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A new method for robust multilinear modelling of fluorescent organic matter applied to Antarctic firn from Patriot Hills, West Antarctica

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Analysis of fluorescent organic matter (FOM) is increasingly applied to ice cores as a sensitive means of detecting ice-bound biomarkers, with these signatures showing great potential as proxies for marine productivity and sea ice changes in the Southern Ocean. A range of instrumentation, including in-situ borehole fluorometers, core scanners such as the Berkeley Fluorescence Spectrometer, and benchtop spectrofluorometers, have been applied in search of FOM within ancient ice. All share a key limitation, impeding species-specific analysis –fluorescing substances (fluorophores) in ice layers will produce overlapping signals that are extremely difficult to deconvolute. Multi-band fluorescence measurements in the form of excitation-emission-matrices (EEMs) have the advantage of encapsulating the entire UV-Vis fluorescence response of an ice core meltwater sample. In this case, multilinear modelling techniques such as Parallel Factor Analysis (PARAFAC) appear to offer a solution to the mixed fluorescence problem by decomposing overlapping signatures into individual fluorophores. However, a key issue in PARAFAC modelling of EEM data is the lack of any tool to quantify per-sample and per-component model fit. In essence, the 'best'model is selected using whole-model metrics, then resolved fluorophores are reported and interpreted without accompanying per-sample information on the effectiveness of the model.
We present, discuss, and apply a tool that quantifies the per-sample and per-component fit of PARAFAC models of ice core fluorescence data. Using contiguous measurements of FOM in Antarctic firn from Patriot Hills in the Ellsworth Mountains, West Antarctica, we demonstrate that intra-model per-sample similarity analysis allows for superior positive identification of ice-bound fluorophores. Subsequently, the technique provides a clear visualisation of where precisely in a contiguous modelled fluorophore record the model fails to adequately represent the underlying fluorescence data. Quantifying fluorescence model variability in this manner will be vital for developing proxy relationships and interrogating the processes (both external and in-situ) that control the presence and intensity of ice-bound fluorophores.

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