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Report

Client: PROCORK

Project number: ONFRPROC19D

Date : 10th December 2019

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Approved by : Charlotte Tournier

Référence : EQ-REA23
Révision : 002
Date : 05/10/2018

Your project

OTR and molecular analyses on wines closed with and without cork coated with Procork Membrane

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REPORT SUMMARY

1 Introduction and purpose

The Procork company developed a membrane technology to control the rate of oxygen entering the wine bottles when closed with natural cork. This membrane made of 5 different layers allows selective permeation of oxygen to allow micro-aeration of grape and oak barrel tannins while blocking bitter cork lignins and taints.

A triangular sensory test has already been conducted by Sensenet using synthetic wines, to confirm the inertness and food neutrality of the Procork membrane. The triangle test compared a synthetic wine which has been in contact with the membrane and the “control” synthetic wine and confirmed the inertness of the ProCork membrane.

To further investigate the impact of the membrane on wines, two 2008 Saint-Emilion Grand cru from Chateau Teyssier wine bottles have been compared: one closed with a natural cork used as a control; the other closed with a cork coated with the Procork Membrane.

Those two bottles have been tasted by the Master of Wine Peter Scudamore-Smith. He mentioned the natural cork bottles was more “flat and bretty”, the Procork bottle was described as “fresher and brighter nose’ and having “more fruit volume and sweeter palate”. “The oxidative regime of natural cork has emphasized Brett, lessened freshness, accelerated ageing and palate dryness, now a poor wine; ProCork has held nose freshness and muted the Brett, allowed ageing without oxidation, kept the wine fresh and the palate able to display aged fruit/tannin complexity.”

To deepen the comparison of those two bottles, Procork asked Sensenet to first measure the OTR (Oxygen Transfer Rate) of the two bottles using an optical/fluorescence Oxygen meter. Objective was to confirm the difference in oxygen supply between the two bottles due to the presence of the Procork Membrane.

In a second time, Sensenet performed molecular analyses (GC-TofMS) on the headspace of the two wine bottles. Those molecular analyses helped to understand the evolution in volatile organic compounds composition between the two bottles.

Additionally, to compare the potential “Brett” character of the two bottles mentioned by the Master of Wine for the natural cork bottle, specific molecular analyses have been performed targeting the typical Brett markers 4-ethylphenol [4-EP], 4-ethylguaiacol [4-EG] and 4-ethylcatechol [4-EC].

This document summarizes the results obtained after OTR measurements and molecular analyses.

2 Services summary

Title: OTR and molecular and analyses on wines closed with cork coated with Procork Membrane		
Experimental Plan		
Number of samples	Two bottles of the same wine: 1 closed with Procork the other as a control (natural cork)	
Sampling		
Protocol	For wine bottle headspace analysis: the wine was introduced into a micro-chamber (at 27 °C. for 10 minutes), the headspace was then trapped on Tenax® tubes by helium scanning. For direct liquid analysis: Direct liquid injection on Tenax® tubes.	
Analyses		
Molecular analyses		
Parameters	**Methodologies**	**Details**
GC-TofMS	Internal method	Headspace analysis: Full scan Direct liquid analysis: targeted analysis on 4-ethylphenol [4-EP], 4-ethylguaiacol [4-EG] and 4-ethylcatechol [4-EC].
Other analyses		
OTR	PROCORK Internal method	Optical/fluorescence Oxygen meter

3 Experimental

The wine used for this study was a red wine: a 2008 Saint-Emilion Grand cru from Chateau Teyssier.

Two different bottles were used: one labelled “N” closed with a simple natural cork and the second labelled “Procork” closed with a cork coated with the Procork Membrane. Those two wine bottles have been stored in the same conditions for eleven years.

3.1 OTR measurements


An Oxygen Transmission Instrument (OTI) has been used to measure oxygen depletion just above the cork. From those values, the Oxygen Transmission Rate (OTR) has been estimated.

An integrated optical oxygen sensor DOpO2 (Spectrecology, St Petersburg, Florida, USA) was used to measure the percentage of oxygen present in the air trapped in a gas measurement cell set above the cork.

The associated Fluorometrics DOpO2 Viewer software was used to collect values.

A measuring cell of known volume was sealed hermetically just above the cork. This measuring cell consisted in a sensor patch put above the cork on a glass plate and sealed on a very low volume chamber. This measuring cell was sealed on the bottle using aluminum foil held in place with epoxy glue.

The oxygen level in the cell has been measured by placing the probe above the measuring cell. Measurements have been performed at days 0, 1, 4, 5, 7, 11, 14 and 21. To ensure repeatability of the measurement marks were drawn on the cell to ensure same positing of the probe for each measurement. The ambient conditions (temperature and pressure) were recorded.

