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A new method to unmix sediment colour data, with specific reference to hematite and goethite abundances

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A number of the magnetic minerals that occur commonly in marine sediments can be difficult to quantify with magnetic methods. Hematite and goethite for example can enter the marine realm from a number of sources such as aeolian dust and ice-rafted debris, but their low spontaneous magnetisation and high coercivity make them difficult to detect at trace levels in many sediments. Diffuse reflectance spectroscopy (DRS) determines the colour of a sediment across the wavelength range of visible light by measuring percentage reflectance at 10 nm increments between 400 and 700 nm. The visible wavelength range can provide information on hematite, goethite, maghemite, clay minerals, carbonate and organic matter. High resolution records (typically a downcore spacing of $<$10 cm) can be obtained easily because the DRS measurement is rapid and requires minimal sample preparation. The DRS spectra do however represent a composite signal from a number of different minerals, therefore it is necessary to "unmix" the data to obtain information on the abundance of phases of specific interest. We will present the details of a new DRS data analysis method, which utilises constrained non-negative matrix factorization to recover the basis vectors from which a data set is composed (effectively the end-member spectra) and the mixing coefficients required to explain the spectra observed for each sample. In order to identify the specific mineral phases present in the sediment the form of the constituent spectra must be compared directly to the curves of reference materials. In turn the downcore mixing coefficients provide a (semi)quantification of the abundance of the minerals which control the colour of the sediment at a given depth. Case studies will be shown where the reflectance data contains information concerning hematite and goethite abundance in recovered sediment cores. Such information can be employed in oceanographic and environmental studies, for example to reconstruct fluxes of aeolian dust entering the oceans or to monitor changes in the intensity of diagenesis.