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Classification of waste wood categories according to the best reuse using FT-NIR spectroscopy and chemometrics

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HIGHLIGHTS

- Waste wood composition is the key-point for deciding the best suited applications.
- Waste wood were divided into three categories according to the best-suited reuse.
- Classification models were developed to separate the material in the three classes.
- Results suggest that Near Infrared Spectroscopy can be used for real-time sorting.

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ABSTRACT

In Europe, the volume of waste wood is increasing. Waste wood can be reused, promoting circular economy and avoiding landfills. It can be used as a bioenergy feedstock reducing the use of fossil fuels, or be reused for producing new composite wood material. Only wood with hazardous substances needs to be disposed. To this aim waste wood samples were collected from a panel board company and several recycling centres in Italy and Denmark. The samples were assigned to waste wood categories and analysed by Near Infrared Spectroscopy. Principal Component Analysis was used to investigate sample variability and Soft Independent Modelling of Class Analogies (SIMCA) for classifying the samples according to the appropriate reuse: energy production, panel board production or landfill. The results are good, with a classification rate of 90% for virgin wood material and 86.7% for treated wood material. The classification of waste wood is key for turning it into a secondary resource.

1. Introduction

Wood represents a valuable, and is one of the oldest, resource and it is used for a wide range of applications, e.g. paper, building, energy production [1]. The utilized wood ends up in waste streams and generates post-consumer waste, better known as waste wood. A recent study has estimated that in the European Union 50 million m^3 of waste wood are generated [2]. By 2030, waste wood is expected to contribute with 59–67 million m^3 to annual European Union wood demand [3].

Because of its relatively high calorific value most of this material is incinerated with energy recovery [2, 4]. However, waste wood may equally meet the requirements for other recycling options, as wood-based panel production. In 2019, the total wood-based panel production was 74.0 million m^3 and the consumption 76.4 million m^3 [5]. One of the most prominent recycling options for waste wood is particleboard, with a European production of 34.8 million m^3 in 2015 [6]. Because of the increasing attention on recycling and the European policy targets encouraging circular economy, waste wood could represent a valuable resource for recycled materials instead of being incinerated or disposed.

In general, most waste wood could be used for energy recovery or recycled for the production of wood engineered products, such as building material [7, 8]. The recycling potential of waste wood is still low because of the presence of contaminants in wood products, which limits considerably its recycling or reuse [9]. In fact, wood is subjected to different treatments, i.e. heat, chemical or mechanical treatments, that involve preservatives containing organic and inorganic contaminants [10, 11]. Those contaminants may represent an issue in the waste wood management, because they can lead to contamination of soil, water or air. In Europe, some preservatives have been banned because they are hazardous (e.g. Chromated Copper Arsenate - CCA, Pentachlorophenol - PCP and creosote), while others are considered

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hazardous only when exceeding specific limits [12]. As a result, in order to be reused for producing wood-based panels waste wood should contain a low level of those contaminants [8]. In general, the end-point for these waste wood materials is the landfill, but it is neither a sustainable nor a cost-efficient option compared to reuse [8].

As a consequence, it is evident that the recycling or reuse of the material could be maximized if the waste wood is properly sorted and handled based on the quality and characteristics of the material itself. Waste wood composition is the key-point for deciding the best suited applications. It is a very heterogeneous material because of the different sources and applications it can come from [13], and a proper sorting based on the quality grade of the material is essential to ensure a high-quality, clean and safe recycling loop.

It is important to consider that also the definition of waste wood categories is not the same across the European countries. For instance, wood with preservatives, paintings or other chemical substances can be used to produce and add value to products such as composites, but not for energy production on the basis of categories and laws of the different European countries [14]. Countries such as Finland, Italy, Germany and United Kingdom have defined the quality indicators for the classification of waste wood in several categories on the basis of their quality and related applications [14]. As an example, glued and painted wood can be used as biofuel in Germany and United Kingdom but it is not allowed in Italy. Finnish classification is similar to the British one, but with some limitations for the energy use of these materials [14]. Regarding Denmark the classification is similar to the German one. The post-consumer waste wood is divided into four quality classes (A1 to A4). The two upper classes are suitable for recycling, the third class (treated wood and wood-based panels) may also be used for particleboard production as long as not exceeding thresholds for selected chemical elements and the last (A4) for disposal of because of hazardous material, due to being impregnated with preservatives or painted. On the contrary, in Germany the third class is sent for incineration [9].

Some studies have already been carried out on the characterization of waste wood composition to determine the suitability for combustion [15-17], and also to check the product quality and safety associated with recycled products [13, 18, 4]. These studies could form the basis for discriminating waste wood according to its quality and deciding the best recycling options. However, the weak point is the use of the traditional lab analysis that employ complex, expensive and long procedures, which make the real-time sorting impossible. In addition, traditional lab analysis requires a sampling of the waste wood material directly along the sorting process or in the waste wood pile and a subsequent transfer of the sample to the lab. Only a few grams of material are used for the lab analysis compared to the tons of waste wood handled, leading to well-known problems of reliability of the results due to the huge variability in material composition [19, 20]. As a consequence, a technique that is rapid, economic, simple, and that can classify directly in the process line is necessary. A good candidate is near infrared spectroscopy (NIRS) [21] which is already widely used in other recycling processes, but with a limited number of studies [22, 23]. However, no studies have been carried out on the discrimination between the different categories of waste wood using spectroscopy, which has huge benefits in terms of real-time quality sorting directly in industrial applications.

The overall aim of this study is to characterize the waste wood material based on its quality and consequently determine its most suited applications. According to the possible applications and recycling options, waste wood has been divided in three main categories: virgin wood, treated wood and disposal wood. Virgin wood can be used either for wood-based panel production or energy applications, treated wood for wood-based panel production or energy applications in big combustion plants provided with gas cleaning filters, and disposal wood should be sent to disposal as the contaminants could persist in sequential recycling loops. A second aim is to investigate the performance of class- and discriminant modelling when applied for sorting problems. In fact, it is well known that these classification tools have similar aims [24], but their application may depend both on the problems studied and the type of material analysed. In the class-modelling approach a set of samples belonging to a specific class (the target class) is modelled. This individual class-model is then used to assign an unknown sample to the target class or not, based on the similarities of the new sample with the target class samples. On the other hand, in discriminant modelling approach, all the possible classes are well known and the model space is divided in different regions based on the differences among the analysed samples. As a consequence, a new and unknown sample is always assigned to one of the classes even if it belongs to none of them.

To reach this aim more than one hundred samples have been collected and analysed by means of Near Infrared Spectroscopy. Principal Component Analysis (PCA) has been used to investigate the variability of the spectral data and Partial Least Squares - Discriminant Analysis (PLS-DA) and Soft Independent Modelling of Class Analogies (SIMCA) for separating the samples in the different waste wood categories. Variable selection has also been applied for improving the classification performance and investigating the most relevant wavelengths responsible for the discrimination among the three waste wood categories. In addition, variable selections emulate the use of an NIR instrument with fewer wavelengths, showcasing how a simpler system, more suitable for industrial processes, could handle such data.

