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Profiling Aldehydes and Furans in White Wine Oxidation: A Systems Perspective on Bottle Geometry, Cork, and Wine Type

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Abstract

Background and goals

The oxidative stability of white wine strongly influences its sensory quality and shelf life. Although bottle closures have been widely studied, bottleneck geometry is an important but still overlooked factor affecting wine composition and quality.

Methods and key findings

By combining bottle geometric measurements with chemical characterization after forced aging, this work presents a preliminary study on the effect of bottleneck heterogeneity (n = 200) on white wine oxidation. Dissolved oxygen, free and total sulfur dioxide (SO_2), and volatile markers were quantified. Results demonstrated that bottleneck heterogeneity had significant effects on oxygen management and SO_2 depletion. Free SO_2 decreased by 50%, with significant variability among bottle types, suggesting bottleneck profile influences oxygen ingress and antioxidant consumption. Aldehyde and furan concentrations increased in all bottles, with hexanal, *trans*-2-hexenal, phenylacetaldehyde, and methional exceeding odor thresholds, thereby affecting wine sensory quality. Additionally, hierarchical cluster analysis revealed strong correlations between bottleneck profile indicators and aldehyde accumulation.

Conclusions and significance

This study demonstrates the effect of bottleneck geometry on oxygen management and SO_2 depletion in wine. The evidence presented here indicates that bottleneck geometry is a key contributor to variability in wine aging and shelf life, suggesting that it is a critical and overlooked factor in wine oxidation, composition, and quality. Stricter manufacturing tolerances in wine bottle production that integrate bottleneck measurements into closure performance assessment should be implemented.

Key words: aldehyde profile, bottleneck, GC-MS, oxygen ingress, sulfur dioxide, wine quality

Introduction

Both the sensory quality and shelf-life of white wine are directly affected by the chemical stability of the wine, especially by the oxidative reactions that occur during its storage (Mercanti et al. 2024). Oxidation in white wine is a complex phenomenon that is driven by the interaction of oxygen with different components of the wine such as polyphenols, sulfur compounds, and volatile aroma molecules (Wang and Kumar 2024). Among these components, carbonyl compounds—particularly aldehydes and furans—are key oxidation markers that when present at elevated concentrations are responsible for both pleasant maturation notes and undesirable off-flavors (Choi et al. 2025). Aldehydes such as hexanal, heptanal, and benzaldehyde are produced by lipid oxidation and amino acid degradation and contribute to nutty or bruised apple aromas (Escudero et al. 2000, Moreira et al. 2013). Furans, including furfural and hydroxymethylfurfural, are associated with caramelized or baked aromas that result from sugar degradation and thermal degradation (Culleré et al. 2009). A comprehensive understanding of the accumulation of aldehydes and furans is critical to predict wine shelf life and optimize storage conditions to prevent premature aging and unpleasant sensory properties.

Recent studies have shown that oxidation extends beyond chemical reactions within the wine and is strongly influenced by the interface between the wine and its environment (Mercanti et al. 2024, Wang and Kumar 2024). Several factors

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contribute to white wine oxidation, including product composition, oxygen ingress during winemaking, and bottling conditions (Karbowiak et al. 2009, Oliveira et al. 2013), but the technological factors driving oxidation during bottle storage are not fully understood. For instance, bottle geometry such as neck dimension and the ratio of volume-to-surface area regulates oxygen ingress and distribution, thereby shaping the oxidative profile of wine (Oliveira et al. 2013). During bottling, oxygen ingress is influenced by several factors, particularly, the amount of oxygen in the bottle headspace and the oxygen introduced during cork compression (Escudero et al. 2000, Silva Ferreira et al. 2003). Additional ingress can occur after bottling through the closure and the cork/bottle interface (Lagorce-Tachon et al. 2016).

Likewise, cork type and quality regulate oxygen transmission rates, leading to variability in exposure of wine to oxygen as well as to interference with varietal composition, phenolic content, and pH, thus resulting in a complex network of factors that determine oxidative pathways (Garcia et al. 2024). In a previous study, the effect of cork stopper compression on oxygen transfer and the role of the glass/cork interface were evaluated; although it was found that compression does not significantly alter the diffusion coefficient of oxygen through raw cork, the effective diffusion coefficient was 50-fold higher when oxygen transfer was assessed in a natural cork, confirming that the main route for oxygen transfer is the glass/cork interface (Lagorce-Tachon et al. 2016). Regardless of cork type, the highest oxygen release occurred during the first month of storage, mainly due to oxygen initially trapped within the cork cells. The contribution of external oxygen ingress became more relevant afterward, progressively decreasing and stabilizing at ~3 mo (Karbowiak et al. 2009, Crouvisier-Urion et al. 2018).

From a systems perspective, the interplay between bottle geometry, cork type, and wine chemistry reinforces the importance of implementing tailored approaches to unravel the mechanisms behind wine oxidation. Conventional methodologies typically determine oxygen uptake or individual volatile compounds (Pinto et al. 2019, Ubeda et al. 2023). Nevertheless, advanced analytical techniques such as gas chromatography-mass spectrometry (GC-MS) enable the quantification of aldehydes and furans, providing sensitive detection of these volatiles and a detailed fingerprint of oxidative changes during storage (Barros et al. 2012). For instance, wines containing high phenolic concentrations may undergo faster aldehyde accumulation, while lighter wines with low phenolic contents are more prone to the formation of furans from sugar degradation (Monforte et al. 2018, 2020). Identification of these patterns is critical for vintners, guaranteeing the wine's freshness and complexity over its shelf life.

Wine composition and quality are influenced by multiple factors arising from winemaking, packaging, and bottling (Figure 1). Oxygen permeation primarily affects the chemical composition of wines during storage; several studies have compared the effects of different cork types on these chemical changes (Brajkovich et al. 2005,

