



Chlorophyll A concentration correlates with organic matter compositions in a stratified drinking water reservoir

Peter Herzsprung (1), Valerie Wentzky (1), Karsten Rinke (1), Norbert Kamjunke (2), Wolf von Tümpling (2), Kurt Friese (1), Bertram Boehrer (1), and Oliver Lechtenfeld (3)

(1) Helmholtz-Centre for Environmental Research UFZ, Department of Lake Research, Brückstraße 3a, D-39114 Magdeburg, Germany, (2) Helmholtz-Centre for Environmental Research UFZ, Department of River Ecology, Brückstraße 3a, D-39114 Magdeburg, Germany, (3) Helmholtz-Centre for Environmental Research UFZ, Department of Analytic, Permoserstrasse 15, D-04318 Leipzig, Germany

Aquatic primary production is the source of autochthonous organic material to be released as dissolved organic matter (DOM). Terrestrial (allochthonous) and autochthonous DOM were traditionally distinguished by the use of fluorescence indices (1,2). However, fluorescence spectra cannot provide high resolution on a molecular level. The observation of DOM quality variations requires due to its exceptional complexity high resolution structural spectrometry and spectroscopy, such as electrospray ionisation (ESI) Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR-MS). In order to identify molecular compositions which are potentially related to primary production Spearman's rank correlation of chlorophyll concentration levels with relative intensity levels of DOM components measured by FT-ICR-MA was used.

High variability of DOM composition was expected by investigating a stratified reservoir at different depths and during different seasons. The number of components showing significant correlations was higher during months with than without thermal stratification. Rather aliphatic components (containing only C, H, O) with low molecular weight correlated positively with chlorophyll concentration. Especially lignin like components of high molecular weight were negatively correlated. The major part of N-containing components (CHON) with low molecular weight were positively correlated. In comparison to CHO and CHON, only few CHOS components were present in all the samples and they mainly did not correlate or few of them correlated negatively.

By the results it can be demonstrated that combining FT-ICR-MS elemental formula data sets with external parameters like fluorescence intensity, UV absorption (3) or chlorophyll concentration (this study) by rank correlation is appropriate for elucidation specific functions of sub-quantities of DOM.

References

- 1) Fellman, J.B., Hood, E., Spencer, R.G.M., 2010. Fluorescence spectroscopy opens new windows into dissolved organic matter dynamics in freshwater ecosystems: a review. *Limnol. Oceanogr.* 55, 2452–2462.
- 2) Zsolnay, A., 2003. Dissolved organic matter: artefacts, definitions, and functions. *Geoderma* 113, 187–209.
- 3) Herzsprung, P., von Tümpling, W., Hertkorn, N., Harir, M., Büttner, O., Bravidor, J., Friese, K., Schmitt-Kopplin, P., 2012. Variations of DOM quality in inflows of a drinking water reservoir: linking of van Krevelen diagrams with EEMF spectra by rank correlation. *Environ. Sci. Technol.* 46, 5511–5518.