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Near- and mid-infrared spectroscopy for the analysis of soils: Where are we and what needs to be done?

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Over several decades, near-infrared reflectance spectroscopy has been shown to be extremely versatile for the rapid analysis of many agricultural materials including forages, foods and grains. More recently, mid-infrared and near-infrared diffuse reflectance spectroscopy (DRIFTS and NIRS, respectively) have come under intense scrutiny for their potential to provide a rapid method for the analysis of soils. This has been especially so for their potential to provide a rapid and inexpensive method for the determination of soil carbon in order to determine carbon sequestration in soils. Research has demonstrated that for the determination of soil C diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) is often more accurate and produces more robust calibrations than near-infrared reflectance spectroscopy (NIRS) when analyzing ground, dry soils under laboratory conditions. However, DRIFTS is known to be affected more by moisture and sample preparation than NIRS even with the spectrometer sealed or purged with dry nitrogen gas to eliminate effects of moisture on the optics, and ambient carbon dioxide and moisture on the spectra. DRIFTS is also not considered to be feasible on samples containing high levels of moisture due to the strong water absorptions in the mid-infrared, although the presence of water is also known to degrade even near-infrared spectra and subsequent calibrations. Thus, while both techniques also offer the potential for the analysis of soils on-site and even in-situ many questions remain to be answered including: 1. What are the advantages and disadvantages of on-site as opposed to analysis in the laboratory; 2. The effect of moisture and particle size on accuracy if samples are to be analyzed on-site; 3. Which spectral range (mid-infrared or near-infrared) is the most effective for in laboratory

and/or on-site analysis; and the effect of different soil types and compositions on the entire process. 4. What analytes can be usefully analyzed by near- and/or mid-infrared spectroscopy. In addition, while DRIFTS has been shown to be advantageous in the laboratory, if samples need to be ground and dried and instruments purged to obtain useable data, it may not be practical for on-site use. Studies were therefore undertaken to determine the effect of ambient atmospheric conditions and soil state (ground, dried, etc.) on DRIFTS and NIRS (Fourier transform and scanning monochromator) calibrations for soil C. Results using a portable Fourier transform mid-infrared spectrometer (FTIR) over a wide range of ambient temperatures and humidity levels have demonstrated that purging of the FTIR is not necessary to obtain calibrations for inorganic or organic C in soils equal to those obtained in the laboratory under ideal conditions. Results will also be shown for the effects of sample state (wet and non-ground, dry and non-ground, and dry and ground) on DRIFTS and NIRS calibrations (Fourier transform and scanning monochromator) for the same samples. Preliminary efforts have already demonstrated that drying of samples on site occurs rapidly under even moderate temperatures (70's) and should not present a problem if dried samples are required.