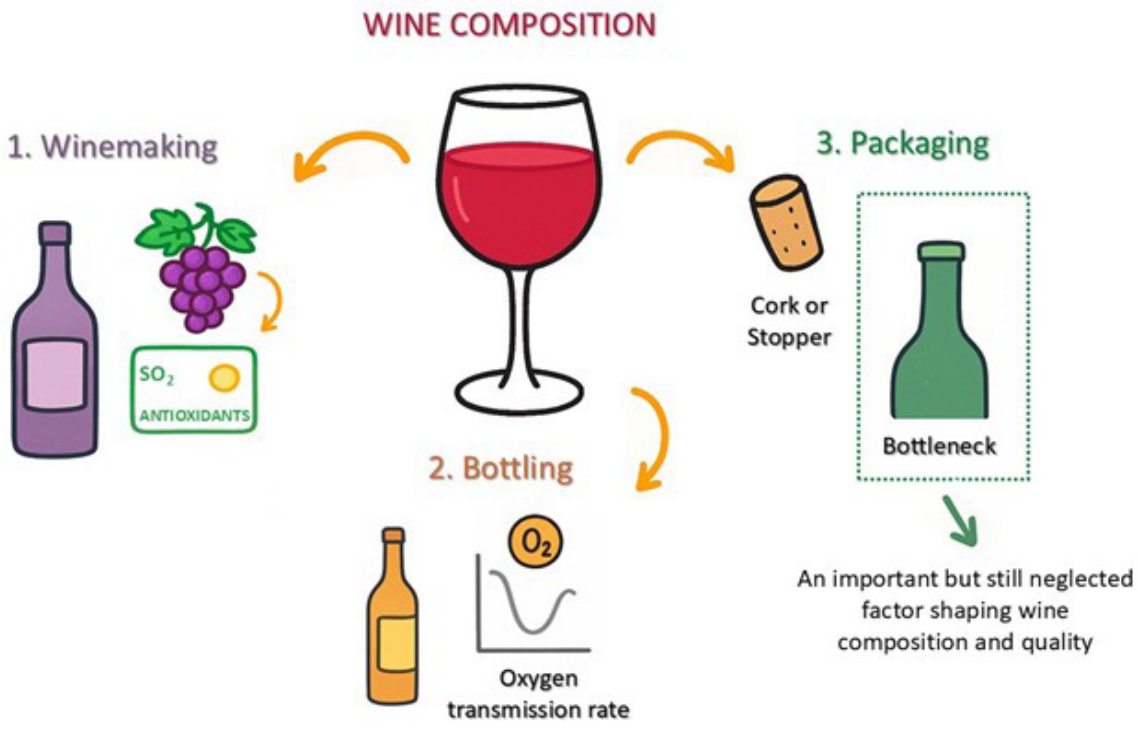

Figure 1 Schematic representation of the principal factors influencing wine composition and quality.

Culleré et al. 2009, Hopfer et al. 2013). The influence of the bottleneck is an important but still overlooked factor affecting wine composition and quality. Profiling aldehydes and furans in white wine through a systems perspective while considering bottle geometry, cork characteristics, and wine type offers a deep understanding of oxidative dynamics, guiding winemakers and industry to anticipate wine aging and optimize storage conditions to preserve the sensory quality of wines. This preliminary study aimed to investigate the impact of bottleneck geometry heterogeneity on the white wine oxidation, exploring the variability of the volatile profile by headspace solid-phase microextraction (HS-SPME) and GC-MS, and the levels of dissolved oxygen, free and total sulfur dioxide (SO_2) as chemical markers of oxidation. Multivariate data analysis was performed to underline the differences between treatment groups. Notably, this integrative approach bridges chemical analysis with practical enology, advancing scientific knowledge and applied wine management.

Materials and Methods

Chemicals

All chemicals, solvents, and standards were of analytical reagent grade (high-purity grade > 99%), used as received or dried by standard procedures, and supplied by Sigma-Aldrich.

Bottles

A total of 200 bottles were selected, including 50 bottles from each of four models under study (Type 1, Type 2, Type 3, Type 4). All bottles had the same characteristics: black glass, volume capacity of 750 ± 10 mL, and internal neck diameter of 18 ± 0.5 mm. Bottles were randomly sampled within each model.

Bottleneck profile analysis

Each bottle's bottleneck profile was characterized using an automated measurement system designed for controlling internal bottleneck dimensions (Egitron PerfilLab; S.I. Instruments). Bottleneck diameter was determined from 2 to 50 mm in depth with a resolution of 2 mm. This interval was selected to accommodate the dimensions of the corks used in the study (45 × 24 mm). Each measurement was performed in triplicate (n = 3).

Bottling and storage

The wine used for bottling was a dry white wine from the Douro region, produced during the 2017 harvest and bottled shortly after fermentation, therefore maintaining the chemical characteristics of a young wine at the time of the experiment. The wine was stored under controlled conditions and opened immediately before the bottling trials. To accelerate oxygen consumption, copper (II) and iron (II) ions were added to the wine at controlled concentrations of 7.5 and 0.4 mg/L, respectively, in the form of $CuSO_4{\cdot}5H_2O$ and $FeSO_4{\cdot}7H_2O$. A single wine (Douro dry 2017) was intentionally selected as a model system to minimize matrix variability and allow a controlled evaluation of the effects of Fe and Cu salt addition on oxidation-related processes. This approach enabled isolation of the metal-induced oxidation effect without the confounding influence of compositional differences between wines.

For the bottling trial, bottles (750-mL capacity) were filled with white wine produced and sealed with natural cork stoppers (45 × 24 mm). The cork stopper was intentionally standardized (24 × 45 mm) to minimize closure-related variability and isolate the effect of bottle geometry, i.e., the primary focus of the current work. Before vacuum insertion into bottles, the cork stoppers were compressed to a diameter of 16 mm. A forced-aging protocol was applied by storing the bottles at 40°C for 1 mo, following an earlier procedure (Silva Ferreira et al. 2002).

Analytical methods

All white wine samples were analyzed for dissolved oxygen, free and total SO_2, and aldehyde and furan profiles at the beginning of the experiment (control) and after 1 mo of storage at 40°C. Each analysis was conducted in triplicate (n = 3).

Determination of dissolved oxygen

Oxygen levels were monitored using PreSens technology, which consisted of oxygen-responsive fluorescent dots (Pst3) affixed to each bottle at mid-height. Measurements were obtained with a fiber-optic system (Fibox 3). Each measurement was made in triplicate.

Determination of free and total SO_2

Free and total SO_2 levels were determined using the Ripper iodometric titration method, following the International Organisation of Vine and Wine (OIV) official procedure (OIV-MA-AS323-04B) which involves acidification of the sample and titration with standardized iodine solution, with free SO_2 quantified directly and total SO_2 measured after alkaline hydrolysis. A standard 0.01 N iodine solution was used for the titration and a 5% (*w*/*v*) starch solution was employed as the endpoint indicator. Total SO_2 was quantified after treating the sample with sodium hydroxide to release bound SO_2.