2. Materials and methods

2.1. Collection of waste wood samples

Waste wood samples were collected in different locations in Italy and Denmark during September and October 2020. The sampling involved three recycling centres in Danish municipalities: Hvidovre (HVI), Audebo Miljøcenter - ARGO (AUD) and Vestamager (VES) and two in Italian municipalities: Ostra (OST) and Pollenza (POL). In addition, samples were collected in a panel board company (Gruppo Mauro Saviola s.r.l. – SAV) and a company producing blocks for pallets (EcoBlocks s.r.l. – ECO). In all the sampling sites waste wood consisted mainly of large pieces of woody material such as items of furniture, fiber board and pallet. The sampling was carried out from static lots, focusing on collecting as many different qualities as possible, with several samples of each waste wood quality. We are well aware that this is far from how a classification could be implemented in the industry, as the whole sampling procedure in itself is an important issue. We have, though, earlier published a study focusing on this important aspect [20], and will therefore not go into that aspect in the current work.

In order to choose the proper reuse of the material according to its characteristics, the collected waste wood was sorted into 12 subcategories as reported in Table S1 (supplementary material). The identification of waste wood category is relevant before deciding the best-suited application and defines possible end-users. Because of this, the 12 sub-categories can be merged into three main waste wood categories according to the possible reuse of the material: i) virgin wood (VW), i.e. clean wood, that can be used both for panel board production and energy applications; ii) treated wood (TW), consisting in wood mixed with glue/resins (panel board, plywood, oriented-strand board, etc.) that can be reused for panel board production or energy applications in big combustion plants provided with gas cleaning filters; and iii) disposal wood (DW), consisting of impregnated and painted wood that needs to be sent to the disposal and cannot be reused.

2.2. Sample preparation

The sample preparation consists in a combination of sample division (reduction of the sample mass) and particle size reduction paying attention to maintain the representativeness of the material, as will be explained in detail below. Since the samples were collected in their original form, ensuring an accurate waste wood characterization, and mainly consist of large pieces, they need to be reduced prior to the NIR analysis to simulate the size of the material during a regular industrial sorting process (around 5 cm).

The size of the material was reduced using a log splitter, as it in this way was possible to obtain the desired particle size of around 5 cm. Unfortunately, we could neither use an industrial/professional shredder (because of the small quantity of material to grind) nor a portable shredder (because of the too small particle size it generates).

As a final step, the sample size was reduced through a quartering process. It consists in piling the sample, dividing it into four, and combining the two opposite fractions. This process is repeated until the wanted sample size is achieved. At the end a total of 117 samples were obtained.

2.3. Near-infrared data

All the waste wood samples were analysed by means of a Foss DS2500 spectrophotometer (Foss A/S, Hillerød, Denmark) equipped with a silicon detector. The Vis-NIR spectrophotometer used an open ring cup cell (large sample cup, 12 cm diameter; FOSS cup) and absorbance was recorded every 2.0 nm from 400 to 2500 nm for a total of 1050 data points. The samples were acquired in diffuse reflectance mode using an integrating sphere and were kept in rotation during the acquisition by means of the spinning cup. During the automatic rotation of the cup 32 spectra were recorded for each replicate. Instead of automatically averaging across these 32 scans, we decided to keep all 32 sub-scans in order to have an improved representativeness of the heterogeneous samples. Each sample was scanned three times, by mixing the analysed aliquot of material with the rest of the sample and picking up another aliquot.

A blank spectrum was collected at the beginning of each sample analysis to remove the random effects associated to the instrument and environment by using a spectralon standard with 100% reflectance as background. All the spectra were collected at room temperature. The resulting dataset consists of 11232 observations (32 spectra × three subsamples × 117 samples) and 1050 wavelengths.

The dataset presented in this study can be found in an online repository. The dataset is uploaded to Zenodo repository with data DOI's assignment (http://doi.org/10.5281/zenodo.7057777).

2.4. Multivariate data analysis

Principal Component Analysis (PCA) was computed to investigate the spectral data and search for groupings and similarities among the different waste wood categories and sub-categories. Any clustering can be helpful for the development of the classification models. For improving the visualization, confidence ellipses were calculated for each waste wood sub-categories using a local PCA on the scores. The loading plot of the two first Principal Component (PCs) was investigated to identify the compounds associated to the distribution of the samples in the score plot. Before any model computation, different standard preprocessing methods were tested, i.e. Standard Normal Variate (SNV), Multiplicative Scatter Correction (MSC), first and second derivative (Savitzky-Golay with 9 or 13 smoothing points and 2nd order polynomial) [25]. In addition, a simple offset correction has been tested (only removing the spectral average).

The data set was split into training and test sets using a constrained random selection. The training set (n = 87 samples) was used to develop the classification model and the test set (n = 30 samples) to validate the model and check its classification performance with unknown samples. The selection was constrained to ensure that all waste wood categories and sub-categories are well distributed both in the training and test sets. The test set remained fixed for all the computations. SIMCA and Partial Least Squares-Discriminant Analysis (PLS-DA) models have been used as supervised classification techniques for separating the samples in the different waste wood categories.

SIMCA models have been developed individually taking into account the three different categories as target class. The position of a new sample was calculated by projecting them on the loadings of the created PCA model. For determining the boundaries around the samples belonging to one particular class Hotelling T^2 and the residual values were considered. Confidence limits were set at $\alpha = 0.05$. If the projected sample is situated within the boundaries of the target class, then it is assigned to that particular class. The classification boundaries/limits have been computed using the formulas:

$$lim_{res} \geq \frac{(m-1)res^2}{X^2_{1-\alpha/2}}$$

$$lim_{T^2} \geq \frac{(m-1)T^2}{X^2_{1-\alpha/2}}$$

where m is the number of samples, res are the residual values, T^2 are Hotelling T^2 values and $X^2_{1-\alpha/2}$ is the chi-squared distribution [26]. Several SIMCA models have been developed using these boundaries and taking into account different number of PCs (up to 8); all the classification results have been stored and the best model has been selected based on the misclassification error in the calibration set.

In order to investigate how the sensitivity of the classification performed according to the set boundary limits, we decided to test different boundary limits by adding an offset to the two limits. This offset is based on the mean Hotelling T^2-value or mean residuals multiplied by a number, n, going from 0.1 to 1.9 in steps of 0.1. The formulas are:

$$new\ lim_{res} = lim_{res} + n^*mean(res)$$

$$new\ lim_{T^2} = lim_{T^2} + n^*mean\left(T^2\right)$$

The accuracy of the classification models was determined using the Receiver Operating Characteristic (ROC) curve. Sensitivity or True-Positive Rate (TPR) and specificity or True-Negative Rate (TNR) values as well as accuracy and misclassification rate were computed to measure the ability of the model to recognize the samples belonging to a given class or reject samples not belonging to that class. The classification results have been stored both considering all the scans individually (as though each scan is a different sample) and counting the number of the correctly classified scans for each sample replicate and, based on that, assigning the sample to a specific class. We have decided to set a classification threshold of 16 or 10 correctly classified scans (out of 32), i.e. 50% and around 30% of the total number of scans. It is imperative for the success of the classification that we allow for a lower threshold than 100%, as there is a high variability in the material [15, 16]. Finally, in order to validate the classification results, and ensure consistency and robustness, 10 different SIMCA models were computed for each category reducing the training set by around 30% and using the same samples as before as a test set.

