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Use of near infrared spectroscopy to predict chemical parameters and phytotoxicity of peats and growing media

Bernard Ludwig [a,*], Gerald Schmilewski [b], Thomas Terhoeven-Urselmans [a]

[a] *Department of Environmental Chemistry, University of Kassel, Nordbahnhofstraße 1a, 37213 Witzenhausen, Germany*
[b] *Klasmann-Deilmann GmbH, Moorgutsweg 2, 26683 Saterland-Sedelsberg, Germany*

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Abstract

Fast and cost efficient tests are required for a screening of chemical parameters of peats and an estimation of a potential phytotoxicity. The objective of this study was to test the usefulness of near infrared spectroscopy (NIRS) for the quality control of peats and growing media. A population of 73 phytotoxic and non-phytotoxic peats from various stockpiles and growing media of different origins was collected and, after storage, characterised for their pH, contents of salt (estimated using the electrical conductivity), P, K, NO_3^- and NH_4^+ and their phytotoxicity using Chinese white cabbage (*Brassica napus* var. *chinensis*) as indicator. For unknown reasons, storage reduced the percentage of phytotoxic peats and growing media from 65 to 16%. Spectra of the visible and near infrared region (400–2500 nm) were obtained for all samples after drying and grinding (variant A) or in a moist state (variant B). A cross validation was carried out using a modified partial least square method which was based on the entire spectra and included the first to third derivate after base line correction. The chemical parameters pH, and contents of salt, P and K were predicted well by NIRS for both variants: the ratios of standard deviation of the laboratory results to standard error of cross validation (RSC) were greater than 2, the regression coefficients (a) of a linear regression (measured against predicted values) ranged from 0.9 to 1.1 and the correlation coefficients (r) were greater or equal to 0.9. Satisfactorily ($0.8 \leq a \leq 1.2$, $r \geq 0.8$ and $1.4 \leq \mathrm{RSC} \leq 2.0$) assessed was the NH_4^+ content in variant A. Nitrate contents and phytotoxicity were predicted unsatisfactorily. However, investigating a less diverse subpopulation of 38 samples which were all growing media for plant propagation from two different origins showed a good prediction accuracy for nitrate contents (variant A) and a satisfactory one for phytotoxicity (variant B). The good and satisfactory predictions reported above indicate a marked usefulness of NIRS in the quality assessment of peats and growing media.

Keywords: Growing media; Near infrared spectroscopy; NIR; NIRS; Peat; Phytotoxicity

1. Introduction

Near infrared spectroscopy (NIRS, 750–2500 nm) is an established analytical technique which has been successfully applied for the investigation of agricultural products, foodstuffs, forage and pharmaceutical products (Norris et al., 1976; Shenk and Westerhaus, 1994; Fahey and Hussein, 1999). Examples are the quantitative determination of the contents of fat, water, protein, total N, glumes, starch, raw fibre, oil and glucan in wheat, free fatty acids and iodine values in plant oils, and amino acids in seeds (Clark et al., 1987; Windham et al., 1988; AOAC, 1990). The determination of the contents of trace compounds is not directly possible with NIRS. Detection limits for direct determinations are generally ranging from 1% (Rager, 2001) to 0.1% (Holroyd, 2003; Fink, 2003).

Resink et al. (2000) and Sharma et al. (2000) showed for different composts that NIRS was useful to determine the contents of water, pH and contents of ash, N, ammonium, neutral- and acid-soluble fibre and raw fibre in a large population sample. Capriel et al. (1999) carried out pot experiments with oats and different organic waste composts. They showed by using cross validation the potential of NIRS to estimate the N uptake and the yield increase due to the compost additions. NIRS measurements before and after incubation experiments indicated that NIRS was useful for the determination of the contents of cellulose, lignin, polypeptides, pectins and labile C in alfalfa, dried maize and laboratory-composted maize, whereas the applicability of NIRS to commercial composts was less satisfactory (Zaccheo et al., 2002).

For peats, however, only a small number of studies exists that report the usefulness of NIRS to predict constituents or

* Corresponding author. Tel.: +49 5542 981631; fax: +49 5542 981633.
E-mail address: bludwig@uni-kassel.de (B. Ludwig).

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characteristics. Prasad and O'Shea (1999) and Prasad et al. (2000) showed the usefulness of NIRS to estimate the changes of cellulose and lignin contents and the breakdown of peats in incubation experiments. Additionally, the applicability of NIRS for the prediction of the moisture content and degree of humification of peat has been reported (McTiernan et al., 1998; O'Mahony et al., 1998). However, to our knowledge, information on the usefulness and limitations of NIRS for prediction of phytotoxicity, self-heating and several chemical parameters of peats are still missing.

