

13TH

IBP PHD CONGRESS

RELOADED



PRESS START



09. April 2021

8:30 AM – 5 PM on Gather.town

12 Talks,

36 Posters

Afterparty on Gather.town

# 13<sup>th</sup> IBP PhD Congress 2021 – **PRESS START**

## Tutorial-Level:

8:30 Login to gather.town

 Gather 

9:00 Welcome by Chairs (Niroshan Gajendra, Surya Gupta)

9:10 Opening IBP Chair (Prof. Nicolas Gruber)

9:15 **Level 1: Talk session – Into the Deep** 

- **Flora Desmet**  
4D marine acidification extremes in the Northeast Pacific: diversity and drivers
- **Eike Köhn**  
Extreme shoaling events of hypoxic waters in the Eastern Pacific
- **Pascal Wiesli**  
Off-Flavour origin, dynamics and mitigation in recirculating aquaculture system producing Atlantic salmon
- **Deniz Dişo**  
Mechanisms behind the spatiotemporal variability in coral reefs: An integrative modelling study

10:30 **Bonus Level: Poster Session A**  Gather

12:00 – Lunch Break –  
13:00

13:00 **Level 2: Talk Session – Sink or Swim** 

- **Benedikt Ehrenfels**  
Hydrodynamics modulate nitrogen fixation in Lake Tanganyika
- **Ma Yingin**  
Intermixing level determines spread of antibiotic resistance during microbial range expansion
- **Kathrin Baumann**  
Microbial Nitrogen potential of two lakes with contrasting trophic states
- **Stephanie Remke**  
Characterizing the chemical nature of long-lived photooxidants produced from dissolved organic matter

14:15 **Bonus Level: Poster Session B**  Gather

15:45

**Level 3: Talk session – Secrets of Soils** 

- **Carla Perez-Mon**  
Microbial responses of alpine permafrost to field-simulated conditions of warming
- **Xu Fang**  
Producing safe rice from As and Cd contaminated paddies via soil management
- **Charlotte Bopp**  
Substrate specificity of enzymatic contaminant oxygenation
- **Charlotte Driesen**  
How potent is the transfer of polychlorinated biphenyls from cow to calf?

17:00

**Apéro & Awards**  **Gather**



**Afterparty**



 **Gather**

**Let's press start!**

We are happy to welcome you to the first online IBP PhD Congress! Brand new research is waiting for you in our custom-made conference world in gather.town. This congress will take you through diverse levels in which you will explore the wide range of research at the Institute of Biogeochemistry and Pollutant Dynamics (IBP) and strengthen interdisciplinary bonds by connecting with each other, scientifically and personally. We're inviting you to get your hands on the keyboard and have a day full of fruitful discussions and fresh ideas!

Enjoy your Apéro Bööxli!

**Organizing committee**



**Katharina  
Sodnikar**



**David  
Haaf**



**Katrin  
Schulz**

**Chairs**



**Surya  
Gupta**



**Nirashan  
Gajendra**

**and with great help from**



**Dr.  
Anouk  
N'Guyen van Chinh**

#### 4D marine acidification extremes in the Northeast Pacific: diversity and drivers

Desmet, Flora

ETH Zürich, Environmental Physics, Institute of Biogeochemistry and Pollutant Dynamics

The ocean uptake of anthropogenic carbon from the atmosphere has led to a 0.1 pH unit decrease of global mean ocean surface pH and a 16% reduction of aragonite saturation state ( $\Omega_A$ ) in the upper 100m of the Pacific since preindustrial times. While mean changes in ocean pH and  $\Omega_A$  have been extensively studied, little is known about episodic extremely low pH- $\Omega_A$  events and their mechanisms. Understanding the dynamic of three-dimensional spatially coherent structures of unusually low pH- $\Omega_A$  levels and their evolution in time is crucial to study the impact of acidification on drifting pelagic organisms. Using a high resolution regional oceanic model coupled to a biogeochemical-ecosystem model (ROMS-BEC) we found that such structures in the upper 100m of the Northeast Pacific occupy up to 240000km<sup>2</sup> a day, being five times the area of Switzerland, and persist up to several years propagating over thousand of kilometers. In the California upwelling system, extremes occurring at surface near the coasts are largely driven by anomalously efficient upwelling while large, long, vertically extended and highly propagating events are at 82% cyclonic eddy-driven. Our findings highlight the importance of subseasonal mechanisms with spatial scales smaller than 100km in forming persistent, large and intense pH- $\Omega_A$  extremes.



Four-dimensional coherent structure of unusually low pH and  $\Omega_A$  at four different dates off the coast of California starting from an upwelling event and persisting due to mesoscale filaments pinching followed by mesoscale eddy trapping.  $\Omega_A$  in the event is given by the yellow-red colorscale.



## Extreme shoaling events of hypoxic waters in the Eastern Pacific

Köhn, Eike E.

Environmental Physics, Institute of Biogeochemistry and Pollutant Dynamics, ETH Zürich,

Climate change-mediated ocean warming drives deoxygenation, the loss of oxygen from the surface ocean. This affects heterotrophic organisms, i.e. those organisms that require oxygen concentrations in respiratory metabolic processes. Their vertical habitat gets sandwiched vertically between well oxygenated surface waters and shallowing subsurface hypoxic waters ( $[O_2] < 60 \text{ mmol m}^{-3}$ ). Superimposed on the long-term trend, natural variability induces periods during which hypoxic waters reach unusually close to the surface. These so-called transient habitat reduction extreme events (THREEs, Fig. 1) can limit food supply, alter food-web interactions, and induce ecosystem shifts on time scales of weeks to months. Yet, little is known about their frequency and characteristics.

Here, we investigate the distribution, drivers and biogeochemical characteristics of THREEs in the Eastern Pacific (EP) between 1979 and 2016, based on a daily hindcast with the coupled physical-biogeochemical ocean model ROMS-BEC. We detect THREEs using a statistical 1st percentile approach and set a minimum duration limit of 5 days. In the tropical EP, most THREEs occur during La Niña conditions, in conjunction with propagating Rossby waves. In the subtropical EP, THREEs are associated with mesoscale eddies. 75% of all THREEs show extremely acidic (low pH) conditions, thus constituting compound events.

