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Emerging techniques for soil analysis via mid-infrared spectroscopy

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Transmittance and diffuse reflectance (DRIFT) spectroscopy in the mid-IR range are well-established methods for soil analysis. Over the last five years, additional mid-IR techniques have been investigated, and in particular:

1. Attenuated total reflectance (ATR)

Attenuated total reflectance is commonly used for analysis of liquids and powders for which simple transmittance measurements are not possible. The method relies on a crystal with a high refractive index, which is in contact with the sample and serves as a waveguide for the IR radiation. The radiation beam is directed in such a way that it hits the crystal/sample interface several times, each time penetrating a few microns into the sample. Since the penetration depth is limited to a few microns, very good contact between the sample and the crystal must be ensured, which can be achieved by working with samples close to water saturation. However, the strong absorbance of water in the mid-infrared range as well as the absorbance of some soil constituents (e.g., calcium carbonate) interfere with some of the absorbance bands of interest. This has led to the development of several post-processing methods for analysis of the spectra. The FTIR-ATR technique has been successfully applied to soil classification as well as to determination of nitrate concentration [1, 6-8, 10]. Furthermore, Shaviv et al. [12] demonstrated the possibility of using fiber optics as an ATR devise for direct determination of nitrate concentration in soil extracts. Recently, Du et al. [5] showed that it is possible to differentiate between 14N and 15N in such spectra, which opens very promising opportunities for developing FTIR-ATR based methods for investigating nitrogen transformation in soils by tracing changes in N-isotopic species.

2. Photo-acoustic spectroscopy

Photoacoustic spectroscopy (PAS) is based on absorption-induced heating of the sample, which produces pressure fluctuations in a surrounding gas. These fluctuations are recorded by a microphone and constitute the PAS signal. The major advantage of this method is that it is suitable for highly absorbing solid samples such as soils without any special pretreatment. This method has been applied successfully to soil classification and to quantitative determination of soil properties such as available nitrogen, phosphorus and potassium, organic matter or calcium carbonate content [2-4].

3. FTIR-based determination of ion concentration using ion-exchange membranes

In addition to the previous direct methods, mid-infrared spectroscopy can also be used to estimate nutrient availability or ion availability indirectly by combining FTIR with ion-exchange membranes. Such membranes are commonly used in studies dealing with nutrient availability, in which standard chemical methods are used to determine the amount of nutrients sorbed onto the membranes. Chemical analysis can be replaced by mid-IR spectroscopy of the loaded membrane, using either the transmittance or photo-acoustic technique depending on the type of membrane [9, 11].

The present work reviews these techniques and the chemometrics tools required for accurate interpretation of the spectra and discusses the potentials and limitations of each method.

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