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Monitoring the homemade fermentation of readymade malt extract using the SCiO NIR sensor: A convergence of technology and tradition

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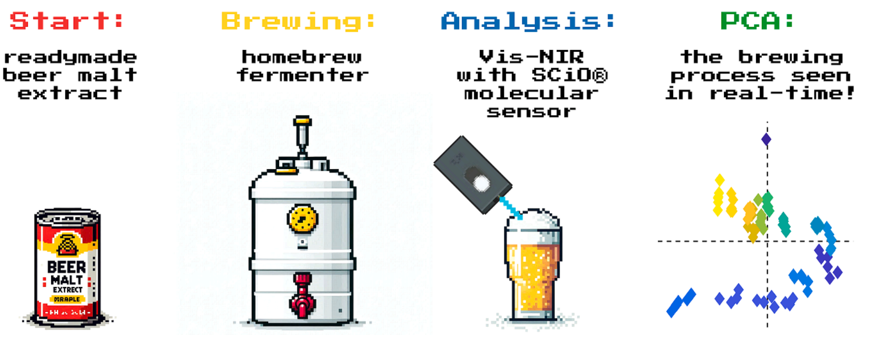
HIGHLIGHTS

- The study examines NIR monitoring of homemade beer fermentation with SCiO sensor.
- The do-it-yourself ethos extends to brewing with portable/handheld NIR instruments.
- Simple data analysis (PCA) reveals brewing stage progression and temperature trends.
- Robust and thoughtful experimental procedures and preprocessing are fundamental.
- Limitations as homebrewing conditions and scattering effects are discussed.

GRAPHICAL ABSTRACT



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ABSTRACT

Miniaturized near-infrared (NIR) instruments are launched on the market to satisfy the need of both researchers and consumers for quick ways of analysing stuff, especially in the food field. Their portability and ease of operation are at the centre of the "do-it-yourself" idea behind providing virtually anyone with the ability of making analytical measurements on their own. In this study, we highlighted the convergence of technology and tradition in two seemingly disparate domains: spectroscopy and homebrewing. Homebrewing is in fact a leisure activity which conceptually shares the do-it-yourself approach: the consumer becomes the producer of his/her own beer.

Hence, in our study, we investigated the analytical possibilities provided by a handheld NIR spectrometer to monitor the homemade fermentation process of a commercial malt extract, over the course of one week. The spectroscopic data, acquired using the SCiO sensor (Consumer Physics), were analysed via Principal Component Analysis (PCA) to investigate temporal trends and relationships with brewing parameters. Our findings reveal that discernible trends, reflective of brewing stage progression and temperature variations, can be captured and unveiled with simple data analysis approaches. At the same time, the detection of scattering effects that can be attributed to bubble formation on the spectrometer's acquisition window confirm the need for robust and reasoned experimental procedures, but also for proper data preprocessing methods.

This rather simple and basic analytical approach could provide the homebrewer the possibility to qualitatively monitor the advancement of the brewing process.

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1. Introduction

What do miniaturized near-infrared (NIR) spectrometers and beer homebrewing have in common? From a conceptual point of view, the "do-it-yourself" motto. Let's break this claim down.

New miniaturized spectroscopic instruments [1,2] are launched on the market for satisfying the need of both researchers and consumers for quick ways for analysing stuff, especially in the food field: these small instruments are frequently operated via smartphone apps, which also often include pre-trained models to quantify specific properties (e.g., fat or protein content). Therefore, the user can, to different extents, employ these instruments to perform measurements and rather easily build tailored calibration models. In a parallel manner, homebrewing has become a very widespread hobby [3], with a wide range of equipment available on the market, allowing people to simply ferment readymade malt extracts, but also to brew more complex recipes, if they were inclined to do so. Standard recipes provided by malt extract producers are generally "optimized": few clear actions must be taken, and few parameters must be controlled to obtain a fairly decent beer.

In our study, we investigated the overlap between these two conceptually connected worlds. The fermentation of a commercial readymade malt extract was followed for one week by means of NIR spectroscopy, using the portable handheld SCiO sensor (by Consumer Physics) equipped with its accessory for liquid measurements.

Spectroscopy in general [4], and NIR spectroscopy in particular, has been used to follow the beer fermentation process [5–9] for monitoring different brewing parameters (also in real-time [10]), such as: ethanol content by volume (or "alcohol by volume", ABV) [5,11–13], soluble solid content [6,7], total cell count [5], specific gravity [5], fermentable sugar content [11,14], nitrogenous compounds [5,15], and pH [6]. Regarding the use of portable/handheld NIR instruments [1,16–18] for the analysis of beer, some examples can be found in literature. This type of instruments has been used for monitoring beer quality parameters, for instance by da Costa Fulgêncio *et al.* who used a MicroNIR (Viavi) instrument to develop an ethanol content calibration model [19] and a screening method for the rapid detection of diethylene glycol contamination [20]. Concerning the evaluation of beer quality during fermentation, Giovenzana *et al.* developed a portable handmade NIR instrument for rapid assessment of the process [21].

