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Feasibility studies and engineering of optical simplified and stand-alone devices for agri-food applications

1. Introduction

The food industry needs to comply with more strict rules (from regulatory agencies) and meet customers' demands for higher quality production. Emerging technologies (from an industry 4.0 approach) for quality and safety inspection are becoming fundamental and needful to fulfil these purposes.
In the winemaking industry, grape maturation control is a complex process that is critical to produce high-quality wines, but currently, maturation control is cumbersome and inefficient. This inefficient control of the maturation is related to a reduced value of the wine.
The current state of the art for grape maturation control is based on multiple wet-chemistry assays that are: (i) destructive, (ii) time consuming, (iii) labour intensive, (iv) performed on a sparse basis and (v) based in on complex sampling process.
Therefore, to shift the current paradigm of grape maturation monitoring (based on lab analysis) it is needed a new technology that: (i) allows a real-time and stand-alone monitoring with a low-cost, (ii) is non-destructive and chemical free, (iii) is capable to drastically reduce the need of manpower and (iv) provides information with temporal and spatial resolution.

2. Scope

This work focused on the development of a fully integrated stand-alone optical device for grape quality monitoring directly in field. The main steps to fulfil the project purpose were:

a) setting up of a miniaturized low-cost and stand-alone optical prototype composed by LEDs suitable for diffuse reflectance measurements, photodetectors (PDs, CMOS), sensors controller and power management;
b) Multivariate predictive models development for the prediction of the main grape ripening parameters;
c) Test the prototype in field conditions.

3. Materials and methods

3.1 Sensor specs

Concerning miniaturization and usability requirements in field, it was developed a "stripe" design in which the spectrometric components were mounted on a long, flexible substrate which can be placed onto or inside the grape bunch. The multiple spectrometers were placed along the stripe (currently 2, module 1, M1 and module 2, M2), enabling simultaneous measurements at different parts of the grape bunch. Figure 1a shows the four optical bands associated to the evolution of the maturation parameters of the grapes such as the development of anthocyanins and sugars, chlorophyll degradation, and decrease of water content. Therefore, four light-emitting diodes (LEDs) were used for illumination of the grape (530 nm, 630 nm, 690 nm and 730 nm). Placed close to these, but optically isolated using an opaque barrier, four photodiodes (with an active area of 520 × 520 μm^2) assembled to allow intensity measurements at the desired wavelengths (the relative spectra sensitivity is reported in figure 1b) have been used.
The light emitted from each LED hits the sample and the diffuse reflectance light is collected by each PD. The electromagnetic signal is converted into electronic signal and expressed in arbitrary units from 0 to 4095. From each sample, 20 readouts were obtained (one readout from each PD at each LED on and one with LEDs off for background info).

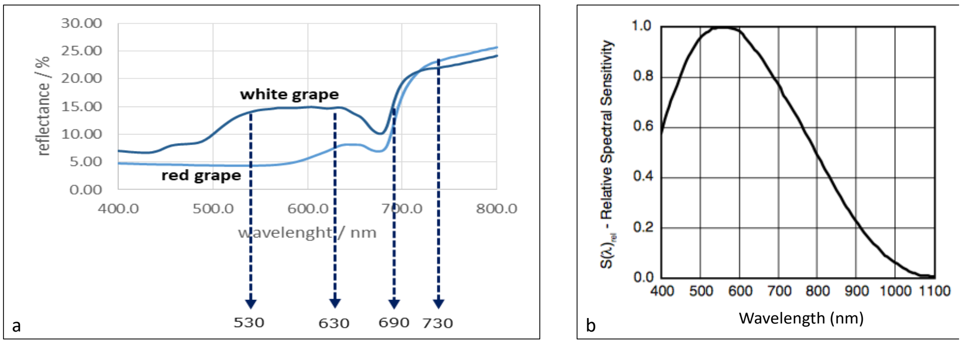

Figure 1 *a) Reflectance spectra from a white and a red grape acquired from benchtop spectrophotometer (Perkin Elmer 950).b) Spectral sensitivity of each PD.*

Concerning the data transmission, the sensors were configurated in order to share the optical outputs coming from the sensors placed in a target parcel to a local IoT gateway LoRaWAN. Then, the local server broadcasts the data to a web app (IoT database) in order to process the data with the chemometric models developed during the sampling campaign 2020 using samples analysed in lab and direct in field (Figure 2).