Aldehyde and furan profiling by HS-SPME-GC-MS

Chromatographic quantification of the target compounds (aldehydes and furans) was carried out according to a previous method (Moreira et al. 2013). A derivatization procedure using O-(2,3,4,5,6-pentafluorobenzyl) hydroxylamine hydrochloride was applied to all samples (Moreira et al. 2013), which were further analyzed by HS-SPME. *p*-Fluorobenzaldehyde was used as the internal standard. The analyses were performed using an EVOQ 436 GC system (Bruker Daltonics) attached to a SCION triple quadrupole mass detector and a Bruker Daltonics

MS workstation ver. 8.2 software. Bruker Compass HyStar ver. 5.1 was used for data acquisition. A Combi-PAL autosampler (Varian Pal Autosampler) was also employed in this analysis. Chromatographic separation was conducted in a GC column CP-Wax 58 FFAP (50 m × 0.25 mm × 0.20 µm film thickness) (Agilent Technologies). Helium C 60 (Gasin) at a constant flow rate of 1.0 mL/min was used as the carrier gas. Before injection, samples were incubated at 40°C for 2 min at 250 rpm of agitator speed. The injector temperature was 250°C (held for 20 min). The samples desorb time was 5 min at the injector penetration depth of 45 mm and speed of 100 mm/sec. The MS detector was operated in electron ionization (EI) mode. The transfer line, manifold, and EI temperatures were 270, 40, and 260°C, respectively. The mass range was 40 to 600 m/z, with a scan rate of 6 scans/sec. The analysis was performed in full scan mode. All samples were analyzed in triplicate.

Data analysis

For each acquired parameter, mean values and standard deviations were calculated, followed by analysis of variance (ANOVA) with post-hoc mean comparisons using Tukey's honest significant difference test, accounting for unequal sample sizes at a 5% significance level. Bottleneck profiles of the 200 bottles were further analyzed by principal component analysis (PCA) to evaluate sample distribution and assess potential clustering by bottle type. A cluster heatmap was applied to classify geometric variables (internal diameters along the bottleneck and the frequency of conicities above 1.5 mm). Quantification of chemical compounds was performed using MATLAB ver. 8.4 (R2014b) software (Mathworks), including all the pre-processing steps (peak detection, peak integration, baseline correction, signal smoothing, calibration curve fitting, and quantification based on internal standard) using built-in MATLAB functions. The main steps of the MATLAB script and the key parameters (thresholds, smoothing window, fitting model) were applied following a previous procedure (Monforte et al. 2021).

Results and Discussion

Bottleneck profile

A wine bottle is divided into five sections (from top to bottom): finish, neck, shoulder, body, and base (Grayhurst 2012). Among these, the finish and neck are particularly important because they are designed to accommodate the cork. The finish, which represents the first step in the bottle-forming process, encompasses all features above the upper end of the bottleneck (Grayhurst 2012). Bottles are broadly classified according to features such as diameter and sealing method. The dimensions of the finish and neck should correspond to the closure dimensions, highlighting the importance of establishing and maintaining strict tolerances during specification and manufacturing (Emblem 2012). Tolerance limits for glass bottles are defined by the International Standard Organization, based on recommendations from the International Technical Centre for Bottling and Related Packaging (Cetie): the average internal diameter should not exceed 1 mm, and to guarantee good sealing performance, the average internal diameter between d_1 and d_2 should not be inferior to the average inlet diameter (ISO 2008). Bottleneck

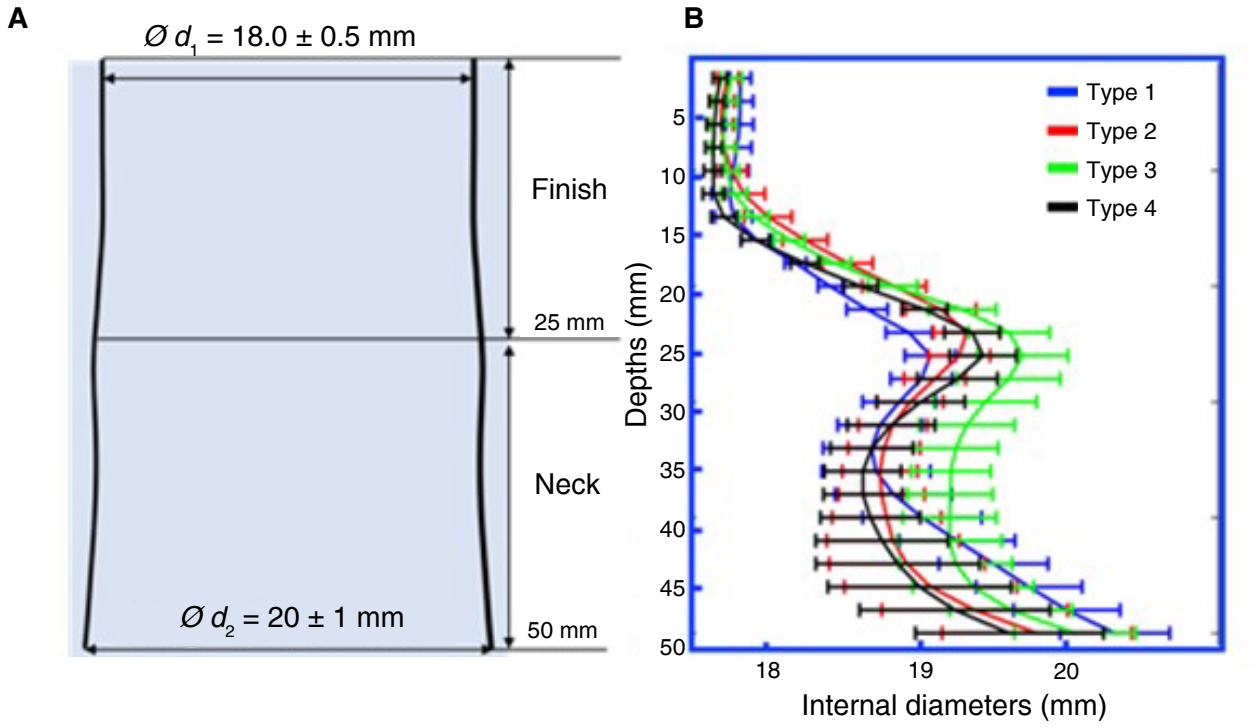

Figure 2 (**A**) Representation of bottleneck profile (2 to 50 mm depth) and (**B**) bottleneck internal diameters for the four types of bottles examined in this study (average ± standard deviation).

profiles and internal diameters for the four bottle types are presented in Figure 2.

The total profile (2 to 50 mm), the finish (2 to 24 mm), and the neck (26 to 50 mm) bottleneck regions were selected for the statistical comparison between bottle types. The bottleneck profile of 200 bottles was measured between 2 and 50 mm, which corresponds to the bottle section where the cork is inserted (Figure 1). In this framework, the finish comprises depths between 2 and 25 mm, while the neck corresponds to the subsequent segment above 26 mm.

