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Quality Assessment of Growing Media with Near-Infrared Spectroscopy: Chemical Characteristics and Plant Assays

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Summary

Quality control of growing media mainly consists of chemical analysis and plant assays, which are time-consuming and expensive. Objectives were to test, if near-infrared spectroscopy (NIRS) is capable to predict several chemical characteristics and plant assay results for a large population of various peat-based growing media having a wide range of humification degrees and characteristics (n=320). Near-infrared measurements (including the visible range, 400–2,500 nm) were done with fresh and with dried and ground growing media in order to predict their chemical characteristics and the results of plant assays using Chinese white cabbage (*Brassica napus* var. *Chinensis*). Spectral manipulations (taking 1st to 3rd derivative after baseline correction), cross-validation and a modified partial-least squares regression method were used to develop equations over the whole spectrum. Generally, NIRS predicted the chemical characteristics of growing media and the yields of fresh weight of Chinese white cabbage and rating better for fresh than for dried and ground samples. The pH and contents of total carbon and nitrogen, salt, P, K, mineral nitrogen, NO_3^-, NH_4^+ and the NH_4^+:NO_3^- ratio were predicted well: the RSC (ratio of standard deviation of laboratory results to the standard error of cross-validation) ranged between 2.0 (NO_3^-) and 4.4 (total carbon), the correlation coefficient (r) of measured against predicted values was higher or equal to 0.9 and the regression coefficient (a) was between 0.9 and 1.1. The good predictions of total carbon content may have been partly due to a clustering of data. Fresh weight yield of Chinese white cabbage was predicted well for the subpopulation of the growing medium with a degree of humification of H2 to H3 on the von Post humification scale (RSC=2.0, r=0.9 and a=0.9). The fresh weight yields for the subpopulations of growing media with H5 to H6 and with H7 were predicted satisfactorily (RSC =1.6 and 1.9, respectively). The prediction of the rating at harvest (overall plant impression) was satisfactorily for two subpopulations (RSC=1.7, r=0.8 and a=0.9 or 1.0) but unsatisfactory for the one with H5 to H6 (RSC=1.3). Overall, NIRS is sufficiently reliable to be used for standard chemical analysis for growing media and it is promising in predicting the results of plant assays.

Key words. Chinese white cabbage – NH_4^+:NO_3^- ratio – NIRS – nitrate – ammonium – passive heating

Introduction

Peat is worldwide the most important growing medium constituent. A reliable and high quality standard to promote plant health is required. Fast and cost-effective methods to predict chemical characteristics and results of plant assays of growing media are desirable.

Near-infrared spectroscopy (NIRS, 750–2,500 nm) is an established analytical technique, which has been successfully applied for the investigation of agricultural products, forage and pharmaceutical products (Williams and Sobering 1993; Fahey and Hussein 1999; Baratieri et al. 2006), composts (Michel et al. 2006) and the determination of various soil characteristics (Chang et al. 2001; Terhoeven-Urselmans et al. 2006a). Advantages are that the method is non-destructive, the sample pre-treatment can be minimal and several constituents can be predicted simultaneously for a large sample set. Detection limits depend on the investigated constituent and range approximately between 0.1 % (Holroyd 2003) and 1 % (Rager 2001), both dry weight.

NIRS bas already been used in peat studies to investigate basic quality constituents. Successful NIRS predictions were made for the determination of peat moisture and the degree of humification (Mc'Tiernan et al. 1998; O'Mahony et al. 1998). Additionally, NIRS predicted the pH and contents of salt, P and K well for a sample collective of 73 growing media (Ludwig et al. 2006). However, the accuracy of the prediction of NO_3^- and NH_4^+ contents was less satisfactory presumably due to a rather small sample number or because of a too diverse population.

Prasad et al. (2000) showed the ability of mid-infrared spectroscopy to predict the breakdown of different peats during an incubation, which lasted from 30 to 208 weeks. They correlated the 1600/1060 wavenumber ratio at the beginning and the end of the incubation with the vertical shrinkage loss (measured in mm) of potted peats. How-

ever, it is not clear, whether their results can be generalized, because they did not consider the impact of particle size on the degree of peat shrinkage.

To our knowledge, NIRS has not yet been used for the prediction of biomass yields of plants cultivated in growing media as a means of quality assessments of such growing media using standard plant assays. However, indications of the usefulness of NIRS for such an application are given by the results of field studies by BABAR et al. (2006) and CHANG et al. (2003). BABAR et al. (2006) used spectral reflectance indices from the plant cover in order to differentiate between various spring wheat genotypes for optimising grain yield. CHANG et al. (2003) used remote sensing (520–920 nm) to predict corn yield. Only early spectral sampling dates, when plant cover was lowest, yielded useful results. The soil spectral information was more important for yield prediction than plant cover spectral information.

