

Research Article

Visible/Near-Infrared Spectroscopy Devices and Wet-Chem Analyses for Grapes (*Vitis vinifera* L.) Quality Assessment: An Environmental Performance Comparison

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Background and Aims. The composition of grapes (*Vitis vinifera* L.) at harvest is a key factor that determines the future quality of wine. The work aimed to evaluate and compare the environmental impact of the most evaluated technological parameters using three approaches: the wet-chem method, the optical method using benchtop devices, and the optical method using a prototype smart and cost-effective device (Technology Readiness Level: 5). **Methods and Results.** The life cycle assessment (LCA) methodology was used to identify the most environmentally sustainable solution in a “from-cradle-to-grave” approach. The functional unit was identified by the execution of the analyses necessary to measure the three technological parameters: TSS, pH, and TA. The findings show that the optical analysis carried out with the prototype is the most suitable and green solution (i.e., with the lowest environmental impact in all the impact categories analysed); in fact, the same technology has proved to be 3.2 times more sustainable than the wet-chem method for the best average environmental performance. **Conclusions.** The research demonstrated the environmental impact advantages of the optical analyses for assessment of grape composition. **Significance of the Study.** Innovations in agriculture and the development of smart solutions represent advantages for managing and monitoring the composition of agri-food products that are a green solution for the industry.

1. Introduction

Grape composition at harvest is a key factor that determines the future quality of wine [1, 2]. By measuring certain grape parameters, such as TSS, reducing sugar, tartaric acid and malic acid, and TA and pH value, it is possible to determine the optimum harvest timing to ensure the production of high quality wines [3]. These parameters are usually obtained through wet-chem analyses, which often require samples to be sent to geographically distant laboratories that can take a long time to return results. These types of analyses have proved to be slow, time-consuming, and destructive, require expert qualified personnel, and do not respond to the demand of the modern wine industry [2, 4]. By considering

more efficient analytical technologies compared to the traditional ones, wineries will increase their efficiency along the production chain [5].

Generally, wine chain production is the responsibility of the oenologist. This professional aims to manage and control all the production processes in the field, starting from the choice of the appropriate cultivar to be planted in the vineyard to the identification of the optimal time for harvesting, and in the winery through the vinification process and finally bottling. The oenologist is also essential to evaluate the composition of the grape through the chemical analyses cited above, with such information being valuable during the decision making to optimise productivity [6]. Even though this role is important because of its professional

experience, the modern wine industry cannot rely on this approach alone but needs more rapid analyses. To satisfy this need, innovative technologies are evolving. In the agri-food industry, spectrophotometers can perform rapid analysis of key composition parameters, giving a precise evaluation of composition. These devices can be used to obtain results in less than 3 min, without using chemical reagents and without having additional costs, even though it requires sample preparation through purification and degasification. In fact, spectroscopy can be used to obtain the chemical composition of a biological product, avoiding destructiveness and slowness. The VIS/NIR spectroscopy consists of the combination of effective sensors with sophisticated mathematical models and computational algorithms to establish relations between selected chemical properties and quality attributes [7]. Essentially, with VIS/NIR technology, the sample is illuminated by light radiation absorbing a certain amount of it and reflecting the remaining part at specific wavelengths. The quantity of light reflected and transmitted is translated into a spectrum by the VIS/NIR detector [8]. The results obtained can be correlated to chemical parameters using chemometric techniques.

In the past, VIS/NIR technology has been used for the determination of the composition of many agricultural products both at a laboratory scale and on-line [9]. The advantages of this technology can also be brought to the wine industry representing a considerable benefit to the sector at different levels: first, by monitoring the composition of the grapes during their growth, it is possible to achieve better management of field practices (e.g., use of water during irrigation) and create a model to monitor the composition of grapes to identify the best harvesting time. Another advantage involves the harvest period during which this technology can be used to identify and separate grapes of different composition so that the value of the final product can be improved [10]. The results derived from VIS/NIR spectroscopy are comparable with those obtained with traditional analytical methods [11–13], with the only difference being that VIS/NIR does not require sample preparation and chemical reagents.

The determination of the composition of incoming grapes in the grading area is also a fundamental step for the overall evaluation of grapes that every winery or grower association needs to consider during winemaking. More than the analysis itself, sampling is the most critical operation, since it is here that the sample, analysed to assess the composition of the entire batch, is obtained and needs to be a representative of the entire load. Nowadays, in the wine sector, truck or bin sampling systems can be used to collect samples with a motorised probe picking up the grapes and crushing them; must is obtained and submitted to analysis to measure main parameters of composition, such as TSS and TA, with a maximum duration of 3 min per truck. Despite that, this type of analysis is defined as destructive due to the fact that the samples analysed are not preserved.

With the shift from conventional to precision agriculture, there are many other proposals on the market to replace wet-chem laboratory instruments, such as simplified portable systems which use a set of discrete commercial

modules, such as LED arrays, white light sources, photodiodes, filters, and microspectrometers. The technology is undergoing rapid development and is moving towards miniaturisation. The consumer electronics industry is driving the convergence of digital circuitry, wireless transceivers, and microelectronic-mechanical systems (MEMS), which makes it possible to integrate sensing, data processing, wireless communication, and power supply into low-cost millimetre-scale devices [14]. The resulting miniaturisation and cost reduction of electronic components are creating a completely new method of data acquisition and management using wireless sensor networks (WSNs) based on small battery-powered nodes. A WSN consists of small and low-cost Internet of Things (IoT) devices in a network of peripheral nodes. The nodes are equipped with sensors and a wireless module for data transmission to an online database, where the data are stored and accessible to the end-user. The nodes are energy independent and are installed in areas which are more representative of the vineyard variability [15]. The WSN technology is widely used to monitor environmental factors, such as temperature, moisture, RH, and leaf wetness, which are essential for the decision making of growers [16]. The availability of miniaturised optical devices, however, is driving the research to develop IoT sensors which are highly sensitive for the detection of substances in an environment, such as chemicals or biological materials. In viticulture, the sensors are directly installed in proximity of the target (vine leaf or grape bunch) to remotely monitor the vineyard during the crop season. These instruments provide a wide range of information, but they require a human operator for data acquisition and are not stand-alone. For future scenarios, they will need to be optimised bringing the laboratory directly into the vineyard, without human intervention for data sampling [17].

