Application of FTIR spectroscopy for evaluation of hydrophobic/hydrophilic organic components in arable soil

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ABSTRACT

The main aim of this study was to determine the intensity of hydrophobic/hydrophilic components of the soil's organic matter as well as its hydrophobicity. Non-destructive Fourier Transform Infrared (FTIR) spectroscopy was used for the diagnosis and characterization of the basic classes of the chemical groups (hydrophilic and hydrophobic components) from which the organic matter in the soils is formed. Soil samples (depth 0–30 cm) were taken from the topsoil of the 70 sampling sites from the experimental field at Prague-Ruzyne (Czech Republic) during 2007–2009, where a conventional soil tillage technology was used. It was found that the variability of the intensity of the hydrophobic components is greater (27.6%) than that of the intensity of the hydrophilic components (6.2%), which correlated significantly with the C_{org} *(r = 0.58; P < 0.05)* and N_t (*r* = 0.65; *P* < 0.05) in the soil. It was proven that the soil samples with a higher proportion of coarse grains are more hydrophobic than those with higher proportions of clay. Data about soil hydrophobicity can help to evaluate the soil quality parameters as well as the soil fertility.

Keywords: organic carbon; soil organic matter; hydrophobic component; hydrophilic component; soil hydrophobicity

The need for the development of more time- and cost-efficient methodologies for soil analysis is increasing. There is a great demand for rapid and predictive soil data to be used in environmental monitoring, soil quality assessment, as well as in both precision agriculture and forestry. The system of precision agriculture, which is included among the sustainable farming systems, demands frequent environmental monitoring, including predictions of soil quality management (Cohen et al. 2005, Viscarra Rossel et al. 2006).

An important aim of sustainable agriculture is to maintain a certain quality of the soil, and thus soil fertility. One way to assess the soil quality, or some of the qualitative parameters of the soil, is by the use of non-destructive FTIR spectroscopy. FTIR spectroscopy was used successfully on whole soils to describe the status of decomposition within the different horizons (Haberhauer et al. 1998, 1999, Chapman et al. 2001). Using multivariate statistics, FTIR data can be used as quantitative indicators of the composition of the soil's organic matter (SOM) in order to distinguish soil horizons (Haberhauer et al. 1999, 2000). This methodology can also be applied on bulk soil samples for the determination of soil hydrophobicity. Soil hydrophobicity is a qualitative parameter that describes the extent of interaction between surface water and soil particles. A certain degree of hydrophobicity of the soil is important from the viewpoint of maintaining the water balance of the soil regime, aggregate soil stability, preventing soil erosion, maintaining soil fertility, and the protection of SOM against microbial degradation (Bachmann et al. 2006). From the measured spectral specific bands that indicate the intensity of the hydrophobic (water repellency) and hydrophilic (wettability) components of SOM are selected. The applicability of this method for soil samples with a different soil sample preparation for measurement (potassium bromide [KBr] pressed discs) was performed on a series of Australian soils by Nguyen et al. (1991). The

applicability of this methodology on soil samples with different preparation of the soil samples for measurement (KBr pressed discs) was performed on a series of Australian soils by Nguyen et al. (1991). Capriel et al. (1995), applied this method to soil samples in order to determine the hydrophobicity of SOM in a wide range of arable soils, with different textures and organic carbon (C_{org}) contents. These authors found a close relationship between the hydrophobicity of the SOM and textures of the studied soils. SOM in sandy soils contained more alkyl C and fewer carbohydrates (CH) and proteins than did clayey soils, i.e. they had a higher hydrophobicity. It is not only the grain size composition that affected the dynamics of the hydrophobic components in the soil, but also the land management and individual interventions in the soils. These mainly include crop rotation, soil preparations (such as intensive cultivation), or *vice-versa* no-till systems, fertilization, grass, etc. Increased levels of SOM contribute to increases of the soil's hydrophobicity. On a number of soil samples from long-term field experiments with various agricultural crops in Germany, Capriel (1997) proved that farming systems clearly affected the number of aliphatic CH components, followed by and the hydrophobicity of the SOM. The decline of C_{org} due to management is accompanied by a decrease in the hydrophobicity, as well as a decrease in both the microbial biomass and soil aggregate stability. Capriel et al. (1995) found that hydrophobicity correlated positively with sand content and negatively with clay content in the soil. Later, Bachman et al. (2006), who assessed the hydrophobicity of many soil samples of sandy, loam, clay, peat, and volcanic ash soils, confirmed that mainly sandy soils (with relatively small specific surface areas) are prone to hydrophobicity. Kubát et al. (2008) confirmed, in a series of soil samples taken from different altitudes and soil types, a similar (or even better) discriminating sensitivity of FTIR spectroscopy, when compared to other qualitative SOM parameters (such as the humic/fulvic acid ratio or A400/A600).