Summarising the findings above, NIRS has been able to predict some basic chemical characteristics of growing media for a rather small population and first attempts were done using NIRS for predictions of complex constituents such as biomass yield in related scientific areas. However, information on the ability of NIRS to predict plant yield of Chinese white cabbage (*Brassica napus* var. *chinensis*) grown in various growing media is missing. Thus, the objectives were to test, if NIRS is capable to predict several chemical characteristics and plant assay results for a large population of various peat-based growing media having a wide range of humification degrees and characteristics.

Materials and Methods

Samples and experiments

Samples. Four peats (P-1 to P-4) and four growing media (GM-1 to GM-4) were used for this investigation. A growing medium which has the same number as the respective peat is based on that peat. The peats and growing media covered a wide range of origins (one weakly decomposed bog peat (H 2–3 on the von Post humification scale) from Finland (P-1), one moderately decomposed (H 5–6) from Ireland (P-2), one strongly decomposed raised bog peat from Germany (P-3) and a mixture of two peats (H 3–5) from Lithuania and Ireland (P-4)) and bulk densities (207 to 577 g L^{-1}). The growing media were obtained by adjusting the pH to 5.0–5.5 and fertilizing the peats with water-soluble complete fertilizer (PG Mix 14-16-18) to a mineral nitrogen level of approximately 175 mg L^{-1}.

Heating experiments. Peat and growing media samples were heated to different temperatures for different periods in order to mimic the effect of unfavourable transport and storage conditions and to obtain a large set with a wide range of plant assays results. The heating experiments are described in detail by (TERHOEVEN-URSELMANS et al. 2006b). Briefly, sub-samples of P-1 to P-3 and GM-1 to GM-3 were filled into three-litre polyethylene tubes (0.15 mm thickness) and compacted. The air was evacuated and the tubes were immediately shrink-wrapped. The samples were kept at 4 (control, only growing media) or heated at 20, 35, 45 and 60 °C for two weeks (experiment (i), total n=54). Heated peats were analysed after heat treatment for mineral nitrogen contents and pH and subsequently fertilized and limed to growing media level. Thus, only growing media were used in Chinese white cabbage test.

Sub-samples of GM-1 to GM-3 were taken and heated at 35 °C for 0 (control), 2, 4, 6, 8 and 10 d. Directly after heating and after five months of storage at 4 °C the test of Chinese white cabbage was conducted (experiment (ii), total n=18).

Additionally, we included a pre-packed growing medium (GM-4) received from a grower who had stored the medium under unfavourable conditions on his premises (experiment (iii), total n=34).

Chemical analysis. . Total organic carbon and nitrogen contents were determined by dry combustion using an Elementar Vario EL Analyser.

The procedures of VDLUFA (1997) were used for the determination of pH (0.01 M $CaCl_2$), salt content (conversion of conductivity to mass of KCl) and P and K content (both CAL).

The contents of soluble NO_3^- and NH_4^+ were determined by adding 200 ml of 0.0125 M $CaCl_2$ to 20 g of peat or growing medium (particle size < 5 mm). Then, the suspension was shaken for 1 h and filtered through a fine-pored filter (VDLUFA 1997). The concentrations of NO_3^- and NH_4^+ were determined colorimetrically.

Chinese white cabbage test. The effect of growing media on plant growth was determined according to VDLUFA (1997). Replicate number was four (experiment (i)) and two (experiments (ii) and (iii)) and the total number of samples was 320. Heated samples were filled into pots and twenty-seven seeds of Chinese white cabbage were sown in all growing media. The pots were kept under constant light (10,000 lux for 16 h d^{-1}) and temperature (16 h at 20 °C, 8 h at 16 °C) conditions and watered regularly by weight. After three weeks, fresh weight yield per pot and the rating of the growth reduction was carried out as described in the Vdlufa method: the best and the worst looking plants within one pot of Chinese white cabbage were taken and graded on a scale from nine (best) to one (worst).

Near-infrared spectral reflectance measurements

Physico-chemical basis of near-infrared spectroscopy. Near-infrared radiation is absorbed by different chemical bonds (e.g. C-H, O-H, N-H, C=O, S-H, CH_2, C-C) and results from primary absorption of radiation in the middle-infrared region (2,500–25,000 nm; OSBORNE and FEARN 1986). The analyses of NIR spectra use mathematical and statistical procedures, but these procedures use the spectral information, which is closely related to the chemical composition. Nevertheless, the assignment of chemical bonds to wavelengths, which were important for the prediction, is not trivial and may be in some cases not definitely possible. Reasons are that (i) compounds absorb at more than one wavelength, (ii) the absorption at a given wavelength can be caused by different absorption features (OSBORNE and FEARN 1986) and that (iii) some correlations are indirect (CHANG et al. 2001).

