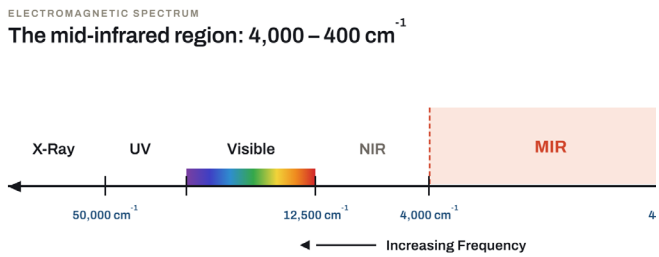
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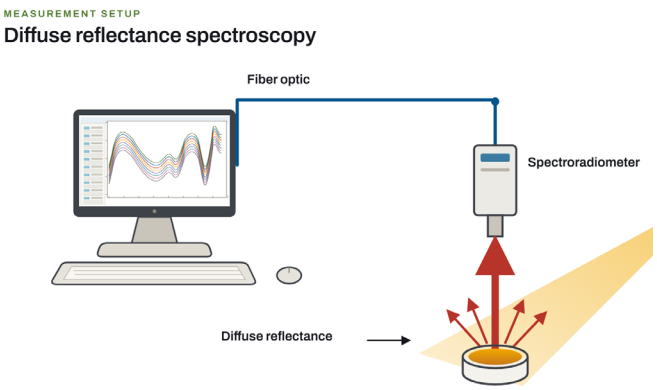
Soil Spectroscopy: Background and Applications

Scientific Basis

Diffuse reflectance spectroscopy has been widely studied as an alternative or supplement to conventional soil testing because it can reduce analysis time and cost by building highly reliable calibrations. (FAO, 2022) Visible, near-infrared (NIR), and mid-infrared (MIR) wavelength regions have all been used for soil characterization, with mid-infrared spectroscopy showing strong performance because it captures molecular vibrations associated with soil minerals and organic matter.



In the simplified diagram below light that is projected onto the surface of the prepared soil sample is reflected and light energy in the MIR range is captured as a digital image of the characteristics of that soil. The reflectance patterns of soil are predictable and the intensity of that energy at specific wavelengths indicates the predominance of different soil characteristics.



This simplified soil spectroscopy schematic from the Open Soil Spectral Library illustrates the typical workflow of a light source, soil sample, spectrometer, and spectral output graph.

In practice, spectroscopy does not replace laboratory analysis rather, spectroscopy relies on the lab work for reference and validation. At the start of creating a soil spectroscopy program, a representative set of soil samples is analyzed by traditional methods and scanned to capture the spectral pattern of each sample. The variations in the spectral patterns are then used to build calibration models that connect the spectral information to the measured soil test properties. To build accuracy into the model, a large set of soil samples and analytical results are used, and every sample is scanned several times. The spectral results are then statistically evaluated against the laboratory reference measurements and used to create prediction models. A second set of validation samples is used to confirm the accuracy of the predicted results.

Applications in Soil Testing

Research has shown that diffuse reflectance soil spectroscopy can accurately predict properties such as total carbon, organic carbon, total nitrogen, carbonate content, cation exchange capacity, soil texture fractions, and water-related indicators. These predictions are most useful when the models are built from a large, representative reference library and are monitored against ongoing laboratory results. (FAO, 2022)

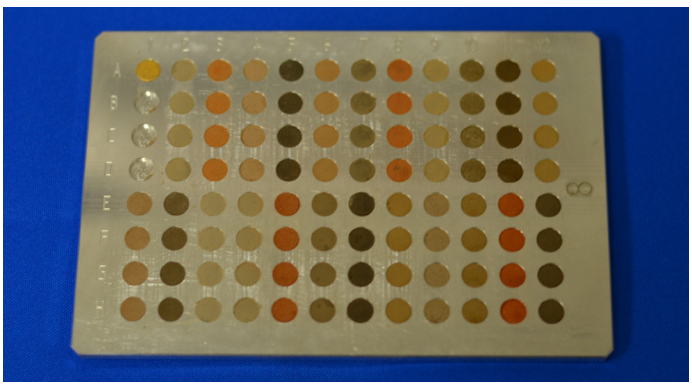
Programs such as the USDA Kellogg Soil Survey Laboratory and international soil spectroscopy efforts have spectra from many thousands of soil samples and demonstrate the value of spectral libraries for routine soil characterization. (Dangal et al., 2019) Their work provided useful background and support for AgSource Laboratories as we evaluated soil spectroscopy as a supplement to routine soil testing and for opportunities of expanded soil health assessment.

Calibration, Validation, and Quality Control

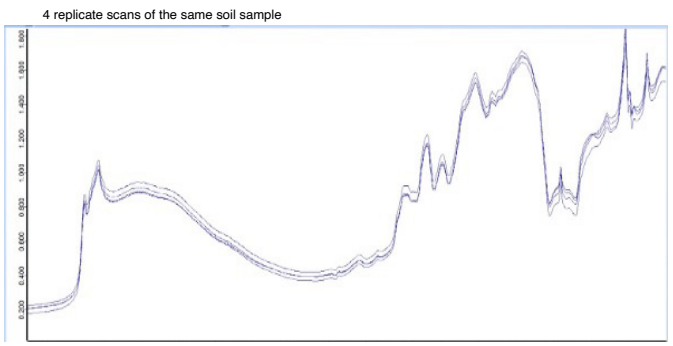
The research and extensive use by the USDA emphasize that calibration quality depends on both the reference laboratory data and the representativeness of the spectral library. (Dangal et al., 2019) The calibration set should span the expected range of soil types, textures, organic matter levels, mineralogy, moisture conditions, and target analyte concentrations. Models developed from narrow or unbalanced datasets may perform well internally but fail when applied to soils that are not adequately represented in the original calibration set. Additionally, grouping samples by regional, geographic or climatic similarities improves the quality of the models.

