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Fluorescence Spectroscopy and Water Quality

FL-28

ELEMENTAL ANALYSIS
FLUORESCENCE
GRATINGS & OEM SPECTROMETERS
OPTICAL COMPONENTS
FORENSICS
PARTICLE CHARACTERIZATION
RAMAN
SPECTROSCOPIC ELLIPSOMETRY
SPR IMAGING

Introduction

Water travels through the environment carrying dissolved organic matter (DOM), made up of various chemical compounds, which have entered the water column from many sources. The amount of DOM in water and its chemical composition vary in space and time. Light's interaction with DOM is a function of its chemical make-up; thus fluorescence spectroscopy can provide information about the amount and type of DOM in a water sample. Because the chemical composition of DOM is determined by its original source material and the processing occurring in the environments through which it travels, DOM characterization using fluorescence spectroscopy can help find the source of DOM, as well as the pathway the water transporting it has followed.[1]

The amount and type of DOM in local water systems is important for urban planning, ecological studies, and understanding effects of trace amounts of organic compounds on living organisms. Fluorescence spectroscopy, especially the excitation-emission matrix (EEM), is becoming more popular for determining the amount of DOM contamination in water. Using EEMs to determine polyaromatic hydrocarbon and "humic substances" (soil-derived compounds) seems especially effective. Brian Bergamaschi and co-workers at the U.S. Geological Survey have been recording EEMs of water sources in California to monitor water quality.[2]

Experimental method

Water samples were quickly filtered in the field through 0.2 µm precombusted glass-fiber filters, chilled, and shipped overnight to the U.S.G.S. laboratory in Sacramento, California.

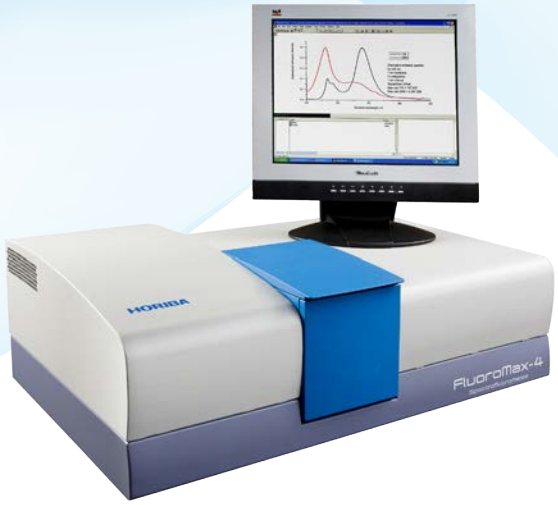

Fig. 1. FluoroMax® spectrofluorometer.

After the sample equilibrated to 25°C, it was placed in a 1-cm2 quartz cuvette inside the sample compartment. An EEM was constructed by measuring a sample's fluorescence via a FluoroMax® spectrofluorometer (Fig. 1) at thousands of combinations of excitation (200–400 nm) and emission (220–600 nm) wavelengths. An automatic shutter protected the samples from photobleaching. While recording fluorescence, the signal was corrected with the reference detector.

[1]Cory, R.M., and McKnight, D.M., Environ. Sci. Technol., 39 (2005), 142–8149, doi:10.1021/es0506962.

[2] Kraus, Tamara E.C., et al., Org. Geochem., 39(9), 2008, pp. 1302–1318; Bergamaschi, B.A., et al., U.S. Geological Survey Scientific Investigations Report 2005-5152, 38 pp. (2005).

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Results and discussion

An example of a typical EEM from a water sample originating in a natural tidal wetland is shown in Fig. 2. Such EEMs can be decomposed into excitation-emission components, representative of fluorophores, via statistical methods. Bergamaschi, et al. used parallel factor analysis (PARAFAC) to decompose data into separate components, and provide values proportional to each component's signal. Fig. 3 is an example of PARAFAC decomposing an EEM. With separate components determined, plots of loading (proportional to signal) versus excitation and emission can be drawn (Fig. 4.).