To the best of the authors' knowledge, the study most similar to ours is the one published in 2021 by França *et al.* [7], even if the latter is characterized by higher complexity. Indeed, França *et al.* followed the beer fermentation process using the tools of multivariate statistics process control with the aim of setting up a multivariate control chart based on NIR spectra (800–2500 nm) to predict the soluble solid content of 8 beer batches [7]. The two main differences between the present study and the one by França *et al.* concern the instrument used for the NIR acquisition and the working spectral range modelled with the tools of chemometrics. Of course, these two aspects are related. In our case a handheld instrument operating in the range 760–1070 nm was used, while in the other study a benchtop Perkin Elmer NIR instrument was employed, but the selected working spectral range was 1000–1840 nm and 2170–2399 nm (the central part of the experimental wavelengths range was removed to exclude the saturated O–H stretching signal around 1900 nm). A very interesting meeting point between the two studies is that the fermentation was in both cases conducted under "normal craft beer conditions using the standard machinery that homebrewers can acquire in any specialised shop" [7].

Our study was conducted at home, where we followed the one-week fermentation of a commercial readymade malt extract using a portable, battery powered, handheld NIR instrument. A small amount of brewing liquid was taken once a day from the fermentation tank, and 30 spectra were acquired each time. Exploratory analysis performed with Principal Component Analysis (PCA) revealed interesting trends that could be globally related to the evolution in time of the homebrewing process and to the recorded temperature of the brewing liquid, both of which might be related to the different stages of maturation of the beer during production. Also, the PCA inspection of the individual time points revealed an interesting trend that could be linked to the formation of bubbles on the acquisition window of the instrument, meaning that the scattering effects on the spectral data caused by the bubbles could be clearly seen and inspected. Due to the simplicity of the analytical approach and experimental setup, we believe that our study and its results could be easily used by curious homebrewers who might want to have a "real time" idea of its (qualitative) evolution in a smart way.

2. Materials and methods

2.1. Experimental setup and liquid sampling

The home brewing experiment was carried out using a commercial plastic fermentation tank equipped with a bubbler (Fig. 1a), to prevent contamination and protect the beer during fermentation, while at the same time highlighting the formation of carbon dioxide. The tank was placed in the cellar of the house to reduce potential thermal shocks during the day, since the experiment was performed during the Summer of 2020. The fermentation tank was initially washed with cold water and a solution of sodium hypochlorite, which was used to repeatedly rinse the inner walls of the tank, but also the tap.

Small amounts of brewing liquid were taken from the tap of the fermentation tank, to avoid contaminations that could ruin the final product. All liquid samples resulted slightly turbid, probably because of the tap's position near the bottom of the fermentation tank, where a solid deposit is present. Knowing this, precautions were taken to avoid moving the tank, and each liquid withdrawal was executed slowly to minimize disturbance to both the liquid inside the tank and the solid deposit at its bottom. The liquid was then placed into a clean kitchen glass (Fig. 1b), where the SCiO liquid reflector tool was then immerged. After calibration the SCiO sensor was placed into the tool, and the spectra were acquired.

The temperature of the liquid was measured immediately after withdrawal using an alcohol thermometer. The tank also had a thermal strip glued to it, which allowed us to quickly assess the general temperature conditions of the brewing process. It is worth noting that the entire experiment was designed to be conducted in the simplest possible manner, utilizing common objects readily available to any homebrewer.

2.2. Brewing broth preparation

The brewing broth was prepared following the standard procedure described by the producer of the readymade malt extract, which was the "Canadian Blonde" produced by Coopers (https://www.diybeer.com/us/, last accessed 28/03/2024). These commercial extracts and their preparation procedures ensure that at least a rather decent beer is obtained, provided that each step is correctly executed with care and sterilized tools (to avoid contaminations which may spoil the beer). Regarding this specific product, the producer describes the extract as such: "Crisp pale malt aromas with a hint of spicy hops, clean pale malt flavours and a light-bodied palate that finishes with obvious hop bitterness. Pale Straw colour." (https://www.diybeer.com/us/canadian-blonde-1–7 kg.html, last accessed 28/03/2024). An aspect worth of notice is that the malt extract is already hopped. No hops infusion was performed during the experiment. Starting from the malt extract can, the brewing broth preparation procedure consists of five main steps (adapted from: https://www.beer101.diybeer.com/canadian-blonde, last accessed 28/03/2024):

1. Remove the label and place the malt extract can in warm water for 10–15 min.
2. Open the malt extract can with a can opener, ensuring cutting end is clean.

3. Pour the malt extract into the fermentation tank, add 2 L of water, and stir.
4. Top up with hot or cold water to 23 L, targeting 21 °C.
5. Add the yeasts by sprinkling it over the top of the brew.

We also decided to add 1 kg of white sugar, to help starting the fermentation and hopefully make the beer a bit stronger than the original Coopers' design. The yeasts (supplied by the producer) were added right after acquiring the spectroscopic measurements of T0. The brewing broth temperature at T0 was 22 °C.