Validation of the models uses samples that are independent from the calibration process and evaluates performance across both common and difficult prediction targets. Studies have reported strong MIR performance, with R2 correlation coefficients above 0.95, for properties such as soil organic carbon, total nitrogen, carbonate, and cation exchange capacity. Other properties with strong correlations are sand and clay soil texture fractions, pH, and water retention, while soil nutrients and characteristics with highly variable reference data may require larger datasets, local calibration, or more cautious interpretation. (Sanderman et al., 2019)

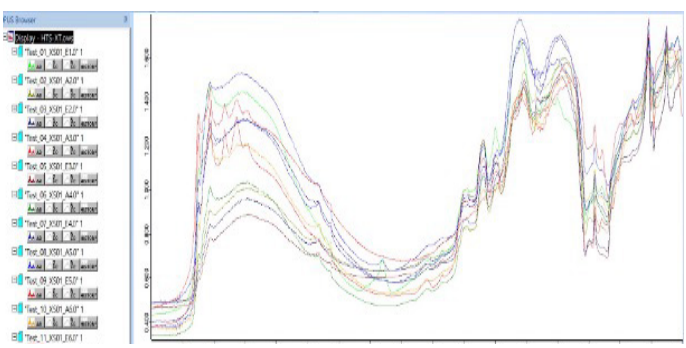
Quality control addresses the full workflow: sample drying and the grinding or milling approach, scan replicates, instrument stability, background corrections, spectral preprocessing, and consistent naming and storage of spectra and reference results. The literature also highlights the need for standardized laboratory protocols so spectra can be compared across instruments, operators, laboratories, and time. (Wijewardane, 2021)



Dried samples are ground with a ball mill to pass an 80 mesh screen (<0.18 mm), desiccated further and pressed into the instrument reader plate. The top left well in every plate is a gold reference followed by 3 blank wells. Then the vertical rows show 4 replicates of the same sample ready for scanning.



Slight differences in the sample preparation are visible in the spectra and evaluated for each sample with the best 3 or 4 lines averaged for each sample.



The average lines for all the samples on each plate are also evaluated for conformity to expectations. While the magnitude of the line (height at each point) will be different because of the quantities of measured variables, the patterns should be similar for soils with similar minerology, and from similar regions and climates. When the pattern does not conform to expectations those samples will be excluded from the data set to be re-tested or analyzed by other analytical methods (note the spectra of the orange lines between 3400 and 3600 cm-1).

With the collection of scans from a reference library of soil samples the relationships of the spectral patterns and the analytical results can be evaluated and used to build statistical predictions of what is in the soil. For example the wavelengths between 3600 and 2500 cm^{-1} and 2270 to 1780 cm^{-1} can accurately predict the Soil Organic Carbon content that would be measured in the lab.

These predictions are continuously verified with periodic check samples and scans of reference library samples. Quality assurance is built upon consistency in sample preparation and routine evaluations of the prediction model against a subset of 5 – 10% of the samples randomly selected for analysis in the laboratory by the wet-chemistry methods. Those spectra and data from the QA samples are added to the models to update the predictions.

Prediction errors are also tracked by soil test property and region or soil group so that the laboratory can identify instrument changes, sample preparation issues, or soil classes that require additional reference samples. When more scans from samples of that region, for example, are collected a new calibration can be developed with those spectra and analytical data. This type of monitoring helps determine when spectroscopy can supplement routine analysis or whether a property or class of samples still requires direct laboratory measurement.

Conclusion

Soil spectroscopy is not a replacement for the high quality analyses that a laboratory can perform on soil samples. Rather it is a supplement of the lab and depends entirely on the analytical work that is done in the laboratory. By collecting spectra from soil samples the many characteristics of that soil are captured in a digital image that can be used again and again to evaluate the soil at that specific point in time. As new prediction models are developed new insights can be gleaned from the spectra that perhaps were not available when the sample was taken. Soil spectroscopy is a stable record of the soil that can be looked at in new ways as we develop new prediction models.

Supporting References

Dangal, S.R.S., Sanderman, J., Skye, W., Ramirez-Lopez, L. (2019). Accurate and precise prediction of soil properties from a large mid-infrared spectral library. Soil Systems, 2019, 3, 11. https://doi.org/10.3390/soilsystems3010011

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Sanderman J, Savage K, Dangal SRS. (2019). Mid-infrared spectroscopy for prediction of soil health indicators in the United States. Soil Sci. Soc. Am. J. 2020;84:251–261. https://doi.org/10.1002/saj2.20009

Wijewardane, N.K., Ge, Y., Sanderman, J., Ferguson, R. (2021), Fine grinding is needed to maintain the high accuracy of mid-infrared diffuse reflectance spectroscopy for soil property estimation. Soil Sci. Soc. Am. J. 2021;85:263-272. https://doi.org/10.1002/saj2.20194