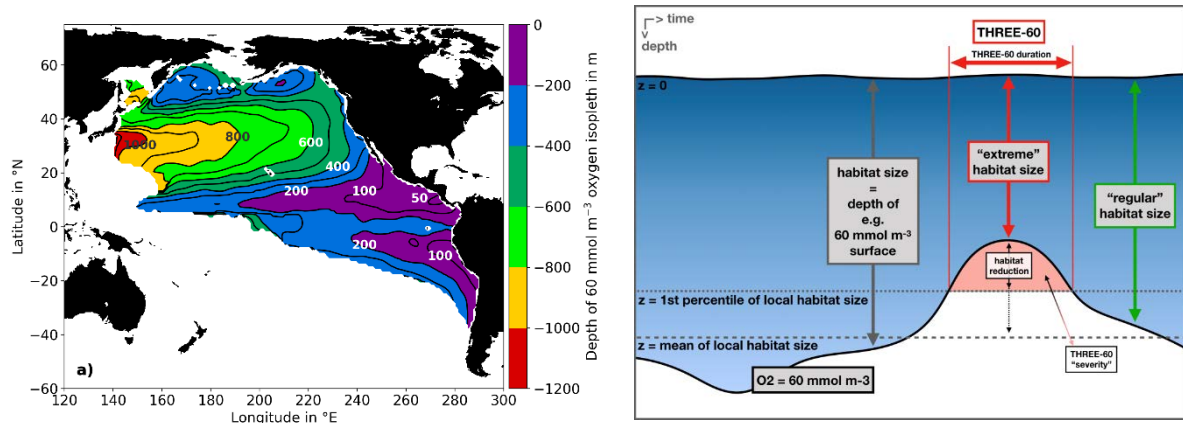


Figure 1: a) Depth of the mean hypoxic interface (HIF, i.e. the  $60 \text{ mmol m}^{-3}$  oxygen isopleth) from World Ocean Atlas 2018 data. b) Conceptual sketch of a transient habitat reduction extreme event (THREE). At each grid point, the threshold depth is calculated as the first percentile of the local HIF depth distribution. As the THREE is detected for the  $60 \text{ mmol m}^{-3}$  oxygen isopleth, it is referred to as THREE-60.

## Off-Flavour origin, dynamics and mitigation in recirculating aquaculture system producing Atlantic salmon.

Wiesli, Pascal

ETH Zürich, Environmental Microbiology, Prof. Dr. Mark Lever

Eawag, Environmental Chemistry, Stable Isotope Lab, PD Dr. Thomas Hofstetter

Over the past decades, the aquaculture sector has grown rapidly to contribute to 50% of the global fish production. While traditional aquaculture systems such as artificial ponds and net-cages can cause well-known environmental problems (eutrophication, use of antibiotics), fish production in recirculating aquaculture systems (RAS) is considered as more environmentally friendly. However, the still developing RAS technology suffers from potential ecological and economic limitations. One major drawback is the accumulation of so-called off-flavour substances, namely geosmin and 2-methylisoborneol in RAS-produced fish, which can cause considerable economic losses.

The objective of my PhD project is to manage off-flavours in RAS by studying their origin and distribution as well as evaluating the implementation of mitigation strategies. High abundances of geosmin producing bacteria were identified in biofilms (qPCR, next generation sequencing), indicating that geosmin recovered in salmon filet in concentrations of up to 20 ng/g derived from the RAS plant. High concentrations of off-flavour were not only measured in biofilm from walls and pipes but also in suspended solids in sludge water collected in the RAS effluent. A large share of geosmin is also bound to dissolved particles after separation of sludge from RAS process water. Recent experiments in RAS pilot plants suggest that this dissolved geosmin fraction can be efficiently removed through a combined treatment with protein skimmer and UV/ozone.



## Mechanisms behind the spatiotemporal variability in coral reefs: An integrative modelling study

Dişa, Deniz

UP Group/IBP/ETH Zurich

The interplay between biological, physical and chemical processes creates substantial amount of spatiotemporal variability in coral habitats. For instance, diurnal fluctuations in seawater pH may reach to 0.2, which is higher than the expected change in world oceans until the end of century. However, the mechanisms behind the variability are poorly understood. To fill this gap, we incorporated a coral physiology model into a 3D coupled biogeochemistry/hydrodynamic model and studied the dynamics of variability under three wave regimes on Moorea island. Our results show that certain reef sections not only experience much more variability, but also fundamentally different mean conditions. The transport of the local signals (i.e. the alteration of the seawater by the underlying corals) creates distinct patterns in the space. Although changes in wave conditions alter circulation and thus seawater chemistry and coral metabolic rates, these spatial patterns remain. The persistence of spatial patterns lead to the formation of distinct biogeochemical niches within the reef, which might translate into differences in coral resilience. Coupling physical, chemical and biological processes, we developed a strong tool to understand the mechanisms behind the spatiotemporal variability in reefs. Our findings are essential to support strategic decisions with regard to ecosystem management options.