2.3. *NIR instrument: The SCiO*

The ultra-portable handheld SCiO molecular sensor (v1.2, Consumer Physics Inc., Tel Aviv, Israel) was employed due to its simplicity of use. The SCiO device can acquire signals in the 740–1070 nm spectral range with 10 cm^{-1} resolution, and a typical scan time of 2–5 s. Spectra collection and management was performed using the SCiO smartphone app (The Lab, version 1.3.1.81). SCiO's data management system is cloud-based: each acquired spectrum is sent via Bluetooth from the sensor to the smartphone app, and then uploaded and stored on the online Consumer Physics Cloud database. Instrumental calibration was performed before the first acquisition of each time point. To acquire measurements on the brew samples, the liquid reflector tool (also called "liquid accessory") for the SCiO sensor was used. It is a plastic container in which the instrument is placed, allowing it to interact with the sample to be analysed through a sealed acquisition window. The light emitted by the instrument interacts with the sample and is reflected by a surface located one centimetre away from the acquisition window. Thus, these measurements can be considered as a transflectance mode, with an optical path of 2 cm. The accessory can be seen in the experimental setup depicted in Fig. 1b.

2.4. *Experimental measurements and time*

The experimental measures were done during August 2020 twice a day for one week, one time in the morning and another time in the evening. The brewing time of one week was set following the standardized instructions indicated by the producer of the readymade malt extract (Section 2.2). A total of 14 time points were acquired, including the initial time point, marked as "T0". At each time point, 6 groups of acquisitions of 5 spectra each were recorded with the SCiO sensor, leading to 30 spectra for each time point.

Two exceptions to this scheme are present in the dataset. For time point T0 only one group of 5 spectra was scanned: at that point the yeasts had not been inoculated yet, and thus, the fermentation process had not started. Therefore, the spectra at T0 were rather straightforward to acquire since no CO_2 bubbles were forming on the SCiO acquisition window. Thus, these measurements correspond to the fermentation broth only containing the water, the malt extract, and the added sugar. The second exception concerns T2, for which twice as many spectra as for the other times were recorded. This is due to an operator's error occurred during the acquisition procedure, since the flashlight used to evaluate the brewing liquid turbidity and bubbles was still on and pointing directly to the liquid and the SCiO sensor. We decided to keep those acquisitions in the dataset to evaluate the possible disturbing effect of such an external light source.

Already from the first measurement session, we became aware that bubbles were forming on the acquisition window. Bubble formation could cause scattering effects which are detrimental to the spectral quality, so their presence was an important aspect to consider in the experimental procedure. The scanning time of SCiO allows to quickly acquire many spectra, which, in theory, would be more and more affected by the bubbles forming and becoming gradually larger (Fig. 2) on the acquisition window. In fact, during the very initial phases of the experiment interesting patterns were noticed with preliminary PCA analyses. These patterns pointed out that something was happening between subsequent acquisitions, i.e., that spectra acquired seconds apart were slightly different following the acquisition sequence (or, more simply, according to time). This effect was consistently found also at other time points, and our interpretation is that it is related to the formation of bubbles. To try to remove as many bubbles as possible, at least temporarily, and to mitigate this phenomenon the instrument was repeatedly moved and tilted between each set of 5 spectral acquisitions. Nevertheless, we noticed that small bubbles were still persistent, but this can be considered as a sort of common effect among all acquired spectra (except for those corresponding to T0).

2.5. *Data analysis*

In line with the spirit of simplicity of the work, also the data analysis was kept as simple as possible.

The spectral data were exported in csv format from the web interface of "The Lab" (SCiO's cloud-based system for spectra management and storage) and imported into MATLAB environment for preprocessing and exploratory analysis. For the analysis of the whole fermentation process (the "global" perspective discussed in Section 3.1) the spectra were averaged according to their acquisition group (5 spectra per group) to provide 6 representative averaged spectra for each time point (remember that T2 has an entire set of "additional" acquisitions, as

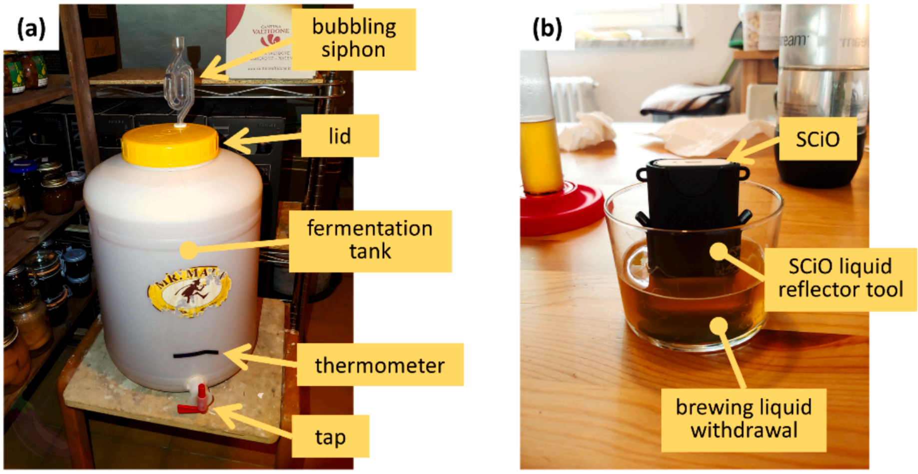

Fig. 1. The experimental setup: (a) the fermentation tank in which the brewing experiment was conducted; (b) the spectral acquisition setup (kitchen glass, SCiO liquid reflector tool and the SCiO instrument placed in it).