PLS-DA models were also developed for classifying the samples in the three different waste wood categories considered in this study. The models were validated both using venetian blind-cross validation (5 segments, keeping scans of the same replicate together in the same segment) and the external test set. A sample is assigned to a category when it scored close to one, using a binary system.

Finally, *ad-hoc* variable selection has been applied to the best SIMCA classification models in order to increase the prediction accuracy and reduce the model complexity.

All the multivariate data analysis was computed using Matlab software (ver. MATLAB R2019b, The MathWorks) with in-house functions based on existing algorithms.

3. Results and discussion

3.1. Spectra

The recorded spectra were visually inspected in order to detect the differences among the three waste wood categories. The spectra were pre-processed with a second derivative (Savitzky-Golay with 9 smoothing points and 2nd order polynomial). The average spectra of virgin wood (VW), treated wood (TW) and disposal wood (DW) were investigated, see Fig. 1. Please note that we have decided to focus on the NIR range of the spectra (1100 to 2500 nm), as the visible part does not contain significant information with regards to the classification task. It is evident that the largest differences occur between the group of virgin/disposal wood and that of treated wood. In order to get a clearer picture of the important differences between the waste wood categories, plots showing the overlap of the variability of pairs of waste wood categories were made, see Fig. 2. This gives a nice overview of the variability of the spectra, and is helpful for highlighting the spectral regions where a higher difference occurs. Some useful spectral dissimilarities between virgin/disposal and treated wood can be noticed in the region between 1450 and 1500 nm, 1950–1980 nm and 2300–2390 nm (Fig. 2A and Fig. 2B). The disposal and virgin wood curves are to a large extent overlapping, but with some differences in the disposal wood curve located at 2140 nm, 2314 and 2352 nm (Fig. 2C). This is probably because the painted or impregnated part consists only of a thin layer on the top of the sample and the core is made of virgin wood. To get an estimate of the similarities/dissimilarities between the categories the percentage of the non-overlapping part of the spectra (area marked in yellow in Fig. 2) was computed and reported in the figure. The percentage of non-overlapping area is the highest between virgin and treated wood (52.2%) and similar between disposal and virgin (38.3%) and disposal and treated wood (34.7%). A higher percentage of non-overlapping area indicates a simpler classification task. Once again it was demonstrated that the most important differences in the curves are related to dissimilarities in chemical composition between treated and virgin wood.

Some of the most important differences in the variability of the waste wood categories, and consequently the most important wavelengths for the discrimination of the three waste wood categories, are reported with grey areas in Fig. 1 and they are:

- Area I between 1450 and 1500 nm: at 1458 nm it is possible to observe a higher peak of the treated wood samples with respect to the others. In addition, it can be noted that DW and VW lines have a minimum at 1470 nm, while in the TW line this minimum is moved forward to 1488 nm.
- Area II between 1950 and 2020 nm: there is a deviation in the TW curve from the DW and VW curves at 1956 and 1972 nm and a shift in TW for the peak at 2010 nm.
- Area III between 2300 and 2390 nm: this is probably the most interesting area with respect to the differences among the three waste wood categories. A minimum and a maximum can be observed in the TW and DW lines at 2314 and 2322 nm, while the VW line is smooth. In addition, the VW curve has two narrow peaks at 2352 and 2362 nm, whereas DW presents just one peak at 2362 nm and TW the same peak at 2362 nm and a smaller at 2350 nm. Furthermore, DW and VW curves have a broader minimum at around 2380 nm, while TW has a sharper minimum at 2388 nm.

Finally, another useful difference is the shoulder in the VW spectrum at 2248 nm, not detected in the other two spectra. The bands associated with virgin waste wood are normally linked to C-bonds, since the lignin and hemicellulose have a higher concentration in the virgin wood, compared to treated wood. Whereas for treated wood we can find N-bonds related to the glue [27].

The assignment of the most important wavelengths reported in Fig. 1 are listed in Table 1. Please consider that for interpretation purposes a negative peak in the 2nd derivative equals a (positive) peak in the raw spectra.

3.2. Principal Component Analysis

A PCA was calculated to investigate the variability of the spectral data. It was of special interest to explore if there are any groupings among the three waste wood categories according to the possible reuse of the material. Spectra were pre-processed with the second derivative, as described in Section 3.1, and were averaged across the 32 NIR measurements to reduce the spectral variation before the model computation. Fig. 3B reports the score plot of the two first PCs. To have a better view of the spectral variability of the samples and their distribution according to the waste wood sub-categories we have also reported the PCA score plot of the pre-processed NIR dataset without averaging the 32 NIR measurements (Fig. 3A).

At a first glance the samples seem to spread across the whole score space without any clear groupings. However, a closer inspection shows some trends in the distribution of the samples, i.e. the treated wood

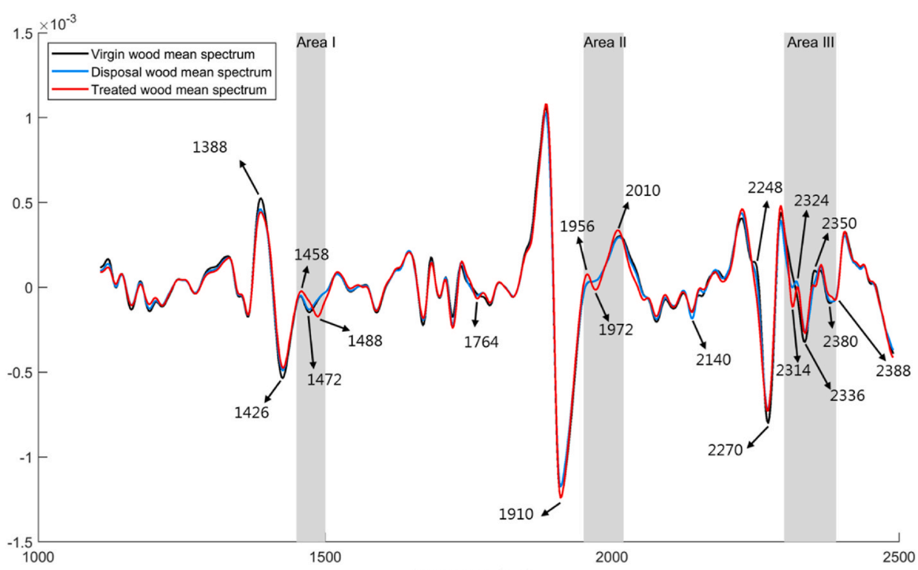

Fig. 1. Mean spectra of virgin, treated and disposal wood samples pre-processed with second derivatives (virgin wood samples: black line; treated wood samples: red line; disposal wood samples: blue line). The numbers refer to the main spectral differences also reported in Table 1. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

