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Testing the uncertainty of diffuse reflectance spectroscopy methods for estimating marine sediment components by full-resolution spectrophotometry and principle component analyses

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ABSTRACT

Estimating terrestrial and biogenic component variations in marine sediment cores provide essential information in paleoceanographic studies. The variations of terrestrial and biogenic components can be used to infer the changes of sediment provenances that are important for understanding what processes have governed the sediment compositional changes in the cores. One non-destructive technique, diffuse reflectance spectroscopy (DRS), is now commonly used to capture high-resolution information on sediment component changes. The DRS method is a quick and cost-effective procedure for sediment core analysis that requires no chemical analysis with complicated procedures. Recently, one DRS device for capturing visible (VIS) color reflectance data (CRD) (400–700 nm) from core surfaces, the Minolta CM-2600d, has become a standard tool in all marine sediment core analysis. However, by capturing the visible wavelength of CRD only, there are uncertainties in the CRD near the ultraviolet (UV) and near-infrared (NIR) obtained by Minolta CM-2600d are poorly known. In this study, we used a full-resolution (FR) DRS device, the Analytical Spectral Device (ASD) LabSpec® Pro FR ultraviolet/visible/near-infrared (UV/VIS/NIR) spectrometer (250–2500 nm) to compare with the CRD obtained from the Minolta CM-2600d, using the marine sediment core MD103264 taken from offshore southwestern Taiwan. We compared the differences in the VIS wavelength range of CRD between the two devices by analyzing the derivatives and a VARIMAX-rotated Principle Components Analysis (VPCA) of the CRD from 420 samples from core MD103264. Our results show significant uncertainties in CRD near the wavelengths of 400–450 and 650–700 nm in the data from the Minolta CM-2600d. These uncertainties could result in biased or erroneous estimates for terrestrial and biogenic components of marine sediment cores. Our experiments indicate that the CRD obtained with any device with VIS wavelength range only should be interpreted with caution, particularly in the 400–450 and 650–700 nm range.

1. Introduction

Diffuse reflectance spectroscopy (DRS) methods have been applied in a wide range of environmental studies, including those in the laboratory and field, and have made important contributions to pharmaceutical, nutraceutical, and analytical chemistry. The DRS methods are now used extensively in the mining, grain, food, dairy, remote sensing, pulp and paper industries. For sediment core analysis, traditional analysis high-resolution sampling and destructive measurements are usually labor-intensive and time-consuming. To overcome this shortcoming, the current techniques of DRS, which are non-destructive methods that allow measurements on the surface of split marine sediment cores, provide a rapid and inexpensive way to extract information on sediment component changes, e.g. in clay mineralogy, iron oxyhydroxides, carbonates, and diatoms and plant pigments (Ali et al., 2012; Balsam et al., 2007, 1999; Balsam and Deaton, 1996; Ortiz, 2011; Ortiz et al., 1999, 2004, 2009; Pan and Chen, 2013; Pan et al., 2014; Rothwell and Rack, 2006; Zhang et al., 2007). The big data set of temporal and spatial patterns of sediment component changes retrieved from DRS methods paves the way for understanding what ocean and climate processes have been responsible for driving the changes in various marine environments. Therefore, the DRS method is now also commonly utilized as an important tool in paleoclimatic and paleoceanographic studies (Debret et al., 2006; Giosan et al., 2002; Mix et al., 1995;

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Nagao and Nakashima, 1992; Nederbragt and Thurow, 2004; Ortiz, 2011; Yang and Ding, 2003; Zhang et al., 2007).

Two types of DRS instruments are now commonly used: the Minolta CM-2600d and the ASD LabSpec® Pro Full-Resolution (FR) ultraviolet/visible/near-infrared (UV/VIS/NIR) spectrometer. The Minolta CM-2600d is a portable, sea-going possible device which simultaneously produces SCI (specular component included) and SCE (specular component excluded) data in the 400–700 nm (10 nm wavelength pitch) wavelength range. The Minolta CM-2600d use 3 pulsed xenon lamps and silicon photodiode array as light source and detector, and which includes changeable apertures of 8 mm and 3 mm, depending on the size of the samples to be measured. These two apertures enable researchers to measure samples of all size and shapes and avoid taking time consuming average measurements on structured surfaces or faulty results on small samples. The Minolta CM-2600d needs approximately 1.5 s (approx. 2 s for fluorescent measurement) to complete one measurement and provides 3-times average data in 5 s. These convenient, rapid and portable functions are suited for a lot of application in the laboratory and the field that had been used in broad researches (Adler et al., 2009; Debret et al., 2006, 2011; Mihindukulasooriya et al., 2015; Ortiz, 2011; Ortiz et al., 2009; Pan and Chen, 2013; Pan et al., 2014; Ranasinghe et al., 2013; Sebag et al., 2013; ST-ONGE and ST-ONGE, 2014; Yurco et al., 2010). Another instrument, the ASD® (Analytical Spectral Devices, Inc.) LabSpec® Pro FR UV/VIS/NIR spectrometer (now produced by the PANalytical Company) provides an innovative methodology that is quick, portable and easy to use with samples in the lab or field and has been successfully applied to examine the sediment components in several studies (Mihindukulasooriya et al., 2015; Nwaodua and Ortiz, 2014; Ortiz et al., 2009; Ranasinghe et al., 2013; Witter et al., 2009). ASD use halogen bulb as light source, silicon array and InGaAs Photodiode as detectors and which appends an ASD high intensity contact probe (HICP, 20 mm aperture) that capable of measuring a much wider wavelength range of 250–2500 nm, 2–10 nm resolution. The ASD® LabSpec Pro FR UV/VIS/NIR spectrometer only needs 0.1 s to complete a full-resolution scan and provides 10-times the average data in 1 s.