This innovative technique allowing non-invasive measurement is being patented by ProCork.

3.2 Molecular analyses protocol

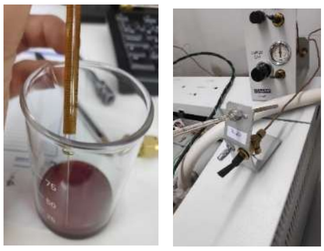
3.2.1 Headspace extraction sampling protocol for volatile organic compounds composition analysis

The headspace of each wine was sampled using an individual Microchamber (M-CTE250, Markes Int) heated at 27°C, to mimic the temperature the wine can reach when placed in contact with the palate. Indeed, during wine degustation some volatile compounds volatilize only when placed in the mouth due to their boiling point.


A defined quantity of wine (40mL) was introduced and confined in the microchamber. To collect samples, an absorbent tube (Tenax/Sulphicarb) was inserted on the top of the microchamber. A total of 1000 mL of headspace volume was collected during 10 minutes. To promote the transport of the volatile organic compounds from the headspace to the tube a nitrogen gas a flow of 10 mL/min (99.999% purity N2) was used. An additional tube, without sample, was prepared in the same sampling conditions as a blank. The sampling was made in duplicate (2 tubes for each sample). The sample tubes were kept closed with two plugs at their ends until the time of analysis.

Initial wine sampling was performed using a glass pipette, just after removing the cork from the bottle to avoid any additional oxidation due to contact of the wine with the air.

3.2.2 Direct liquid injection sampling protocol for Brett markers analysis



A defined quantity of wine (1 µL) was directly injected on a Tenax® tube using a glass syringe and Markes Calibration Solution Loading Rig (CSLR, Markes, UK).

3.2.3 Molecular Analyses

Our instrument is composed of a gas chromatograph (Agilent 7890 model, US), Time-of-Flight mass spectrometer (BenchTOF-dx model, Almsco, Germany) and thermal desorption unity (Unity2, Markes, UK).

The desorption Tenax® tubes were connected to the thermodesorption unit of the GC-ToFMS instrument. They were individually subjected to high temperatures during an initial phase to desorb the VOC captured during sampling. Afterwards, VOCs were entrained by a flow of helium carrier gas (99.9999% purity He) to a cold trap at low temperature by thermoelectric cooling, where they were again retained. Then, the cold trap was heated drastically to release and drag all VOCs into the GC for subsequent chromatographic separation. At the end of the tour of the GC column, once separated, the compounds reached the mass detector at different times, being ionized and by the Time-of-Flight (ToF) selector. The TargetView V3 software (ALMSCO, Germany) has been used to carry out deconvolution process providing the chemical identification from the GC-MS data.

Due to the high amounts of alcohols and esters leading to coelution phenomenon between the peaks, the analysis and processing of the samples was made three times using different analysis conditions; a filament delay of 12 minutes has also been used.