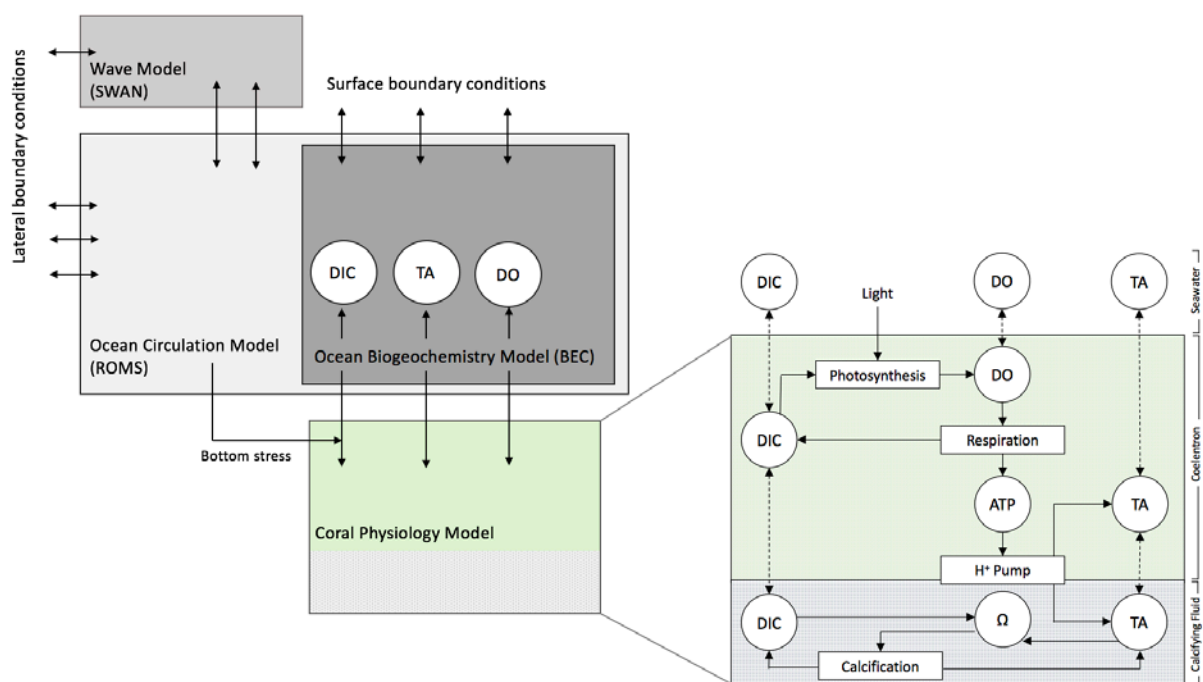


Figure 1 Conceptual diagram of the coupled model structure

## Hydrodynamics modulate nitrogen fixation in Lake Tanganyika

Ehrenfels, Benedikt

Department Surface Waters – Research and Management, Eawag

Marine and freshwater low-oxygen environments are hotspots of nitrogen cycling. Climate change alters hydrodynamic regimes worldwide, and additional information is needed on how hydrodynamic conditions affect nitrogen cycling in low-oxygen waters. Here, we present basin-scale budgets of nitrogen fixation for Lake Tanganyika, the largest anoxic freshwater body. Our biogeochemical analysis combines stable isotope tracer experiments, natural abundance stable isotope analyses, and metagenomics. Both aerobic and anaerobic nitrogen fixation were lower in the upwelling-driven south compared to the heavily stratified north and central basins. Upwelling promoted high nutrient fluxes to the nitrogen-depleted euphotic zone supporting a heterotrophic diazotroph community, whereas the slow nitrate resupply in the the north basin was associated with high nitrogen fixation by filamentous cyanobacteria. In the anoxic zone, the stable water column in the north enabled the formation of an anoxic chlorophyll maximum hosting a high potential for anaerobic nitrogen fixation by autotrophs. In contrast, the more dynamic water column in the south prevented the development of an anoxic chlorophyll maximum, leading to a lower potential for anaerobic nitrogen fixation and a largely heterotrophic diazotroph community. We suggest that upwelling and mixing constrain both aerobic and anaerobic nitrogen fixation in Lake Tanganyika and alter the diazotroph community.



Sampling on board M/V Maman Benita, facing the Tanzanian coast of Lake Tanganyika.



## Intermixing level determines spread of antibiotic resistance during microbial range expansion

Yinyin, Ma

Eawag Umik & ETH USYS

Range expansion is a general feature of surface-attached microbes. It involves the non-random self-arrangement of microbes across space. This process is referred as spatial self-organization (SSO), which is determined by local environmental conditions and interactions occurring between genotypes. Intermixing is an emergent property of SSO that results in various magnitudes of cell-cell contacts, the greater intermixing, the more contacts. Here we hypothesize that intermixing level is an important determinant of conjugation-mediated horizontal gene transfer (HGT) within microbial communities. We predict that spatial patterns with greater intermixing between genotypes will promote spread of plasmid-borne antibiotic resistance. In order to test this prediction, we performed range expansion experiments using a synthetic microbial community consisting of two strains, one of whom carries plasmid and the other does not. We modified the mode of interaction between these two genotypes, either competing or cross-feeding to manipulate intermixing level between them, and quantify the spread of transconjugants who can be identified by distinct colour under confocal microscopy. In the end, we did not find any transconjugants on population level in competing group, but we did find them in cross-feeding group due to much higher intermixing level caused by mechanical cell-shoving.

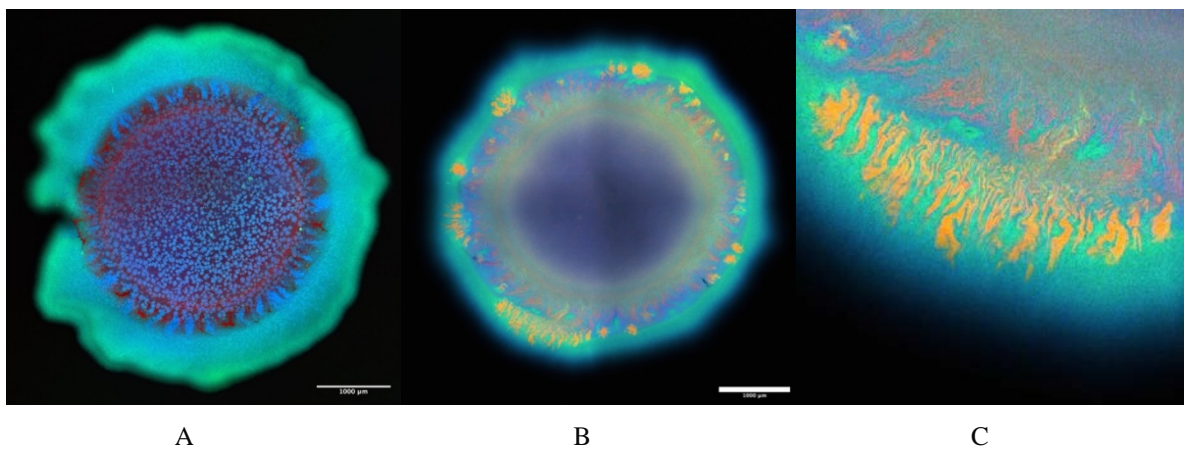


Figure 1. Cyan represents donors, red represents recipients, yellow represents transconjugants. Initially cyan and red are mixed 1:1 and compete in A and cross-feed in B. Only yellow (transconjugants) are found in B. C is zoom-in picture of B left-bottom part.





## **Microbial Nitrogen potential of two lakes with contrasting trophic states**

Baumann, Kathrin B.L.

EAWAG/SURF

The nitrogen (N) cycle is of global importance as N is an essential element and occasionally limiting nutrient in terrestrial and aquatic ecosystems. Increasing anthropogenic nitrogen input results in eutrophication of lake catchments and downstream coastal ecosystems. Freshwater lake sediments remove excess N through various microbial N transformation processes. However, the microbial N cycling community and the driving environmental parameters in lake sediments are not sufficiently understood.