(i) The predictions of the contents of C_t and N_t are commonly used applications and absorption bands oc-

cur e.g. for alkyl and O-alkyl C in soils between 800 and 1,250 nm, 1,350 and 1,450 nm, 1,700 and 1,800 nm and 2,250 and 2,500 nm. Main nitrogen absorptions bands of amino and acid amid groups occur between 1,000 and 1,050 nm, 1,450 and 1,600 nm and 1,950 to 2,200 nm (MILLER 2001). The important wavelengths can vary depending on the investigated type of sample. DALAL and HENRY (1986) showed that the wavelengths 1,702, 1,870 and 2,052 nm were useful in determining soil nitrogen. BOGREKCI and LEE (2005) found for common soil phosphates the following absorbing wavelengths: 2,548 nm for $Mg_3(PO_4)_2$ x 2 H_2O and 2,516 nm for $CaPO_4$.

(ii) Other compounds like NO_3^- and NH_4^+ are as well spectrally active (VOGT and FINLAYSON-PITTS 1994). For NO_3^- one major peak is at 1,942 nm (EHSANI et al. 1999), whereas it is found for NH_4^+ between 1,600 and 1,650 nm (SHRINER et al. 1998). However, the main obstacle to accurately measure NO_3^- is the interfering band of carbonate (LINKER et al. 2004).

(iii) Even though sodium chloride has no specific absorption bands in the NIR wavelength region, salt analysis is possible because of the perturbation of the water band by sodium chloride (LIN and BROWN 1993)

Sample preparation and near-infrared measurements. From all samples, which were used in the test of Chinese white cabbage, sub-samples were taken after the heat treatments. They were measured (A) fresh as received (stored at 4 °C until the measurement) and (B) dried (60 °C) and finely ground and calibrated against the chemical characteristics and the test results of Chinese white cabbage. Absorbance spectra (log [1/reflectance]) in the near-infrared range (including the visible range, 400–2,500 nm) were recorded in 2 nm steps using a Foss NIRSystems spectrometer (Silver Spring, USA). Two measurements per sample were done and averaged, if their spectral difference did not exceed a root mean square of (A) 10,000 or (B) 3,000. Otherwise, measurements were repeated again.

Spectral manipulation, cross-validation and regression procedure. Spectra were manipulated using scatter correction SNV (standard normal variate) and detrend (BARNES et al. 1989), taking derivates of 1st to 3rd order, defining the gaps over which derivates were calculated and smoothing the spectra in order to find fine absorption bands. The gaps and the smoothing width ranged between one and twenty (Table 2). The cross-validation equation was calculated using a modified-partial-least squares regression method (MPLS; SHENK and WESTERHAUS 1991). The number of terms (x) used in the MPLS were calculated according to the following formula:

$$x = (n/10) + 2 \qquad (1)$$

where n is the sample number.

The number of outlier elimination passes was two. The outliers were defined as samples with a spectrum out of the population of spectra (H-outliers) or for which the difference between the reference and the predicted value were much larger than the standard error of cross-validation (SECV; t-outliers). The limits were set to 10 (H-outliers) and 2.5 (t-outliers) as suggested by the WinISI II

Table 1. Chemical characteristics of growing media (GM) and the test results of Chinese white cabbage. Sample number (N) refers to all samples minus the outliers obtained in the cross-validation procedure. The results refer to the variant using fresh samples.

Constituent	Unit	N	Range	Mean	Standard deviation
C_t content	% dry matter	306	39.6 – 50.2	45.7	3.2
N_t content	% dry matter	306	0.9 – 1.2	1.0	0.1
pH-value		310	4.1 – 5.6	5.1	0.4
Salt content	g L^{-1}	310	0.4 – 1.3	0.8	0.2
P content	mg P_2O_5 L^{-1}	305	97 – 266	176	49
K content	mg K_2O L^{-1}	310	119 – 340	223	72
Mineral nitrogen content	mg L^{-1}	312	9 – 205	124	45
NO_3^- content	mg NO_3-N L^{-1}	307	2 – 139	56	37
NH_4^+ content	mg NH_4-N L^{-1}	312	4 – 113	68	31
NH_4^+:NO_3^- ratio		304	0.0 – 36.3	4.2	7.3
Rating at harvest		301	4 – 9	7.5	1.2
Rating at harvest (GM-1)		79	2 – 9	7.8	1.4
Rating at harvest (GM-2)		77	6 – 9	7.7	0.6
Rating at harvest (GM-3)		78	5 – 9	7.9	1.0
Fresh weight yield	g pot^{-1}	310	6.1 – 26.1	16.3	4.1
Fresh weight yield (GM-1)	g pot^{-1}	80	6.1 – 25.2	16.9	4.7
Fresh weight yield (GM-2)	g pot^{-1}	79	8.4 – 22.2	15.5	3.7
Fresh weight yield (GM-3)	g pot^{-1}	81	8.4 – 24.0	17.2	4.5

Table 2. Cross-validation statistics for the chemical characteristics of the growing media (GM) and the test results of Chinese white cabbage. The mathematical treatment, the number of outliers, the standard error of cross-validation (SECV), the ratio of the standard deviation of the laboratory results to SECV (RSC) and the correlation coefficient (r) and the regression coefficient (a) of a linear regression (measured against predicted values) are given. The results refer to the variant using fresh samples.