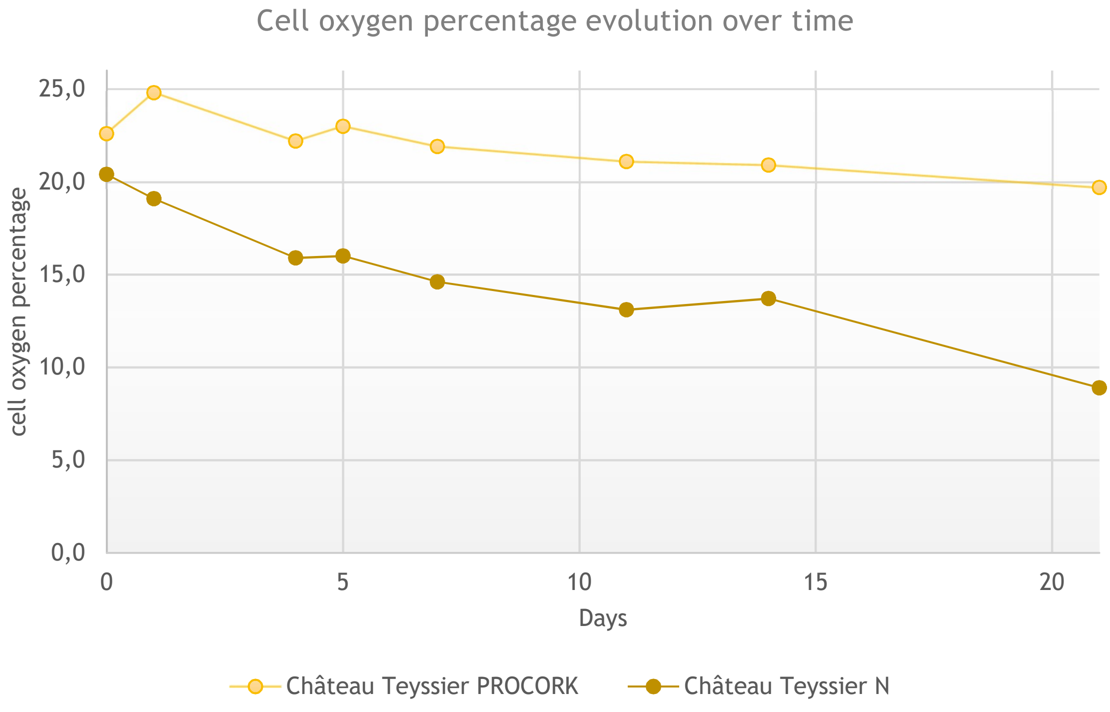
4 Results and discussion

4.1 OTR measurements results

The table below presents the cell oxygen percentage measured in the two bottles over time:

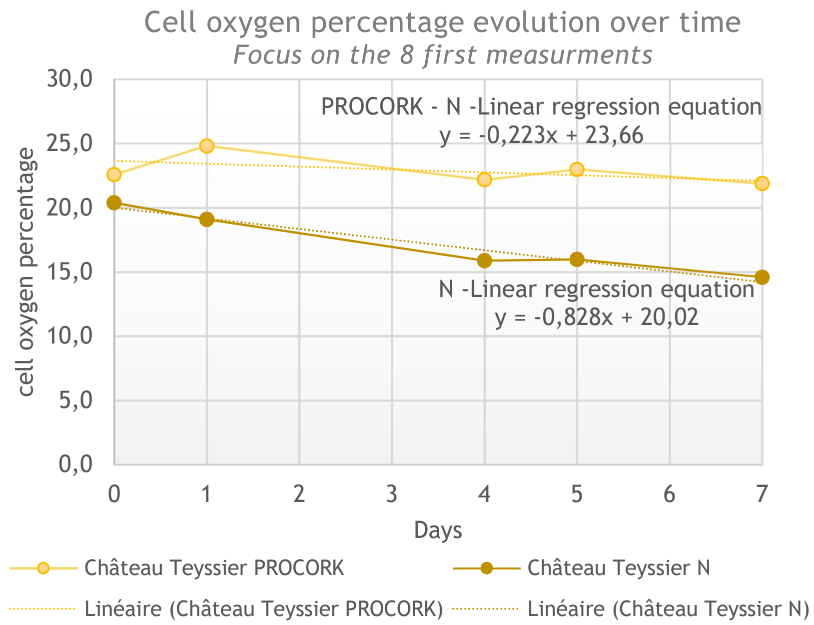
Sample	Days							
	0	1	4	5	7	11	14	21
Château Teyssier PROCORK	22,6%	24,8%	22,2%	23,0%	21,9%	21,1%	20,9%	19,7%
Château Teyssier N	20,4%	19,1%	15,9%	16,0%	14,6%	13,1%	13,7%	8,9%

The graphs below show the evolution with time of oxygen level in the measuring cell placed above the N bottle and the PROCORK one.



This graph clearly indicates the rate of evolution is higher in the N bottle compared to the PROCORK one. After 21 days, the oxygen percentage in the N bottle cell decreased to 8,9% whereas it was still of 19,7% in the PROCORK bottle cell.

To estimate the approximate OTR values of the two bottles, cells volumes and oxygen depletion rate have been used. Oxygen depletion rate has been estimated using linear regression modelling of the curve. Only the initial measurement points have been used for linear regressions. Indeed, with time the decrease in the oxygen level of the cell leads to a slight decrease of the driving force. Considering only the first 8 days would give a more robust estimation of the oxygen depletion rate.