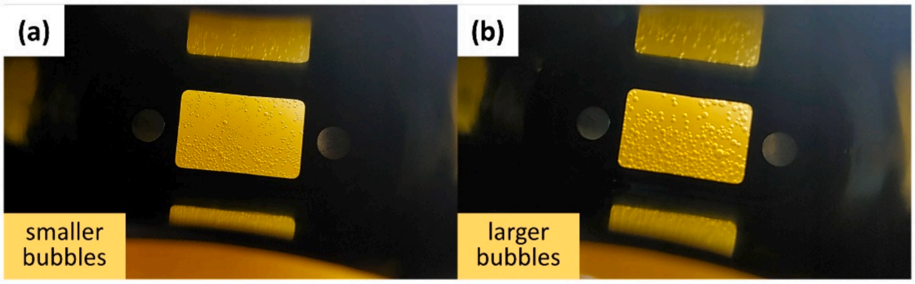

Fig. 2. Example of bubbles formation (at T5): picture of the acquisition window with smaller bubbles at the beginning (a) and at the end (b) of the acquisition of a group of 5 spectra at T5.

described and discussed in Section 2.4). Then, the spectra were preprocessed using standard normal variate (SNV, [22]) normalization followed by mean centering. The application of this sequence of preprocessing steps can be seen in Fig. 3. Regarding the focus on the individual time points to study the scattering effects due to the bubbles' formation, for all time point's individual PCA models no preprocessing was applied, not even mean centering.

Exploratory analysis was performed with principal component analysis (PCA, [23]), the exploratory cornerstone of chemometrics.

2.6. Software

Data analysis was carried out on MATLAB 2021a (Mathworks, Natick, MA, USA). Data preprocessing and PCA modelling were performed using the functions included in the PLS_Toolbox (version 9.0, Eigenvector Research Inc., Manson, WA, USA). In-house written routines were used to import, manage, and assess the raw data and organize the data analysis workflow. The smartphone app "The Lab" (version 1.2.1 for most of the experimental data acquisition; https://play.google.com/store/apps/details?id = com.consumerphysics.researcher or https://apps.apple.com/us/app/the-lab-dev-toolkit-for-scio/id965758603, last accessed 28/03/2024) used to control the SCiO sensor was installed on an Android phone. The acquired SCiO spectra were managed and downloaded from the web interface of "The Lab".

3. Results and discussion

During the week spent brewing and analysing the beer under development, some exploratory PCAs were carried out, to observe whether the SCiO was capturing interesting information about the brewing process evolution. Our expectation was that the spectra acquired at the different time points would be grouped together, and a time trend would have been discovered. These expectations were correct, and the related results are reported in Section 3.1. Regarding the formation of bubbles on the acquisition window (as described in Section 2.4), the detection and modelling of the bubbles-induced scattering effects on the spectra is reported and discussed in Section 3.2.

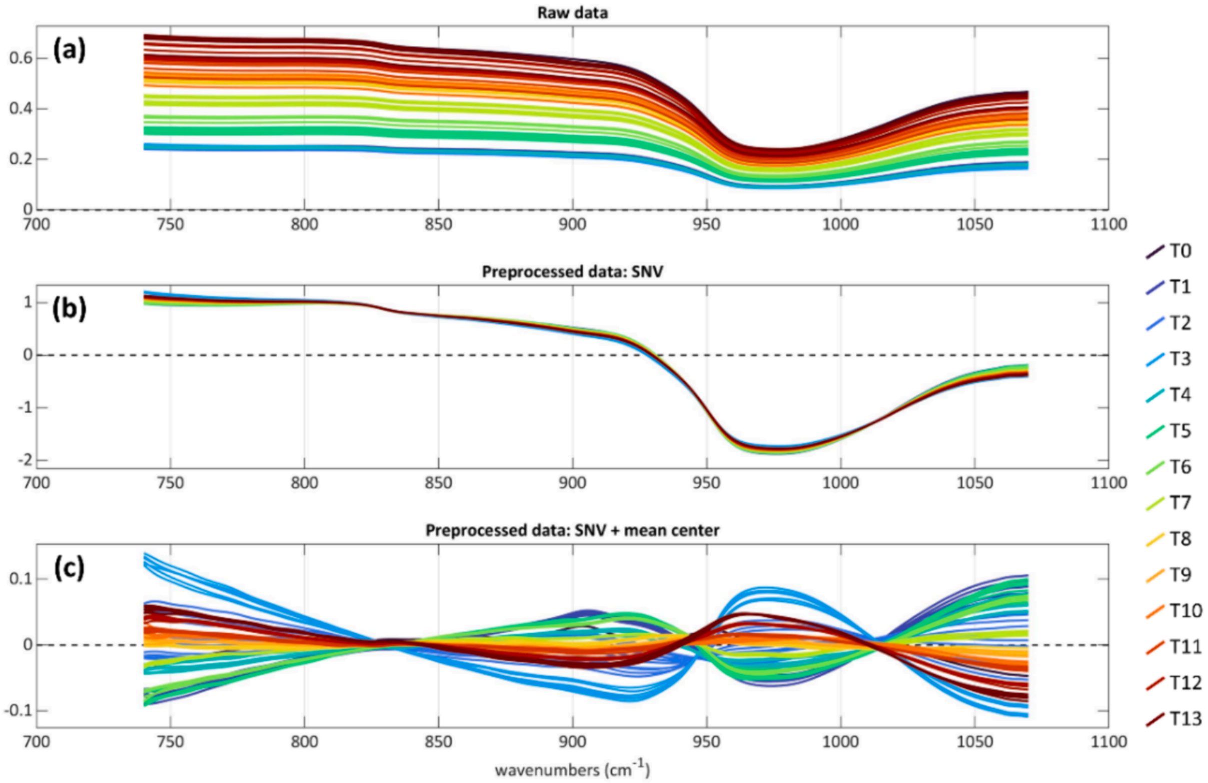

Fig. 3. The data: (a) raw data (no preprocessing), (b) data preprocessed with SNV, (c) data preprocessed with SNV and mean center. The spectra are colored according to the time.