Constituent	Mathematical treatment [a]	Outliers	SECV	RSC	r	a
C_t content	1,15,1	14	0.73	4.4	0.97	1.00
N_t content	1,10,10	14	0.02	3.6	0.94	0.98
pH value	1,10,5	10	0.10	3.9	0.97	1.00
Salt content	1,5,5	10	0.08	2.6	0.92	0.96
P content	1,5,1	15	13.80	3.6	0.95	0.99
K content	1,5,5	10	22.20	3.2	0.96	0.98
Mineral nitrogen content	3,15,5	8	19.60	2.3	0.90	0.91
NO_3^- content	1,5,5	13	18.40	2.0	0.87	0.95
NH_4^+ content	2,20,1	8	9.50	3.2	0.95	0.97
NH_4^+:NO_3^- ratio	1,10,5	16	3.40	2.2	0.88	1.11
Rating at harvest	2,10,1	19	0.85	1.4	0.67	1.01
Rating at harvest (GM 1)	1,15,1	5	0.79	1.7	0.81	1.01
Rating at harvest (GM 2)	3,20,5	7	0.44	1.3	0.35	0.70
Rating at harvest (GM 3)	3,5,5	6	0.58	1.7	0.79	0.94
Fresh weight yield	1,1,1	10	2.89	1.4	0.71	0.91
Fresh weight yield (GM 1)	2,15,1	4	2.33	2.0	0.88	0.87
Fresh weight yield (GM 2)	1,5,5	5	2.28	1.6	0.77	0.99
Fresh weight yield (GM 3)	1,5,1	3	2.40	1.9	0.82	0.95

[a] The first number of the mathematical treatment is the order of the derivative function, the second one the segment length in data points over which the derivative was taken, and the third one the segment length over which the function was smoothed.

software and TILLMANN (2000). The SECV was calculated as follows:

$$SECV = \sqrt{\frac{\sum (X_i - Y_i)^2}{n-1}} \qquad (2)$$

where y are the NIRS-predicted values of a growing medium property, x are the measured growing medium properties and n is the total number of samples (TILLMANN 2000).

The number of excluded outliers obtained in this way was maximal 19 (6 % of the total sample set) for the contents of K and total carbon for dried and ground samples and rating at harvest for fresh samples (data not shown, Table 2). All outliers in this study, except for six, were t-outliers. The outliers excluded during the MPLS procedure were included again in the graphs of measured against predicted values (Fig. 2, 4) and in the calculations of the correlation coefficients (r) and regression coefficients (a) in order not to overrate the potential of NIRS.

The best mathematical treatment was found by carrying out a trial and error procedure. The criteria were the smallest SECV and the highest RSC (the ratio of the standard deviation of laboratory results and SECV). According to Chang et al. (2001) and LUDWIG et al. (2002) the accuracy of NIR predictions can be described as follows: good predictions have a RSC greater than 2, a correlation coefficient (r) greater or equal to 0.9 and a regression coefficient (a) in the range from 0.9 to 1.1. Satisfactory results are obtained for $1.4 \leq RSC \leq 2.0$, $r \geq 0.8$ and $0.8 \leq a \leq 1.2$.

Wavelength assignment. The WinISI II software computed the correlation coefficients for the different constituents

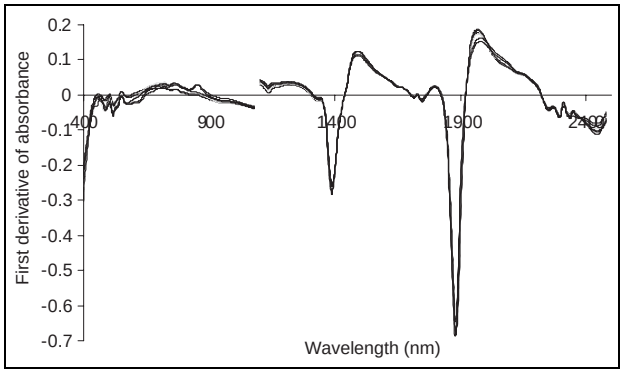


Fig. 1. First order derivative of absorbance spectra for six selected growing media, which cover the spectral range of the sample set. The derivative was calculated including scatter correction, using a segment length of five data points over which the derivative was taken and smoothing the spectra over five data points.