The aim of this paper was to find the intensity of the hydrophobic and hydrophilic organic components in the soil samples with similar texture and SOM content for a subsequent determination of its hydrophobicity. Obtained knowledge about hydrophobicity should help to better estimate the soil properties. Detailed and accurate information about the soil allows more precise control of the state of soil properties and more accurate distribution of inputs to the soil.

MATERIAL AND METHODS

The experimental data for this study were obtained from an experimental field of 11.5 ha located at the Prague-Ruzyně (50°05'N, 14°18'E), Czech Republic pilot farm. The field is located in a sugar beet production area. The average slope of the field is approximately 3°, and most of the field has a southern aspect. The elevation ranges from 338.5 m to 357.5 m a.s.l. The experimental field is represented by Haplic Luvisol soil. The average precipitation over a year is 472 mm, and the average temperature is 8.5°C. The precipitation and temperature data for this area was provided by the Agrometeorology station at the Crop Research Institute in Prague-Ruzyně. Our experiment included data from 2007 through 2009. Since 2001 the crop rotations have been: sugar beet (2001), spring barley (2002), winter wheat (2003), winter rape (2004), winter wheat (2005), oat (2006), winter barely (2007), winter rape (2008), and winter wheat (2009). Conventional soil tillage technology was used on this field. Precision farming has been practiced in this experimental field since 2002. Since 2003, site-specific application of nitrogen has been used, with the aim of studying its impact on the variations of yields (Kumhálová et al. 2008, Matějková et al. 2010). The 70 locations measured with DGPS were created on a regular grid of 40 × 40 m. These locations were sampling points for the soil samples. The soil samples, taken from depths of 0–30 cm, were analysed for total nitrogen (N_t), C_{org} content, as well as particle size distribution. Particle size distribution was only determined for 28 sites because the accurate, but expensive, sedimentation method (ISO 11277) was chosen for this purpose. C_{org} content and N_t content were determined on a VARIO MAX analyser (Elementar Analysensysteme GmbH, Hanau, Germany).

Field-moist soil samples from each sampling point were sieved through a 2 mm sieve and then air-dried. For the FTIR analysis, the soil samples (300 mg) were mixed with 900 mg KBr (FTIR grade 99%, Aldrich, Germany), and then ground in an agate mortar. The homogenous mixture was transferred to a diffuse reflectance cup (12 mm diam.) without any pressure, and then levelled with a microscope glass slide. The FTIR spectra were measured on a Thermo Nicolet Avatar 320 FTIR spectrometer (Thermo Nicolet Corporation, Madison, WI, USA), equipped by a Smart Diffuse Reflectance accessory (Nicolet, Madison, USA). Three FTIR spectra were collected for each soil sample (absorption mode, KBr background, 256 scans,

Table 1. Basic descriptive statistics of hydrophobic and hydrophilic components of soil. Intensities are derived from 3000–2800/cm (hydrophobic component) and 1740–1600/cm (hydrophilic component) areas of absorption bands of the FTIR spectra

Soil component	Mean	Minimum	Maximum	SD	*CV* (%)
Hydrophobic (intensity)	0.80	0.41	1.37	0.22	27.6
Hydrophilic (intensity)	7.17	6.12	8.17	0.45	6.2
Hydrophobicity	0.11	0.06	0.18	0.03	27.2

n = 70

data spacing 1.929/cm). The FTIR spectra were analysed at two absorption bands, which indicate the hydrophobic (CH-groups), and the hydrophilic (CO-groups) functional groups. The C-H bands occurred at the 3000–2800/cm signal area, while the C-O bands occurred at 1740–1600/cm signal area. The areas of the absorption bands of the hydrophobic and hydrophilic groups in the FTIR spectra were integrated with Omnic, version 6a, spectrometer software (Thermo Fisher, Waltham, USA) and they were defined as intensities. The hydrophobic/hydrophilic functional groups ratio was calculated and defined as the parameter of the soil's hydrophobicity.

