Technical Note

ANALYSIS OF SOILS USING NEAR INFRA-RED SPECTROSCOPY (NIRS)

Introduction

NIRS provides a rapid and cost effective alternative to conventional wet chemistry tests. Hill Labs (HL) has developed this methodology for analysis of soil for Total Nitrogen, Total Carbon, Total Sulphur and Anaerobic Mineralisable Nitrogen as well as Extractable Organic Sulphur and Anion Storage Capacity. As from July 2022, Hot Water Extractable Carbon has been added to the list and HWEONNIr was added in July 2023. This technical note outlines the general test performance and the trade-offs compared to the reference method. For simplicity, the example of Total Nitrogen (tNNir) is used here, but very similar principles apply to the other analytes measured by this technique at Hill Labs.

NIRS has been used very successfully for over thirty years for analysing feedstuffs. Soil testing, however, is much more challenging, because of the diverse nature of soils, i.e. ranging from lignified plant material (peat) to almost pure sand. At Hill Labs, we have put in considerable effort over the last decade to create reliable calibrations for several soil tests. Initially, we worked in collaboration with the Machine Learning Group at Waikato University, and in recent years, we have continued the development with our own small team of in-house chemometricians.

What is Near Infra-red Spectroscopy?

Near Infra-red is the region of light immediately adjacent to the visible range, between 700 and 3000 nanometers in wavelength. This region of light corresponds to the energy of molecular vibrations and will therefore selectively absorb NIR light, depending on the molecules present. The resulting absorbance spectra can be interpreted with high level chemometrics to characterize the chemical composition of the sample. Calibration models are built by collection of many thousand spectra and relating these against reference chemistry values for the same samples – the models are then used to “predict” results for samples of the same type.

Some of the key features of our service are:

- Very large calibration databases. Some workers use only a few hundred samples to build calibrations, which limits their reliability. Our Total N calibration set has in excess of 30,000 soils, for example.
- Use of the ‘nearest neighbours’ approach to utilise only very similar soils (typically 500) to build the NIRS calibrations ‘on-the-fly’.
- Use of sophisticated algorithms.
- Developing robust ways to assess how ‘good’ a prediction is.
- Automatically reverting to the reference wet chemistry for questionable predictions.
- Regularly incorporate these outliers into the calibration database, thereby continually strengthening it for future samples.

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Quality Assurance

We run an expanded Quality Assurance program, where perhaps one in ten or twenty samples are re-analysed by the reference wet chemistry. The differences between these results and the predictions are continually monitored, to ensure acceptable accuracy of the NIRS system. Should the results fall 'out of control', we revert immediately to 100% wet chemistry testing, and our chemometricians respond to resolve the problem.

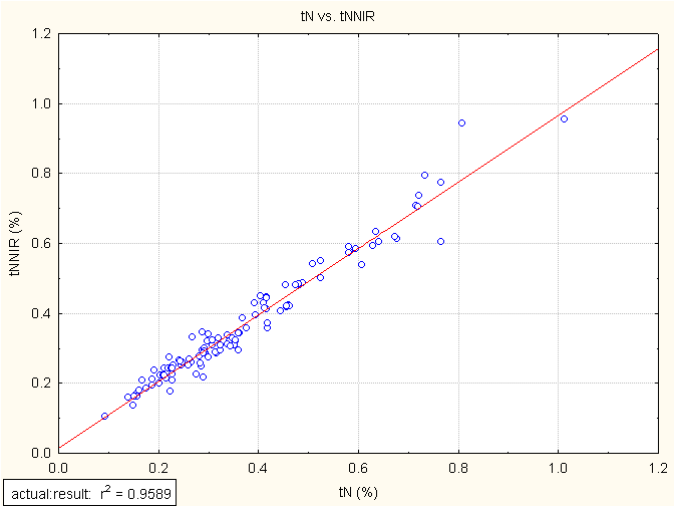

Fig 1. Combustion and NIR results on "new" samples after application of sample qualification rules.

A higher Uncertainty of Measurement (UoM)

This rapid spectroscopic method does introduce higher UoM over the reference chemistry, and a trade-off is required between the precision achieved vs the % of samples being redirected to wet chemistry. We propose the cut-off be set at accepting a doubling of the UoM. At this level, approximately 85% of the predictions are accepted and 15% of the samples are analysed by wet chemistry.

We are mindful that the tests must be fit-for-purpose, but given the much larger uncertainties that occur when collecting a sample, we are confident this test will still be fit-for-purpose.

What's in it for the client?

While the benefits of using NIRS are very real for the lab, what is in it for the customer? Turnaround-time from sample receipt to reporting of results can be significantly improved e.g. the anaerobic mineralisable nitrogen (AMN) conventional method requires a 7-day incubation, whereas the NIRS result is ready within 2-3 days. We are happy to share the efficiency benefits, by reducing the price of the tests via the Organic Soil Profile (OrgSP) and now for Total N (tNNir). It is hoped a price reduction for some of the other tests will be possible in the future also, once the technique becomes routine in the laboratory.

Hill Labs are pleased to be offering this new service, and intend to roll out further NIRS soil tests in the future.

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