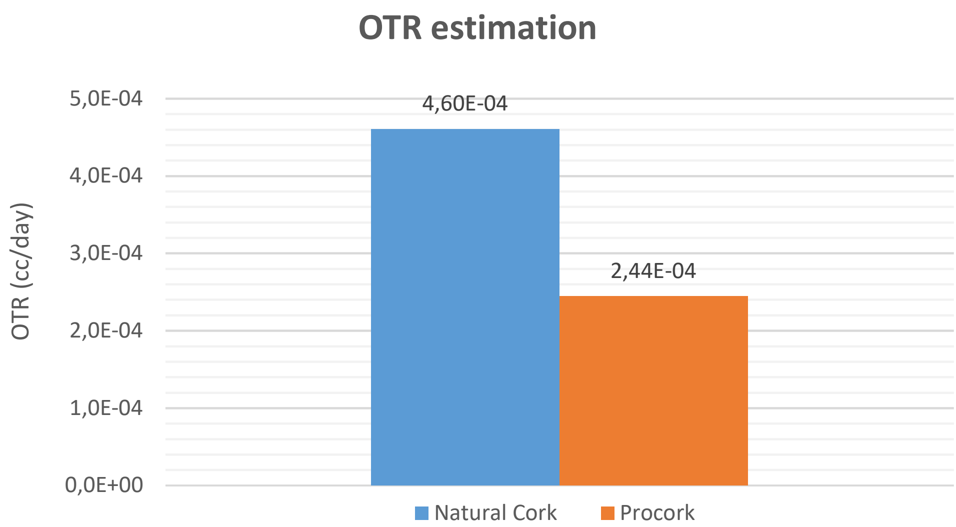


This oxygen depletion rate and the free volume of the measuring cell have been used to estimate the approximate OTR of the two bottles, corresponding to the volume of oxygen drawn into the bottles during 24 hours. The following formula has been used for such calculation:

$$OTR = \frac{\text{Cell volume x | linear regression slope |}}{100}$$

Sample	Absolute value of linear regression slope	Volume (cc)	OTR (cc/day)
Chateau Teyssier PROCORK	0,223	0,109556256	$2{,}44.10^{-4}$
Chateau Teyssier N	0,828	0,055608887	$4{,}60.10^{-4}$

The approximate OTR calculated from those values are presented in the graph below.



Those results show that the OTR of the N bottle (4,60.10^{-4} cc/day) is 1,9 times higher than the one of the PROCORK bottle (2,44.10^{-4} cc/day). This confirms the efficacy of the Procork membrane in controlling the level of oxygen entering in the wine bottles.

4.2 Molecular analysis results

4.2.1 Volatile organic compounds composition comparison

GC-TofMS analyses have been performed on the samples collected on the two wine bottles. The table on next page presents the main results of the analyses by GC-TofMS (identification and quantification of the volatile organic compounds present). Compounds present in quantities greater than their theoretical olfactory threshold (OTV) or in notable concentrations as well as totals by chemical families are summarized here. Full results are provided in ANNEX 1.

A comparison of the measured concentrations with the olfactory thresholds of the compounds (OTV) (if available) is proposed. This theoretical OTV corresponds to the mass of compound that can just be perceived when evaporated in a m3 of neutral air. An order of the number of times by which the measured concentration is greater than the theoretical olfactory threshold (OTV) is indicated. The colour coding below helps to understand the potential participation of the compound to the overall product odour.

COLOUR CODE:

<1 x Theoretical olfactory threshold (OTV)
1-10 x Theoretical olfactory threshold (OTV)
10-50 x Theoretical olfactory threshold (OTV)
50-100 x Theoretical olfactory threshold (OTV)
100-1000 x Theoretical olfactory threshold (OTV)
>1000 x Theoretical olfactory threshold (OTV)