Though the DRS method is powerful enough to rapidly detect the primary sediment compositions from the color reflectance data (CRD) measured from the split surface of marine sediment cores, the degree of uncertainty in the CRD near the ultraviolet (UV) and near-infrared (NIR) obtained by the Minolta CM-2600d is not

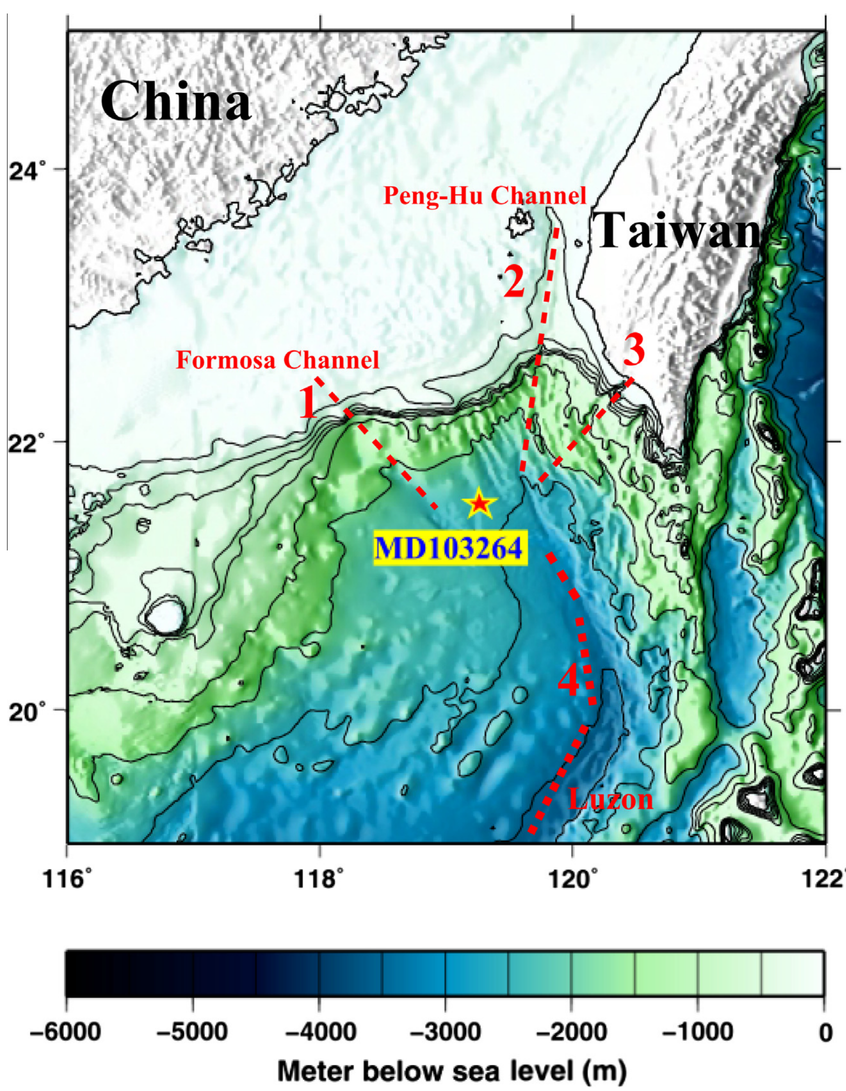

Fig. 1. Map of MD103264 core location used for testing the uncertainty between Minolta CM-2600d and ASD LabSpec® Pro FR ultraviolet/visible/near-infrared (UV/VIS/NIR) spectrometer. Four major sediment sources and transport paths to this site are: 1. Southeast China shelves and slopes via the Formosa Channel; 2. Peng-Hu Island through Peng-Hu Channel; 3. The southwestern Taiwan through Kao-Ping River and submarine canyons; and 4. Volcanic products from the Luzon Island through surface currents.