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Usefulness of near-infrared spectroscopy to determine biological and chemical soil properties: Importance of sample pre-treatment

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Abstract

Near-infrared reflectance spectroscopy (NIRS) is known for its inexpensiveness, rapidity and accuracy and may become a useful tool for the assessment of soil quality. Objectives were (i) to evaluate the ability of NIRS to predict several chemical and biological properties of organically managed arable soils as well as the properties of grain yield from winter cereals for a closed population and (ii) to test whether the use of field-moist and pre-treated (quick-freezing followed by freeze-drying and grinding) samples will generate similar results. One hundred and sixteen soil samples from nine organically managed farms from Germany sampled in 2005 and 2006 were used for this investigation. Spectra of the near-infrared region (including the visible range, 400–2500 nm) from field-moist (<2 mm) or pre-treated soil samples were recorded. A modified partial least-square regression method and cross-validation were used to develop an equation over the whole spectrum (first–third derivation). For the pre-treated soils, good predictions were obtained for pH, contents of organic C, total N, plant-available P (Olsen) and exchangeable K (calcium-acetate-lactate (CAL)), contents of microbial biomass C and N (C_{mic} and N_{mic}) and ergosterol, basal respiration, metabolic quotient, the ratio of organic C/total N, the grain yield of winter cereals and grain nitrogen uptake. The RSC (the ratio of standard deviation of laboratory results to standard error of cross-validation) was greater than 2.0, the correlation coefficients (r) of a linear regression (measured against predicted values) were greater than or equal to 0.9 and the regression coefficients (a) ranged from 0.9 to 1.1. Similar good predictions were obtained if field-moist samples were used, with the exception of P (Olsen), K (CAL), metabolic quotient, grain yield of winter cereals and grain nitrogen uptake (satisfactory predictions) and ergosterol content (unsatisfactory prediction). Good predictions of the contents of Mg ($CaCl_2$) and microbial biomass P (P_{mic}) were achieved for field-moist but not for pre-treated samples. Despite sample preparation, only satisfactory predictions were obtained for the ratios of C_{mic}/N_{mic} and ergosterol/C_{mic} and grain nitrogen content ($1.4 \leqslant RSC \leqslant 2.0$, $r \geqslant 0.8$ and $0.8 \leqslant a \leqslant 1.2$). However, unsatisfactory predictions for field-moist and pre-treated samples were achieved for the content of P (CAL), the nitrogen mineralisation rate and the ratios of C_{mic}/P_{mic} and basal respiration/nitrogen mineralisation rate. Our results demonstrate that biological soil properties can be predicted with NIRS for closed populations in both sample states. The pre-treatment should be used if samples have to be stored prior to infrared measurements for periods longer than a month.

Keywords: Plant nutrition; Soil biology; Microbial biomass; Ergosterol; Yield prediction; NIRS

1. Introduction

Agricultural research often relies on the determination of chemical and biological soil properties and yield properties of field crops. Moreover, results of some biological soil properties, e.g. ergosterol content, may change with time due to longer storage of the field-moist sample or exposure

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to short unfavourable conditions like hot conditions or drying (West et al., 1987).

Visible (VIS, 400–750 nm) and near-infrared spectroscopy (NIRS, 750–2500 nm) is known for its rapidity, accuracy, reliability and low costs in many scientific areas (Norris et al., 1976; Fahey Jr. and Hussein, 1999). During the last decade, NIRS has become important in soil-landscape modelling (Brown, 2006). Advantages are that the method is non-destructive, the sample pre-treatment can be minimal and several properties can be predicted for a large sample set simultaneously. The detection limit depends on the investigated compound and ranges approximately between 0.1% (Holroyd, 2003) and 1% of dry matter (Rager, 2001).

Several studies suggested that soil chemical properties can be predicted well or satisfactorily with NIRS. These studies used air-dried and ground soils. For instance, Moron and Cozzolino (2002) predicted the contents of organic C and total N and pH values successfully. Predictions of microbial biomass C and N (C_{mic}, N_{mic}) were done for arable and forest soils (Chang et al., 2001; Ludwig et al., 2002) and they were successful only in one study (Chodak et al., 2002; RDP (ratio of standard deviation of laboratory results to standard error of prediction) $= 2.2$ and $r = 0.9$). Ergosterol content was predicted well ($r = 0.9$) with NIRS for freeze-dried samples of forest organic layers (Pietikainen and Fritze, 1995).