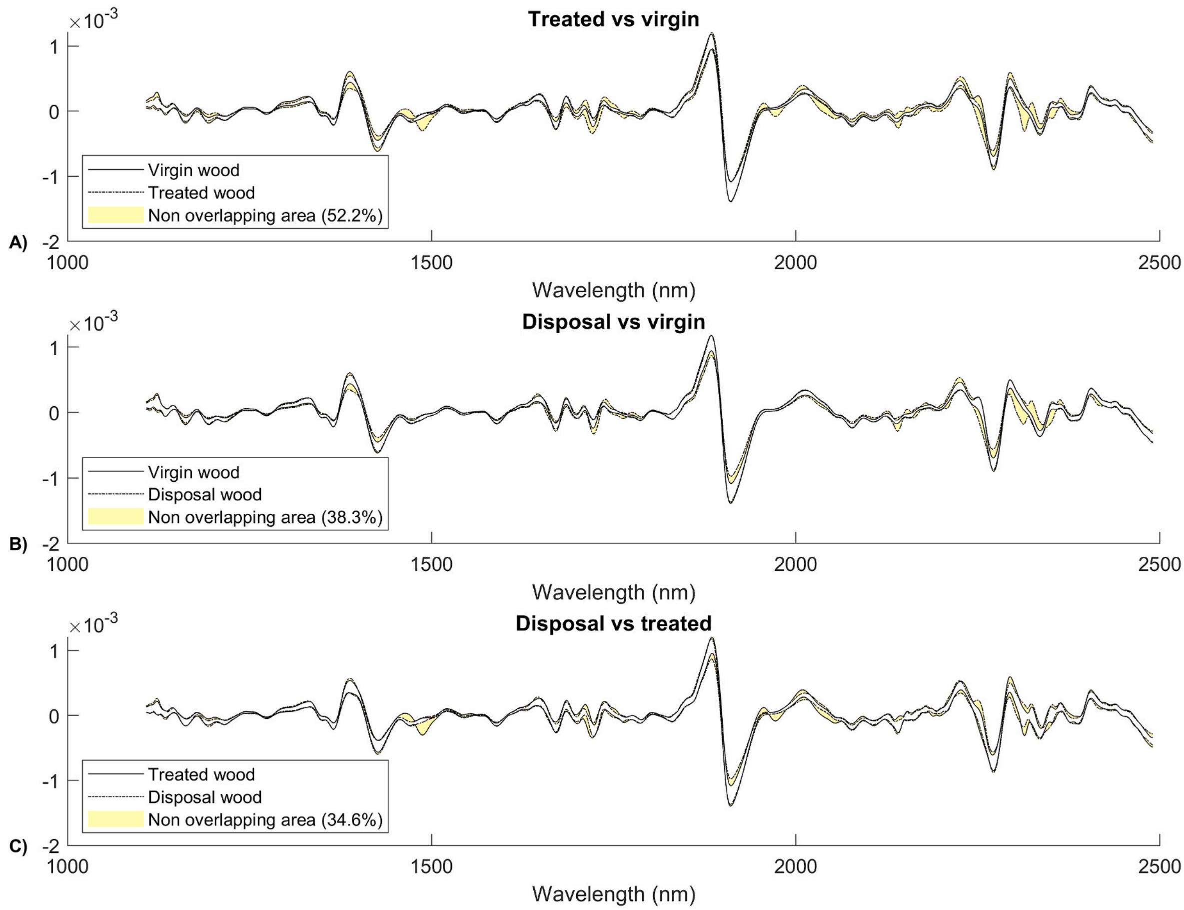

Fig. 2. Comparing the confidence intervals at each wavelength of the pair-wise comparison of the three different waste wood categories: A) treated vs virgin wood; B) disposal vs virgin wood and C) disposal vs treated wood. Non-overlapping areas are highlighted in light yellow, and the sum of this area compared to the total area between the highest and lowest confidence limits are given in the legend of each individual figure. Larger numbers indicate simpler classification task. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

samples are mostly located in the negative part of PC1 while the virgin wood samples are to the positive direction. To make a clearer picture of the differences among the waste wood categories considered in this study, confidence ellipses were computed using the standard error for each waste wood sub-category. Fig. 3C reports the same plot as Fig. 3B, but now with confidence ellipses instead of each individual subsample being plotted. The plot clearly shows some groupings among the waste wood categories. The virgin wood samples are located in the upper right corner of the score plot, while the treated wood samples are located in the lower left corner of PC1 and PC2. The samples with negative values for PC1 have a higher degree of glue (they are mainly composite wood), while the ones placed in the bottom right part of the score plot (positive PC1 and negative PC2 values) present a lower degree of contamination/higher presence of virgin wood. These latter samples belong to the categories of fruit boxes (PB – type 12), floor (FL – type 7) and solid wood furniture (FT – type 2), in other words, the moderate treated wood. Finally, the disposal wood samples are spread in the PCA score space. Impregnated wood (IW) is placed in the area of the virgin wood, while the painted wood (PW) is almost at the centre of the PCA score plot. This nicely confirms the findings of the small differences between DW and VW found in section 3.1. We will discuss further about the similarities of the waste wood sub-categories in section 3.4.

As a note, it can be mentioned that we also have computed the PCA testing different pre-processing methods, where both Multiplicative Scatter Correction (MSC) and offset correction gave similar results (results not shown).

The loadings are inspected to understand which variables characterize the different waste wood categories and identify the compounds associated to the discrimination between the three categories. The first two loadings were considered as they cover 62.67% of the explained variance and they are able to detect most of the characteristic spectral bands, as marked in Fig. 1. In fact, in Fig. 3D it is possible to observe that the first loading shows the main bands at 1422, 1468, 1906, 1922, 2274 and 2326 nm, and the second loading at 1706, 1742, 1886, 2226 and 2292 nm. The first loading is mostly related to differences between virgin and treated wood samples, while the second loading shows differences between the treated wood and disposal wood samples. The third component describes further differences between the virgin and treated wood (Fig. S1 of supplementary material).

3.3. Classification models

Both SIMCA and PLS-DA models have been used as supervised classification techniques for separating the samples in the different waste wood categories. Several PLS-DA models were developed testing different pre-processing methods, but without obtaining any satisfactory results. This is in-line with the findings of Malyjurek et al. [41], who also found that PLS-DA was insufficient in a case where the classes were not linearly separated. The best model was developed using 5 LVs and second derivative as pre-processing, achieving a misclassification error of 19.66%. The NIR scans have been averaged across the replicate before model computation. Due to this result, this manuscript will focus on the SIMCA classification models.

SIMCA classification models were developed using offset correction

Table 1
Absorption band assignment associated with the main spectral differences between the three waste wood categories. The rows marked with '*' refer to the wavelengths located in the three grey areas reported in Fig. 1. (str.: stretching; bend.: bending; OT: overtone; L: lignin; H: hemicellulose; C: cellulose; E: extractives). The bibliography wavenumbers (cm^{-1}) have been converted into wavelengths (nm) (reported in italic in the table) for a better comparison with the measured wavelengths.