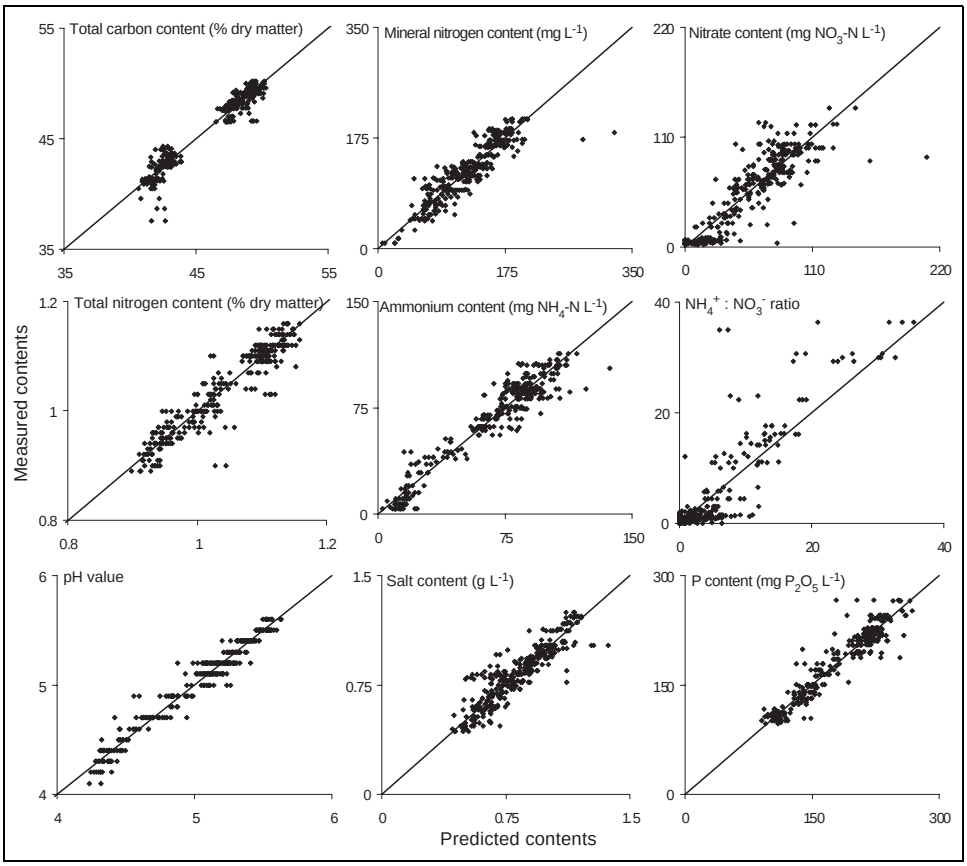


Fig. 2. Measured against predicted contents for the chemical characteristics of the growing media. The results refer to the variant using fresh samples. The lines indicate 1:1.

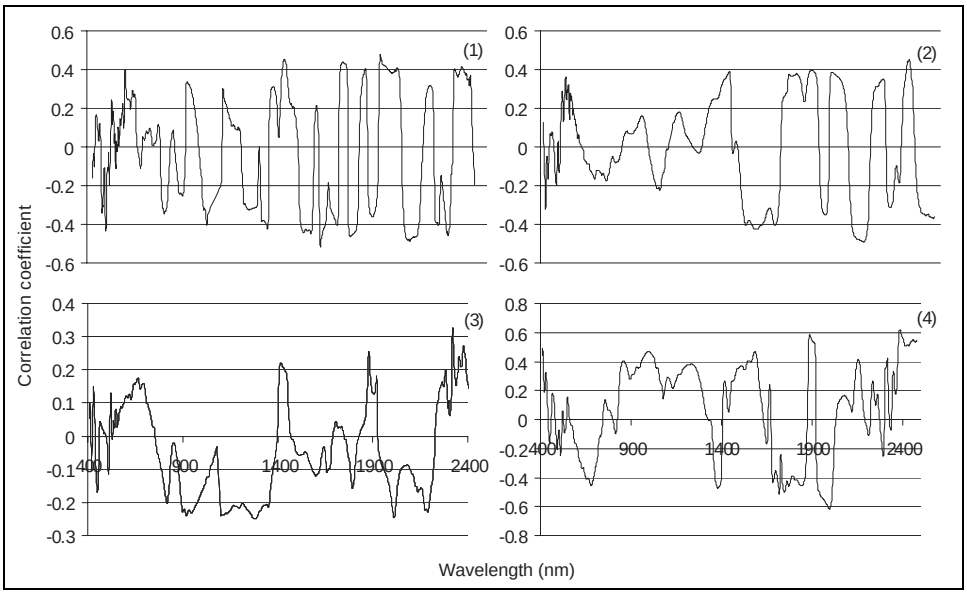


Fig. 3. Correlations as a function of the wavelength for (1) the fresh weight yield (growing medium 1, GM-1), (2) the rating at harvest (GM-1), (3) the contents of NO_3^- (all growing media) and (4) the contents of salt (all growing media). Spectra were manipulated with SNV and detrend and the mathematical treatments are given in Tab. 2. The results refer to the variant using fresh samples.