All four bottle types examined in this study showed heterogeneity in their bottleneck profiles, with a higher incidence observed at depths between 20 and 50 mm, corresponding to the finish and neck regions (Figure 2). ANOVA revealed significant differences between bottle types ($p < 0.05$) when considering the entire bottleneck profile (0 to 50 mm), as well as within the finish and neck regions. Boxplots of the average internal diameters across the three regions are shown (Figure 3).

The trends varied among bottle types depending on the region. According to Tukey's test, Types 1 and 2 showed similar bottleneck dimensions which differed from Types 3 and 4. For the finish region, Types 2 and 3 were similar in average diameters, although distinct from the other two bottle models. In contrast, the neck region showed a different pattern in which Types 2 and 4 were more similar, whereas Types 1 and 3 had distinct neck dimensions.

These observations demonstrate that bottleneck profile is heterogeneous and varies across specific regions (bottleneck, neck, and finish). According to the literature, the bottleneck is the part of the bottle where most defects occur during fabrication due to the challenges of handling its narrow structure (Carrasco and Mery 2011). However, no standardized reference measurements are currently available for quality control of wine bottles. The only specification provided by the manufacturer about bottleneck measurements is that the internal diameter of the finish should be 18 ± 0.5 mm. Our results align with this specification, with internal diameters in the finish region ranging from 18.4 to 18.6 mm.

Nonetheless, wine companies perform inspections of bottles and based on specific recommendations, a criterion has been established on conicity, defined as the difference between the inlet diameter and the internal diameter along the bottleneck. Bottles with a high frequency of conicity values exceeding 1.5 mm may not have efficient sealing (Cetie 2008). In the bottles analyzed in our study, the frequency of conicity values higher than 1.5 mm ranged from 0 to 7 (Figure 4). Types 1 and 4 had the highest number of bottles with frequencies above 3. A graph is presented showing the frequency of conicity values above 1.5 mm, in relation to the Cetie criterion that the average internal diameter should not exceed the average inlet diameter by more than 1 mm (Figure 4). Samples with a frequency above 4 also exhibit a Cetie index greater than 0.8 mm. Interestingly, some bottles with a large difference between the inlet and internal diameters exhibit a low frequency of conicity values (<1.5 mm). These observations suggest that a single parameter is insufficient to fully evaluate the quality of the bottleneck profile.

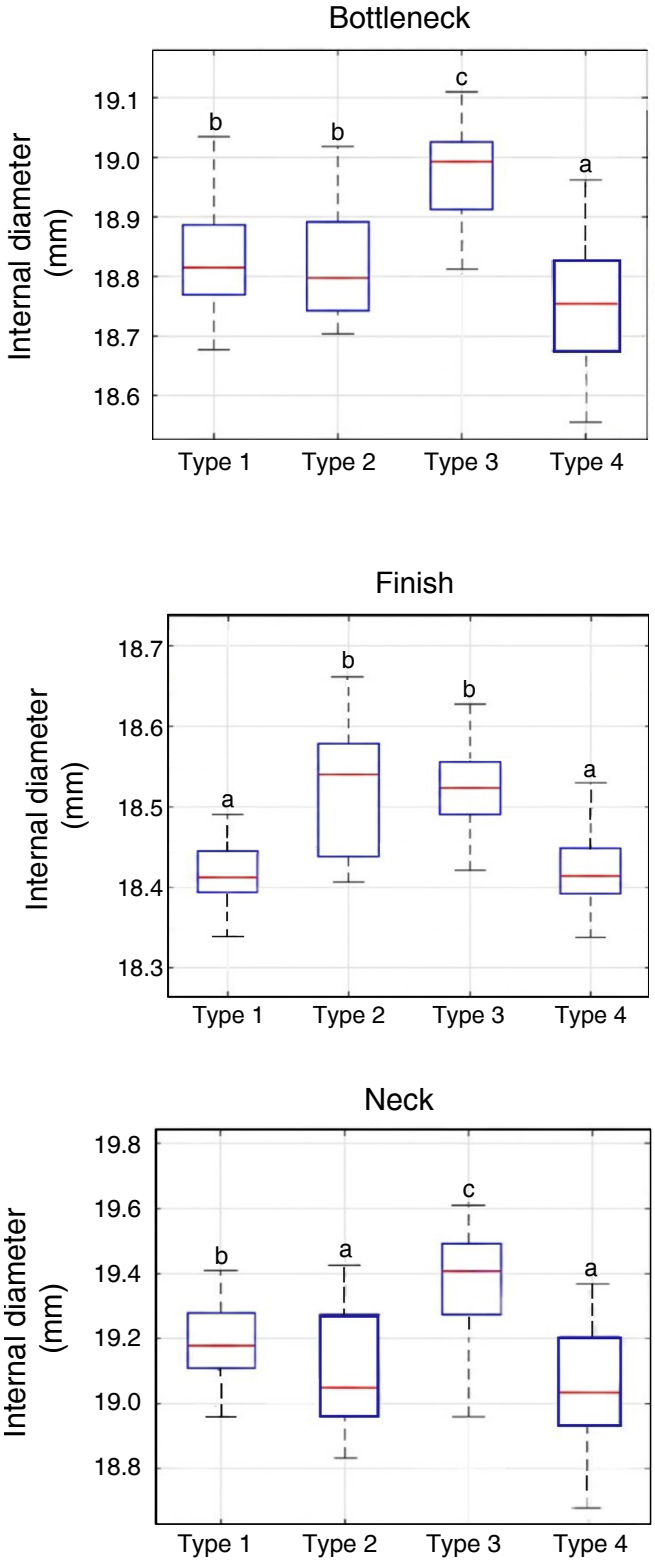

Figure 3 Box plot representation of average internal diameters for bottleneck, finish, and neck regions, including minimum, maximum, median, and quartile distribution by bottle model. Different letters indicate statistically significant differences ($p < 0.05$) among bottle types (analysis of variance followed by Tukey's multiple comparison test, $\alpha = 0.05$), while the same letter denotes no significant difference.