Data analysis was done with Statistica Cz 8.0 (Stat Inc., Tulsa, OK, USA). The variability of the intensity of the hydrophilic component, hydrophobic component, as well as hydrophobicity were expressed by the variation coefficient (*CV*).

RESULTS AND DISCUSSION

A high *CV* (27.6%) of the intensity of the hydrophobic components of SOM was found from the measured results of the FTIR spectroscopy. On the contrary, the *CV* of the intensity of the hydrophilic components in the soil was lower (6.2%); these elements in the soils predominate, are stable, and less affected by soil tillage and mineral or organic fertilization (Kaiser et al. 2007). The difference between value of the maximum and minimum intensity of the hydrophilic components of the soil was 2.054, and it was 0.953 for hydrophobic components (Table 1). The hydrophobic components are more responsive to soil tillage and the addition of organic matter containing substantial amounts of hydrophobic components to the soil, for example, can increase soil hydrophobicity, and thus its stability (Piccolo and Mbagwu 1999). Harper et al. (2000) and McKissock et al. (2003) showed that farming which increased the C_{org} content in the soil might increase the hydrophobicity (water repellency) and reduce the soil wettability. The results in Table 2 indicate that there are significant correlations between the grain size composition of the soil and the soil hydrophobicity. The content of finer grains correlated negatively with hydrophobicity ($r = -0.494$, $P < 0.05$), while the content of coarse grains is correlated positively with hydrophobicity ($r = 0.424$, $P < 0.05$). Thus, the hydrophobicity of soil containing grains smaller than 0.01 mm is reduced; and the hydrophobicity of soil containing soil grains in the range of 0.25–2 mm is increased. It follows that those soils containing a higher proportion of finer grains (higher clay content) are less hydrophobic than are soils with a higher proportion of coarse grains (sandy soils). Table 3 shows the correlation between hydrophobicity and the C_{org} as well as the N_t in the soil. The results show that the hydrophilic SOM

Table 2. Relationships between grain size composition and soil hydrophobicity

Variable	Mean	Hydrophobicity *r*
Grain < 0.001 mm (%)	20.0	−0.37
Grain < 0.01 mm (%)	36.7	−0.49*
Grain 0.01–0.05 mm (%)	25.6	−0.25
Grain 0.05–0.25 mm (%)	23.3	0.31
Grain 0.25–2.00 mm (%)	14.4	0.42*

n = 28; *the values are significant at *P* < 0.05; *r* – correlation coefficient

Table 3. Correlation between hydrophobicity, hydrophilic, hydrophobic component, C_{org} and N_t

Variable	N_t *r*	C_{org} *r*
Hydrophobicity	0.28*	0.14
Hydrophobic component	0.43*	0.27*
Hydrophilic component	0.65*	0.58*

n = 70; *the values are significant at *P* < 0.05; *r* – relation coefficient

content correlated significantly with C_{org} ($r = 0.577$, $P < 0.05$), but not with hydrophobicity ($r = 0.139$, $P < 0.05$). The correlation between C_{org} and the hydrophilic organic components in the soil suggests that a larger part of SOM is hydrophilic, and thus the correlation is stronger. Kubát and Lipavský (2006) wrote that soil C_{org} is site specific, and that it is mainly affected by the land use history such as tillage, crop rotations, and fertilization. On the other hand, hydrophobicity of many soil samples (given particularly by hydrophobic component) may vary and is more influenced by the amount and the content and quality of SOM at the sampling site.

In our work, we received detailed information about spatial variability of soil hydrophobicity in field where the precision agriculture is practiced. The results showed that SOM contains more hydrophilic components than hydrophobic components. This information should mainly contribute to sensitive soil management and environmental protection. Thus, farmers can optimize all of the production inputs into the field exactly where they are needed, on the basis of detailed knowledge about the soil properties of that particular field.

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