over the whole spectrum. The value of the correlation coefficient at a single wavelength describes how important this particular wavelength for the prediction of the given constituent was (Fig. 3). The original spectra were transformed prior calculations using the optimum mathematical treatment for each constituent. The maximum or null correlations were selected for the wavelength assignment in dependence of the order of the derivative functions of the cross-validation function: for the first and third derivative, null correlations between the highest absolute values refer to a peak in the original spectrum (see Fig. 3, chart (4), 1922 nm for salt prediction). Oppositely, the highest correlations for the second derivative refer to peaks in the original spectrum. The assignment of functional groups to the wavelengths with the highest correlation coefficient was done using the WinISI II software and the information provided by MILLER (2001).

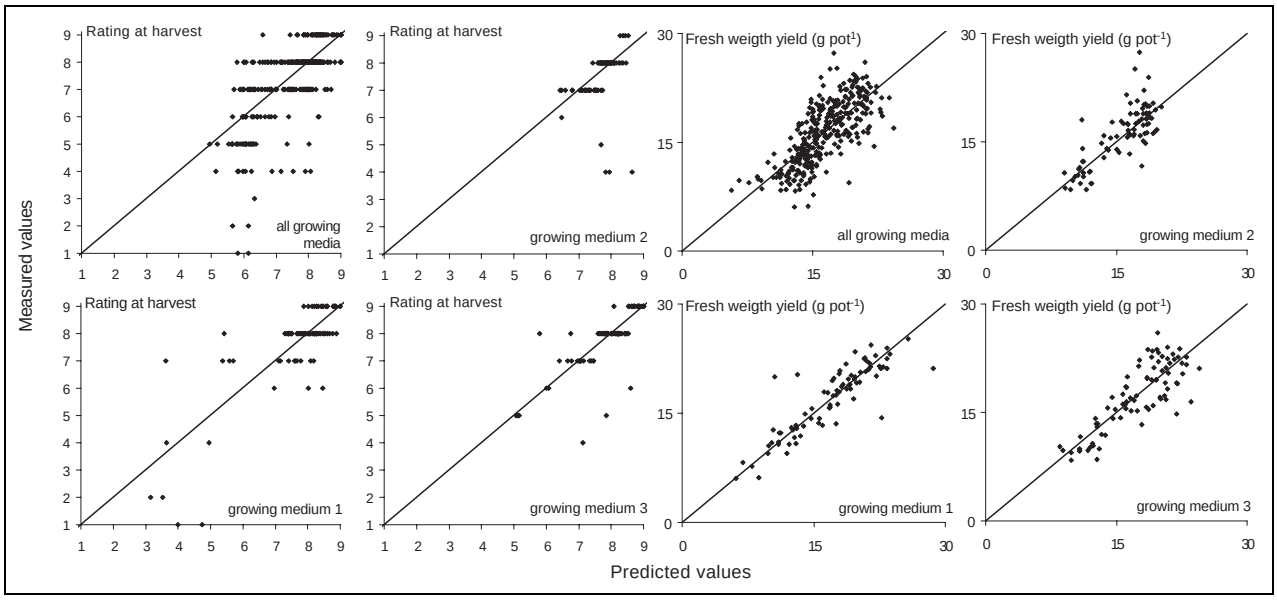


Fig. 4. Measured against predicted values for the test results of Chinese white cabbage. The results for all samples and separated for each growing medium refer to the variant using fresh samples. The lines indicate 1:1.

Results and Discussion

Spectra of the growing media

The first derivative spectra of selected samples shown in Fig. 1 cover the spectral range of the sample set. The two most visible features in the original spectra were the water peaks with maxima at 1438 and 1922 nm, which are zero in the first derivative (Fig. 1). A marked variability between the spectra was observed in the visible range from 430 to 900 nm and from 1940 to 2500 nm. Some important wavelengths reported for peats are 864 nm (unidentifiable organic material), 2396 (absorption of *Sphagnum papillosum*) and 2476 nm (absorption of *Sphagnum magellanicum*; Mc'Tiernan et al. 1998).