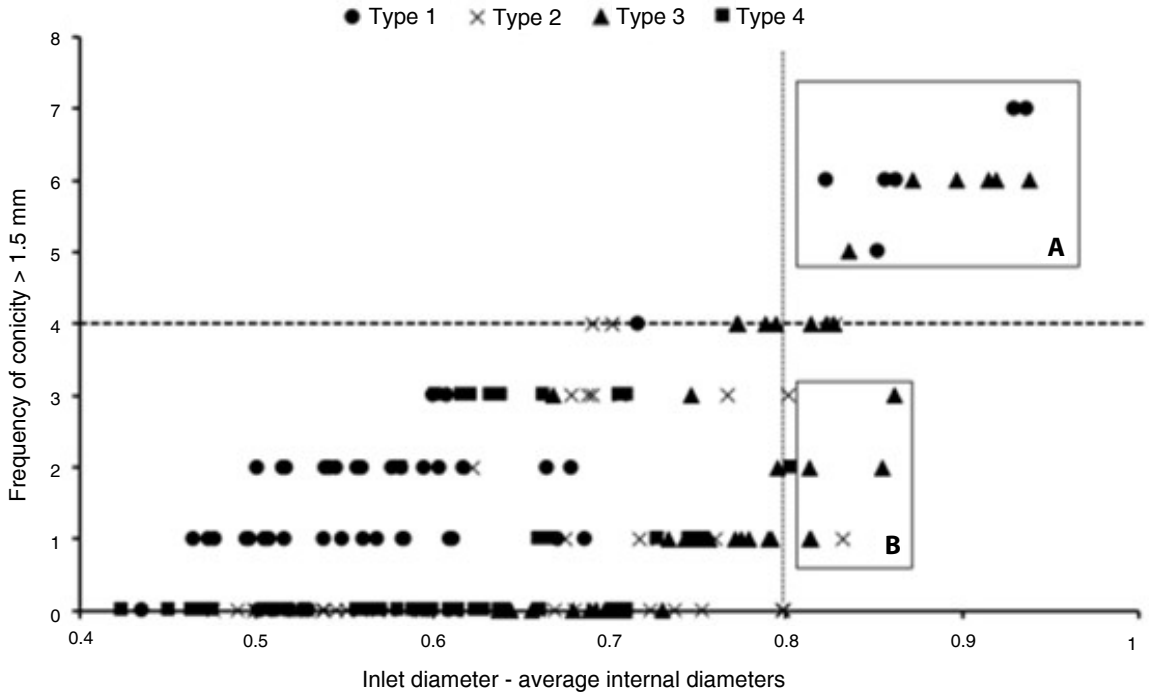

Figure 4 Frequency of conicity >1.5 mm versus Cetie (International Technical Centre for Bottling and Related Packaging) index (difference of inlet diameter and average internal diameters), marked according to bottle type. Inset panels show the bottles with the highest (above 4; **A**) and the lowest (below 3 and above 1; **B**) frequencies of coinicity.

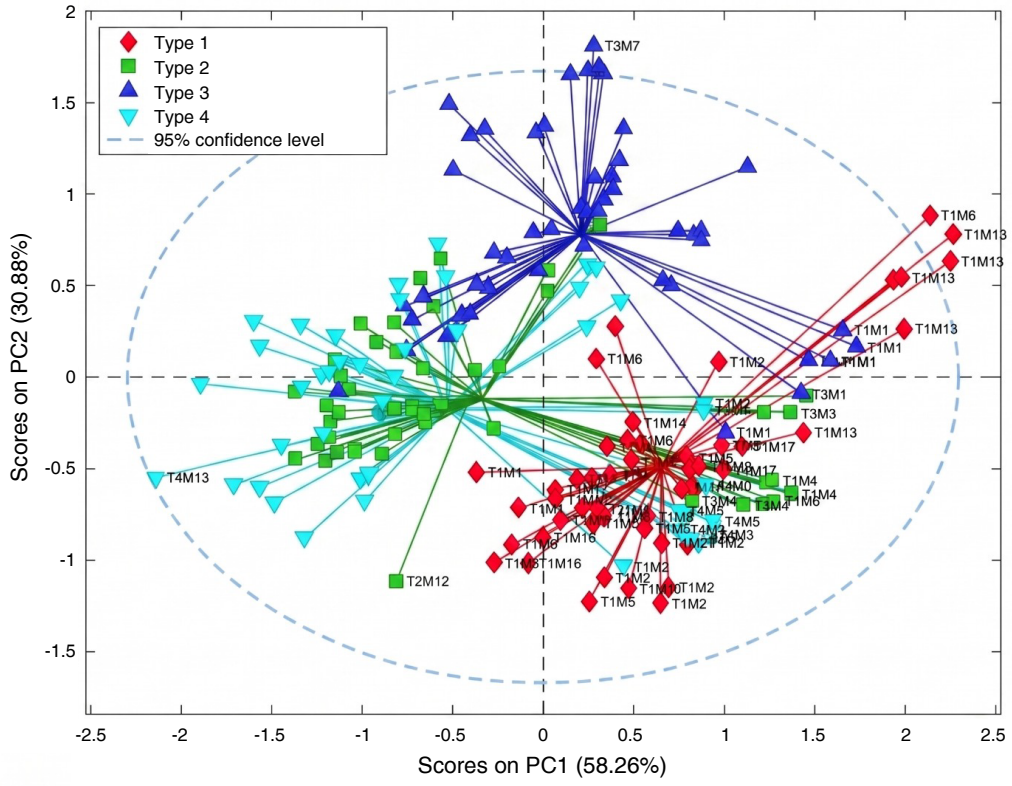

Figure 5 Principal component analysis plot of sample scores (PC1 versus PC2), grouped by bottle type.

PCA applied to bottleneck profile

PCA was applied to observe any possible cluster within the four types of bottles and to reveal patterns in the measured responses (Figure 5). Principal components 1 and 2 (PC1 and PC2, respectively) account for 89.1% of the cumulative variance. The PCA plot revealed distinct clustering patterns along the PC1 and PC2 axes. Type 1 clustered separately from the other groups along PC1, mainly influenced by the neck region; Type 3 separated from the other bottle models along PC2 due to differences in finish internal diameters; and both Types 2 and 4 showed similar bottleneck profiles. PCA loadings represent independent sources of variance in the bottleneck profile. PC1 is associated with the neck, while PC2 is related to the finish. This confirms the statistical analysis performed on the average diameters, which demonstrated that different regions are affected independently. Lastly, some bottles from specific groups clustered with bottles of other groups, suggesting similarities in bottleneck profiles regardless of bottle type.