GC-TOFMS MAIN RESULTS

Compound	CAS No.	Concentration (ug/m3) N bottle	Concentration (ug/m3) PROCORK bottle	OTV available?
Alcohols				
2-Propanol, 2-methyl-	75-65-0	**0,0**	9,2	yes
1-Propanol	71-23-8	**1 543,6**	**1 118,4**	yes
1-Propanol, 2-methyl-	78-83-1	**5 327,2**	**5 525,3**	yes
1-Butanol	71-36-3	113,5	**124,3**	yes
1-Butanol, 3-methyl-	123-51-3	**7 279,2**	**9 818,0**	yes
1-Butanol, 2-methyl-	137-32-6	**3 656,2**	**3 787,8**	yes
1-Pentanol	71-41-0	**0,0**	0,9	yes
1-Hexanol	111-27-3	**124,6**	**125,9**	yes
Phenylethyl Alcohol	60-12-8	**0,0**	52,5	no
	Total Alcohols	**18103,3**	**20577,3**	
Aldehydes				
Propanal, 2-methyl-	78-84-2	**66,1**	**18,5**	yes
Methacrolein	78-85-3	**172,1**	**76,3**	yes
Butanal, 3-methyl-	590-86-3	**1 005,6**	**602,5**	yes
2-Butenal, 2-methyl-, (E)-	497-03-0	79,6	33,0	no
	Total Aldehydes	**1379,4**	**740,3**	
Aliphatic Hydrocarbons				
	Total Aliphatic Hydrocarbons	**29,8**	**15,0**	
Amines				
Cyclobutylamine	2516-34-9	40,9	**0,0**	no
Methylamine	74-89-5	1,7	**0,0**	yes
	Total Amines	**42,6**	**0,0**	
Aromatic Alcohol				
Phenol	108-95-2	**0,0**	8,5	yes
	Total Aromatic Alcohol	**0,0**	**8,5**	
Aromatic compounds				
Ethylbenzene	100-41-4	1,9	11,0	yes
p-Xylene	106-42-3	4,3	12,5	yes
	Total Aromatic compounds	**7,4**	**27,3**	
Esters				
Ethyl Acetate	141-78-6	**8 503,1**	**8 425,5**	yes
Propanoic acid, ethyl ester	105-37-3	**168,5**	**152,0**	yes
Propanoic acid, 2-methyl-, ethyl ester	97-62-1	**397,4**	**291,9**	yes
Isobutyl acetate	110-19-0	**1 041,4**	**83,1**	yes
Diethyl carbonate	105-58-8	**0,0**	2,3	no
2-Propen-1-ol, 2-methyl-, acetate	820-71-3	**0,0**	4,3	no
Butanoic acid, ethyl ester	105-54-4	**191,0**	**146,1**	yes
Acetic acid, butyl ester	123-86-4	19,6	**0,0**	yes
Propanoic acid, 2-hydroxy-, ethyl ester, (S)-	687-47-8	934,0	900,5	no
Butanoic acid, 3-methyl-, ethyl ester	108-64-5	**133,8**	**94,3**	yes
1-Butanol, 3-methyl-, acetate	123-92-2	**1 692,9**	**312,1**	yes
1-Butanol, 2-methyl-, acetate	624-41-9	**1 228,1**	62,0	yes
Hexanoic acid, ethyl ester	123-66-0	502,5	382,3	no
Octanoic acid, ethyl ester	106-32-1	**169,2**	**226,1**	yes
Decanoic acid, ethyl ester	110-38-3	**0,0**	32,1	yes
	Total Esters	**15517,7**	**11506,6**	
Ethers				
	Total Ethers	**69,2**	**72,5**	
Furans				
	Total Furans	**69,2**	**89,8**	
Ketones				
	Total Ketones	**2,0**	**3,2**	
Oxygen-containing compounds				
	Total Oxygen-containing compounds	**15,2**	**58,7**	
Sulfur-containing compounds				
Thiophene, 3-methyl-	616-44-4	23,1	**0,0**	no
Diethyl disulfide	110-81-6	**17,3**	**0,0**	yes
	Total Sulfur-containing compounds	**40,4**	**0,0**	
Terpenes				
	Total Terpenes	**0,0**	**6,0**	
	Total COV	**35276,3**	**33105,4**	

The concentrations in bold and red exceed the odour threshold value (OTV)

The concentrations in bold and green don´t exceed 0.1 ug/m3

Chemical inertness of the Procork Membrane

The results of the GC-TofMS analyses performed show that no additional compounds related to the membrane composition were detected in the Procork bottle compared to the natural one. It confirms the absence of molecules released by the Procork membrane into the wine. This study thus demonstrated the chemical inertness of the Procork membrane even after eleven years of storage.

Impact of Procork Membrane on wine organic volatile composition

In total 64 chemical compounds have been identified by GC-TofMS. Some of them are present only in one of the bottles. Some others are present in both bottles but in different concentrations.
The main chemical families represented are: alcohols, esters and aldehydes. The total COV concentration is higher in N bottle (35 276, 3 µg/m3) than in PROCORK bottle (33 105,4 µg/m3).

Alcohols

The PROCORK sample contains higher quantities of fusel alcohols (also called higher alcohols) (20 577,3 µg/m^3) than the N bottle (18 103, 3 µg/m^3). Except for 1-Propanol concentration which is higher in N bottle than in PROCORK bottle, the concentration of those complex alcohols (1-propanol, 2-methyl-1-propanol, 3-methyl-1-butanol, ...) is higher in the PROCORK bottle.
Particularly the concentrations of 3-methyl-butanol (isoamyl alcohol) and 2-methyl butanol (active amyl alcohol) are higher in the PROCORK sample. Those compounds are known for bringing respectively cheese/balsamic and roasted/onion/fruity notes and for influencing the aromatic complexity of a wine.

For both samples, the concentrations of 1-Propanol (Bouquet/Ripe fruity odour), 2-methyl-1-Propanol (Solvent like odour), 3-methyl-butanol (cheese/balsamic notes) and 2-methyl butanol (roasted/ onion/fruity notes) are above the theoretical OTV.

Three alcohols have been detected only in the PROCORK sample: 2-methyl-2-propanol (Camphor-like odour; 9,2 µg/m^3), 1-Pentanol (Fresh/Alcohol character; 0,9 µg/m^3) and Phenylethyl Alcohol (Rose-like notes; 52,5 µg/m^3).

Aldehydes

The PROCORK sample contains much lower quantities of aldehydes (740,3 µg/m3) than the N bottle (1379,4µg/m3). The three aldehydes present in higher concentrations are: Isobutyraldehyde (2-methyl propanal (fruity/pungent)), Isovaleraldehyde (3-methyl butanal (Fruity/Rancid/Sour)) and Methacrolein (Floral)). For those three compounds the concentrations measured are above the theoretical OTV in both samples.