Chemical characteristics of growing media

The chemical characteristics of the growing media covered wide ranges (Table 1). The pH (4.1–5.6) and contents of P (97–226 mg P_2O_5 L^{-1}) and K (119–340 mg K_2O L^{-1}) were sufficient for undisturbed plant growth. Mineral nitrogen levels (9–205 mg L^{-1}) were the most important chemical characteristics regarding the prediction of plant yield.

All chemical characteristics of the growing media were predicted well by NIRS: the RSC ranged between 2.0 and 5.0 for the pH and contents of total carbon (C_t) and nitrogen (N_t), K, P, salt, NO_3^- and NH_4^+ and the NH_4^+:NO_3^- ratio and (r) and (a) of a linear regression of measured against predicted values were in the range of 0.87 to 0.97 and 0.91 to 1.11, respectively (Table 2, Fig. 2).

The good predictions for the pH and contents of P, K and salt correspond to the results of Ludwig et al. (2006), who used a rather small set of growing media (n=73) with special characteristics (known or assumed phytotoxicity). The predictions of the contents of P, K and salt in our investigation yielded better results for fresh samples (Table 2) than for dried and ground ones (data not shown). Only pH prediction was better for dried samples (RSC=5.0) than for fresh samples (RSC=3.9). However, the reason for this remains unclear. In agreement with this, Ludwig et al. (2006) also reported more accurate predictions for P and K using fresh material and for pH using dried and ground material, whereas for the salt content, opposite results were reported. Correlation analysis indicated that the most important wavelengths for salt prediction were in our study 1,922 nm (vibrations of -C=O, -$CONH_2$-, O=C-O-, and -OH) and 1,874 nm (vibration of water, Table 3). The –OH group was amongst others also important for salt prediction in fermented soybean food (Lin and Brown 1993; Lu and Han 2005). The prediction of P and K is of statistically nature, because the assigned wavelengths (Table 3) are not connected to any P or K absorbing compounds.

For N_t, which was predicted well (Table 2), correlation analysis showed that the most important wavelengths were 660 nm (red) in the visible region and 960 (vibrations of -OH, HC=O and HC-OH) and 1650 nm (vibrations of –NH) in the near-infrared region.

The predictions of the contents of mineral nitrogen, NO_3^- and NH_4^+ and of the NH_4^+:NO_3^- ratio were better for fresh samples (Table 2, Fig. 2) than for dried and ground ones (data not shown). In contrast to the good predictions in this study, Ludwig et al. (2006) achieved only satisfactory predictions for the NH_4^+ contents, whereas NO_3^- contents were predicted unsatisfactorily for their small sample set (n=73). Reasons were most probably (i) that the sample number in our study was much higher (320 in comparison to 73 samples) and (ii) that the spectral diversity in our study was less, since the number of growing media origins was smaller, even though the range of humification degrees was similar. Predictions of NO_3^- are likely more promising in the middle-infrared region (Jahn et al. 2006). Nevertheless, one of the assigned wavelengths (1,928 nm, Table 3) is close

Table 3. Assignments of the near-infrared absorption bands with the highest correlation coefficients of those constituents, which were predicted well. See Table 1 for units.

Constituent	Wavelength (nm)	Chemical bond origin
C_t content	1870	C=O
	686	Red light
	1348	CH_3, CH, CHO, C=CH, C=OH
N_t content	660	Red light
	960	OH, HC=O, HC-OH
	1650	NH, C≡O
pH value	1668	C=C
	1918	C=OH, OC=NH_2, OC-OH, OC-Cl
	2052	OC-NH, -OH, NH
	772	Not assigned
Salt content	1922	C=O, $CONH_2$-, O=CO, OH
	1874	Water
	1406	OH, CH_3, CH_2, CH
P content	834	Not assigned
	1660	C=CH, aromatic C
	2040	=CH_2, NH_2, NH, CONH, OH, COOH
	1926	CO, COH, $CONH_2$, COOH, phenolic groups, OH
K content	838	Not assigned
	1672	C=CH, aromatic C
	2070	=CH_2, CONH, NH_2, NH, OH, COOH, water
Mineral nitrogen content	2094	=CH_2, NH_2, NH, OH, COOH, water
	2260	CH_3, CH_2, CH, C=CH, NO_2
	1404	CH_3, CH_2, CH, C=CH, COH, CONH, phenolic groups, water
	798	Not assigned
NO_3^- content	2228	CH_3, NH_3 aquatic
	1928	COH, $CONH_2$, COOH, OH, phenolic groups, water
	1398	CH_3, CH_2, CH, C=CH, COH, CONH, water
NH_4^+ content	1598	NH_2, NH, OH, phenolic groups, water
	1716	CH_3, CH_2, CH, C=CH
NH_4^+:NO_3^- ratio	2218	Close to 2228 nm from NO_3^- prediction
	742	Not assigned
	1388	Close to 1398 nm from NO_3^- prediction
Fresh weight yield GM 1	1626	Not assigned
	2098	Close to 2094 nm from Mineral mitrogen prediction
	1940	Close to 1928 nm NO_3^- prediction