Casson et al. [18] demonstrated that VIS/NIR technology can be defined as a sustainable solution to monitor the composition of olives and that the analyses carried out to monitor the composition of grapes are different; as a result, they considered that the issue of the sustainability of the technology in the wine sector remains to be determined. Overall, innovation in agriculture activities tends to propose smart solutions that can represent advantages of managing and monitoring agri-food product composition, but the sustainability level of these solutions remains a knowledge gap.

This work aims to evaluate and compare the environmental impact of three scenarios based on two different methods, chemical and optical, used in the wine sector to measure the main composition parameters of grapes: TSS, TA, and pH value. For each of these parameters, chemical methods and VIS/NIR spectroscopy, located in benchtop instrumentation and using an innovative smart solution (optical in-field prototype), will be analysed and then compared. The life cycle assessment (LCA) methodology and estimation performance were carried out to identify the most sustainable solution and to propose actions to reduce waste and the impact along the wine supply chain.

2. Materials and Methods

The basic idea of LCA is that all the environmental burdens connected with a product or service must be assessed, back to the raw materials and through to waste removal. This method is developed according to the international standard ISO 14040-14044 [19, 20].

2.1. Goal and Scope Definition. The goal of this study was to evaluate and compare the environmental impact of two types of method, chemical and optical, used in the wine sector to measure the composition of grapes. Three main quality parameters were considered: TSS, determined by a digital refractometer; TA, analysed by volumetric titration; and pH value measured with a pH meter [21]. The definition of the environmental impact was performed for both the chemical methods (destructive analyses) and the VIS-NIR spectroscopy (nondestructive analysis).

Specifically, for the nondestructive analyses, two technologies were considered: benchtop spectroscopy and the prototype of a simplified and portable device which incorporates sensors and is used to measure the same three compositional parameters cited above. Such a technology, compared with the benchtop, can be used directly in the field and allow the creation of a measurement database based on a cloud system [17].

2.1.1. Functional Unit. According to the ISO 14040 standard, the functional unit represents the performance of the outputs of a product system providing a reference to which inputs and outputs are related [19, 20]. In this comparative study, the functional unit was identified by the pool of analyses carried out for the three different parameters, that is, three chemical analyses for the wet-chem analyses and one single nondestructive analysis for the optical analysis to estimate the three grape composition parameters.

2.1.2. Definition of the System. The system under study included all the procedures related to the chemical analysis, traditionally used in laboratories, and the VIS/NIR technology. For the former, all activities necessary to obtain three replicates for the three parameters were considered. The latter consisted of one single optical measure carried out three times to obtain results for the three parameters simultaneously.

All the inputs and outputs necessary to complete the study were collected through some interviews at the laboratory of the Università degli Studi di Milano, which specialises in analysis of grape composition. The instruments are used only for this purpose; during other periods of the year, the instruments are not used. Considering this usage pattern, the laboratory capacity should be defined as equal to 450 analyses/year, defining the average number of analyses carried out in a day equal to five.

2.1.3. System Boundaries. The system boundaries determine which unit processes are included within the LCA (Figure 1). In this study, a “cradle to grave” approach was used, which

considers all the inputs of the process: from the extraction of the raw materials; through the construction of the laboratory materials and analytical tools; the chemicals; and the calibration of the VIS/NIR technology including energy, electricity, and water supply. In addition to that, the system boundaries considered the outputs of the process, thus the disposal of every single material used during the analysis (exhausted plastic, paper, chemicals, and sample).

The laboratory carried out the wet-chem analyses for 3 months during the maturation period (July to September), and all the tools were not used for other tasks or in another period. Instead, the VIS/NIR technology was considered as an alternative method to measure the same compositional parameters but without the destructiveness of the sample.

2.2. Life Cycle Inventory (LCI). Inventory analysis involves data collection and calculation procedures to quantify relevant inputs and outputs of a product system [20]. All the inputs and outputs collected in the study should be interpreted, depending on the goals and scope of the LCA. The data within LCI also constitute the starting point to the life cycle impact assessment.

For this study, the information necessary for the inventory phase should be referred to the methods of the Organisation Internationale de la Vigne et du Vin (OIV); despite that, the data collection of the procedures of each analysis was obtained through interviews carried out with the laboratory personnel of the Università degli Studi di Milano.

All the materials used and described in the interviews were analysed: from analytical tools and laboratory materials up to reagents, the quantity of the sample and energy, in addition to all the waste generated along with the procedures.

For the LCI, it was also necessary to indicate the lifetime of the analytical tools and the laboratory materials expressed in years, in addition to the number of analyses carried out by each machine during their lifetime. All the analytical tools have a lifetime of 15 years with a total of 6750 analyses, while the laboratory materials last 10 years with 4500 complete analyses.

For the present study, the inventory of every single analysis was performed separately and reported.