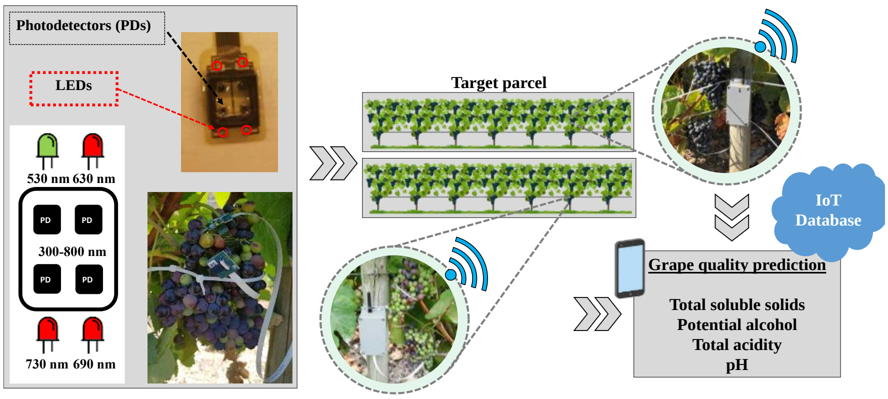

Figure 2 *Sensor technical features, installation and data transmission.*

3.2 Reference analysis

The experimental activity took place in the viticulture area of the Douro Valley (Sogrape's owned Quinta do Seixo, Portugal) from the end of July to mid-September for a total of six sampling dates. Sampling was performed on *cv.* Touriga Nacional (TN) and Touriga Franca (TF) (from 18 parcels) using the optical prototype without any sample preparation.

The reference analyses of (i) Total Soluble Solids (TSS, °Brix), (ii) Potential Alcohol (PA, % vol), (iii) Titratable Acidity (TA, $g_{tartaric\ acid}$ dm^{-3}), (iv) Total Poliphenols (TP, mg dm^{-3}) (Ough & Amerine, 1988), (v) Extractable Anthocyanins (EA, mg dm^{-3}) (Ribéreau-Gayon *et al.*, 2006) and (vi) pH were performed.

3.3 Optical analysis

The optical acquisitions were managed considering: (i) the environmental noise, (ii) the berries physical features, (iii) the increase in size of the bunch, (iv) the variable optical gap and (v) the position of the field sensor which change during the ripening process. In order to minimize these issues and maximize the info picked from the sensors, the measurements were performed overnight (for in field analysis) and using a dark room (for in lab analysis). The readouts coming from each PD were analysed individually as a variable in order to obtain the maximum information that can be collected. Therefore, a total of 16 optical variables (light emitted by 4 LEDs read by 4 PDs) were used for the model building.

3.4 Models development

A multivariate analytical approach was followed exploring the information using PCA. A latent variable modelling using the PLS method, which maximizes the covariance among the sensor readouts and the reference qualitative parameters (TSS, PA, pH and TA), was performed (Oliveri *et al.*, 2019). Model accuracy was evaluated (in calibration, cross-validation and prediction) using the RMSE, as well as bias and R^2.

4. Results

4.1 Sensor output

Figure 3 shows the optical outcome from the lab and field sensor (figure 3b and 3c) used for modelling. While for a better understanding of the grape optical behaviour, the general mean readouts coming from the reading by each PD at all LEDs (including LED off) have been reported in figure 3a.