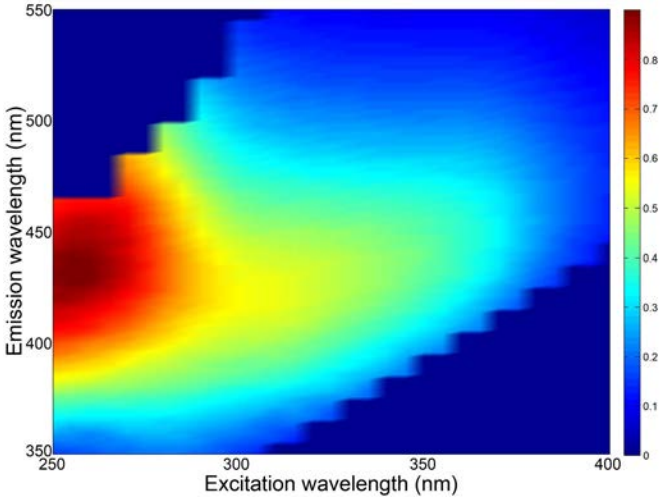

Fig. 2. EEM recorded from water in a natural tidal wetland.

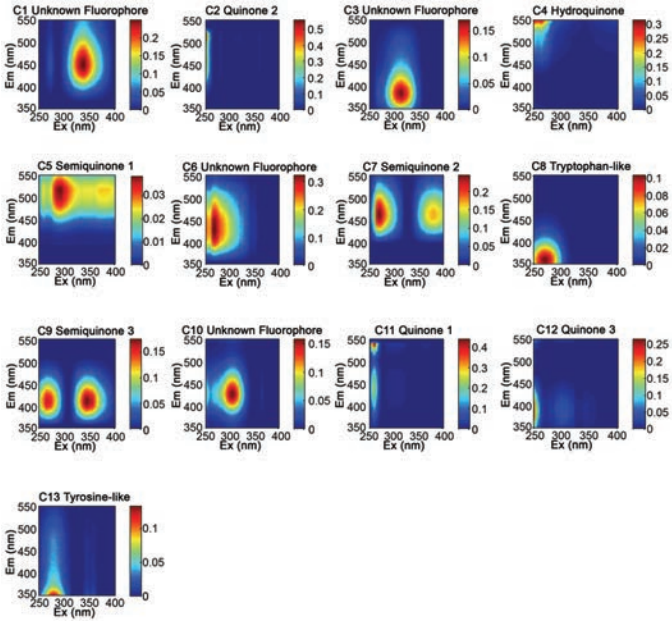

Fig. 3. PARAFAC analysis on the EEM in Fig.2. Thirteen separate modeled components describe 98% of the variability.

Conclusions

Ecological and geological studies by means of parallel factor analysis of EEMs has been shown to be a useful application involving HORIBA Jobin Yvon spectrofluorometers.

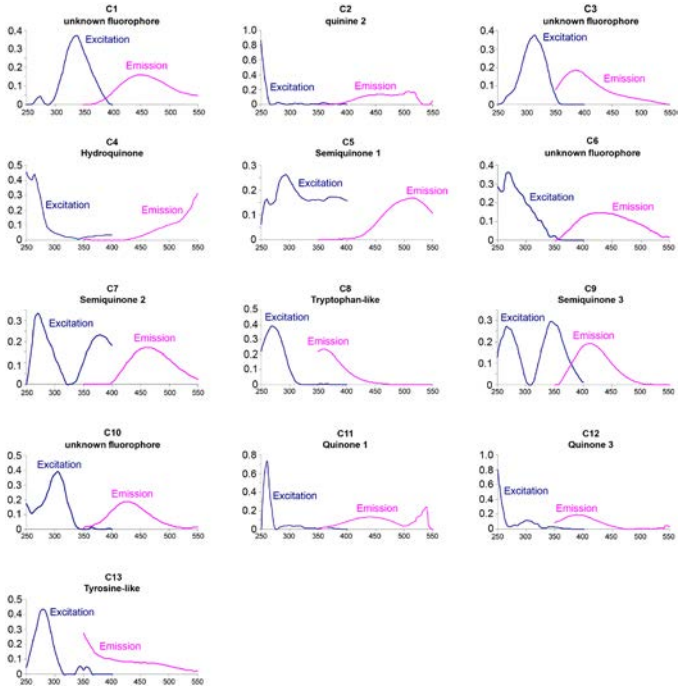

Fig. 4. Loading (y-axis) vs. wavelength (x-axis) for the components in Fig. 3.

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