2.2.1. Allocation Procedures. According to the International Organization for Standardization [19], allocation is the tool for partitioning the input/output flows of a process or a product system between the product system under study and one or more other product systems. During laboratory analyses, many analytical tools or laboratory materials are used for more than one type of analysis (i.e., computer, automatic volumetric titrator, and pipettes), so it was necessary to adopt a procedure that consisted in allocating all the inputs of every chemical and optical analyses (benchtop and prototype) to a specific value, as reported in a previous study [22]. This value is known as the amount per analysis and requires different variables to calculate it: the allocation factor (A_f) ranging from 0 to 1, the quantity of input (Q) in

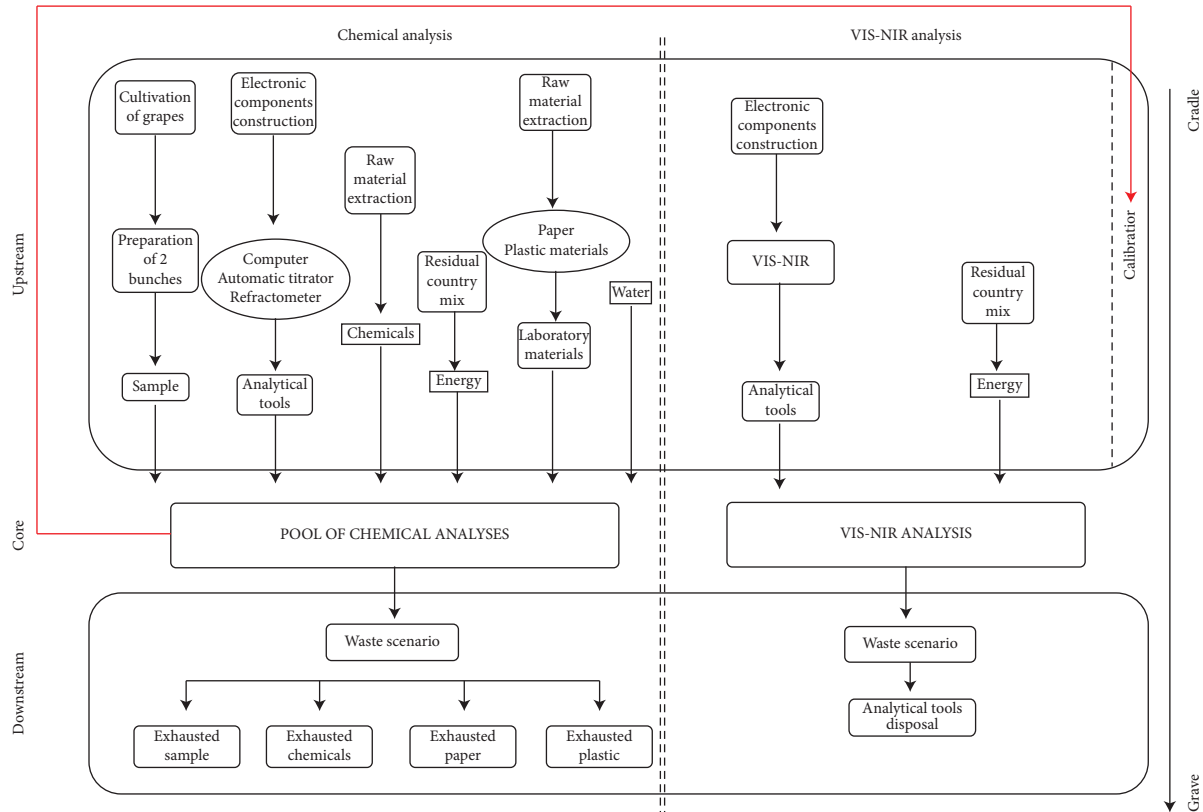


FIGURE 1: System boundaries and elements flow. *Calibration = chemical analysis + benchtop analysis/prototype analysis.

terms of mass, volume, energy, and the number of analyses (Noa) performed during the lifetime of the product under study.

$$\text{Amount per analysis} = \frac{Q * Af}{\text{Noa}}. \quad (1)$$

2.2.2. Preparation of the Sample LCI. For the preparation of the sample used in the chemical analysis, two bunches of grapes were collected from the field and squeezed manually in a plastic bag (20 × 30 cm) to obtain 100 g of must. A solution of 0.2% sodium azide (NaN₃) (1 mL) was added to avoid fermentation and alterations in must and to guarantee storage of the sample for long periods (weeks or even months). For this study, must was stored at room temperature for 2 weeks until analysed in the laboratory. Input and output data related to this procedure are reported in Table 1.

2.2.3. Total Acidity Determination LCI. Total acidity, expressed in g/L, was determined with an automatic volumetric titrator, associated with an autosampler and a computer. The automatic volumetric titrator used 0.1 N sodium hydroxide as the titrant. Starting from must, 7.5 mL was collected, and 50 mL of deionised water was added to start the analysis with the autosampler and titrator. All the inputs and outputs related to this analysis are summarised in Table 2.

2.2.4. Determination of pH LCI. Similar to the TA, pH was determined with an automatic potentiometric titrator. In this case, 50 mL of must sample and two buffer solutions were used. The titrator performed the analysis automatically, and no more chemicals or reagents were used. Water was accounted for the routine procedure of washing analytical tools and workspace. The input and output concerning this chemical analysis are illustrated in Table 3.

2.2.5. Determination of TSS LCI. Must TSS was determined with a digital refractometer: for each sample analysed, about 100 μL of must was placed within the analytical tool and the TSS measured. This procedure can also be carried out in the field without extra sample preparation. Considering the aim of the study, the worst scenario was analysed. The input and the output related to the determination of TSS are reported in Table 4.

2.2.6. Benchtop VIS/NIR Spectroscopy LCI. The use of visible and near-infrared spectroscopy (VIS/NIR) can provide an objective, repeatable, rapid, accurate, and nondestructive method for the evaluation of the composition of grapes. Without any sample preparation, the undamaged grape samples were analysed using the light from the VIS/NIR spectrophotometer.