	Measured nm	Bibliography		Assignment	Compound	Reference
		nm	cm^{-1}			
1	1388	1386		1st OT OH str.	–	[28]
				1st OT CH str. + CH def.		
2	1426	1428		1st OT OH str. + H_2O	C/H_2O	[28]
		1428	7008	1st OT OH stretching (amorphous region in cellulose)	C	[29,30]
3*	1458	*1455*	6874	1st OT OH str. (phenolic groups)	L	[31]
4*	1472	*1470*	6802	2nd OT and combinations modes of NH stretches	glue	[32]
		1470		1st OT NH asymmetric stretching	resin	[30]
5*	1488	1489		1st OT OH str.	C	[28]
		1490				[30]
		1489	6718	1st OT OH str.	C	[33]
		1488	6720			[29]
		1485	6720	1st OT NH symmetric stretching	resin glue	[30,34]
		1488				
		1485	6736	Second overtone of NH stretching from urea, amine, or amide	resin	[35]
		1484	6737	2nd OT and combinations modes of NH stretches	glue	[32]
6	1764	1765		1st OT CH str.		[28]
		1767	5660	1st OT CH str.	glue	[29]
7	1910	1910		2nd OT C=O str.	H	[28]
		1902	5257 (?)	1st OT CN functional groups	glue	[27,36]
		1908		OT NH str. of urea	glue	[37]
8*	1956	1960		NH combination bands		[38]
9*	1972	*1967*	5084	NH stretching and bending of OH combination band	glue	[35]
		1978	5055	NH asymm. + NH amide II	glue	[34]
10*	2010	*2016*	4960	Associated with $C{=}ONH_2$ groups	glue	[35]
		1989–2020	4950–5028	combination modes between the N–H	glue	[32]
				stretches and rocking and bending modes of the NH_2 groups		
11	2140	2134		C_{ar}-H str. + C=C str.	L/E	[28]
		2134		CH str. + C=O str.	H	[28]
		2134	4685	Combination CH str. and C=O str. in acetyl groups	H	[39]
12	2248	*2253*	4439	CH str. and CH bending combination band	Resin	[35]
		2248	4449	Stretching-bending combination	urea	[32]
		2247	4450	CH_2 combination of methylol	glue	[27,40]
				Group		
		2247		CH_2 combination band of the methylol group	glue	[30]
13	2270	2270		OH str. + CO str.	C	[28]
		2267		OH str. + CO str.	L	[28]
		2271	4404	CH_2 stretching + CH_2 deformation	C	[33]
14*	2314	*2314*	4322	Urea	glue	[37]
		2313	4324		C	[39]
15*	2324	2328		CH str. + CH def.	H	[28]
16*	2336	2336		CH str. + CH_2 def.	L	[28]
		2336	4280	CH str. + CH def.	C	[33]
		2336	4281	Xylans	C/H	[39]
		2335		CH str. + CH_2 def. combination band	C	[30]
17*	2350	2343		CH str. + CH def. and/or 2nd OT C–H def.	C	[28]
		2347		CH (1st OT CH_2 symmetric stretching and δ CH_2) combination	C	[30]
18*	2380	2380		2nd OT OH def	Holo	[28]
		2384	4195	OH stretching and CO stretching, as well as CH str and CC str		[31]
19*	2388	2384		Not assigned	L	[28]
		2382	4198	2nd OT CH def.	C/H	[33]

as pre-processing. Other pre-processing gave good results for TW-SIMCA and/or VW-SIMCA models, but we decided to use the offset correction as it simplifies the model complexity, and to keep the same pre-processing for both SIMCA models. The samples have been split in training and test sets by constrained random selection as explained in section 2.4, ensuring the representativeness of the collected samples in both datasets.

SIMCA was applied to discriminate between the three waste wood categories. Treated wood and virgin wood classes were modelled separately by selecting the best performing confidence limits (n between 0.1 and 1.9) and the appropriate number of PCs necessary to describe each class (up to 8 PCs). We also tried to develop a SIMCA model with disposal wood as target class, but without obtaining any good results. This is probably because of the similarity of these samples with both VW and TW classes as also reported in the previous sections. However, the disposal wood samples can be recognized as the samples not belonging to either the virgin wood nor the treated wood target classes.

As a first approach in the SIMCA models, they were made based on averaging the spectra across each sample replicate and across each sample. However, this gave inferior results (results not shown), and as such was omitted from further investigation. This could be related to the similarity between some waste wood subcategories. In fact, averaging the NIR scans diminishes the differences between the classes, as the chemical differences between the samples are not observed homogenously across a sample, but rather in specific areas, and thus the chemical details are found in the specific scans, and not at the average level.

Table 2A summarizes the classification parameters for the SIMCA model on VW samples as target class, at scan, replicate and sample levels (VW-SIMCA). The model was developed on a total of 8352 spectra (2688 in the target class), corresponding to 87 samples (28 in the target class), and has been validated on a total of 2880 spectra (960 in the target