Chemical characterization

Dissolved oxygen

The sealing integrity of wine bottles is essential for preserving wine quality and bottleneck profile plays a critical role in the closure efficiency (Lagorce-Tachon et al. 2016). The heterogeneity of the bottleneck profile can compromise the sealing capacity, potentially leading to oxygen ingress and consequently, a decline in wine quality (Lagorce-Tachon et al. 2016, Garcia et al. 2024). At the beginning of the experiment, all bottles were saturated with oxygen (8.2 ± 0.5 mg/L), with no significant differences observed among the bottles. After 1 mo of storage at 40°C, oxygen consumption was also similar across all bottles (4.1 ± 0.7 mg/L). Regardless, these outcomes do not exclude the possibility of slight variations that could affect wine quality over extended storage periods.

Previous research has proposed that oxygen ingress into wine bottles occurs through various pathways, including the closure material and the glass/cork interface (Mercanti et al. 2024). For instance, multiple oxygen ingress routes using different closures were found in one study, emphasizing the complexity of this wine bottling process (Lopes Cardoso et al. 2022). Furthermore, the oxygen ingress was directly dependent on the bottleneck profile, with narrower bottlenecks contributing to higher oxygen ingress rates (Lopes Cardoso et al. 2022). These results indicate that even minor variations in bottleneck dimensions could influence oxygen transmission rate and consequently, the wine's exposure to oxygen (Lopes et al. 2006).

The role of oxygen in wine aging is well-documented, with controlled oxygen exposure leading to the development of desirable characteristics such as high aromatic complexity and integration of flavors (Karbowiak et al. 2009). In contrast, excessive oxygen can accelerate oxidative spoilage, resulting in the formation of off-flavors, loss of freshness, and degradation of wine quality (Ferreira et al. 2014). Although our study did not detect significant variations in dissolved oxygen levels across bottle types, the effect of bottleneck profile heterogeneity on oxygen ingress should be further investigated. Future studies should address long-term experiments to evaluate the cumulative effects of oxygen ingress on wine quality, considering the complex interplay between bottleneck geometry, closure material, and storage conditions.

Free and total SO_2

SO_2 plays a pivotal role in winemaking, acting as an antimicrobial agent that inhibits the growth of undesirable microorganisms and as a potent antioxidant that protects wine against oxidative spoilage (Ough and Crowell 1987). The concentrations of free and total SO_2 in wines are critical indicators of wine stability and quality; in our study, these concentrations were determined by iodometric titration.

Free SO_2 concentrations ranged from 10 to 32 mg/L and total SO_2 concentrations ranged from 65 to 120 mg/L (Figure 6). After 4 wk of storage at 40°C, free SO_2 decreased by an average of 17 mg/L, corresponding to a 50% loss. Significant differences ($p < 0.05$) were observed among different bottle types, which may be associated with heterogeneity in the bottleneck profile. The pronounced decline in free SO_2 observed in our study is consistent with previous findings that report substantial SO_2 losses during the early stages of wine storage (Vidal et al. 2015). This decrease is mainly attributed to the consumption of free SO_2 via the reaction with dissolved oxygen present at bottling and oxygen ingress through the closure over time.

The substantial differences in SO_2 loss among different bottle types reinforce the influence of bottleneck profile heterogeneity on oxygen ingress and therefore, on SO_2 depletion (Lopes et al. 2006). Thus, factors such as oxygen ingress, bottleneck profile heterogeneity, and closure properties play key roles in SO_2 depletion. This finding underscores the importance of standardized bottleneck profiles to guarantee consistent oxygen management and preservation of wine quality; future studies should focus on developing predictive models that integrate these factors to control SO_2 dynamics in bottled wines.

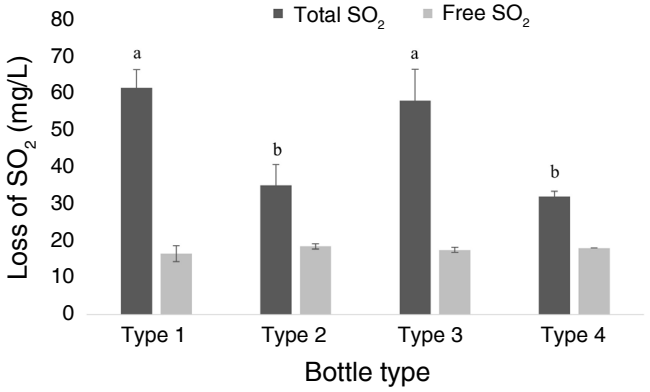

Figure 6 Loss of free and total sulfur dioxide (SO_2) between bottling and 1 mo of storage at 40°C across all bottles tested. Different letters indicate significant differences ($p < 0.05$) among the same variable.

Aldehyde and furan profiling

Volatile composition of wine plays a pivotal role in shaping its sensory attributes, with aldehydes and furans contributing to desirable aroma complexity and to the development of oxidative off-flavors, depending on the concentrations of aldehydes and furans and their interactions with other components (Moreira et al. 2013, Ferreira et al. 2014). Aldehydes and furans were identified and quantified in the wines from the different bottle types (Table 1).

A total of 17 volatile compounds were quantified in wines from various bottle types, including six alkanals, three alkenals, six Strecker aldehydes, and two furans. All compounds exhibited increased concentrations after 1 mo of storage at 40°C, indicating oxidative processes and potential interactions with bottle closure characteristics (Table 1). Among the alkanals, butanal, pentanal, hexanal, octanal, nonanal, and decanal were quantified in wine stored in the four bottle types analyzed. Among alkanals, significant differences ($p < 0.05$) were observed only for hexanal and octanal, with maximum concentrations of 13.3 and 0.5 µg/L, respectively, for wine stored in bottle Type 1. Otherwise, the lowest concentrations were reached for the control bottle at time 0 with 6.8 and 0.2 µg/L for hexanal and octanal, respectively. These aldehydes contribute to grassy and waxy notes in wine and their high concentrations may indicate increased oxidation rates (Catalano et al. 2024).

For alkenals, *trans*-2-hexenal, *trans*-2-octenal, and *trans*-2-nonenal were quantified in wines from all bottle types. However, significant differences ($p < 0.05$) were observed only for *trans*-2-hexenal and *trans*-2-nonenal. For both *trans*-2-hexenal and *trans*-2-nonenal, concentrations exceeded their odor thresholds, estimated at 17 and 0.6 µg/L, respectively (Watkins and Wijesundera 2006); the highest concentrations of these volatile molecules were found in wine stored in bottle Type 1, reaching 20 and 3.1 µg/L, respectively. *Trans*-2-hexenal provides a green leafy aroma, while *trans*-2-nonenal imparts fatty waxy notes (Catalano et al. 2024). When these compounds' concentrations are high in wine, specific factors (i.e., oxygen ingress and seal integrity) should be assessed, given their role in aldehyde formation.