The basic concept of VIS/NIR spectroscopy is that the light coming from the instrument is reflected by the grapes and the spectra obtained are then analysed and visualised by

TABLE 1: Quantity, allocation factor, lifetime, and amount per analysis for the preparation of the sample.

	Unit	Quantity (Q)	Allocation factor (Af)	Lifetime (years)	Lifetime (no. analyses)	Amount per analysis [†]
Input						
Must	g	100	0.33	n.a.	1	33.333
Plastic container (100 mL)	g	15.91	0.33	10	4500	0.001
Plastic tops	g	4.06	0.33	10	4500	0.000
Plastic bags (20 × 30)	g	6.57	0.33	n.a.	1	2.190
Sodium azide (0.2%)	g	1	0.33	n.a.	1	0.333
Paper towel (for materials cleaning)	g	2.03	0.33	n.a.	1	0.677
Deionised water (for materials washing)	g	5	0.33	n.a.	1	1.667
Manual pipettes (100–1000 μL)	g	83.42	0.33	10	4500	0.006
Pipette caps (100–1000 μL)	g	0.787	0.33	1	1	0.262
Output						
Sample waste	g	230	n.a.	n.a.	n.a.	n.a.
Plastic waste	g	7.36	n.a.	n.a.	n.a.	n.a.
Paper waste	g	2.03	n.a.	n.a.	n.a.	n.a.

[†]Quantity × allocation factor/no. of analyses.

TABLE 2: Quantity, allocation factor, lifetime, and amount per analysis for the TA determination.

	Unit	Quantity (Q)	Allocation factor (Af)	Lifetime (years)	Lifetime (no. analyses)	Amount per analysis [†]
Input						
Must	g	7.5	1.00	1	1	7.500
Automatic volumetric titrator	g	20 × 10 ³	0.50	15.00	6750	1.481
Computer	g	13 × 10 ³	0.33	15.00	6750	0.642
Plastic glasses	g	2.27	5.00	1	1	11.350
Deionised water	g	270	1.00	1	1	270.000
NaOH (0.1 mol/L) as titrant	g	17.5	1.00	1	1	17.500
Buffer solution (pH 4)	g	50	2.00	1	1	100.000
Buffer solution (pH 7)	g	50	2.00	1	1	100.000
Manual pipettes (1–10 mL)	g	114.81	1.00	10	4500	0.026
Pipettes caps (1–10 mL)	g	5.85	0.10	1	1	0.585
Water (for cap washing)	g	5	1.00	1	1	5.000
Electricity	kWh	0.059	1.00	n.a.	1	0.059
Output						
Plastic waste	g	17.1	n.a.	n.a.	n.a.	n.a.
Chemical waste	g	240	n.a.	n.a.	n.a.	n.a.

^{††}Quantity × allocation factor/no. of analyses.

TABLE 3: Quantity, allocation factor, lifetime, and amount per analysis for pH determination.

	Unit	Quantity (Q)	Allocation factor (Af)	Lifetime (years)	Lifetime (no. analyses)	Amount per analysis [†]
Input						
Must	g	50	1.00	n.a.	1	50.000
Automatic volumetric titrator	g	20 × 10 ³	0.50	15.00	6750	1.481
Computer	g	13 × 10 ³	0.33	15.00	6750	0.636
Plastic glasses	g	2.27	3.00	1	1	6.810
Deionised water (for workspace washing)	g	200	0.10	n.a.	1	20.000
Deionised water (for instrument washing)	g	200	0.20	n.a.	1	40.000
Buffer solution (pH 4)	g	50	2.00	1	1	100.000
Buffer solution (pH 7)	g	50	2.00	1	1	100.000
Electricity	kWh	0.059	1.00	n.a.	1	0.059
Output						
Plastic waste	g	6.81	n.a.	n.a.	n.a.	n.a.
Chemical waste	g	210	n.a.	n.a.	n.a.	n.a.

^{††}Quantity × allocation factor/no. of analyses.

TABLE 4: Quantity, allocation factor, lifetime, and amount per analysis for TSS determination.

	Unit	Quantity (Q)	Allocation factor (Af)	Lifetime (years)	Lifetime (no. analyses)	Amount per analysis [†]
Input						
Must	g	0.2	1.00	n.a.	1	0.200
Digital refractometer	g	200	1.00	15	6750	0.030
Manual pipettes (20–200 μ L)	g	80.6	1.00	10	4500	0.018
Pipettes caps (20–200 μ L)	g	0.38	1.00	1	1	0.380
Paper towel (for instrument cleansing)	g	2.03	0.33	n.a.	1	0.677
Water (for instrument washing)	g	0.015	1.00	n.a.	1	0.015
Output						
Plastic waste	g	0.38	n.a.	n.a.	n.a.	n.a.
Paper waste	g	0.892	n.a.	n.a.	n.a.	n.a.

[†]Quantity \times allocation factor/no. of analyses.

TABLE 5: Quantity, allocation factor, lifetime, and amount per analysis for VIS/NIR spectroscopy analysis.

Input	Unit	Quantity (Q)	Allocation factor (Af)	Lifetime (years)	Lifetime (no. analyses)	Amount per analysis [†]
VIS-NIR spectrophotometer	g	15×10^3	1.00	15	6750	2.22
Computer	g	13×10^3	1.00	15	6750	1.926
Calibration	n	2100	0.015	15	6750	0.004666667
Electricity	kWh	0.0564	1.00	n.a.	1	0.0564

[†]Quantity \times allocation factor/no. of analyses.

software for model calibration within a computer. From the spectral result, a wide range of information can be deduced after only a single analysis.