Esters

Esters concentrations are most of the time higher in N bottle than in PROCORK bottle. Esters can contribute positively to the aroma of the wine bringing, at low concentrations, fruity and floral character. However, present at too high concentrations they can mask the aroma complexity of the wine. High concentrations may thus negatively impact the wine. Both ethyl esters and acetate esters have been identified. The concentrations of the following esters are above their theoretical OTV values: Ethyl acetate, Ethylpropanoate, Methylethylpropanoate, Isobutyl acetate, Ethylbutanoate, Methylethylbutanoate and 3-methyl-butylacetate, 2-methyl-butylacetate, Ethyloctanoate.

Ethyl acetate, a typical oxidation marker, has been found in both samples. However, its concentration is higher in N bottle (8 503,1 µg/m3) than in PROCORK bottle (8 425,5 µg/m3). This compound has a sweet and fruity smell at low concentrations but at higher concentrations it brings solvent and nail polish remover unwanted notes.

Aromatic compounds

Concentrations of aromatic compounds (ethylbenzene, p-xylene, 1,3-dimethylbenzene) are 3 to 5 times higher in the PROCORK sample compared to N sample.

Sulphur and Amine compounds

One of the major differences between the two samples is related to the presence of amine and Sulphur compounds only in the natural cork (N) sample. Indeed, biogenic amines (cyclobutylamine 40,9 µg/m3, methylamine 1,7µg/m3) and volatile Sulphur compounds (3-methylthiophene (23,1µg/m3 and diethyl disulfide 17,3 µg/m3) have been identified only in this N sample.

Those type of compounds generally bring unpleasant aromas to wine: Methylamine is known for bringing Pungent/Fishy/Ammonia odour; 3-methyl-thiophene brings Fatty/Winey character whereas Diethyl disulfide is responsible for strong onion/burnt rubber notes.

4.2.2 Brett markers analysis

Ethyl phenols can have a negative effect on wine quality when present in excessive levels, bringing unpleasant animals/horse/mouse/barnyards character to the wine. They are related to the presence of contaminating *Brettanomyces* yeasts. To confirm whether the “Brett” character mentioned by the Master of Wine was related to the presence of these ethyl phenols, targeted molecular analyses have been performed on the liquid wine contained in both bottles.

The table below presents results of the targeted GC-TofMS analyses performed to identify the common Brett markers.

		Concentration (ug/m3)		
Compound	CAS No.	N bottle	PROCORK bottle	OTV available?
4-Ethylphenol	123-07-9	-	-	no
4-Ethylguaiacol	2785-89-9	-	-	no
4-Ethylcatechol	1124-39-6	-	-	no

(*) The concentration of methyl alcohol, acetaldehyde, carbon sulfide and carbon disulfide cannot be determined accurately
The concentrations in bold and red exceed the odour threshold value (OTV)

The results indicate that none of the three Brett markers targeted (4-Ethylphenol (4-EP), 4-Ethylguaiacol (4-EG) and 4-Ethylcatechol (4-EC)) have been identified neither in the N bottle nor in the PROCORK one.

This mouse/animal character could thus maybe be more related to the presence of amine and Sulphur compounds mentioned above.

4.2.3 Results interpretations

The two bottles present quite different chemical profiles. The different profiles are the result of different wine evolution processes in the two bottles. The N bottle which had an oxygen transfer rate (OTR) 1,9 times higher than the PROCORK bottle presented higher concentrations of esters, aldehydes, sulphur and amine compounds. It is possible that those two latter types of compounds have been generated by microbial activity stimulated by the higher rate of oxygen ingress. The PROCORK bottle with lower oxygen supply had higher quantities of complex alcohols and aromatic compounds and lower quantities of esters and aldehydes.

Peter SCUDAMORE-SMITH, Master of Wine, in 2019 made the following tasting notes on the Teyssier 2008:

"2008 Bordeaux/ natural cork: aged, flat, bretty, palate extracted, dried out, past any drinking window, Brett more obvious.
2008 Bordeaux/ ProCork: fresher and brighter nose, molasses fruit/oak development, more fruit volume, sweeter palate.

COMPARISON…The oxidative regime of natural cork has emphasized brett, lessened freshness, accelerated ageing and palate dryness, now a poor wine; ProCork has held nose freshness and muted the brett, allowed ageing without oxidation, kept the wine fresh and the palate able to display aged fruit/tannin complexity."