Among the Strecker aldehydes, 2-methyl-1-propanal, 2-methyl-1-butanal, 3-methyl-1-butanal, phenylacetaldehyde, methional, and benzaldehyde were quantified in all bottle types as products of amino acid degradation and indicators of oxidative stress in wine (Monforte et al. 2018). Phenylacetaldehyde, methional, and benzaldehyde showed significantly higher concentrations ($p < 0.05$) than the control sample across all wines, with levels exceeding their odor thresholds (25, 0.5, and 200 µg/L, respectively) (Escudero et al. 2000, Culleré et al. 2009). Phenylacetaldehyde, which imparts floral and honey-like aromas, showed concentrations ranging from 26.2 µg/L in bottle Type 2 to 39.5 µg/L in bottle Type 3, representing a variation of nearly 50%, depending only on the bottle type. The highest concentration of methional, which contributes to a cooked potato aroma, was detected in wine from bottle Type 1 (50.3 µg/L) and the lowest was found in wine from bottle Type 4 (36.0 µg/L). Benzaldehyde, which contributes to almond-like notes, had concentrations varying from 12.1 µg/L (in wine stored in bottle Types 2 and 4) to 16.2 µg/L (in wine stored in bottle Type 1), which corresponds to a variation of over 50% across bottle types. The formation of Strecker aldehydes can result from several mechanisms, however, oxygen exposure is broadly recognized as a key factor in their formation (Ferreira et al. 2014, Monforte et al. 2019). Notably, the formation of Strecker aldehydes is closely linked to oxygen exposure, which facilitates the Maillard reaction and subsequent amino acid degradation (Monforte et al. 2019). Recent studies have shown that increased oxygen ingress leads to higher aldehyde concentrations, which affects the sensory quality of wine (Escudero et al. 2002). In this study, the variability observed among bottle types suggests that sealing integrity and oxygen permeability are critical factors in controlling oxidative pathways.

Finally, two furans, 2-furfural and 5-methylfurfural, were detected in wines from all bottle types. However, significant differences ($p < 0.05$) were detected only for 2-furfural, with the highest concentration achieved in bottle Type 1 (115 µg/L) and the lowest in bottle Type 3 (89.5 µg/L). The 5-methylfurfural concentrations remained relatively consistent across all bottle types. These furans are typically formed through Maillard reactions and caramelization processes, and their

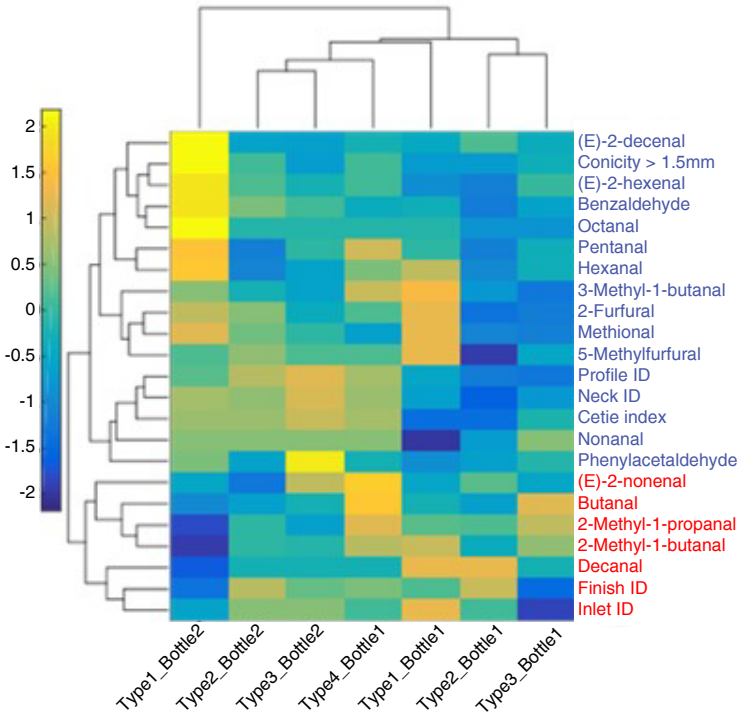

Figure 7 Hierarchical cluster analysis and heatmap of the relationship between volatile compounds and bottleneck profiles across all bottle types. For each bottle type, data correspond to the mean values obtained from the analysis of 50 bottles. The two sets of columns for bottle Types 1 to 3 represent the technical replicates or independent analytical runs.

presence indicates ongoing oxidative processes and potential interactions with packaging materials (Seok et al. 2015).

These findings emphasize the effect of bottle type and sealing traits on the volatile composition of wine. The variations in aldehyde and furan concentrations indicate that factors such as oxygen ingress, seal integrity, and packaging material have a significant influence on the oxidative stability and sensory quality of wine. Notably, these outcomes align with previous studies on the aroma profile of wine (Ferreira et al. 2014, Monforte et al. 2018, 2019). Further studies should explore the sensory effects of specific volatile compounds and their interactions, to offer new insights into wine quality and consumer preferences.

Relationship between volatile compounds and bottleneck profile by hierarchical cluster analysis (HCA)

The integration of HCA with bottleneck profile measurements provides a robust framework for identifying the effect of structural variations of bottle closures on the volatile composition of wine. An HCA heatmap of volatile compounds and bottleneck measurements across all bottle types is presented (Figure 7). For each bottle type, data correspond to the mean values obtained from the analysis of 50 bottles. The two sets of columns for bottle Types 1 to 3 represent technical replicates or independent analytical runs.

In this study, HCA revealed that volatile compounds and bottleneck profile indicators are grouped into two main clusters. One cluster comprises key Strecker aldehydes (phenylacetaldehyde, methional, and benzaldehyde), alkanals (hexanal and octanal), furans (2-furfural and 5-methylfurfural), bottle profile indicators (neck and total bottle profile), and the Cetie index, indicating that a higher Cetie index (reflecting poor sealing efficiency) is correlated with increased aldehyde concentrations. The second cluster encompasses some volatile molecules and two bottle profile measurements (finish and inlet).

The Cetie index, which reflects the sealing efficiency of wine bottle closures, is a critical factor influencing oxygen ingress during storage. Previous studies have demonstrated that closures with higher Cetie index values allow greater oxygen transmission, thereby accelerating oxidation in wine (Mercanti et al. 2024, Suhas et al. 2025). This increased oxygen exposure facilitates the formation of aldehydes through various pathways—primarily the Strecker degradation of amino acids (Monforte et al. 2018).