The only devices necessary for this type of technology are the VIS/NIR spectrophotometer and the computer; in addition to that, no chemicals are required, and the samples can be analysed directly in the field without producing any waste; thus, no outputs were considered in the VIS/NIR inventory. The input concerning the optical analysis is reported in Table 5.

A fundamental matter concerning VIS/NIR technology is the calibration phase that allows reliable results to be obtained, although they are not a direct measurement of the quality parameters, but only their estimation. The calibration is designed to be a process that entails 700 conventional analyses per parameter, which correspond to 700 optical analyses conducted on the same sample. Five hundred calibration analyses were performed at the beginning of the optical method, with the other 200 analyses used as a validation test. In this study, three models for TA, pH, and TSS were allocated to the 6750 analyses undertaken in 15 years.

2.2.7. Simplified and Portable VIS/NIR Prototype LCI. Another type of optical method used a simplified and portable LED-based prototype. This prototype device (technology readiness level equal to 5) is composed of tuned photodiode arrays, interference filters, LEDs, and optics. In detail, the device incorporates two digital sensors (ams-OSRAM, models AS7262 visible and AS7263 NIR, Premstätten, Austria) for spectral measurement in the visible (VIS) and short wave near-infrared (SW-NIR) region. The VIS and SW-NIR sensors are 4.5×4.4 mm in size and are classified as ultra-low power consumption sensors. They

have 12 independent on-device optical filters to detect reflectance light at 450, 500, 550, 570, 600, 610, 650, 680, 730, 760, 810, and 860 nm [17].

Optical data were acquired on both bunches and single berries directly in the field without any sample preparation. Data were collected using the LED fully integrated prototype to avoid sample degradation. The inputs referring to this optical analysis are collected in Table 6. Also, for this analysis with the portable device, a calibration procedure was based upon the benchtop device calibration model.

2.2.8. Performance Characterisation Factor. As described above, the two optical instruments (benchtop and prototype) do not provide a direct measurement of the compositional parameters, only their estimation; chemical procedures, however, do provide a direct measurement. Thus, the prediction capacity of the instruments was considered an important aspect that contributes to the final environmental impact interpretation. To obtain the performance values of the two instruments, two common main factors were considered: the mean and the root mean square error of cross-validation (RMSEcv). Both instruments were used on the same grapes; regarding the benchtop VIS/NIR device, the values of the mean and the RMSEcv were taken according to Casiraghi et al. [23]; while, the same two factors referred to the prototype were collected from Pampuri et al. [17].

2.2.9. Life Cycle Impact Assessment (LCIA). The impact assessment phase of LCA aimed at evaluating the significance of potential environmental impacts using the results of the life

TABLE 6: Quantity, allocation factor, lifetime, and amount per analyses for portable device.

Input	Unit	Quantity (Q)	Allocation factor (Af)	Lifetime (years)	Lifetime (no. analyses)	Amount per analysis [†]
Prototype	g	130	1.00	15	6750	0.019
Calibration	n	2100	0.015	15	6750	0.004666
Electricity	kWh	0,000093	1.00	n.a.	1	0.000093

[†]Quantity × allocation factor/no. of analyses.

TABLE 7: Impact categories, acronyms, and unit of the ReCiPe 2016 midpoint (H) method.

Impact category	Acronyms	Unit
Global warming	GWP	kg CO ₂ eq
Stratospheric ozone depletion	ODP	kg CFC11 eq
Ionising radiation	IRP	kBq Co-60 eq
Ozone formation–human health	HOFP	kg Nox eq
Fine particular matter formation	PMPF	kg PM _{2.5} eq
Ozone formation–terrestrial ecosystems	EOFP	kg Nox eq
Terrestrial acidification	TAP	kg SO ₂ eq
Freshwater eutrophication	FEP	kg P eq
Marine eutrophication	MEP	kg N eq
Terrestrial ecotoxicity	TETP	kg 1.4-DCB
Freshwater ecotoxicity	FET	kg 1.4-DCB
Marine ecotoxicity	METP	kg 1.4-DCB
Human carcinogenic toxicity	HTPc	kg 1.4-DCB
Human noncarcinogenic toxicity	HTPnc	kg 1.4-DCB
Land use	LU	m ² a crop eq
Mineral resource scarcity	SOP	kg Cu eq
Fossil resource scarcity	FFP	kg oil eq
Water consumption	WCP	m ³

TABLE 8: Environmental impact percentage responsibilities of the three chemical analyses.

Impact category	Unit	Total Pool of three chemical analyses	Percentage responsibility (%)		
			TA	pH	TSS
GWP	kg CO ₂ eq	1.66	50.7	49.0	0.3
ODP	kg CFC11 eq	2.40 × 10 ⁻⁶	45.1	54.8	0.1
IRP	kBq Co-60 eq	6.69 × 10 ⁻²	58.8	40.4	0.9
HOFP	kg Nox eq	2.16 × 10 ⁻³	47.0	52.5	0.5
PMPF	kg PM _{2.5} eq	1.45 × 10 ⁻³	47.5	51.9	0.6
EOFP	kg Nox eq	2.26 × 10 ⁻³	47.0	52.5	0.5
TAP	kg SO ₂ eq	3.72 × 10 ⁻³	45.9	53.5	0.6
FEP	kg P eq	4.45 × 10 ⁻⁴	49.1	50.4	0.5
MEP	kg N eq	2.89 × 10 ⁻⁴	20.4	79.1	0.5
TETP	kg 1.4-DCB	3.39	49.0	50.6	0.4
FET	kg 1.4-DCB	1.25 × 10 ⁻¹	39.9	59.7	0.4
METP	kg 1.4-DCB	1.23 × 10 ⁻¹	48.5	51.1	0.4
HTPc	kg 1.4-DCB	4.61 × 10 ⁻²	47.4	52.2	0.4
HTPnc	kg 1.4-DCB	1.84	42.4	57.0	0.5
LU	m ² a crop eq	1.76 × 10 ⁻¹	16.6	82.2	1.2
SOP	kg Cu eq	1.39 × 10 ⁻²	48.3	51.6	0.2
FFP	kg oil eq	3.15 × 10 ⁻¹	50.6	49.0	0.5
WCP	m ³	4.71 × 10 ⁻²	23.0	76.6	0.4

Impact categories and acronyms are defined in Table 7.

cycle inventory analysis. In general, this process involves associating inventory data with specific environmental impacts and attempting to understand those impacts. The level of detail, choice of impacts evaluated, and methodologies used depend on the goal and scope of the study [19].