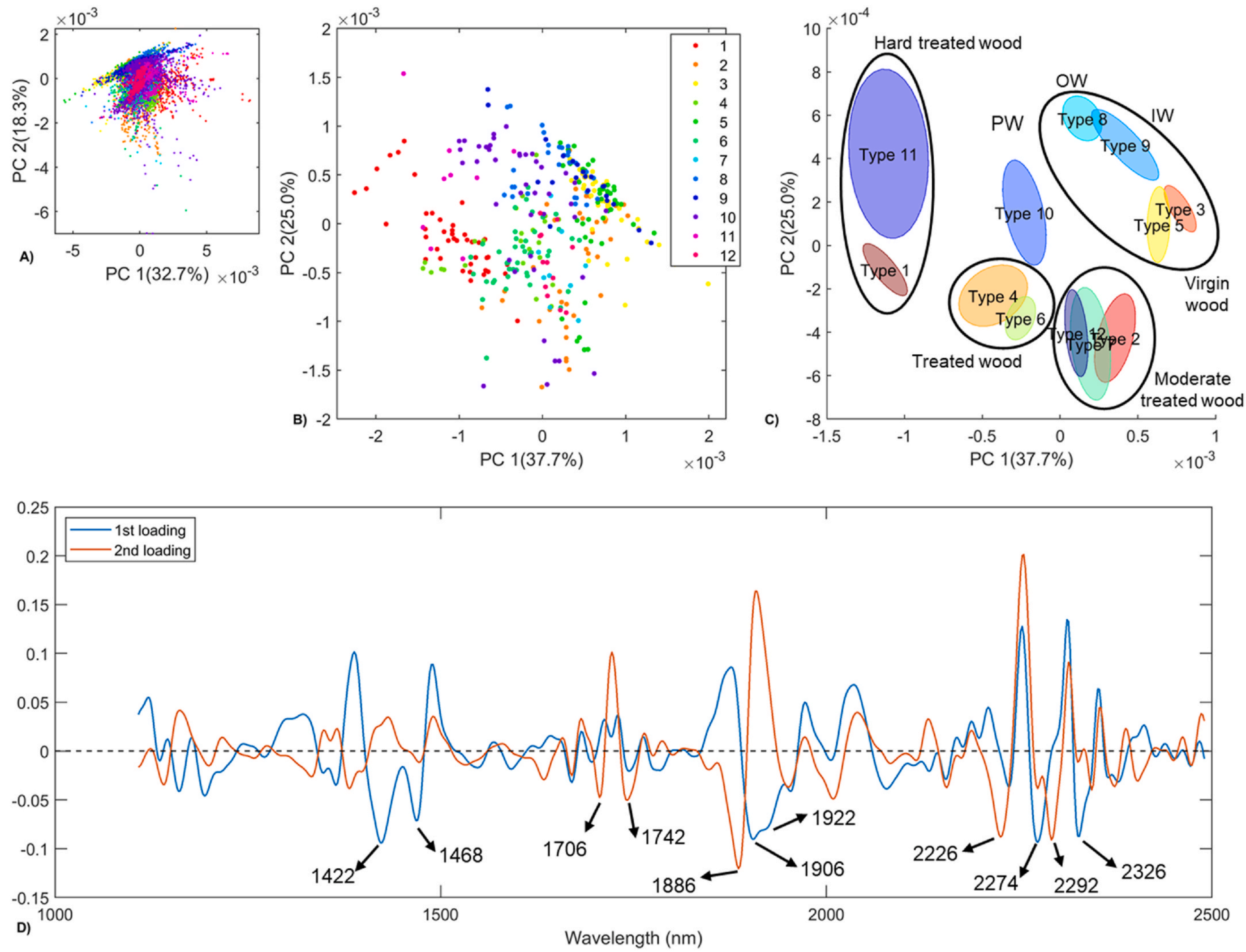

Fig. 3. A) PCA score plot of the two first PCs on the pre-processed spectra (without averaging the 32 NIR measurements) colored according to waste wood sub-categories. B) PCA score plot of the two first PCs on the pre-processed spectra (averaging the 32 NIR measurements) colored according to waste wood sub-categories. C) PCA score plot of waste wood sample with standard error ellipses for each waste wood sub-categories. (IW: impregnated wood; OW: old wood; PW: painted wood). D) The two first PCA loadings. Important wavelengths for the discrimination among the waste wood categories are marked with arrows in the plot.

class), corresponding to 30 samples (10 in the target class). For the model calibration a total of 8 PCs (99.83% explained variance) and a confidence limit $n = 1.4$ was found to be the optimal based on the calibration set (which includes 59 samples not used for making the PCA model).

The results clearly show how the classification performs better by moving from the scan level to the sample level. This is expected because of the high variability of the material. In fact, a scan of the same sample could be classified in one class rather than another simply by changing the spot of the sample surface analysed with NIRS (confirming the high variability of the material). Instead, at the replicate and sample levels a sample is classified in a class considering the majority voting of scans/replicates belonging to that specific class. The best model has been developed at the sample level with a misclassification error of 4.6% and 10.0% in the calibration and validation phase, respectively. At the replicate and scan levels the VW-SIMCA model recognizes the TW samples easier than the DW samples, and this could be related to the similarities of the IW samples with the virgin wood samples (see section 3.2).

Table 2B summarizes the classification parameters for the SIMCA model on TW samples as target class at scan, replicate and sample levels (TW-SIMCA). The model has been developed on a total of 8342 spectra (4598 in the target class), corresponding to 87 samples (48 in the target class), and has been validated on a total of 2880 spectra (960 in the target class), corresponding to 30 samples (10 in the target class). Ten outlying spectral scans have been removed from the training set of the TW-SIMCA before model computation because they have high residuals. For the calibration of the model only 1 PC (74.66% explained variance) and a confidence limit $n = 0.6$ have been used. (Fig. S2 reports the ROC curve for the first 8 PCs and the different classification limits for TW-SIMCA model showing how PC 1 is describing how treated wood is unique, while the higher PCs start describing wood in general). Also in this case, the classification results improve by moving from the scan level to the sample level. The best model has been developed at the sample level with a misclassification error of 8.0% and 13.3% in the calibration and validation phase, respectively. In general, at the replicate and scan levels TW-SIMCA model recognizes the DW samples better than the VW samples. The spectra of the moderate treated wood samples are close to the virgin wood spectra, meaning that the model detects some spectral similarities between treated and virgin wood classes (see section 3.2).

At the end, based on the obtained results it was also possible to

Table 2
A) Class performance parameters for the SIMCA model considering virgin wood as target class. (TNR: True Negative Rate; TPR: True Positive Rate; TW: treated wood; DW: disposal wood). B) Class performance parameters for the SIMCA model considering treated wood as target class. (TNR: True Negative Rate; TPR: True Positive Rate; VW: virgin wood; DW: disposal wood).

A)	Calibration				Validation			
	Scans	Replicate (16 scans)	Replicate (10 scans)	Sample (10 scans)	Scans	Replicate (16 scans)	Replicate (10 scans)	Sample (10 scans)
TNR	80.9	91.7	97.6	100.0	77.4	83.3	90.0	90.0
TPR (Total)	82.1	84.7	91.0	93.2	72.9	80.0	91.7	90.0
TPR (TW)	85.1	88.2	90.3	91.7	77.5	80.0	90.0	90.0
TPR (DW)	69.0	69.7	93.9	100.0	68.3	80.0	93.3	90.0
Accuracy	81.7	87.0	93.1	95.4	74.4	81.1	91.1	90.0
Misclassification error	18.3	13.0	6.9	4.6	25.6	18.9	8.9	10.0

B)	Calibration				Validation			
	Scans	Replicate (16 scans)	Replicate (10 scans)	Sample (10 scans)	Scans	Replicate (16 scans)	Replicate (10 scans)	Sample (10 scans)
TNR	63.6	64.6	84.7	87.5	67.5	66.7	83.3	90.0
TPR (Total)	70.0	75.2	94.9	97.4	48.5	41.7	80.0	85.0
TPR (VW)	73.8	81.0	97.6	96.4	49.7	46.7	76.7	80.0
TPR (DW)	60.3	60.6	87.9	100.0	47.3	36.7	83.3	90.0
Accuracy	66.4	69.3	89.3	92.0	54.8	50.0	81.1	86.7
Misclassification error	33.5	30.7	10.7	8.0	45.2	50.0	18.9	13.3

estimate the percentage of correctly classified disposal wood, as the samples never classified in the virgin wood nor treated wood classes of the two SIMCA models. We obtained a misclassification rate of 0% and 10% in the calibration and validation phases, respectively.

A total of 10 repeated SIMCA classification models were computed with reduced training sets and using the same fixed test set. The results clearly demonstrate the consistency and robustness of the developed models and suggest that the good classification performance is not related to random effects. Table S2 (supplementary material) reports the mean and standard deviation values of the 10 developed TW-SIMCA and VW-SIMCA models for each class performance parameter at the sample level. In general, the standard deviation is slightly smaller in the validation step with respect to the calibration step for the VW-SIMCA model and has an opposite trend for the TW-SIMCA model. It can be observed that for the VW-SIMCA model the highest standard deviation values are associated with the True Positive Rate (TPR) (DW) parameter (std = 6.0 in the calibration phase and std = 4.8 in the validation phase), while for TW-SIMCA model the highest standard deviation values are associated with TPR (VW) parameter (std = 6.3 in the calibration phase and std = 10.5 in the validation phase). This probably indicates the similarity of some waste wood sub-categories; VW with some DW samples (mainly impregnated wood), and the moderate treated wood with virgin wood (see section 3.4).