Lake Baldegg and Sarnen are representative eutrophic and oligotrophic lakes, respectively. Using metagenomics in combination with pore water chemistry and process rate measurements, we investigated the spatial and seasonal differences in the N cycle.

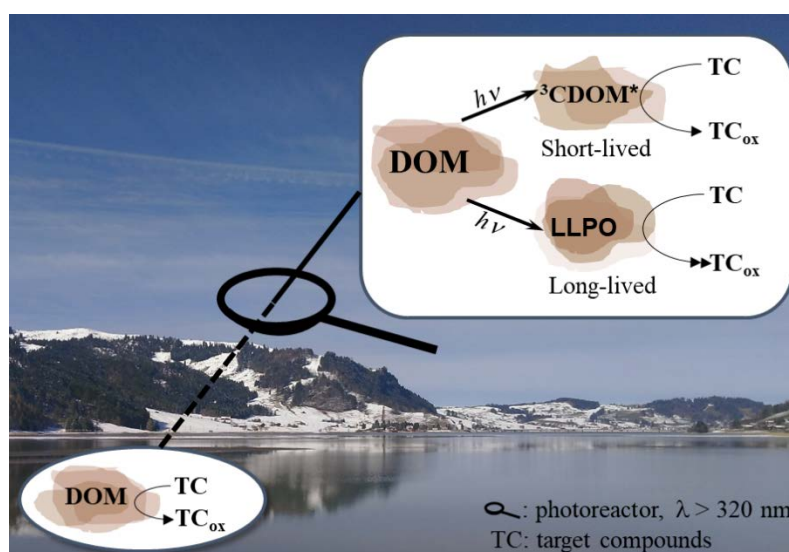
The potential denitrification and nitrification rates were two fold higher and the N removal efficiency three fold higher in Lake Baldegg. The microbial community data, and N cycling gene composition show a clear difference between the lakes and suggest more distinct spatial compared to seasonal variations. Results indicate that the biological basis for N processing differs considerably in sediments of lakes of different trophic status and that sampling schemes should take spatial heterogeneity into account.

## Characterizing the chemical nature of long-lived photooxidants produced from dissolved organic matter

Remke, Stephanie C.

Eawag, Water Resources and Drinking Water W&T

Sunlight irradiation of dissolved organic matter (DOM) leads to the formation of photochemically produced reactive intermediates, which can induce the indirect phototransformation of a variety of aquatic organic contaminants. A previously observed enhancement effect in the indirect phototransformation of electron-rich phenols at submicromolar concentration was ascribed to so far unexplored long-lived photooxidants (LLPO). Such LLPO, having estimated lifetimes  $\tau \sim 100 \mu\text{s}$ , are hypothesized to occur concomitantly with the shorter-lived excited triplet states of DOM,  ${}^3\text{DOM}^*$  ( $\tau \sim 2 \mu\text{s}$ ). In the present study we further characterized the chemical nature of LLPO by steady-state irradiations, chemical model systems and laser flash photolysis. By comparing the transformation rate constant at a high ( $5.0 \mu\text{M}$ ) and a low ( $0.1 \mu\text{M}$ ) starting concentration, LLPO were observed to enhance the transformation of electron-rich compounds out of various chemical classes, namely phenols, anilines and phenylureas. The one-electron oxidation potential of LLPO was estimated to be in the range of 1.0-1.3 V vs SHE. Chemical model systems consisting of a photosensitizer and an electron-poor phenol produced an analogous enhancement effect on transformation rates of electron-rich compounds, supporting the hypothesis that electron-poor phenolic moieties of the DOM are plausible LLPO precursors.



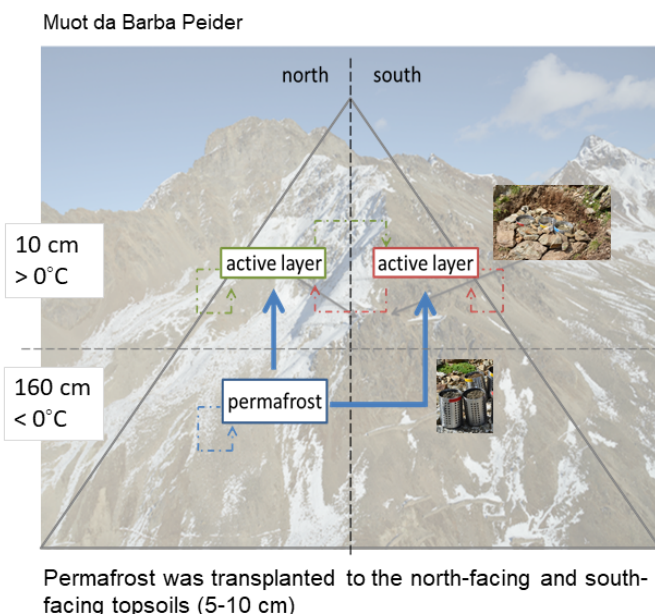
Conceptual model illustrating the formation of long-lived photooxidants in the DOM-photosensitized transformation of target compounds.

## Microbial responses of alpine permafrost to field-simulated conditions of warming

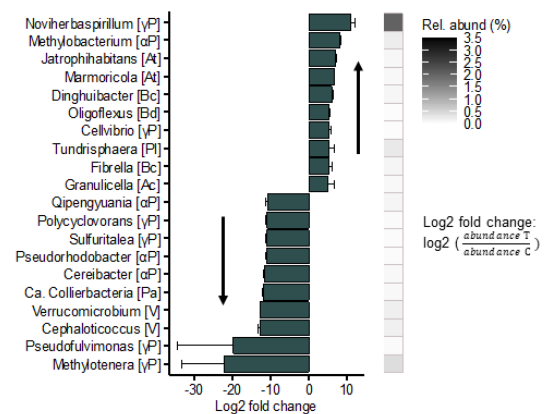
Perez-Mon, Carla

Forest Soils and Biogeochemistry, Swiss Federal Institute for Forest, Snow and Landscape Research WSL, Birmensdorf, Switzerland

Warming is accelerated in mid-latitude alpine permafrost regions. Yet, the effects of the increasing soil temperatures, moisture and C and nutrients on the alpine permafrost microbiome (i.e. prokaryotes and fungi), and its consequences for the soil ecosystem functioning, are poorly understood. We evaluated the responses of an alpine permafrost microbiota to warming, by transplanting permafrost soils from a depth of 160 cm to the topsoil (5-10 cm), at the mountain summit of “Muot-da-Barba-Peider” (Swiss Alps, 2979 m. a. s. l.). After three years of transplantation, the transplanted permafrost showed a decline in prokaryotic  $\alpha$ -diversity and significant structural shifts of both the prokaryotic and, to a minor extent, the fungal communities. Fast-growing and metabolically versatile bacterial taxa (e.g. *Noviherbaspirillum*) benefited from the transplantation-simulated warming, whereas slow-growing and poorly characterized parasitic bacteria (e.g. *Patescibacteria*) were negatively affected. Saprotrophic and pathogenic fungi benefited from warming. Substrate-use assays and enhanced soil bacterial and fungal abundances in the transplanted soils suggested the warming-stimulated growth of the permafrost microbiota, utilizing a wider range of C-substrates. Overall, our findings indicate the fast acclimation of the permafrost microbiota to the changing alpine environments, where the increase of copiotrophic microorganisms could result in alterations in the soil C dynamics.