3.1. The fermentation process, globally

Starting with the results about the whole fermentation process, the acquired spectral data were averaged in sets of 5 scans, i.e., 6 representative spectra for each time point (except T0 which only had one spectrum) were obtained. The rationale for acquiring these groups of 5 scans is based on the possible scattering effects due to bubbles formation, and it is discussed in Section 2.4 and then deepened in Section 3.2. The data were SNV-corrected and mean centered before PCA modelling.

Considering the evolution in time of the brewing process as described by PC1 and PC2 (Fig. 4b, combined explained variance = 99.42 %), a clear trajectory emerges. Starting from an isolated T0 at high PC2 scores values, a sudden shift brings the process to positive PC1 scores values (T1) and then to the lower part of the plot (T2-T4), at negative PC2 values. Thus, the evolution in time appears non-linear, and large movements along both PC1 and PC2 occur. In this perspective, T0 can be viewed as a “reference” time point, being far away from all other measurements and different by definition, as the fermentation was not yet started. We noted that already at T1 the fermentation process was active since the siphon on top of the tank was bubbling vivaciously. Twenty-one hours had passed between T0 and T1, with a temperature increment of about 3 °C. The additional replicates of T2 do not appear to be significantly different from the “correct” ones, so the error of pointing the flashlight directly at the sampled liquid and the SCiO sensor did not cause any noticeable effects on the spectra (group of samples in the bottom-central part of Fig. 4b). As for the evolution of the process toward the end point (T13), the main changes between time points occur along PC1, from right to left. It is important to consider that the experiment was not carried out for longer than one week (Section 2.4), as indicated by the producer of the readymade malt extract. A longer study would probably show further differences, potentially across more PCs, as more information would be collected: however, the authors wanted to be able to taste the beer, not only for personal enjoyment, but also to be able to propose a study in which the product would be genuinely good and consumable.

The interpretation of the results according to the signals is rather difficult since not many univocally assigned NIR bands are present within the SCiO’s spectral range. However, the different time points appear well grouped, suggesting that it could be possible to identify some stages of maturation of the beer.

Regarding the additional information about the temperature of the fermentation liquid (PCA scores colored accordingly in Fig. 4c), two main groups of time points can be identified. Their separation can be mainly ascribed to PC2, and these two groups correspond to the beginning of the fermentation characterized by higher temperatures (T2-T3), followed by a maturation phase in which the temperature seems to decrease (from T4 on) slightly but homogeneously. Once again, T0 appears to be different: in this case, this point corresponds to the lowest temperature, when the brewing broth was cooled down to room temperature. As opposed to T0, T2-T3 correspond to the maximum recorded temperature: this happened at the transition between days 1 and 2, after which the temperature became lower and more stable, in the range 23–25 °C. This initial spike can be linked to the yeast activity ramping up, and continuously changing the liquid’s composition.

Regarding the interpretation of the signals related to the time and temperature trends detected by PC1 vs PC2, some signals in particular stick out. It is interesting to note that no signals related to ethanol are present in the SCiO’s operative wavelengths range [24,25], but still the different time points describing the brewing process (during which ethanol is produced up to 4–5 % in volume) appear nicely grouped, drawing a clear trajectory.

One of the most influent signal is related to the water combination band at 960 nm ($2\nu_1 + \nu_3$, [13,24–26]), as it can be clearly noted in the negative direction of PC1 loadings (in blue in Fig. 4d). However, its