To analyse the environmental impact, the SimaPro v 9.1.1.1. (PRé Sustainability, Amersfoort, The Netherlands) software was used. ReCiPe 2016 midpoint (H) was used as the method to calculate the environmental impact related to the chemical and the optical analyses for the measurement of the three compositional parameters of grapes. ReCiPe 2016 considers 18 impact categories that are reported in Table 7.

3. Results and Discussion

According to the purpose of the study, the chemical analysis and the optical analysis with benchtop instrument spectroscopy and with the prototype were first analysed separately and then compared with each other. The results included the hotspot identification criterion for the single study of the three approaches. For the comparison, a numerical and quantitative concept was needed including all the three possible solutions together (chemical analysis, optical analysis with the benchtop spectrometer, and optical analysis with a portable device).

3.1. Conventional Methods LCIA. Table 8 represents the environmental impact in percentages, highlighting the main hotspots deriving from the inputs and outputs of the pool of chemical analyses. To better interpret the results of this method, the final environmental impact was divided into the three chemical analyses that allow the three compositional parameters of grapes to be obtained.

Among these three chemical analyses, the ones that appear to have the highest environmental impact are the determination of pH and TA, which has an impact range of 40–50% in almost every impact category. This result is explained by using a certain quantity (100 g) of buffer solution that is fundamental for the calibration of the automatic potentiometric titrator, used for TA and pH analyses. Only three impact categories (MEP, LUs and WCP) see the pH determination as mainly responsible for the environmental impact reaching values of 79.1, 82.2, and 76.5%, respectively, and therefore define a lower level of environmental responsibility for the determination of TA. For TSS, the environmental responsibility reaches a maximum of 1% in all the impact categories, thus not appearing environmentally significant, due to the use of a simplified system such as the refractometer for its determination.

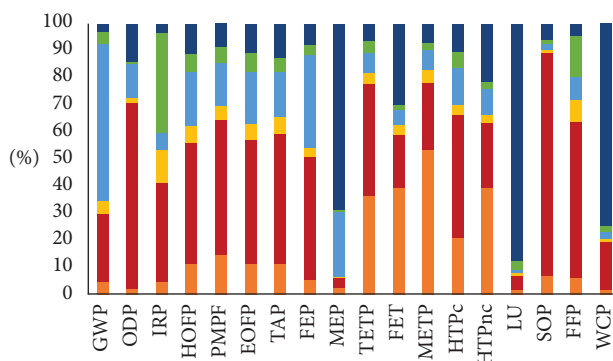


FIGURE 2: Hotspots for the pool of chemical analyses based on a factor subdivision. Impact categories and acronyms are defined in Table 7. Analytical tools (orange), chemicals (red), energy (yellow), waste (light blue), laboratory materials (green), sample (dark blue), and calibration (brown).

Table 8 underlines the most environmentally impactful analysis, although it is unable to convey the reason. Thus, according to the goal of the study, the three wet-chem analyses must be treated as a single chemical analysis represented by a pool. To interpret the results derived from the pool, its inputs and outputs were subdivided into seven factors (analytical tools, chemicals, energy, waste, laboratory materials, sample, and calibration) allowing the identification of the main hotspots.

As shown in Figure 2, the use of chemicals is the most impactful factor among those cited above in almost all the impact categories (9 out of 18) with values ranging from 45% to 70%. This factor refers to all the solutions and reagents used during chemical procedures, such as deionised water, sodium hydroxide, and all the buffer solutions used to calibrate the automatic potentiometer.

Only for the WCP, LU, and MEP categories, the main factor responsible for the environmental impact is the preparation of the sample, which is mainly influenced by the impact related to obtaining the grapes. In fact, due to the use of fertilisers and pesticides during the cultivation phase, grape cultivation reaches 69% responsibility in the marine eutrophication impact category (MEP). The same behaviour can be seen in the land use impact category (LU), where the sample has a percentage value of 88% due to the occupation of the field for the growth of the grapes. Regarding to water consumption, an impact of 75% is observed, justified by the consumption of water for irrigation of the vineyard.

3.2. Benchtop VIS/NIR and Prototype Optical Analyses LCIA.

The VIS/NIR approach does not require the same inputs and outputs as the conventional method; thus, only three factors needed to be identified, according to the subdivision criteria: analytical tools, energy, and calibration. Figure 3 represents the main responsible hotspots of the environmental impact of the benchtop technology and of the prototype. The hotspot with the highest environmental responsibility in all the impact categories considered is the calibration phase, which requires a high number of chemical analyses to calibrate the predictive model to define the quality parameters for the grapes. The energy

appears to be the second hotspot for the benchtop technology due to its low consumption during the optical procedure.