Bacterial genera that increased ( $\uparrow$ ) or decreased ( $\downarrow$ ) in abundance in the transplanted permafrost (T) compared with the control (C)



Ac: Acidobacteriota, At: Actinobacteriota, Bc: Bacteriota, Bd: Bdellovibrionota, Pa: Patescibacteria, Pl: Planctomycetota, αP: α-Proteobacteria, yP: γ-Proteobacteria, V: Verrucomicrobiota

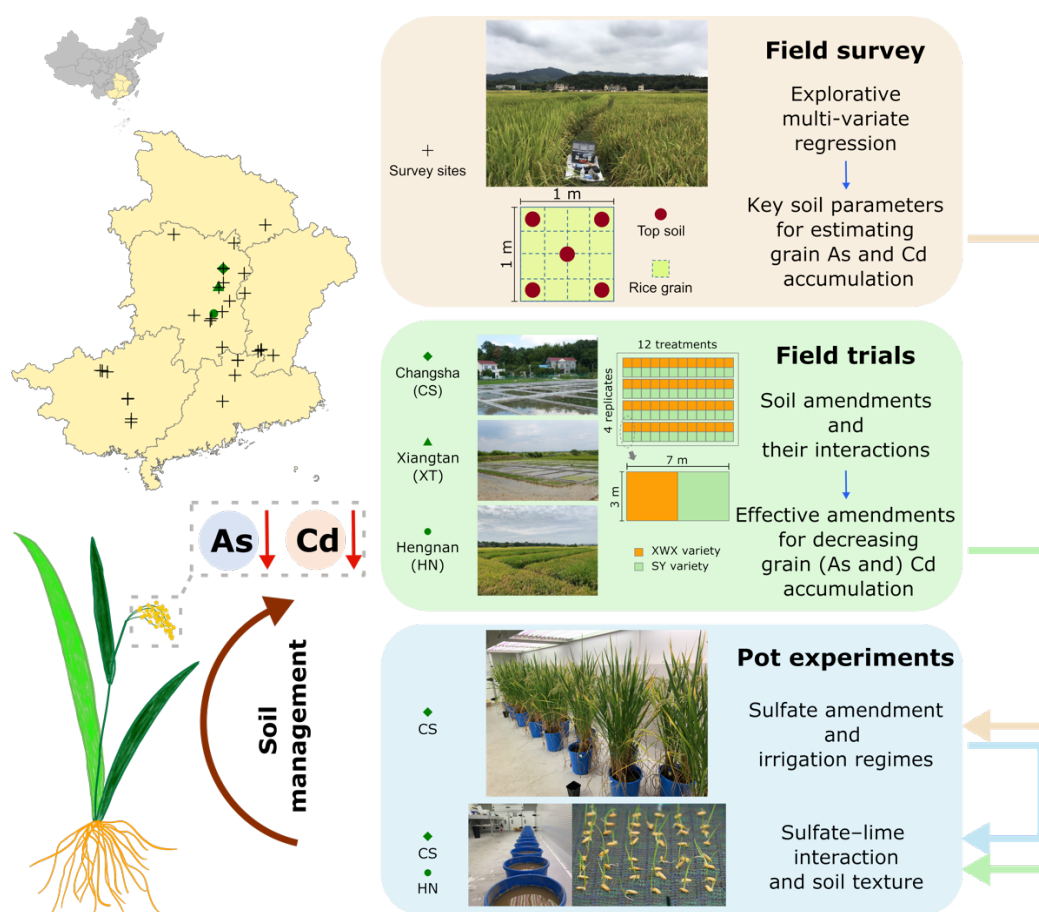


## Producing safe rice from As and Cd contaminated paddies via soil management

Fang, Xu

Soil Chemistry Group, ETH Zentrum

Contamination of agricultural soils threatens food safety. In southern China, the widespread As and Cd contamination has been observed to result in elevated As and Cd concentration in rice grains which often exceed food safety limits. Water management strongly affects grain accumulation of both As and Cd but, unfortunately, in opposite ways. Thus, additional soil amendments are required to produce rice free of As and Cd contamination simultaneously. In this project, we combined a field survey of 31 sites across southern China, field trials at three experimental stations, and pot experiments in a growth chamber to develop efficient soil management strategies for simultaneously decreasing As and Cd accumulation in rice grain. From field trials, we found soil amendments decreasing soil Cd availability or/and increasing soil Mn availability could greatly decrease grain Cd levels. In a pot experiment, we found that sulfate amendment to a sandy soil significantly decreased the accumulation of inorganic As in rice grain under intermittent flooding but not under continuous flooding. Both field trials and pot experiment agreed with the key soil parameters extracted from regression models developed in the field survey. Therefore, combining liming, sulfate amendment and intermittent flooding may be a promising solution for safe rice production on As and Cd contaminated paddy soils.