The objective of this study was to determine the accuracy of NIRS for the quality assessment of peats and growing media using a population of 73 phytotoxic and non-phytotoxic samples of different origins and composition and with varying horticultural characteristics.

2. Materials and methods

2.1. Samples

A population of peats from stockpiles in the Baltic States and pre-packed growing media of which some were known or assumed (because they were from the same stockpile as the phytotoxic ones) to be phytotoxic and others known to be non-phytotoxic were collected and stored in a closed, unheated storehouse in order to obtain a sample number which is sufficient for this near infrared (NIR) study. Phytotoxicity (plant response of Chinese cabbage) was determined for each sample directly after collection and after the whole set of 73 samples was obtained, which took about 1 year. Initially, 65% of the 73 samples were slightly, moderately or strongly phytotoxic. During storage, the characteristics of the peats and growing media were determined (Table 1). For unknown reasons, storage reduced the phytotoxicity of the samples to 16% (12 out of 73 samples). Nevertheless, the samples covered a wide range of the contents and phytotoxicity studied (Table 1).

2.2. General characteristics of the sampled peats and growing media

For the pH determination, 20 cm^3 of peat or growing medium (moisture content as received and <5 mm) were suspended in 50 ml of 0.01 M $CaCl_2$. The suspension was stirred twice within one hour and pH was determined afterwards with a glass electrode (VDLUFA, 1997).

We obtained the salt content as follows: 200 ml of distilled water were added to 20 g of the peat or growing medium (<5 mm) and the suspension was shaken for 1 h. Then, the solution was filtered through a fine-pored filter and the conductivity was measured. We calculated the salt content on a basis of mass KCl/100 g substrate by using the equation and correction factors provided by VDLUFA (1997).

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 (<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 measured colourimetrically.

Table 1
Characteristics of the peats and growing media

Constituent	n	Treatment[a]	Median[b]	Range[b]
NO_3^- content (mg N kg^{-1} DM)	59	A, B	138	16.7–1100
NO_3^- content for a subpopulation of 38 samples (mg N kg^{-1} DM)	38	A, B	238	16.7–1100
NH_4^+ content (mg N kg^{-1} DM)	59	A	308	30.8–900
		B	308	30.8–617
K content (mg K_2O kg^{-1} DM)	59	A	1058	200–3100
		B	1058	200–3400
P content (mg P_2O_5 kg^{-1} DM)	59	A	815	183–1762
		B	815	183–1783
Salt content (g kg^{-1} DM)	59	A	4.00	1.67–9.58
		B	4.00	1.67–8.46
pH	59	A	4.70	2.80–5.70
		B	4.70	2.80–5.90
Phytotoxicity	73	A, B	1	1–4
Phytotoxicity for a subpopulation of 38 samples	38	A, B	1	1–4
Self-heating (°C)	10	A, B	28	18–60
Odour	10	A, B	1	1–3

The units given in the second column refer to the median and range of measured values.
[a] Treatment A refers to the NIR measurement of dried and ground samples and treatment B to the measurement of samples with a moisture content as received.
[b] The data refer to all samples minus the outliers (see Table 2).

P and K contents were obtained using the CAL method. One hundred milliliter of a CAL solution (0.05 M calciumacetate, 0.05 M calciumlactate, 0.3 M acetic acid) were added to 5 g of sample (<5 mm). The suspension was shaken for 90 min and filtered through a fine-pored filter. The P and K concentrations were determined photometrically (VDLUFA, 1997).

2.3. Phytotoxicity

Phytotoxicity was determined according to VDLUFA (1997). Peat (only for this purpose pH-adjusted to pH 5.5 ($CaCl_2$) and fertilized with 1.2 g l^{-1} water-soluble complete fertilizer) or the ready-to-use growing medium (<5 mm) was filled to the rim of plastic pots (diameter: 11.5 cm, height 7.5 cm) and compacted slightly. Thirty seeds of Chinese white cabbage (*Brassica napus* var. *chinensis*) were distributed evenly on the surface of all media (three replications per medium). The seeds were then covered with a thin layer of medium and the medium was subsequently moistened. Then, the pots were covered with watchglasses and kept under constant light and temperature conditions and watered regularly. After 3 weeks, the classification of the phytotoxicity was carried out, as a modification of the VDLUFA method, according to the degree of damage symptoms (chlorosis, stunted growth): 1 – no damage symptoms, 2 – slight degree of damage symptoms, 3 – moderate degree, 4 – severe degree.