How to use *UltraFine+® Next Gen Analytics* FTIR data

What is FTIR data?

Fourier transform infrared spectroscopy or *FTIR* spectroscopy is a tool that is used for the study of mineral and organic components in soil samples. The mid-infrared spectrum (which is obtained using an FTIR spectrometer) provides chemical information to help understand your soil samples in relation to landscape settings and to potentially be used to identify false positive geochemical anomalies in mineral exploration. The method attenuated total reflectance (ATR) spectroscopy has been used to measure the ultrafine soil samples and all ATR-FTIR studies are performed in the region between 4000 to 360 cm^{-1} (2.5 to 27 μm). When you submit your soil samples to the *UltraFine+® Next Gen Analytics* project via LabWest, you will receive five parameters from the mid-infrared spectrum that contain specific information on the composition and chemical properties of the ultrafine soil. This information can help to better understand the influence of ultrafine soil composition on the mobile element uptake and adsorption.

What does this data mean?

FTIR spectroscopy gives you semi-quantitative information on a number of components in your ultrafine soil sample such as the clay, carbonate, quartz and organic carbon content. In addition, it provides information about the absence or presence of gibbsite along with an estimate of the gibbsite quantity. It is important to note that the FTIR data does not give an accurate description and classification of soil type given that only the ultrafine fraction was analysed rather than the original bulk soil sample. However, it does provide relative trends in the chemical content of various components (i.e., clay, carbonate, quartz, organic carbon and gibbsite) and this may be used to help explain variations in metal uptake or to understand false positive geochemical anomalies. When comparing FTIR data from one ultrafine soil sample to the next, generally, differences that are greater than 20 % (for high clay, quartz, carbonate or organic carbon contents) should be considered significant.

Parameter	Definition	Applications & Limitations
Clay_wt%	Estimate of total clay content	It is sensitive to certain clay groups (i.e., kaolinite, montmorillonite/smectite, illite, muscovite) but it does not distinguish between different clay species. The FTIR results on samples that have clay contents of < 20 % are less reliable and are limited to samples with low (<20 %) quantities of gibbsite (a NULL or 1 result in the Gibbs_Index). The quantification error can vary by up to ± 10 wt. % (depending on the clay content).
Qtz_wt%	Estimate of quartz content	It is sensitive to quartz and is limited to samples with low amounts of feldspar (<10 %). Quartz contents of <1 % and above 10 % are less reliable. The quantification error can vary by up to ± 1 wt. % (depending on the quartz content).
Carb_wt%	Estimate of total carbonate content	It is sensitive to a range of carbonates, but it does not distinguish between different carbonate species. Carbonate contents of <1 % and above 40 % are unreliable. If large quantities (>20 %) of carbonate are measured, further processing can separate some carbonate types, but this is very uncommon in UltraFine+ soil samples and is not part of the standard output. The quantification error can vary by up to ± 4 wt. % (depending on the carbonate content).
TOC_wt%	Estimate of total organic carbon content	It is sensitive to a range of organic matter, but it does not distinguish between different types of organic matter. The TOC values <1 % or >15 % are less reliable and it is limited to samples with a low carbonate content. Typically, samples with <15 % carbonate will not influence the result but can

Parameter	Definition	Applications & Limitations
		be cross checked with Carb_wt% result. The quantification error can vary by up to ± 2 wt. % (depending on the TOC content).
Gibbs_indx	A classification that provides an approximate amount of gibbsite abundance	Limited to samples with a low metal hydroxide content. Typically, samples with >10 % metal hydroxide may influence the result and can be cross checked with the VNIR data.

Why are there so many NULLs in my data?

NULLs may be observed in the FTIR data, and this is due to either (a) the amount of various components (i.e., clay, carbonate, quartz, organic carbon or gibbsite) being below the detection limit, (b) spectral interferences/variations which occur due to the nature of the sample that result in less accurate data, and/or (c) the abundance values may be outside the linear concentration range. Data that falls into any of these three categories is unreliable and should be disregarded. To ensure that only reliable data is used, these values are automatically replaced by NULLs. Note that your shape file and the final data in your Data Package contain "-9999" and empty cells, respectively, rather than NULLs.

How do I read the Gibbsite Index?

Gibbsite Index	Definition	Actual values
NULL	Excluded data	values <0.019
1	Low	values between 0.02 to 0.19
2	Medium	values between 0.20 to 0.59
3	High	values >0.6

We use the gibbsite index as a proxy for gibbsite abundance, and generally a larger index value is indicative of a higher gibbsite content in your ultrafine sample. We currently use an index to estimate the gibbsite quantity rather than providing the decimal numbers, because the exact abundance (in wt. %) has not yet been established with known gibbsite standards. However, we can confidently measure abundance trends (i.e., low, medium, high).

How do I use FTIR data?

In addition to the raw data that you and can plot and interrogate as you wish, you will also receive a shapefile of your FTIR data that can be dropped into ArcGIS® or other spatial data plotting software. We recommend plotting the Gibbsite Index as *categories* and all other data as *quantities*. In addition, you may want to use the data to create ratios (first-pass ratios are also being developed as part of the *UltraFine+® Next Gen Analytics* data package).

FTIR application for surface exploration – normalisation of Au concentrations by total organic carbon (TOC)

"Scavenging" phases such as clays, organic compounds and various oxides/oxyhydroxides preferentially adsorb metals. Hence, the concentration of many metals relates to the abundance of such phases in a given soil sample. FTIR parameters can aid in the identification of patterns and areas of unique soil types to better interpret anomalies. Which parameter to use may be dependent on soil type, landscape context and deposit style.

Given the high adsorption capacity of organic matter, it is worth considering whether an anomaly of a metal of interest is present in organic-rich or -poor soils and normalise the geochemical data accordingly to up- or downgrade targets.

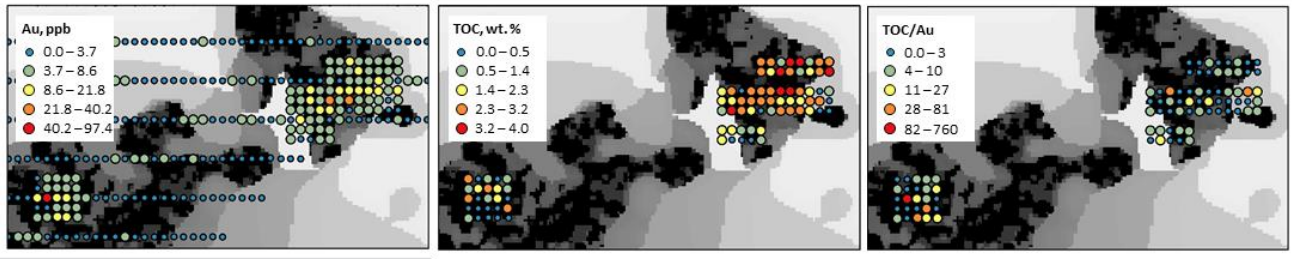

Figure 1: Au concentration, total organic carbon content, and Au normalised by total organic carbon content over depth of cover (grey scale). The normalised data has effectively reduced the Au target size in the two main areas of interest.

References

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