A possible correlation between the analytical results and some of the sensory descriptions made by the Master of Wine can be tentatively proposed:

- The "sweeter palate" and "more fruit volume" of the PROCORK bottle may be related to the presence of higher quantities of fusel alcohols,

- The "molasses fruit/oak development" and "aged fruit/tannin complexity" of the PROCORK bottle may be related to the presence of higher quantities of aromatic compounds,

- The "fresher and brighter nose" character described may be linked to the lower quantities of aldehydes present in the PROCORK bottle. Aldehydes are generally known to make the wine "flatter" and less fruity,

- The Brett or mousiness character of the natural cork bottle may be related to the presence of the sulphur and amine compounds identified. The direct liquid injection molecular analysis confirmed the absence of 4-EP, 4-EC and 4-EG in the wine. The mousiness character of the N bottle would thus not be related to these Brettanomyces markers but could be related instead to the presence of the sulphur and amine compounds. It is known that mousiness can also be related to the presence of amine compounds produced by lactic bacteria particularly lactobacilli.

5 Conclusion

The Oxygen Transfer Rate (OTR) on two bottles of the same wine (a 2008 Saint-Emilion Grand cru from Chateau Teyssier), one closed with a cork coated with the Procork membrane, the other closed with a natural cork (N), has been estimated using an innovative technique. The values obtained confirmed the ProCork bottle had a lower OTR than the N bottle (1,9 times lower). This highlights the efficacy of the Procork membrane in controlling the level of oxygen entering the wine bottles.

Molecular analyses on the same two bottles have been performed by GC-TofMS (using both headspace extraction and direct liquid injection). The objective of the study was to compare the chemical composition of both wines and see if any correlation could be made with the sensory profile of the wines established by the Master of Wine Peter Scudamore-Smith. After tasting, he declared: "The oxidative regime of natural cork has emphasized Brett, lessened freshness, accelerated ageing and palate dryness, now a poor wine; ProCork has held nose freshness and muted the Brett, allowed ageing without oxidation, kept the wine fresh and the palate able to display aged fruit/tannin complexity." A possible correlation has been tentatively proposed for further investigation.

Analyses performed after headspace extraction showed that no additional chemical compounds are released from the membrane into the wine. It thus confirmed the chemical inertness of the Procork membrane towards this red wine, even after ten years of storage. This study also evidenced the different chemical profile of the Chateau Teyssier 2008 bottle closed with natural corks compared to the one closed with Procork technology. This difference may be related to higher oxygen ingress into the natural cork bottle as demonstrated with OTR values estimations. The higher oxygen supply in the natural cork bottle could lead to more oxidation and also activation of bacteria and yeasts present in the wine. The microbial processes could participate in the formation of amine and sulphur compounds, potentially responsible for the "animal/mousiness" odours and flavours described by the taster as "Brett".