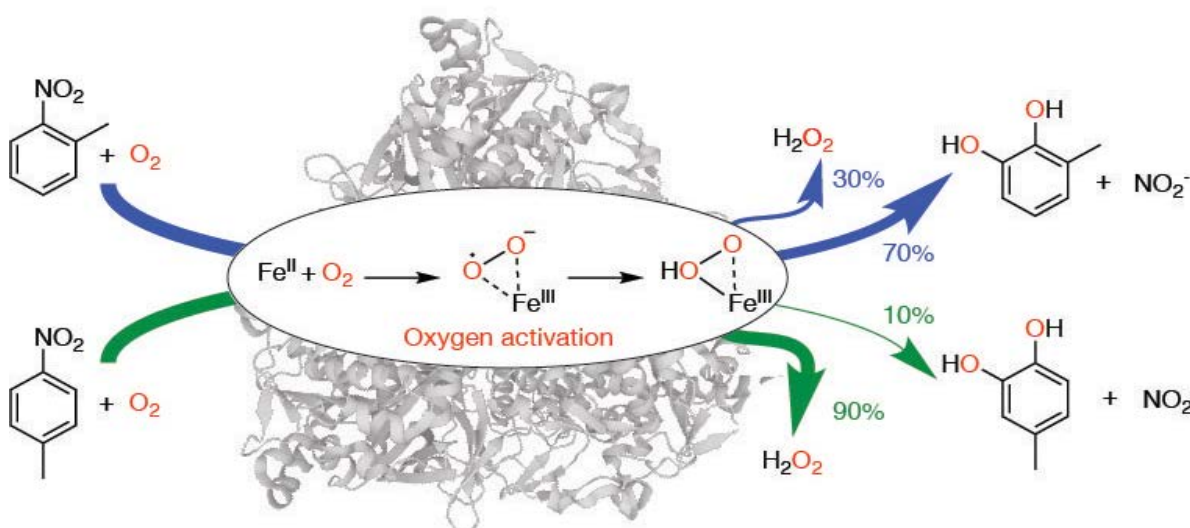
## Substrate specificity of enzymatic contaminant oxygenation

Bopp, Charlotte E.

Eawag/Department Environmental Chemistry

Oxygenases initiate the biotransformation and biodegradation of many organic compounds from persistent chemicals in contaminated soils and sediments to micropollutants in sewage treatment plants. To assess rates of biotransformation and predict the products formed, environmental (bio)chemists exploit knowledge of enzyme expression and function. However, it is often neglected that enzymatic O<sub>2</sub> activation is a chemically complex reaction with inefficient substrate and O<sub>2</sub> turnover. Instead, unproductive O<sub>2</sub> activation can be toxic because of the generation of reactive oxygen species (ROS) that can damage the enzyme and trigger cellular responses leading to enzyme evolution.

In my PhD project, I investigate the catalytic mechanism and O<sub>2</sub> activation of Rieske non-heme iron dioxygenases (RDO), the class of enzymes that initiates the degradation of aromatic hydrocarbons. Studying a wide range of structurally related compounds, I found that RDOs are quite inefficient at oxygenating these substrates with so-called O<sub>2</sub> uncoupling ranging from 30 to 100%. <sup>13</sup>C- and <sup>18</sup>O-isotope effects of organic substrates and O<sub>2</sub> revealed a general mechanism of O<sub>2</sub> activation in that RDO produce Fe-peroxo species as a critical intermediate. These results reveal the importance of considering O<sub>2</sub>-uncoupling in the assessment of overall transformation rates by enzymatic oxygenations and warrants more research into cellular and evolutionary responses to ROS generation from exposure to contaminants.



**Figure 1:** Two nitrotoluene isomers are transformed to methylcatechol by a Rieske non-heme iron dioxygenase. While both substrates trigger the same mechanisms of O<sub>2</sub> activation, the share of activated O<sub>2</sub> successfully transferred onto the substrate differs by 60%.



## How potent is the transfer of polychlorinated biphenyls from cow to calf?

Driesen, Charlotte

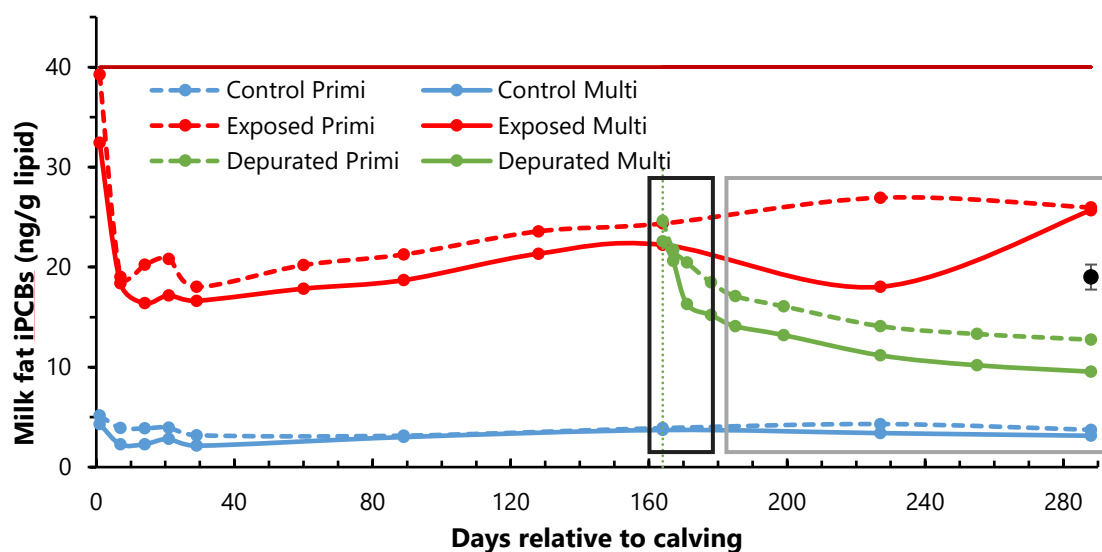
Empa, Laboratory for Advanced Analytical Technologies

Agroscope, Ruminants Research Unit

Polychlorinated biphenyls (PCBs) are toxic, persistent and bioaccumulative. Despite their worldwide ban in 2004, consumption of bovine products accounts for >70% of the total exposure. This is of concern since 50% Europeans exceed the tolerable weekly intake, but occasionally results as in herd/product destruction given an accidental contamination. To improve chemical safety, the PCB-transfer from feed to cows/calves over the end of gestation and full lactation was examined.

Twelve Simmental cow-calf pairs were monitored from 113 days before parturition until 288 days in milk (DIM). Calves were fed milk of their respective mother. Four cows received control grass silage and 8 a PCB-loaded soil-grass silage mix. After 164 DIM, latter was divided into 4 exposed and 4 decontaminated. The PCB kinetics were analyzed via HRGC-MS.

The exposed diet had a 6 to 11-higher PCB concentration compared to the control diet, resulting in a 4 to 8-fold higher milk level. Switching exposed cows to clean feed resulted in a 2-phased exponential decline of the milk PCB concentration. Calf serum was 2 to 3-fold higher in PCB concentrations compared to cow serum. These results will help to assess the predictive capability of physiological-based toxicokinetic models, to ensure their use in risk assessment and management.