Our findings align with previous studies, reinforcing the effect of closure-related oxygen ingress on wine composition. For example, one study emphasized the role of oxygen in the formation of aldehydes in wine, highlighting the importance of closure integrity in preserving wine quality (Ferreira et al. 2014). Likewise, another study proved that variations in closure performance may lead to significant discrepancies in the volatile profile of wines, corroborating the present results (Monforte et al. 2019).

Application of HCA elucidated the relationship between closure features and wine composition, providing a valuable tool to predict the effect of closure quality on wine aging and shelf life. These insights could pave the way for optimizing closure design and selection to improve the preservation of wine quality during storage.

Table 1 Aldehyde and furan concentrations (µg/L) in wines from the four bottle types analyzed.

	t0 (Control)	Type 1	Type 2	Type 3	Type 4	*p* value
Alkanals						
Butanal	2.7 ± 0.18	2.9 ± 0.13	2.9 ± 0.23	3.2 ± 0.36	3.5 ± 0.10	ns[a]
Pentanal	2.1 ± 0.22	4.0 ± 0.43	3.3 ± 0.20	3.7 ± 0.35	4.1 ± 0.01	ns
Hexanal	6.8 ± 0.68	13.3 ± 1.1	9.7 ± 0.32	10.6 ± 0.53	12.0 ± 0.40	***>0.001***
Octanal	0.2 ± 0.06	0.5 ± 0.17	0.3 ± 0.06	0.3 ± 0.06	0.3 ± 0.01	***>0.001***
Nonanal	0.6 ± 0.02	0.7 ± 0.14	0.8 ± 0.08	0.8 ± 0.05	0.8 ± 0.03	ns
Decanal	0.2 ± 0.05	0.4 ± 0.11	0.5 ± 0.06	0.4 ± 0.05	0.4 ± 0.01	ns
Alkenals						
Trans-2-hexenal	2.0 ± 0.29	20.0 ± 5.6	17 ± 2.7	17.7 ± 0.76	18.5 ± 0.15	***>0.001***
Trans-2-octenal	0.1 ± 0.01	0.3 ± 0.02	0.3 ± 0.12	0.4 ± 0.12	0.60 ± 0.01	ns
Trans-2-nonenal	1.4 ± 0.29	3.1 ± 1.4	2.1 ± 0.45	1.8 ± 0.21	2.0 ± 0.14	***>0.001***
Strecker aldehydes						
2-Methyl-1-propanal	21.0 ± 2.2	35.2 ± 8.0	40 ± 2.1	40.4 ± 5.0	46.5 ± 0.60	ns
2-Methyl-1-butanal	21.2 ± 2.1	35.0 ± 4.1	35.5 ± 1.5	36.3 ± 2.3	37.5 ± 2.1	ns
3-Methyl-1-butanal	37.3 ± 1.0	95.9 ± 5.7	89.1 ± 4.1	87.3 ± 1.8	96.1 ± 2.0	ns
Phenylacetaldehyde	8.6 ± 0.83	29.1 ± 6.9	26.2 ± 1.5	39.5 ± 10.1	29.4 ± 0.70	***>0.001***
Methional	8.0 ± 0.42	50.3 ± 0.7	38.3 ± 6.3	36.2 ± 4.8	36.0 ± 2.9	***>0.001***
Benzaldehyde	6.9 ± 0.34	16.2 ± 4.4	12.1 ± 3.1	12.6 ± 1.5	12.1 ± 0.40	***>0.001***
Furans						
2-Furfural	18.6 ± 1.7	115 ± 6.4	94.7 ± 13.5	89.5 ± 6.4	102 ± 4.2	***>0.001***
5-Methylfurfural	1.6 ± 0.28	3.7 ± 0.4	3.3 ± 0.48	3.4 ± 0.2	3.5 ± 0.10	ns

[a]ns, not significant.

Conclusion

This study presents preliminary results on the effect of bottle geometry on the oxidative stability of white wines. The combination of bottleneck measurements with chemical and volatile profiling provides evidence that small variations in bottleneck dimensions may significantly influence sealing efficiency, oxygen ingress, and consequently, the formation of oxidation-related molecules in wine. Although dissolved oxygen levels decreased during storage across all bottle types, free SO_2 losses varied markedly, reinforcing the role of bottleneck heterogeneity in oxygen management. The substantial depletion of free SO_2 within the first month of storage supports its role as an early oxidation marker. Furthermore, a significant increase in carbonyl compound concentrations was detected after storage. Among these, hexanal, *trans*-2-hexenal, phenylacetaldehyde, and methional exceeded their odor thresholds, proposing a direct effect on wine aroma and quality. The variability observed across bottle types underscores the role of seal integrity in modulating oxidative pathways. In addition, HCA revealed that Strecker aldehydes clustered closely with the Cetie index, emphasizing the strong relationship between bottleneck and aldehyde accumulation. Although these results corroborate previous reports on closure oxygen transmission, they also highlight for the first time the importance of bottleneck geometry as a crucial and overlooked factor of wine oxidation.

Overall, this work demonstrates that bottleneck heterogeneity is a key contributor to variability in wine aging and shelf life. From an applied perspective, these findings strengthen the importance of implementing stricter manufacturing tolerances in wine bottle production, integrating bottleneck measurements into closure performance assessment. Future studies should focus on long-term storage and sensory evaluation to correlate chemical markers with consumer perception, aiming to optimize packaging design and guarantee wine quality. Additionally, expanding this work to include multiple wine varieties with distinct chemical characteristics (particularly reductive thiol-rich wines) and different cork lengths and types would allow a more comprehensive assessment of the effect of Fe and Cu salts and cork stoppers on oxidation behavior. Antioxidant capacity (evaluated by the 2,2'-azino-bis-(3-ethylbenzothiazoline-6-sulfonic) acid [ABTS] assay) could also provide complementary information about the overall redox status of wine, while phenolic profiling and color analysis may further elucidate the role of phenolic composition in oxidation behavior.

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CRediT Authorship Contributions

DP, AM, and CR: Formal Analysis; DP and AM: Methodology; DP and ASF: Software; DP, AM, CR, and ASF: Validation; DP and AM: Writing – Original Draft; AM and CR: Investigation; CS, AF, and ASF: Resources, Supervision, Writing – Review & Editing; CS and AF: Visualization; ASF: Conceptualization, Data Curation, Funding Acquisition, Project Administration

Conflict of Interest

António César da Silva Ferreira declares that his affiliation with Cork Supply had no influence on the design, analysis, interpretation, or reporting of the results presented in this paper. All other authors declare no competing interests.

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Data Availability

The data underlying this study are available on request from the corresponding author.

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