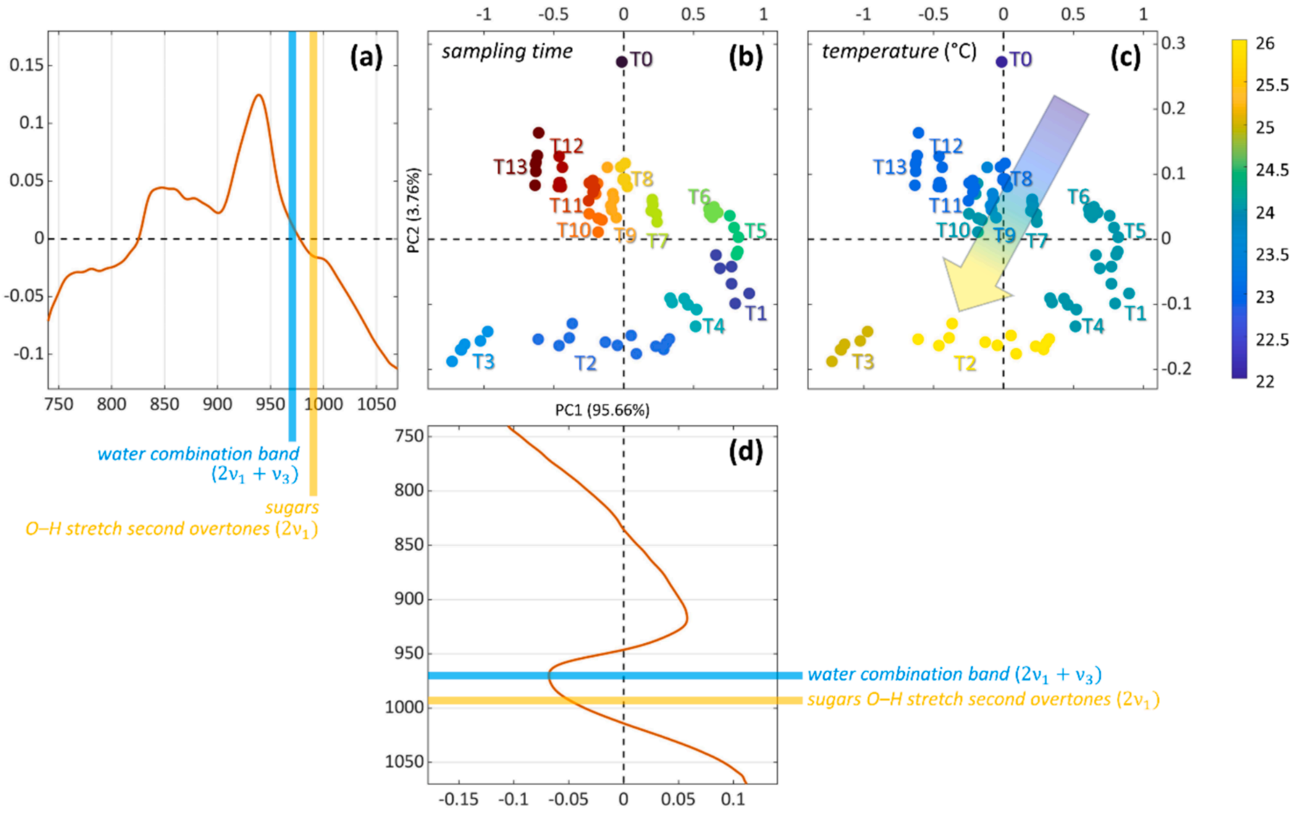

Fig. 4. The fermentation process, globally: PC1 vs PC2 scores plots (b-c) and the two PCs’ loadings plots (a and d). The central scores plot (b) is colored according to the time point, while the scores plot on the right (c) is colored according to the measured temperature of the analysed liquid sample. Some band assignments are also reported on the loadings plots (a and d).

interpretation is rather confusing: it seems like T1 is characterized by lower contributions from this water signal, which increases moving to T2 to become extreme at T3, to become lower again at T4-5, to gradually increase again up to T13. To complete the review of the water signals within the experimental range, the "small in-depth peak at 760 nm" related to the third overtone of OH stretching reported by Giovenzana *et al.* [21] could not be directly noticed, even if it could be covered by other larger variations in the loadings.

A lot of chemical changes are occurring during the brewing process, and the most influential signals, the water combination band and the large contribution of the wavelengths related to color (the first shades of red in the visible interval, 740–800 nm), are probably indirectly describing all these mutations in composition.

Other chemical compounds that could be expected to give rise to signals during the brewing process are the sugars, but since the origin of their associated NIR bands at around 990 nm can be ascribed to O–H stretching, just like water (neighbouring this signal with an intense band at about 960 nm), no clear evidence can be found from the inspected loadings (in orange in Fig. 4a,d). If the sugars' signals are present, they probably contribute little to the whole spectral signal.

Sharing the same OH functional group, the alcohols could give rise to contributions in the range 940–980 nm (2nd O–H stretching overtone), also very close to the contributions due to the methylene group (CH=CH, 3rd C–H stretching overtone), as reported by Workman [27]. The intense and rather narrow band in the PC2 loadings (Fig. 4a) at about 930 nm can probably be interpreted from this point of view, relating the signal both to the presence of alcohols being produced during the fermentation process and to the presence and growth of the yeasts. The methylene signals could indeed be related to the yeasts' presence, revealed by the absorption of their structural unsaturated fatty acids. The very general signal of the amines (2nd N–H stretching overtone, [27]) at around 1000 nm does not seem to show up in PC2 (Fig. 4a), but it could rather be contributing to the negative signal in PC1 (Fig. 4d). Also, the fact that the time points at positive PC2 scores are the latest ones seem to support this interpretation, as at the final stages of the fermentation ethanol (and other alcohols, [28]) has increased, together with the growth of the yeasts. For more information on the composition of yeasts like *Saccharomyces cerevisiae*, especially regarding the percentage of proteins, fats, α-amino nitrogen compounds and solids, we suggest the work by Tao *et al.* [29].