**Figure | Milk fat indicator PCB concentration during lactation.** The mean milk concentrations in primiparous and multiparous control, exposed and deperuted cows are displayed. The red horizontal line represents the max regulatory level in milk. The two rectangles highlight the 2-phased decontamination process (●).



## Poster Session A – Overview

- A01 Amy Macfarlane – The microstructure of snow on sea ice measured by micro-computed tomography**
- A02 David Haaf – Understanding effects of anthropogenic pressures on groundwater arsenic contamination in Hanoi, Vietnam**
- A03 Roman Schefer – Effect of weathering towards eco-corona formation on plastic**
- A04 Francesco Parrella – Settling dynamics of microplastics in freshwater systems**
- A05 Joel Rüthi – Plastic in cold soils selects for a specific plastisphere microbiome**
- A06 Andrew Grigg – Ferrihydrite transformation in flooded rice paddy soils with diffusion limited Fe(II) supply**
- A07 Rachel London – Alternatives to PFAS and the regulation of very persistent substances**
- A08 Natalie Wichmann – Exploring the potential of wastewater enzymes to biotransform peptide-based antibiotics**
- A09 Anne-Marie Wefing – Annual variability of the long-lived anthropogenic radionuclide <sup>236</sup>U in the Fram Strait**
- A10 Domitille Louchard – The imprint of the Amazon River on the marine carbon cycling**
- A11 Jana Härrri – The interannual variability of marine N<sub>2</sub> fixation in the Western tropical Atlantic**
- A12 Sophie Bogler – Singlet oxygen production in aqueous organic aerosols: seasonality and predicting molecular markers**
- A13 Jon Went – Salts affect the ice nucleating ability of macromolecules beyond freezing point depression**
- A14 Emanuele Fara – The role of the Lambda prophage in a cross-feeding microbial community**
- A15 Joëlle Kubeneck – Mn<sup>2+</sup> and Mg<sup>2+</sup> incorporation in the ferrous phosphate mineral vivianite**
- A16 Maya Amacha – Assessing the contribution of ketones to DOM photochemistry through selective chemical trapping**
- A17 Joanna Houska – Quantification of Oxidant-Reactive Carbonous Sites in Dissolved Organic Matter**
- A18 Astrid Stubbusch – Interbacterial Killing in the Oceans**



## Poster Session B - Overview

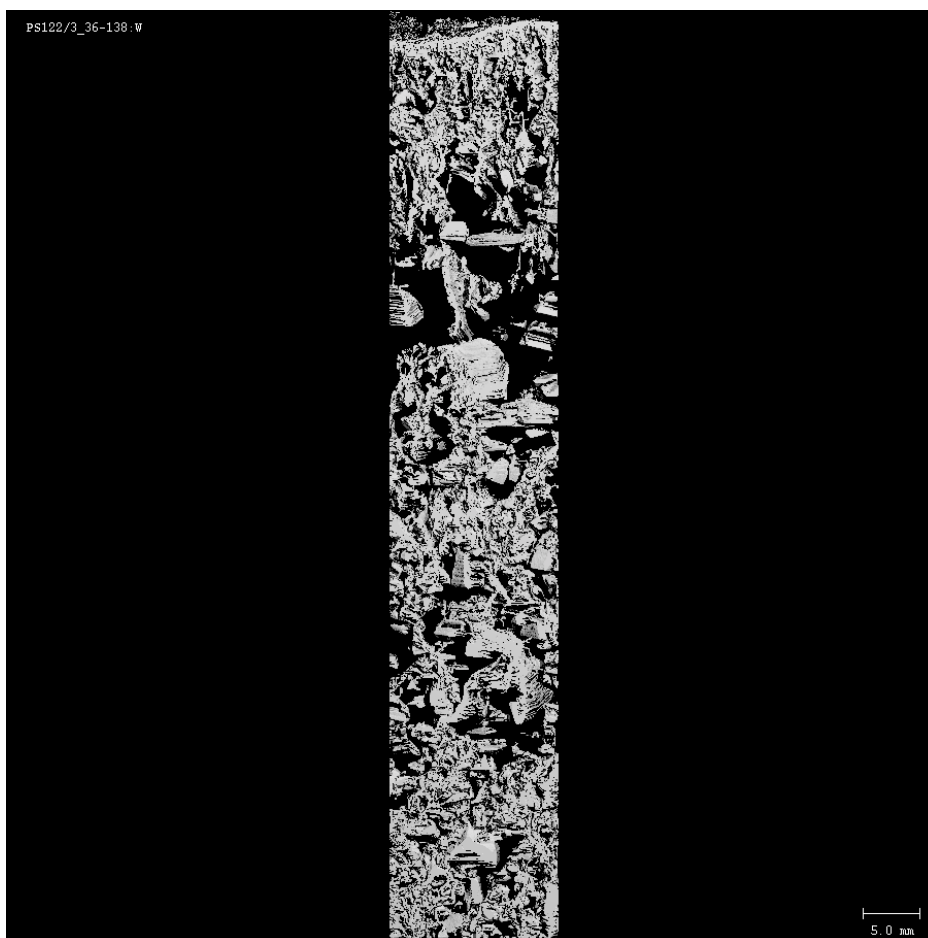
- B01 **Joel Meng Cheng Wong** - Marine heatwave detection in the global ocean
- B02 **Mattia Cerri/Silvan Arn** - Biodegradation of polyester mulch films: comparison between model systems and agricultural fields
- B03 **Nikola Obradović** - Electron donating capacity of particulate organic matter from ombrotrophic bogs
- B04 **Esther Breuninger** - Ultratrace level speciation of Se, As and S in atmospheric deposition
- B05 **Sahar Naim** - Investigating the mechanism of methane sulfonic acid formation from photosensitized degradation of Methionine
- B06 **Emma Chollet Ramampandra** - From data science to mechanistic modelling to gain knowledge about community assembly
- B07 **Katie Platt** - Photochemical Reactivity of Phenylenediamines and the Toxic Degradation Product Causing Fish Kills
- B08 **Ville Nenonen** - Formation and transformation of iron(III) and calcium precipitates: Consequences for phosphate trapping
- B09 **Donghe Zhu** - Revision of the eMLR(C\*) Method to Determine the Oceanic Uptake of Anthropogenic CO<sub>2</sub> in the 2010s
- B10 **Lena Bakker** - Deep Sea Mnammox: Could it be and how can we see it?
- B11 **Jill Bachelder** - Which organic fertilizers may increase Zn, but not Cd, in wheat grains?
- B12 **Niroshan Gajendra** - What controls the fate of carbohydrates in lake sediments?
- B13 **Benedikt Lauper** - Toxicokinetics of pesticides in Gammarus under field conditions: Different to laboratory data?
- B14 **Hassan Almoammar** - A Synthetic Ecology Approach to Elucidate the Causes of Microbial Nitrous Oxide Release during Denitrification
- B15 **Marie-Sophie Maier** - Insights from mapping noble gases in the Danube Delta
- B16 **Urs Hofmann Elizondo** - Individual-based modelling of shelled pteropods
- B17 **Zoè Le Bras** - TD-GC-ICP-MS as novel analytical method to study marine Se and S emissions