Properties of grain yield may mainly depend on the nutrient availability in the soil, which is dependent on chemical and biological soil properties. However, properties of grain yield are also influenced by other factors such as the level and type of fertilisation, the amount of rain, the rain distribution over the vegetation period and plant pests. Thus, NIRS predictions of yield properties are assumed to be weaker than predictions of soil properties. Predictions of grain yield, determined with dried and ground rice soils, were unsatisfactory (RDP $= 1.0$ and $r = 0.2$; van Groenigen et al., 2003).

Summarising the findings above, NIRS was capable of predicting several chemical soil properties successfully, biological soil properties satisfactorily and only yield properties unsatisfactorily. Nearly all investigations used dried soils, which were dried at room temperature or warmer conditions prior to NIRS measurements. We propose that measurements with field-moist samples should improve predictions for biological soil properties markedly, because experiences showed that air-drying reduced, e.g. the ergosterol content by 70–88% (West et al., 1987). Moreover, we assume that quick-freezing with liquid nitrogen and subsequent freeze-drying of the soil samples is the fastest drying method that inhibits changes of the microbial community, which takes place during drying at warm temperatures. Finally, we assume that predictions for those constituents, which are predicted indirectly (the constituent is not spectrally active, but correlated with spectrally active constituents), especially the yield properties, may not be transferable to samples outside the sample set from which the calibration samples are chosen (closed population).

Objectives of this study were (i) to evaluate the ability of NIRS to predict several chemical and biological properties of organically managed arable soils as well as the properties of grain yield from winter cereals for a closed population and (ii) to test whether the use of field-moist and pre-treated (quick-freezing followed by freeze-drying and grinding) samples will generate similar results.

2. Materials and methods

2.1. Soil samples and reference analysis

2.1.1. Sites and samples

Soil samples were taken from the arable land of nine organically managed farms in Germany (see for details Table 1). The farms are located in Lower Saxony, Hesse, Bavaria and Baden-Wuerttemberg. The long-term annual mean temperature for the sites ranges from 7.1 to 9.8 °C and the annual precipitation ranges from 620 to 900 mm. The sites are located from 25 to 650 m a.s.l. Soil texture varied strongly: contents of clay varied between 3% and 62%, contents of silt between 11% and 92% and contents of sand between 2% and 84%, respectively. The moisture content of the samples ranged from 14% to 28% (w/w). The parent material of the soils differed as well as their origin: they were glacial sands, loess, new red sandstone, granite, gneiss, mica shale, mari and mudstone (personal communications of the farmers).

Soil samples were taken in March 2005 and 2006 at 0–20 cm soil depth. Two to six different fields per farm, each cultivated with winter cereals, were chosen (Table 1). Three separate sub-samples, with a distance of 15 m from each other, were taken per field ($n = 116$). Sub-samples were a mixture of eight samples taken within a circle of 2 m radius. Samples for biological characterisation were stored for some days to a maximum of 2 weeks at 4 °C and sieved (<2 mm) prior to analysis. The samples for soil chemical analysis were air dried and sieved (<2 mm).

2.1.2. Soil chemical analysis

Contents of organic C and total N were determined after drying and grinding on a Vario EL CN autoanalyser. Carbonate content was determined volumetrically as CO_2 (Schlichting et al., 1995). Organic C content was calculated by difference. Soil pH was measured in a solution of soil and 0.01 M $CaCl_2$ at a ratio of 1:2.5 (Hoffmann, 1991). Plant-available P (Olsen) was determined colorimetrically using standard methodology (Kuo, 1996). Exchangeable P and K were extracted in a solution of calcium-acetate-lactate (CAL) at a ratio of 1:20 (pH 4.1). After filtration, P was measured with a spectral photometer at 580 nm as molybdenum blue (Schüller, 1969). Potassium was measured with an atom-emission spectrometer at 767 nm (Hoffmann, 1991). Exchangeable Mg was extracted in a solution of soil and 0.0125 M $CaCl_2$ at a ratio of 1:10.