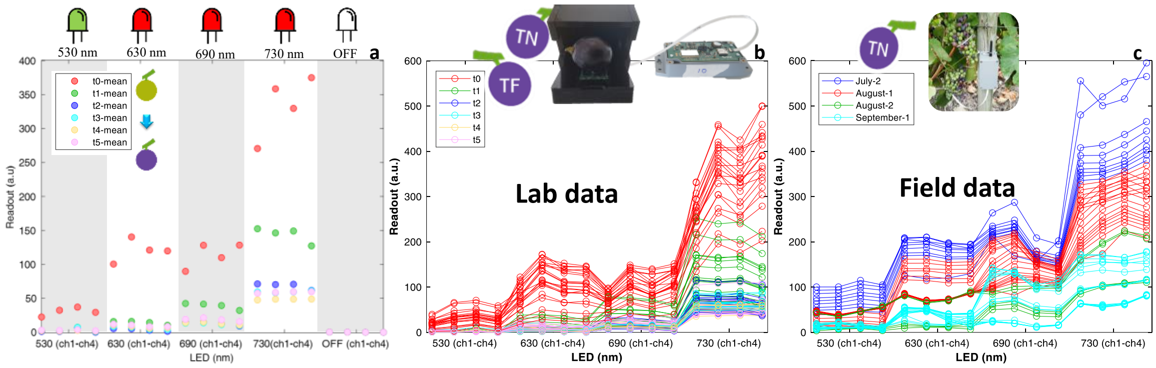

Figure 3 *Sensor readouts of each LED read by each PD. a) mean optical outputs obtained each sampling time (background included); (b) lab readouts (samples labelled according to the sampling times) and (c) field readouts (samples labelled according to rang of weeks).*

4.2 Modelling

The wet-chemical descriptive statistics are summarized in figure 4. Overall, the technological maturation curve of TN and TF grapes is well described by the sampling campaign performed during the crop season 2020. Each sample was analysed optically (by lab sensor) and chemically (by the reference instruments) to proceed with the models calculation. In addition, a reference measurement needs to be associated also to the optical outputs from the field sensor in order to develop general predictive models computing data from both lab and field. Therefore, the wet-chem outcome was used to develop the evolution curve (for each specific parameter) to extrapolate for each day the reference values to be associated with the optical outcomes deriving from the field sensor.

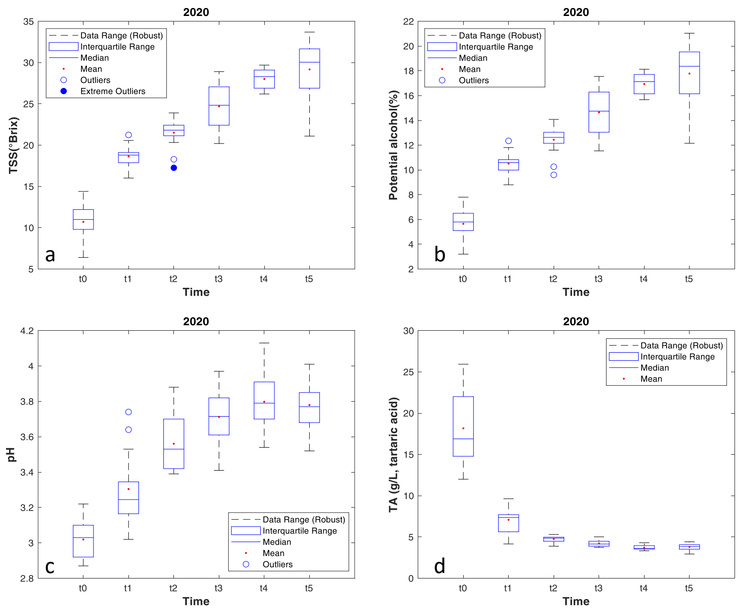

Figure 4 *Wet-chemical descriptive statistics for TSS (a), PA (b), pH (c) and TA (d).*

PLS models were developed for the prediction of the qualitative parameters of interest. The 70% of the total amount of the data were used for calibration and 30% for the external validation (prediction).