Martelo-Vidal *et al.* provide an exhaustive list of assignments for many compounds like lactic, acetic, tartaric, and malic acids (the first two being linked to spoilage of beer [30]), ethanol, glucose, and glycerol [25]. However, only tartaric acid would give rise to a signal within the SCiO interval (856 nm, [25]), but no evidence from literature relating this compound to the natural fermentation of beer could be found. Another interesting "indication from absence" regards the amine compounds: as reported by Barba *et al.* an absorption band around 1033 nm can be attributable to the stretching vibration of the –NH bond [31]: also in this case, the potential signal is probably covered by more intense neighbouring bands, so it could not be located in the loadings plots.

Since the SCiO can record signals belonging to the visible interval it was also checked whether by selecting the 740–800 nm wavelength range (which corresponds to "extreme" shades of red) any information connecting the brewing time/evolution and the color of the brewing liquid would have been found. However, no clear trend was detected, which suggests that the brewing liquid might undergo changes in its colored mixture of chemical compounds that cannot be interpreted or modelled based on the SCiO's "red wavelengths" alone.

3.2. *Focus on the individual time points*

Local time trends were detected by analysing the data before averaging out the individual spectral replicates. Fig. 5a depicts the PC1 scores of the time-point specific PCA models built with the replicates of each individual time point. Coloring of the figure corresponds to the PC1 scores value of each sample. For all PCA models no preprocessing was applied, not even mean centering (even though the scores would have looked the same, but vertically shifted). This was done to preserve the scattering effects, which are usually removed by applying SNV to the data. By doing so, we could directly inspect these effects, which were unexpectedly captured by PC1 (consistently describing high amounts of explained variance, 99.996 ± 0.008 %). As a further proof that the data structure captured by PC1 can be related to the scattering, when SNV is applied to the data prior to PCA modelling the descending pattern completely disappears, as reported in the Supplementary Materials (Fig. S1).

By inspecting the loadings (Fig. 5b) it can be clearly seen that for all models they all look basically the same. In all cases the loadings are completely positive (keep in mind that no mean centering was applied), and the wavelengths corresponding to flatter and less rich in signals areas also show the most positive loadings values, meaning that these areas are the most affected by scattering.

Regarding the pattern in the scores, as shown in Fig. 5a, from T5 on it can be noticed that the trend followed by each group of 5 replicates follows the same "descending" pattern. In some cases, the different groups of 5 spectra result more similar (T7, T9) and in other cases some groups are more different (T10, T13). The descending pattern can be explained by considering the refraction and reflection effects caused by the bubbles forming: smaller particles might deviate light to a larger extent and could be more numerous, whereas larger bubbles are likely fewer on the same window surface. Additionally, the score values of subsequent groups of replicates at individual time points appear to have increasing averages, which likely correspond to stronger scattering effects. This group-pattern is particularly clear at T5, T7, and T11. This drift also appears to be time-related: between each group of 5 replicates, the SCiO was shaken and moved to remove as many bubbles as possible from the acquisition window. It is possible that smaller bubbles were not fully removed from one group to the next, causing a "carry-over" effect. This could have led to the next group of acquisitions starting from a point where small bubbles were already present. Also, the latest groups of acquisitions appear more similar between each other than compared to the other groups, suggesting that a surface saturation effect might also develop.

Considering then the time points from T0 to T4 – not so unexpectedly – different patterns were found. At T0, as already mentioned, the fermentation process has not started yet, so no bubbles were forming (and during the spectra acquisition their absence was visually noticed), therefore no scattering effects possibly linked to the bubble formation are present. From T1 to T4 the fermentation process was in its initial stages, with higher temperatures and the yeasts' activity was probably at its highest. The scattering patterns within the same group of replicates can also be observed, but for unknown reasons, in some cases, the direction shows increasing score values, or the pattern is very weak. Once again, the additional replicates of T2 do not appear to be different from the "correct" ones, so the flashlight pointed at the liquid under examination did not cause any effect on the spectra.

All these considerations support the decision that was taken of acquiring more spectral replicates, but also to acquire more groups of replicates for each time point (1 time point = 5 representative spectra × 6 groups). Of course, the application of SNV to the data is fundamental for getting rid of the scattering effects, also avoiding wasting the first principal component of a PCA model. Therefore, the combination of reasoned experimental design and chemometrics preprocessing proved to be the right solution for studying the overall time evolution of the fermentation process. It is important to notice that the acquisition of these large numbers of spectra within a very short measurement time could be done thanks to the measurement speed of the SCiO sensor.