As observed in Table 8 for the determination of TSS, the use of simplified systems permits a significant reduction of the environmental impacts. Therefore, this study included also this type of system for the determination of the three quality parameters simultaneously and not only for one single parameter as in the conventional analysis. Therefore, regarding the optical methods, not only the benchtop device was considered but also a portable prototype. In Figure 3, the environmental impact of this second type of optical method is also reported highlighting the main responsible hotspots for the procedure, and the subdivision follows the same as the benchtop device (analytical tools, energy, and calibration). The calibration factor is the principal hotspot also for this kind of optical system in all the impact categories with a percentage responsibility that in some impact categories reaches values of 100%. The analytical tools instead have an impact percentage so small (less than 5%) that they were considered as a negligible factor.

To compare the environmental impact of the conventional analysis, the optical analysis with benchtop VIS/NIR and with the prototype, a quantitative evaluation is needed. Table 9 reports the comparison of the three methods showing their environmental responsibility, in addition to the ratio values for each impact category, which consider the pool of three chemical analyses compared with one optical analysis with the benchtop technology and with the portable technology. The chemical analyses have the highest environmental impact in all the impact categories; instead of the optical analyses with the benchtop instrument and the prototype, the environmental impacts are similar, even though the benchtop VIS/NIR solution appears to have a higher impact due to the necessity of having a computer to analyse the spectra obtained by the instrument, the portable device, on the other hand, does not require a PC because it is used directly in the field and as shown in Figure 3 (the analytical tools are not significant in terms of environmental impact). In addition to the environmental impact, the ratio % results highlight the differences between the two optical analyses even though there is no wide variability. It can be observed that an average ratio of 37% is related to the benchtop technology concerning the

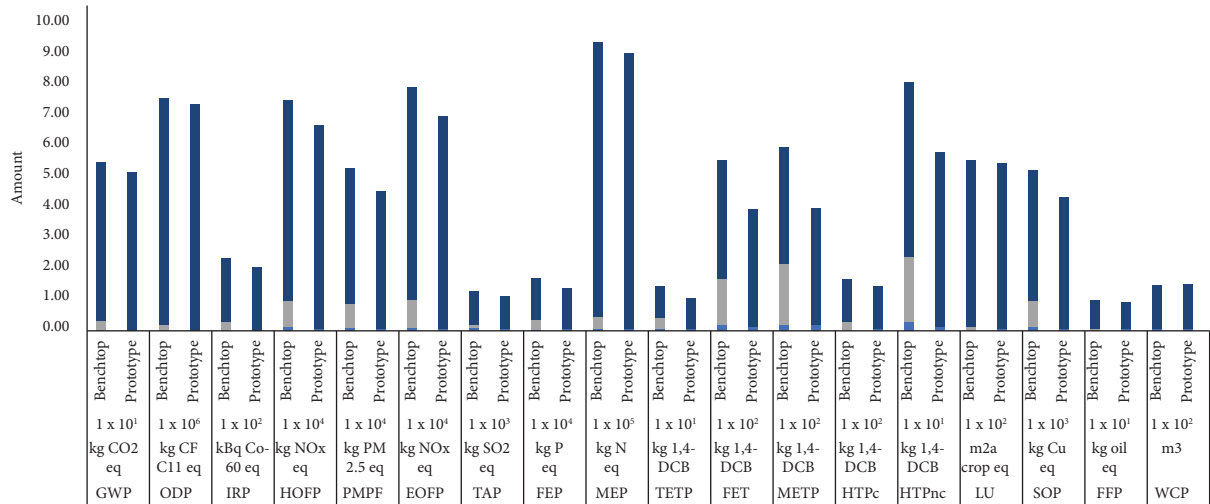


FIGURE 3: Hotspots for the benchtop VIS/NIR and the prototype devices based on the reference parameters. Impact categories and acronyms are reported in Table 7. Analytical tools (■), energy (■), laboratory materials (■), and calibration (■).

TABLE 9: Impact values related to the execution of the three methods, chemical, optical with benchtop device, and optical with portable device, to measure the three reference parameters to characterise grapes.

Impact category	Unit	Pull of three chemical analyses	Ratio % benchtop	Ratio % prototype
GWP	kg CO ₂ eq	1.66	33	31
ODP	kg CFC11 eq	2.40×10^{-6}	32	31
IRP	kBq Co-60 eq	6.69×10^{-2}	36	31
HOFP	kg Nox eq	2.16×10^{-3}	35	31
PMPF	kg PM _{2.5} eq	1.45×10^{-3}	37	31
EOFP	kg Nox eq	2.26×10^{-3}	35	31
TAP	kg SO ₂ eq	3.72×10^{-3}	35	31
FEP	kg P eq	4.45×10^{-4}	39	32
MEP	kg N eq	2.89×10^{-4}	33	31
TETP	kg 1,4-DCB	3.39	43	32
FET	kg 1,4-DCB	1.25×10^{-1}	45	32
METP	kg 1,4-DCB	1.23×10^{-1}	49	32
HTPc	kg 1,4-DCB	4.61×10^{-2}	37	31
HTPnc	kg 1,4-DCB	1.84	44	32
LU	m ² a crop eq	1.76×10^{-1}	32	31
SOP	kg Cu eq	1.39×10^{-2}	38	31
FFP	kg oil eq	3.15×10^{-1}	34	31
WCP	m ³	4.71×10^{-2}	32	31

environmental impact of the pool of the three chemical analyses; while for the prototype, an average value of 31% is considered. These results identify once again the advantages of using the prototype technology, which allows different parameters to be obtained with one single analysis due to a simplified system.

The results reported in Table 9 underline the importance of having a simplified device as it is the greenest solution among those evaluated in this study, allowing a general reduction of the environmental impact in all the impact categories. Nevertheless, this statement cannot be assumed as completely reliable due to the fact that the performance of the instrument can be identified as a limiting factor. To evaluate the change of impact deriving from taking into consideration the performance of the optical devices, a normalisation of the results concerning this limiting factor was performed.