Figure 5 summarize the models figure of merit in pure prediction of the external validation. The external validation samples set were labelled in red (TF) and in green (TN) for the samples coming from lab analysis and field samples labelled in blue (B01).
In detail, it was concluded that:

- The best models were obtained for TSS, and consequently PA considering an R^2 about 0.90 and RMSEP of 2.22 and 1.54, respectively using 6 LVs.
- A very promising model was also obtained concerning the TA with an R^2 equal to 0.93 and RMSEP of 1.39 (using 4 LVs).
- The pH model (using 4 LVs) showed a lower performance than previous parameters (R^2 of 0.76 and RMSEP 0.15) but still with potential for being used with further improvements.

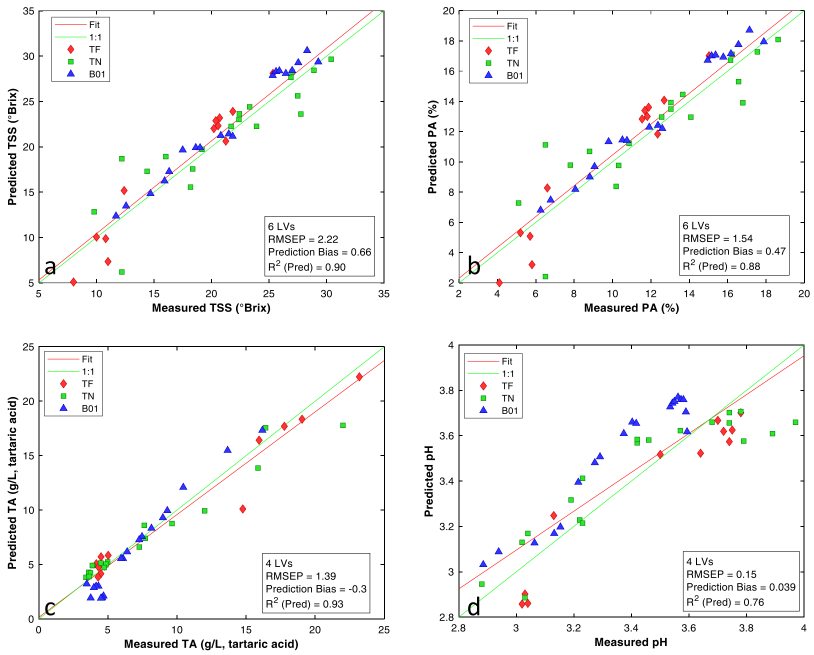

Figure 5. *Figure of merit of the PLS models. Prediction results expressed in terms of Root Mean Squared Error in prediction (RMSEP), R^2 and prediction bias. Lab samples labelled in red (TF) and in green (TN) and field samples labelled in blue (B01)*

5. Conclusions

To conclude, a good prediction capability has been reached for each qualitative parameter envisaging a real application of this device in a more sophisticated network of sensors in order to give the possibility to the wine industry to bring the laboratory to the field. However, further experiments must be carried out and different operational strategies to obtain reliable optical data need to be fine-tuned.
In order to spread the application of this sensor for the whole viticulture sector, other models for the prediction of qualitative parameters need to be calibrated to include white grape varieties into the package of potential applications of this new type of sensors.
Moreover, given the low capability of these sensors (which work in diffuse reflectance in the vis/NIR range) to give back optical outputs strongly related to the concentration of polyphenols and anthocyanins (performance is consistent with previous works reported in literature), the development of a fluorescence module is currently under study and it will be taken in consideration for a future sensor upgrade.

References

Oliveri, P. *et al.* (2019) ‘The impact of signal pre-processing on the final interpretation of analytical outcomes – A tutorial’, *Analytica Chimica Acta*. Elsevier Ltd, 1058, pp. 9–17. doi: 10.1016/j.aca.2018.10.055.
Ough, C. S. and Amerine, M. A. (Maynard A. (1988) *Methods analysis of musts and wines*, *Methods analysis of musts and wines*. doi: 10.1002/9780470114735.hawley15337.
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