Annex 1: Detailed GC-TofMS results

Compound	CAS No.	Concentration (ug/m3) N bottle	Concentration (ug/m3) PROCORK bottle	OTV available?
Alcohols				
2-Propanol, 2-methyl-	75-65-0	0,0	9,2	yes
1-Propanol	71-23-8	1 543,6	1 118,4	yes
2-Buten-1-ol, 3-methyl-	556-82-1	2,7	2,5	no
1-Propanol, 2-methyl-	78-83-1	5 327,2	5 525,3	yes
1-Butanol	71-36-3	113,5	124,3	yes
1-Butanol, 3-methyl-	123-51-3	7 279,2	9 818,0	yes
1-Butanol, 2-methyl-	137-32-6	3 656,2	3 787,8	yes
3-Pentyn-1-ol	10229-10-4	51,5	7,9	no
1-Pentanol	71-41-0	0,0	0,9	yes
1-Pentanol, 4-methyl-	626-89-1	4,8	4,7	no
1-Hexanol	111-27-3	124,6	125,9	yes
Phenylethyl Alcohol	60-12-8	0,0	52,5	no
	Total Alcohols	**18103,3**	**20577,3**	
Aldehydes				
Propanal, 2-methyl-	78-84-2	66,1	18,5	yes
Methacrolein	78-85-3	172,1	76,3	yes
Butanal, 3-methyl-	590-86-3	1 005,6	602,5	yes
Butanal, 2-methyl-	96-17-3	48,5	5,5	no
2-Butenal, 2-methyl-, (E)-	497-03-0	79,6	33,0	no
2-Butenal, 3-methyl-	107-86-8	7,5	4,5	no
	Total Aldehydes	**1379,4**	**740,3**	
Aliphatic Hydrocarbons				
Pentane, 3-ethyl-	617-78-7	1,0	1,0	yes
Hexadecane	544-76-3	28,9	14,0	yes
	Total Aliphatic Hydrocarbons	**29,8**	**15,0**	
Amines				
Cyclobutylamine	2516-34-9	40,9	0,0	no
Methylamine	74-89-5	1,7	0,0	yes
	Total Amines	**42,6**	**0,0**	
Aromatic Alcohol				
Phenol	108-95-2	0,0	8,5	yes
	Total Aromatic Alcohol	**0,0**	**8,5**	
Aromatic compounds				
Ethylbenzene	100-41-4	1,9	11,0	yes
p-Xylene	106-42-3	4,3	12,5	yes
Benzene, 1,3-dimethyl-	108-38-3	1,2	3,8	yes
	Total Aromatic compounds	**7,4**	**27,3**	
Esters				
Acetic acid, methyl ester	79-20-9	158,1	124,7	yes
Ethyl Acetate	141-78-6	8 503,1	8 425,5	yes
Propanoic acid, ethyl ester	105-37-3	168,5	152,0	yes
n-Propyl acetate	109-60-4	110,0	15,0	yes
Propanoic acid, 2-methyl-, ethyl ester	97-62-1	397,4	291,9	yes
Isobutyl acetate	110-19-0	1 041,4	83,1	yes
Diethyl carbonate	105-58-8	0,0	2,3	no
2-Propen-1-ol, 2-methyl-, acetate	820-71-3	0,0	4,3	no
1-Butanol, 3-methyl-, formate	110-45-2	0,7	8,6	no
Butanoic acid, ethyl ester	105-54-4	191,0	146,1	yes
Acetic acid, butyl ester	123-86-4	19,6	0,0	yes
Propanoic acid, 2-hydroxy-, ethyl ester, (S)-	687-47-8	934,0	900,5	no
Butanoic acid, 2-methyl-, ethyl ester	7452-79-1	66,7	43,9	no
Butanoic acid, 3-methyl-, ethyl ester	108-64-5	133,8	94,3	yes
Propanoic acid, 2-methylpropyl ester	540-42-1	1,1	0,0	yes
1-Butanol, 3-methyl-, acetate	123-92-2	1 692,9	312,1	yes
1-Butanol, 2-methyl-, acetate	624-41-9	1 228,1	62,0	yes
Hexanoic acid, ethyl ester	123-66-0	502,5	382,3	no
Octanoic acid, ethyl ester	106-32-1	169,2	226,1	yes
Butanedioic acid, diethyl ester	123-25-1	107,8	188,5	no
Decanoic acid, ethyl ester	110-38-3	0,0	32,1	yes
1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	84-69-5	91,6	11,4	no

	Total Esters	15517,7	11506,6	
Ethers				
Oxetane, 3-(1-methylethyl)-	10317-17-6	2,6	0,0	no
1,3-Dioxolane	646-06-0	0,9	0,0	yes
1,3-Dioxolane, 2,4,5-trimethyl-	3299-32-9	34,6	39,5	no
Pentane, 1-ethoxy-	17952-11-3	8,3	10,1	no
Propane, 2-ethoxy-	625-54-7	22,9	22,9	no
	Total Ethers	69,2	72,5	
Furans				
Furan, 2-methyl-	534-22-5	9,5	14,4	no
Furan, tetrahydro-3-methyl-	13423-15-9	12,1	31,3	no
Furan, 2,2'-[oxybis(methylene)]bis-	4437-22-3	47,6	44,1	no
	Total Furans	69,2	89,8	
Ketones				
2-Butanone, 3-methyl-	563-80-4	2,0	1,7	yes
2-Butanone	78-93-3	0,0	1,6	yes
	Total Ketones	2,0	3,2	
Oxygen-containing compounds				
Propanoic acid, 2-oxo-, ethyl ester	617-35-6	15,2	25,4	no
(+)-Dibenzoyl-L-tartaric acid anhydride	64339-95-3	0,0	20,9	no
Ethanone, 2-(formyloxy)-1-phenyl-	55153-12-3	0,0	12,4	no
	Total Oxygen-containing compounds	15,2	58,7	
Sulfur-containing compounds				
Thiophene, 3-methyl-	616-44-4	23,1	0,0	no
Diethyl disulfide	110-81-6	**17,3**	0,0	yes
	Total Sulfur-containing compounds	40,4	0,0	
Terpenes				
1,3-Cyclopentadiene, 5-(1-methylethylidene)-	2175-91-9	0,0	6,0	no
	Total Terpenes	0,0	6,0	
	Total COV	**35276,3**	**33105,4**	

(*) The concentration of this compound cannot be determined accurately

The concentrations in bold and red exceed the odour threshold value (OTV)

The concentrations in bold and green don´t exceed 0.1 ug/m3

****** too much quantity**

Colour code:

<1 x theorical olfactory threshold

1-10 x theorical olfactory threshold

10-50 x theorical olfactory threshold

50-100 x theorical olfactory threshold

100-1000 x theorical olfactory threshold

>1000 x theorical olfactory threshold

Annex 2: Chromatograms