Eawag
Überlandstrasse 133
8600 Dübendorf
Switzerland
Phone +41 (0)58 765 53 61
Fax +41 (0)58 765 53 75
info@eawag.ch
www.eawag.ch

Eawag Seminar Invitation

Linking dissolved organic matter composition with photoreactivity using high-resolution mass spectrometry

Speaker **Prof. Christina K. Remucal**
University of Wisconsin-Madison, USA

When **March 22, 11.00 – 12.00 a.m.**
Where **Forum Chriesbach, room C20, Eawag Dübendorf**

Abstract The composition of dissolved organic matter (DOM) determines its photochemical reactivity and ability to form photochemically produced reactive intermediates (PPRI). We collected water samples in the St. Louis River in the United States, which includes of variety of DOM sources and processing. Bulk characterization techniques, such as measurements of total organic carbon and ultraviolet-visible spectroscopy, show the quantity of DOM, apparent molecular weight, and aromaticity all decrease downstream in the system. Characterization at the molecular level using Fourier-transform ion cyclotron resonance mass spectrometry (FT-ICR MS) reveals that saturation of DOM generally increases downstream. Photochemical experiments measuring quantum yields for PPRI formation show that upstream samples are more efficient at producing hydroxyl radical, while downstream samples are more efficient at producing triplet DOM and singlet oxygen. Spearman rank correlations were used to correlate formula intensities, as determined by FT-ICR MS, to observed quantum yields for PPRI formation and to photodegradation rate constants of target contaminants (atorvastatin, carbamazepine, DEET, and venlafaxine). These analyses indicate that the more saturated DOM pool most strongly correlated to formation of triplet DOM and singlet oxygen is the same pool of DOM correlated to photodegradation of atorvastatin, carbamazepine, and venlafaxine. In contrast, highly aromatic DOM formulas are strongly correlated to hydroxyl radical formation and DEET photodegradation. Together, these results demonstrate how DOM composition affects photoreactivity and contaminant fate.