3.4. The challenging samples

As noted in the previous sections some waste wood sub-categories are more difficult to classify than others. This is due to their similarities in the chemical composition (also indicated by the large overlap in the PCA score plot) and in this section we will try to understand how the classification models could be improved and which are the most problematic samples to be classified. The main challenges for the waste wood classification are i) the partial overlap between DW (more specifically impregnated wood) and VW categories and ii) the high variability among the different treated wood sub-categories, with the moderate treated wood closer to the virgin wood category.

As already mentioned, DW spectra are very heterogeneous because the painted or impregnated part of the wood are located only in the external portion of the sample while the core part is made of virgin wood. This can be seen in Fig. 3B, showing the PCA score plot colored according to the waste wood sub-categories. Some DW scans are similar to VW scans in the PCA space, while others are more spread in the scores space. To better investigate this issue, we decided to colour the PCA according to the waste wood categories and the two subcategories of DW: impregnated wood (IW) and painted wood (PW) (see Fig. S3 in the supplementary material). We found that the impregnated wood is located close to the virgin wood category while the painted wood is more spread. This is nicely confirmed by Fig. 4A showing the mean spectrum of the VW, TW, IW and PW. It can be observed that IW and virgin wood samples are very similar, while PW and treated wood samples have a similar trend. The main differences can be observed in the three absorbance areas marked in grey in the figure where the characteristic absorbance bands of TW differ from the PW samples. In addition, a peak at 2140 nm can be observed in the PW curve, while IW is close to VW. This is also evident by looking at Fig. 4B, C & D, reporting a zoom of the specific wavelength regions marked in Fig. 4A where the main differences among the different types of wood occur. Fig. 4A explains the position of the impregnated and painted wood samples in the PCA score plot and why they are difficult to be classified in the SIMCA models.

Another subset of samples difficult to classify are the moderated treated wood samples. The treated wood samples present a high variability among the different waste wood sub-categories as also shown in Fig. 3. It can be observed that the main differences are related to the degree of glue and presence of virgin wood. To explore this, Fig. 4E reports the mean spectra of the moderate treated wood samples, the rest of the treated wood samples and the virgin wood samples. Fig. 4F, G & H report a zoom of the specific wavelength regions marked in Fig. 4E where the main differences among the different types of wood occur. It can be observed how the moderate treated wood samples have a mean spectrum more similar to virgin wood than to the treated wood samples confirming the outcomes of the previous sections. To investigate this even further, we have reported the results of the VW-SIMCA and TW-SIMCA models developed removing the moderate treated wood sub-categories. Both models improve; in the validation phase the misclassification error of VW-SIMCA model (sample level) decreased from 10.00% to 6.67% and for TW-SIMCA model (sample level) the misclassification error decreased from 13.33% to 3.33%.

3.5. Variable selection

As shown in Fig. 2 some parts of the spectra show higher chemical differences among the three waste wood categories. We used this knowledge to perform variables selection to remove areas in the spectra

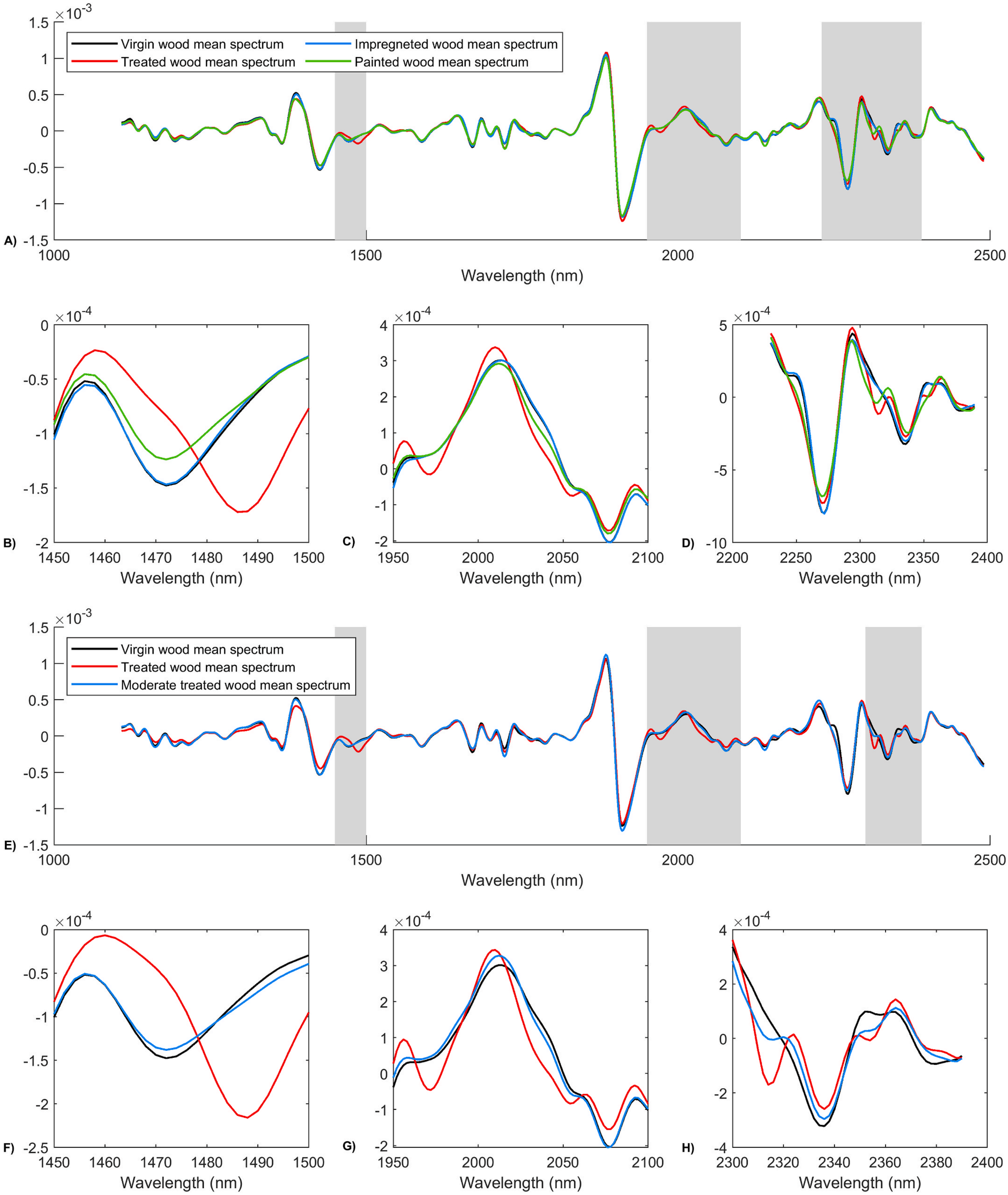

Fig. 4. A) Mean spectra of virgin, treated, impregnated and painted wood pre-processed with second derivatives (virgin wood samples: black line; treated wood samples: red line; impregnated wood samples: blue line; painted wood samples: green line). B), C) & D) plot of specific wavelength regions marked in A) where the main differences among the different types of wood occur. E) Mean spectra of virgin, moderate treated and treated wood samples pre-processed with second derivatives (virgin wood samples: black line; treated wood samples: red line; moderate treated wood samples: blue line). F), G) & H) plot of specific wavelength regions marked in E) where the main differences among the three types of wood occur. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

where there are only minor differences between the classes, thus increasing the model accuracy. Furthermore, variable selection enables a model based on a smaller number of wavelengths, making the interpretation of the relationship between the chemical structure of the waste wood categories and the spectral information easier.