4. Conclusions

In our study we tried to apply our technical and statistical knowledge

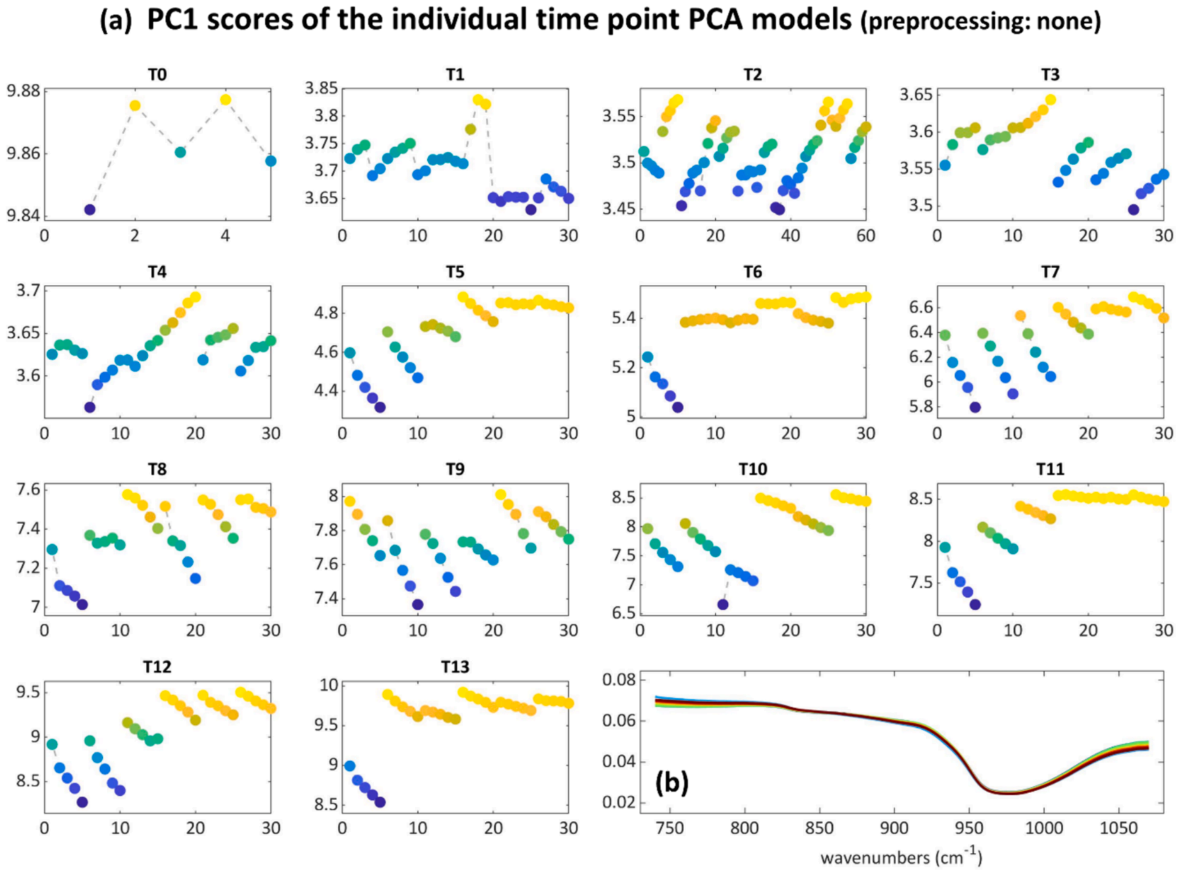

Fig. 5. The "descending" trends detected in the PC1 scores of individual PCA models (built on the raw data), one for each time point (a). Coloring highlights the scores values, while the 6 groups of 5 spectra acquired for each time point are connected using dashed lines. The initial time point T0 only has one group of acquisitions due to the absence of scattering effects probably due to bubbles formation (the fermentation process was not started yet). The loadings plots of individual PCA models (on built on the raw data), one for each time point, are reported in the same plot in (b): they all basically look the same.

in the simplest – but robust – way to an everyday leisure activity: beer homebrewing. We think that the study proved that simple and portable NIR instruments coupled with chemometrics can be used for tackling "everyday problems", at least from a qualitative point of view.

The SCiO sensor proved reliable and easy to use, providing clear signals. It revealed time trajectories, temperature trends, and the scattering effect from bubbles formation on the acquisition window, highlighting the importance of sound experimental procedures and proper data preprocessing for generating and modelling spectral data. The interpretation of the most interesting signals surely deserves further development to be possibly matched with more specific phenomena and/or stages of beer maturation during the brewing process. Precise or unique assignments are however rather difficult to achieve with the SCiO, since within its spectral window very few combination and overtone signals can occur.

Some aspects of our experimental setup can be seen both as limitations and as strong points: for instance, due to the basic homemade setup, reproducibility could prove very reduced. The evolution in time of the measured temperature should also be further investigated: in a replicate of the study the temperature should be measured directly on the liquid in the fermentation tank, instead of on the withdrawn sample. New experimental runs with the same simple procedure should also be executed to test the consistency and robustness of the information extracted by PCA: a clear time trend was found, and some tentative explanations were attempted, based both on the knowledge about the brewing process and the most relevant spectral NIR signals. However, it can be figured out that changes in the materials (different malt extracts, both from different producers and for different beer styles) or the conditions (different period of the year for brewing, different storage temperature and light conditions) could result in very different outcomes.

Considering the computational aspect of the study it is important to consider that a potential user would need an app to run PCA or other process monitoring analyses on such data. The prospect of providing users with a smartphone app that enables easy and automated collection and interpretation of process data is very promising. Indeed, this is already somewhat possible with the SCiO "Applets" within the "SCiO Pocket Molecular Sensor" app, but no process control is currently possible with the customizable applets available in the SCiO app. Regarding the extended applicability that could result from this study, an important further development could be building calibration models to describe and predict brewing parameters of interest such as alcohol content, gravity, pH, colour, and bitterness.

Hence, to conclude, if the readers have access to a SCiO and a passion for homebrewing, we warmly invite them to try replicating our analysis and then get back in contact with us. And hopefully share some of the brewed beer.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.saa.2024.125126.

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