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A RAPID AND NON-DESTRUCTIVE FOURIER TRANSFORM NEAR-INFRARED SPECTROSCOPY (FT-NIRS) METHOD TO RECONSTRUCT ORGANIC CARBON, CARBONATE AND OPAL RECORDS FROM MARINE AND LACUSTRINE SEDIMENTS

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Total organic carbon (TOC), $CaCO_3$ and Opal are bulk geochemical parameters representing a major share of most aquatic sediments and also coal beds. Analysing all three components traditionally requires separate analytical methods and intense sample preparation which are time consuming and expensive if performed at high depth resolution and over long study sections, typically required for high-quality climate records. Near Infrared Spectroscopy (NIRS) has been known for over 100 years, although recent enhancements in technology has meant that this method now has routine applications in environmental science, medicine, agriculture and pharmaceuticals amongst others. Fourier transform near-infrared spectroscopy (FT-NIRS) is a fast, non-destructive and inexpensive technique with the potential to provide accurate key elemental data on natural samples and thus partly replace wet chemical analyses in marine and climate research (e.g. Chang et al., 2005). Here we expand on this approach and report the application of FT-NIRS to a wide range of natural sediments including modern and Quaternary marine sediments, Eocene lacustrine deposits, and Cretaceous black shale.

The marine sediments used in this study were taken from the Equatorial Atlantic and covered deep sea, continental margin, river fan, upwelling and Cretaceous black shale environments. Samples from the Equatorial Atlantic were chosen not only for their wide diversity but also for their importance in understanding tectonics, global carbon budgets as well as past and present climate systems. Lake Messel was chosen as a paleolacustrine setting since it has over one million years of consistent sedimentation and also the presence of a kerogen Type I oil shale with exceptionally high TOC concentrations.

Analyses were performed on a Nexus 870 FT-IR/FT-NIR spectrometer, fitted with a Smart UpDrift accessory (ThermoNicolet Corp.) which allows measurements on powdered samples in diffuse reflection mode, with a quartz sample window to reduce scatter effects. Analyses were carried out over a wavelength range of 875-2500nm at 1nm resolution, yielding 1625 raw data points per sample. Although near infrared spectra display characteristic absorption peaks and troughs relating to specific vibrations from molecular

bonds, their complex, broad overlapping nature relating to overtone and combination bands means that multivariate statistics are needed to relate absorptions at specific wavelengths with chemical data of interest. In this study we used Partial Least Squares Regression (PLSR) as a numerical technique to calibrate and, importantly, predict element concentrations. All data were subject to various spectral pre-treatments to determine the best calibration equations, defined by the lowest RMSEP and the highest R^2 value.

The calibrations developed show strong predictive ability for all three constituents (R^2>0.9) in all of the different settings, providing evidence that FT-NIRS has wide potential for the rapid analysis and prediction of element data of a very wide range of sediments. As one example we show the results for TOC measurement in Figure 1. The plot shows a fully internally cross validated calibration set of conventionally measured (using a Leco CS244 instrument) versus FT-NIRS predicted TOC data using 405 samples from all study sites covering a range of TOC concentrations from 0.04 % to 41 % wt.

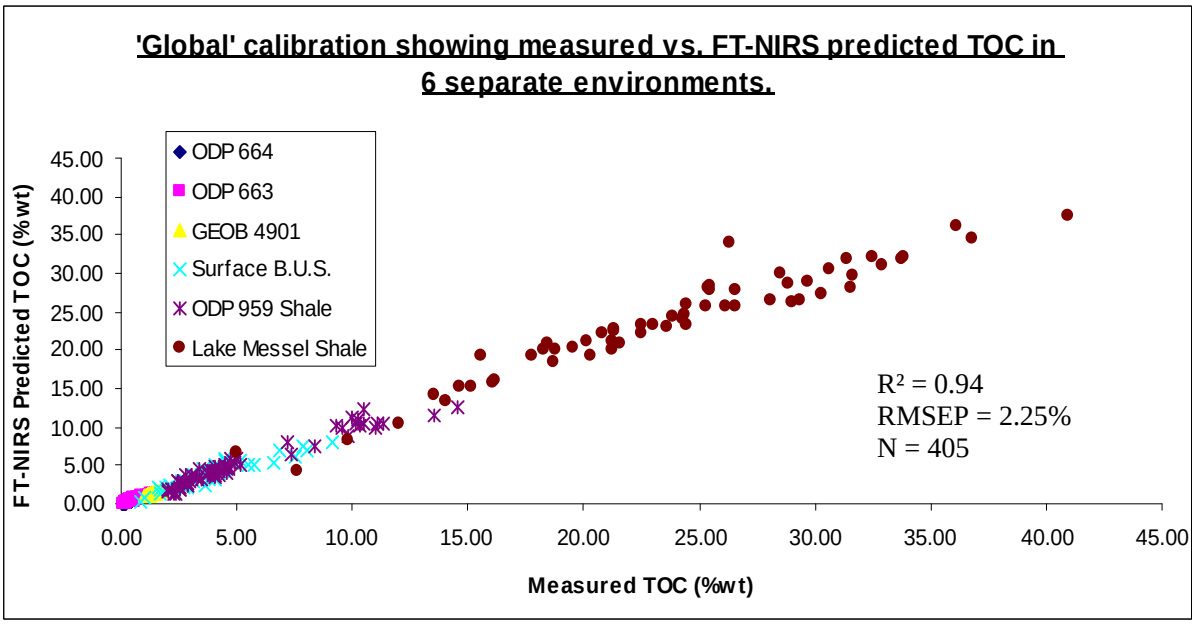

Figure 1. Comparison of measured (Leco) and predicted (FT-NIRS) TOC data for a range of marine and lacustine sediments. Modern: Benguela Upwelling System; Quaternary: ODP 663/664 and GeoB 4901; Eocene: Lacustrine Messel oil shale (courtesy P. Hofmann, Cologne); Cretaceous black shale: ODP 959

We conclude that this technique has the potential to be developed into a fully automated non-destructive scanning technique providing a novel tool for a broad range of environmental and marine applications, in particular for high-resolution climate research and petroleum geology.

REFERENCES

Chang, C-W., You, C-F., Huang, C-Y., & Lee, T-Q. (2005) Rapid determination of chemical and physical properties in marine sediments using a near-infrared reflectance spectroscopic technique. *Applied Geochemistry* 20: 1637-1647.