3.3. Performance Adjusted/Based Functional Unit.

Considering environmental aspects, the prototype appears to be the best choice in determining the three compositional parameters for the characterisation of grapes, but its performance may not be so reliable in obtaining precise and trustworthy results. For this reason, as cited in the inventory phase for the optical analyses, the performance factor was also included. Therefore, the study compared the conventional analyses with the two optical methods (benchtop and prototype) in order to observe how results change if the attention is focused not only on the environmental impact but also on the performance of the devices.

Table 10 represents the performance of the three scenarios analysed. Three main factors were taken into consideration: the mean, the root mean square error of cross-validation (RMSEcv), and the final performance of the

TABLE 10: Mean, root mean square error of cross validation, performance, and correction factor of the three methods under study.

Method	TSS			TA			pH			Pull of three analyses Ap (%)	CF
	<i>m</i>	RMSEcv	<i>P</i> (%)	<i>m</i>	RMSEcv	<i>P</i> (%)	<i>m</i>	RMSE cv	<i>P</i> (%)		
Benchtop	21.45	0.7	97	10.22	1.09	89	3.215	0.08	98	95	1.06
Prototype	22.9	1.31	94	6.9	0.83	88	3.33	0.09	97	93	1.07

Ap, average performance; CF, correction factor; *M*, mean; *p*, performance; RMSEcv, root mean square error of cross validation.

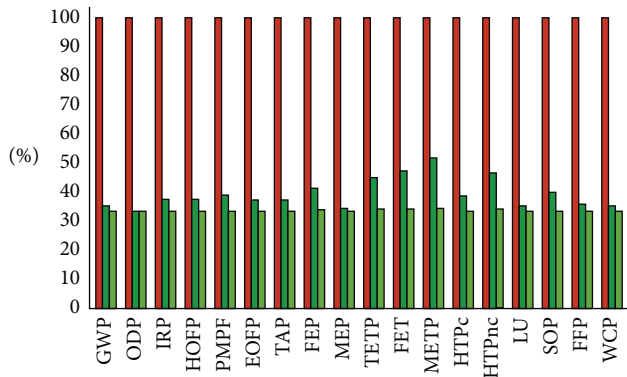


FIGURE 4: Comparison between the environmental impact of the two optical analyses, benchtop (■) and prototype (■), compared to the pool of the three chemical analyses (■) after the performance evaluation.

procedures. The three chemical methods were considered as the best choice in terms of reliability of results assuming an error equal to zero and a performance that reaches a value of 100%. Assuming that the three chemical analyses are the best solution to obtain results without errors, between the two optical methods, the benchtop device appears to have a better performance in determining all the three quality parameters (97% for TSS, 89% for TA, and 98% for pH) with respect to the prototype device that appears to be less precise. The last column of Table 10 reports also the correction factor (CF) which was calculated by relating the average performance (Ap) of the chemical analyses (equal to 100%) with the average performance (Ap) of the benchtop and prototype, respectively. For the benchtop, a correction factor of +6% must be applied to reach the same performance as the chemical analyses, while for the prototype solution, the CF is equal to +7%. These results highlight how the benchtop technology is an effective choice that produces similar and precise values to those obtained with the conventional method compared to the prototype, even though the LCA study recognises it as the better solution in terms of environmental impact.

According to the normalisation of the results concerning the performance of the two optical instruments, the gap between the pool of the three chemical analyses and the two optical solutions decreases. Despite this change in the gap and even if the benchtop technology has a higher performance with percentage points between +1% and +3% compared to the performance of the simplified system, the prototype is once again the most convenient solution

compared to the benchtop because it requires a lower number of analyses to reach the same results as those obtained from the pool of the three chemical analyses.

The environmental impacts of the two optical analyses compared to the pool of the three chemical analyses after the performance evaluation are reported in Figure 4, which recognises the prototype device as the best solution in terms of environmental impact compared to the benchtop instrument.

4. Conclusions

The optical analyses are already validated systems in food production to reduce the environmental impact along the chain by adopting not only benchtop solutions but also portable and simplified technologies. The environmental impact of wet-chem analyses, optical with benchtop, and optical with the simplified prototype were analysed and compared in this study to characterise and evaluate the quality of grapes. The results obtained from the study highlight that the use of chemicals during the procedures of the wet-chem analyses is the main driver of the environmental impact, while for what concerns the optical analyses with the two different instruments, the calibration phase is the most impactful factor. At the end of the study, it was possible to define the optical analysis with the prototype as the most suitable and greenest solution to obtain the three quality parameters. Nevertheless, the study did not consider the variability of results due to the performance of the two optical devices; therefore, an additional observation was made normalising the results obtained with respect to a performance factor. Considering only the performance, the benchtop solution is the best choice because it produces similar and precise values to those obtained with the conventional method, even though it has a higher environmental impact compared to the prototype device. After this evaluation, results were normalised to the performance of the two devices and the results showed how the optical analysis with the portable device is once again the best solution to obtain much more reliable measurements compared to the benchtop instrument. Research should consider the environmental advantages of these optical analyses relating them to a performance evaluation to identify the best solution in terms of both performance and environmental impact. This study could be a starting point for further works, which will consider a similar environmental comparison but applying it to different agri-food products that need other kinds of quality analyses.

Innovations in agriculture and the development of smart solutions could represent advantages of managing and monitoring agri-food product quality and propose actions to reduce waste and the impact of the agri-food supply chain in a view of agriculture 4.0.

Data Availability

The data that support the findings of this study are available from the corresponding author upon request.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Authors' Contributions

All authors contributed significantly to the manuscript and are in agreement with the manuscript.

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Supplementary Materials

Figure S1: Graphical abstract of the study. (*Supplementary Materials*)

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