to 1,942 nm, which is an absorption feature for NO_3^- (Ehsani et al. 1999). The assigned wavelength 1,589 nm for NH_4^+ prediction is very close to the range of NH_4^+ absorbing features (1,600 and 1,650 nm, Shriner et al. 1998). The NH_4^+:NO_3^- ratio prediction was based on wavelengths, which were used for the NO_3^- prediction (Table 3). Interestingly, the assigned wavelengths for contents of mineral nitrogen and NO_3^- and the NH_4^+:NO_3^- ratio exhibited between 2218 and 2260 nm absorptions for aqueous ammonia (Table 3). However, correlations with the C_t (NH_4^+: r=0.51, P<0.01) and the N_t content (NH_4^+: r=0.16, P<0.01; NO_3^-: r=0.13, P<0.05) were only small or absent (NO_3^- with C_t: r=0.01; data not shown).

The good prediction of C_t (Table 2, Fig. 2) has not been reported before for peat. Prasad and O'Shea (1999) found only a rough estimate for two carbon fractions (contents of lignin and cellulose) with infrared spectroscopy. Nevertheless, our result has to be taken cautiously, because a clustering of data occurred in respect to the different peat sources. Similar to our results, predictions of carbon contents were satisfactory for a sample population of composts, which was rich in carbon and even more heterogeneous (Michel et al. 2006) than our population of peat samples. In the present investigation, two assigned wavelengths for C_t prediction were 1,870 (-C=O vibrations) and 1,348 nm (vibrations of -CH_3, -CH-, -CHO, -C=CH-, Table 3).

Overall, our results suggested that predictions of chemical characteristics of growing media may be done using fresh samples. The only constituent, where drying and grinding gave considerably better results was pH, but both treatments had RSC values which were well above two.

Chinese white cabbage test

Plant growth in the greenhouse depends mainly on the supply of water and nutrients, the absence of plant pests and the climatic conditions. In our study, the only variation was the differing nutrient concentration, especially the mineral nitrogen content (Table 1), which was caused by the different heat treatments. This is supported by the assigned wavelength for fresh weight yield prediction of GM-1, because it is based on very similar wavelengths as the NO_3^- and mineral nitrogen predictions (Table 3, Fig. 3)

For the entire population of growing media, the prediction of fresh weight yield was satisfactory regarding the RSC (1.4) but not regarding the correlation coefficient (r=0.7, Table 2, Fig. 4).

Better predictions for the fresh weight yield were obtained by separating the growing media by their origin. Fresh weight yields were predicted well for GM-1 (Table 2, Fig. 4). The RSC was 2.0. We explained more than three-quarter (r^2=0.77) of the variation in fresh weight yield with the spectral information of GM-1 (Table 2). The RSC was 1.6 and 1.9 for GM-2 and GM-3, respectively, and thus the predictions were satisfactory, since also (r) was equal to 0.8 for both subpopulations. The better performance of NIRS for the subpopulations is not surprising, since it is known that differing peat origins are spectrally different. For instance, MIARA (1992) identified different peat classes with the spectral information of satellite data. The good prediction performance for GM-1 (in contrast to the satisfactory one for GM-2 and GM-3) may be explained as follows: GM-1 had the lowest degree of humification and hence a lower content of humic substances. This resulted in a lower molecular complexity and less interacting functional groups.

Rating at harvest was predicted satisfactorily regarding the RSC, but unsatisfactorily regarding (r) for the entire population (Table 2). The accuracy of predictions of rating at harvest may have been enhanced, if the ratings were more evenly distributed over a wide range (i.e. more values of three and lower). Nevertheless, rating at harvest was predicted satisfactorily for GM-1 and GM-3 (for both RSC=1.7 and r=0.8; Table 2, Fig. 4).

Overall, NIRS predictions of the results of the plant assay using Chinese white cabbage were generally better for fresh samples than for dried and ground ones. One explanation is that peat shrinks during drying. This process changes its properties, namely increasing the hydrophobic characteristics (MICHEL et al. 2001). The better performance for fresh samples than for dried and ground samples is not surprising, because the sample number in our study was high enough to compensate for the possible negative particle size effect of fresh samples (SLAUGHTER et al. 2001).

Conclusions

NIRS was well suited to characterize growing media chemically. Moreover, NIRS showed a marked potential to predict the fresh weight yield of Chinese white cabbage for all three subpopulations of differing origins.

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