TW-SIMCA and VW-SIMCA models have been computed again using offset correction as pre-processing and different combinations of wavelengths range selected by looking at the spectral regions where a higher difference in the variability of the three waste wood categories occur (see Fig. 2). The best VW-SIMCA model was developed considering the wavelengths range 1356–1502 nm and 1850–2498 nm. The model improved by applying the variable selection demonstrating that the removed variables are not containing useful information for the discrimination of the three waste wood categories. In the validation, the misclassification error of the model decreases from 10.00% to 3.33%. A good VW-SIMCA model could also be obtained considering less variables, i.e. 1356-1502 nm, 1652–1782 nm and 1932–2382 nm. In this case the misclassification error of the model decreases from 10.00% to 6.67%, but we are reducing the number of variables to 366 instead of the 700 for the total model and 399 of the previous one.

On the other hand, the TW-SIMCA model is a tad worse compared to the full-model, demonstrating that some of the deleted variables are somehow important for the discrimination (once again this could be explained by the higher variability of the treated wood samples). The best TW-SIMCA model has been developed considering the wavelengths range 1442–1492 nm, 1942–1972 nm and 2292–2382 nm. The model does not improve; in the validation, the misclassification error of the model increases from 13.33% to 16.67%. Other spectral ranges have been tested and with some of them we have obtained similar results, i.e. i) 1100–1360 nm, 1400–1900 nm and 2000–2498 nm; ii) 1100–1900 nm and 2000–2498 nm; iii) 1442–1492 nm, 1942–1972 nm and 2240–2390 nm. In any case the first TW-SIMCA has been chosen because of the lower number of variables (only 88) in comparison to the others (632, 651 and 118 respectively). (Table S3 reported in the supplementary material reports all the class performance parameters for the TW and VW SIMCA models using variables selection).

3.6. Discussion

The current separation of waste wood, i.e. clean wood from treated wood and other contaminants, is mainly based on visual, mechanical, magnetic or gravity sifting techniques. The application of spectroscopic techniques combined with chemometrics is highly innovative and already applied in other sorting facilities [22, 23]. Online NIR sorting techniques have the potential benefit of 'scanning' all the material in a rapid and low-cost way, thus improving the wood separation performance. This innovative sorting approach could be the solution for removing impurities and divide waste wood according to the appropriate reuse. In addition, the sector operators could benefit of greater efficiencies and better product quality.

Nowadays, the recycling potential of wood-based material could be expanded and one of the main obstacle is the lack of an efficient sorting of the material. Other studies have investigated the characterization of waste wood composition but mainly using conventional lab analysis instead of NIR spectroscopy.

In their study Huron et al. confirmed the heterogeneity of treated wood material, with properties quite different among the different classes of the waste wood characterized. The difference can be found in the chemical elements present in the different samples and depending on the treatments undergone by the samples [15]. Edo et al. assessed the chemical and physical characteristics of 500 waste wood samples collected at a co-combustion facility in Sweden. The knowledge of the chemical composition of such material is essential for ensuring a fuel with higher quality and lower potential for the formation of pollutants when combusted [16]. Similarly, Gehrmann et al. aimed at testing the suitability of waste wood as feedstock in an industrial combustion unit. An extensive characterization of properties relevant for combustion was performed on two samples of waste wood and one sample of natural wood for comparison revealing the differences in the combustion reactor [17]. Other authors demonstrated that contaminant and concentration levels vary significantly according to wood waste type and source, confirming the high variability of the material and the necessity of its characterization before material sorting [9]. Recently some authors examined the possibility to use NIR spectroscopy for sorting waste wood material from Amazonian species to improve the efficiency of the carbonization process and consequently charcoal production [42].

In general, the presence of contaminants in wood products limits considerably its recycling or reuse because of environmental contaminations. Given the current European (and global) ambition for more circularity, greater resource productivity, and the high demand from panel board companies, it is essential to recover as many recyclable materials from waste wood as possible and NIR spectroscopy is able to increase the waste wood separation performance. In addition, this study demonstrates how class modelling approach can be used not only for authentication and detection purposes but also for sorting problems. In fact it is well known that waste wood presents a high inherent variability [20] and materials other than wood could be part of the waste wood material and need to be properly handled in the sorting facilities. For this reason, the classical discriminant approach cannot be applied for this purpose, since a non-wood sample would be incorrectly assigned to one of the three classes considered in this study. On the other hand, class-modelling identifies non-wood sample as belonging to none of the waste wood classes.

4. Conclusions

More than one hundred waste wood samples were collected in different locations in Denmark and Italy and were analysed with NIR spectroscopy with the aim to study the sample variability and develop classification models based on modelling approach for deciding the best suited reuse of the material. Two SIMCA models were developed to recognize the virgin wood samples and the treated wood samples resulting in a validated misclassification error of 10.0% and 13.3% respectively. The disposal wood samples can be recognized as the samples neither belonging to the virgin wood or the treated wood classes, and gave a misclassification error of 10.0%. Variable selection was applied for improving the classification performance and decreasing the model complexity with good results for VW-SIMCA model, decreasing the misclassification from 10.00% to 3.33%, while no improvement was seen for the TW-SIMCA model.

A natural next step would be to move this application closer to the sorting line. This can be achieved by hyperspectral imaging including the near-infrared range. Such an approach can be used for the sorting of high volumes of waste wood.

Classification of waste wood samples is a key-point for improving the reuse of the material and avoiding expensive landfill. The recycling potential could be expanded with an adequate sorting of the material based on their quality and characteristics. The definition of the waste wood properties could also help in deciding the best recycling option and, in case of energy use, the best suited combustion process in order to avoid environmental problems related to such biofuel.

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CRediT authorship contribution statement

Manuela Mancini: Conceptualization, Methodology, Validation, Formal analysis, Investigation, Resources, Data curation, Writing –

original draft, Visualization, Funding acquisition. **Åsmund Rinnan:** Conceptualization, Methodology, Validation, Formal analysis, Resources, Writing – review & editing, Visualization, Supervision, Funding acquisition.

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

The dataset is uploaded to Zenodo as written in section 2.3

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.aca.2023.341564.

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