol (molar mass 88 g/mol; vapour pressure 635 Pa; log P 1.22), octanoic acid (molar mass 144 g/mol; vapour pressure 3 Pa; log P 2.74), ethyl octanoate (molar mass 172 g/mol; vapour pressure 30 Pa; log P 3.9), hexanoic acid (molar mass 116 g/mol; vapour pressure 21 Pa; log P 1.72), hexyl acetate (molar mass. 144 g/mol; vapour pressure 185 Pa; log P 2.83), ethyl hexanoate (molar mass. 144 g/mol; vapour pressure 221 Pa; log P 2.83), isobutanol (molar mass 74 g/mol; vapour pressure 1200 Pa; log P 0.76), methionol (molar mass 106 g/mol; vapour pressure 21 Pa; log P 0.4),and 2-phenylethanol (molar mass 122 g/mol; vapour pressure 10 Pa; log P 1.36) were purchased from Sigma-Aldrich, France, and hexanol (molar mass 102 g/mol; vapour pressure 126 Pa; log P 1.86) from Prolabo, France. Dichloromethane, and 4-nonanol, the internal standard were provided by Sigma-Aldrich, France. Anhydrous sodium sulfate was provided by MERCK, France.

2.2. Wine

Wine used was a Rosé Cinsault from South of France. It was produced in 2011 and kindly supplied by UCCOAR — Val d'Orbieu (Carcassonne, France). Wine pH was 3.23, its ethanol content was 12% (v/v), its total acidity was 3.54 g/L, and volatile acidity 0.12 g/L.

2.3. Packaging, filling and storage conditions

The filling was carried out in the spring of 2012. The wine was packed in 0.75 cl bordelaise glass bottles (BSN Glasspack SA, Villeurbanne, France) and in 0.75 cl virgin polyethylene terephthalate bottles containing 1% and 3% of oxygen scavengers (1osPET and 3osPET respectively) supplied by SIDEL Blowing Service (France). The materials used were authorized to food contact and tests of global and specific migration are confirmed that the materials were in agreement with European Food Safety Authority requirements (personal data). The O_2 permeability of 1os and 3osPET measured at 20 °C and at 95% relative humidity were found equal to 1.47 and 0.6×10^{-17} mol/(m.s.Pa) respectively (Dombre et al., 2014). The weight of both PET bottles was 38 g, the thickness was 350 μm for the bottle body, increasing to 470 μm in the lower part and 700 μm in the top of the bottle shoulder. The same kind of closure was used for PET and glass bottles: a polypropylene cap with a multilayer connective joint (Novatwist® TM from Novembal) with an oxygen transfer rate of 0.0016 mg/caps.day^{-} at 23 °C and 60% HR.

Filling was performed by the Experimental Unit of Pech Rouge (UEPR, INRA, Gruissan, France). Bottles were filled using a "Perrier filler" equipped with a WineBrane® filtration system (INOXPA) (membrane porosity 1 μm for pre-filtration and 0.65 μm for final filtration). The bottles were capped using a Zalkin TM3 machine. There was no headspace flushing and then the oxygen concentration corresponded to the dissolved oxygen and the oxygen in the headspace The headspace volume is equal to 15.3 ± 1 ml for PET and 17.2 ± 0.4 mL for glass bottles. After bottling, total oxygen of wine was equal to 4.83 ± 0.34 mg/bottle and free and total SO_2 to 32.3 ± 1.15 and 130 ± 5 mg/L respectively.

The wine bottles were stored for 12 months at 20 °C and under a 400 lx light to mimic storage conditions in supermarket.

2.4. Extraction and analysis of aroma compounds of wine

The qualitative and quantitative analysis of aroma compounds were carried out just after filling (t0) and after 3, 7, 9 and 12 months of storage at 20 °C for wine in glass and 1osPET bottles and after 7 and 12 months for wine in 3osPET. Aroma compounds were extracted by a liquid–liquid method developed in our laboratory using dichloromethane as solvent (Schneider, Baumes, Bayonove, & Razungles, 1998). The extraction was carried out twice on 100 mL of wine, using the same volume of dichloromethane (25 mL) and after addition of a known quantity of 4-nonanol, the internal standard (100 μL of a solution at 2.17 mg/mL). The mixture was placed in a closed container and shaken by magnetic stirring during 20 min at 500 rpm and both phases were separated by centrifugation during 30 min at 7000 g. The resulting organic phase was dried on anhydrous sodium sulfate. Identification and semi-quantitative determination were performed using Gas Chromatography–Mass Spectrometry (GC–MS). The GC–MS used was an Agilent 1530 coupled to a quadrupole mass spectrometer (5973 MSD Hewlett Packard) equipped with a ZBWAX column (30 m × 0.25 mm, 0.25 μm). Helium was used as carrier gas with a flow rate of 1 mL/min. The oven temperature stayed at 60 °C for 3 min, then was raised by 3 °C/min to 250 °C and was kept at 250 °C for 10 min. The injector was maintained at 245 °C. Injection was done in split mode with a 1:10 ratio. The electron impact energy was 70 eV and the MS source was maintained at 230 °C. All the analyses were carried out in SCAN mode, using the National Institute of Standards and Technology (NIST), the Wiley and the interne INRA library. A response factor equal to 1 toward the internal standard (4-nonanol), was adopted for the semi-quantitative analysis. The results were expressed in mg of equivalent 4-nonanol/L. Three replicates were done for each experiment.