**A01 – The microstructure of snow on sea ice measured by micro-computed tomography.**

Macfarlane, Amy

WSL Snow and Avalanche Research SLF

Snow on sea ice governs much of the heat exchange during winter, and its melting during summer. The microstructure has a key role in the thermal heat resistance and in the albedo. We installed a micro-CT on board of the research icebreaker Polarstern during the MOSAiC-expedition. The MOSAiC expedition drifted for a full year in the Arctic Ocean. We could measure every week 1-2 full snow profiles between 0.1-0.3 m deep. We extracted, mostly in-situ, cores of 48-78 mm diameter and of about 0.1 m length, and scanned with 18-28  $\mu\text{m}$  resolution. The goal of these measurements was to understand the formation and metamorphism of the snowpack in detail, and to derive detailed geometrical and physical properties from the samples. First examples will be presented and an overview of characteristic snow profiles from leg 1 – 4, spanning the winter, spring and melt season, and the evolution of the sea ice from solid ice towards the formation of the surface scattering layer, a snow-like ice cover. We could also observe the inclusion of brine in some snow samples, especially in first year ice. Until now it was not known how brine is included in the ice structure of snow.



The microstructure of snow on sea ice taken on 4/19/2020

## A02 – Understanding effects of anthropogenic pressures on groundwater arsenic contamination in Hanoi, Vietnam

Haaf, David

Inorganic Environmental Geochemistry/Eawag W+T

Natural contamination of groundwater with the toxic and cancerogenic element arsenic (As) is a global health problem affecting over 200 million people, mainly in Southeast (SE) Asia, including the Red River Delta and Hanoi in Vietnam. The main mechanism responsible for the widespread release of As from aquifer sediments to groundwater in SE Asia is microbially induced reductive dissolution of iron (oxyhydro) oxides in young (Holocene), fine-grained aquifers rich in organic material. In comparison, As concentrations in older (Pleistocene) coarse-grained aquifers were generally reported to be below the World Health Organization (WHO) guideline value of 10 µg As/L. However, more recent studies in Vietnam have shown that deep and presumed As free aquifers can be highly contaminated, potentially due to increased groundwater abstraction for domestic water supply. Based on these findings, two contamination mechanisms of deeper aquifers in relation to increased groundwater pumping have been hypothesized:

1. Advection of As/As mobilizing solutes from Holocene aquifers to Pleistocene aquifers
2. Release of As/As mobilizing solutes from adjacent aquitards potentially in relation to clay compaction

In this study, the proposed As contamination hypotheses are analyzed for Hanoi by investigating spatiotemporal relationships between hydrochemical, hydrological, geological and land-use information with various geostatistical approaches.

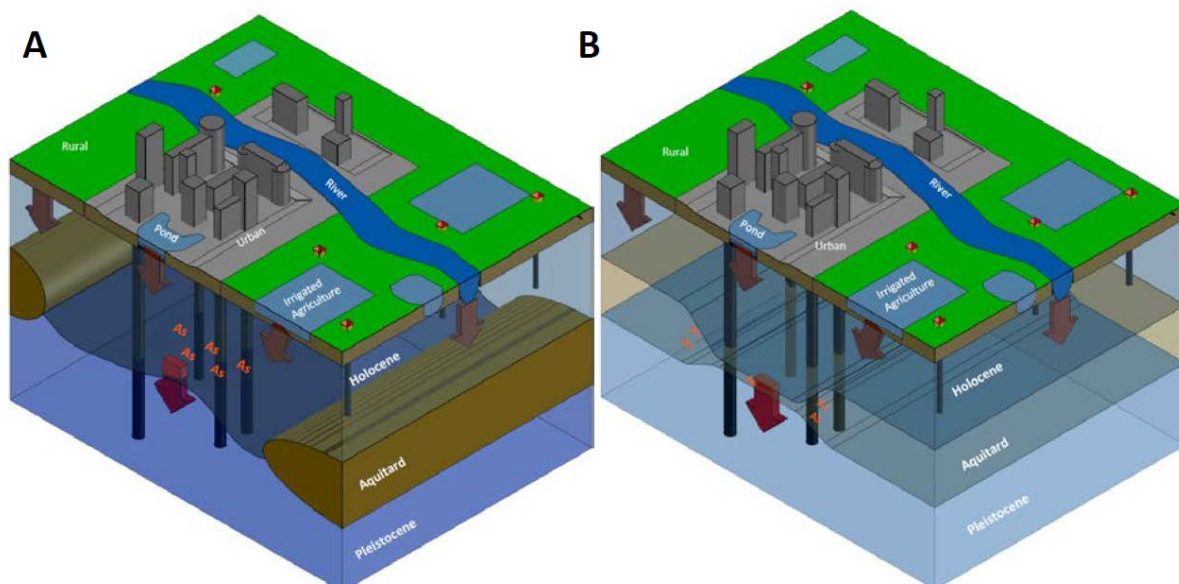


Figure 1: Schematic diagram of processes potentially affecting As mobilization in aquifers of Hanoi, either directly (surface inputs; brown arrows) and/or indirectly (potential groundwater pumping; black cylinders). In A, drawdown advection (Hypothesis 1) is represented. In B, releases from aquitards in relation to clay compaction (Hypothesis 2) are shown.



### A03 – Effect of weathering towards eco-corona formation on plastic

Schefer, Roman

IBP/Environmental Chemistry/Denise Mitrano's group

Concerns about environmental implications of particulate plastics (nano- and microplastic particles) are continuously rising. Nevertheless, the understanding of plastic behaviour in freshwater environments is still quite meagre. Organic biomolecules are omnipresent in freshwater systems and lead to the formation of so-called “eco-coronas” around plastics and other natural particles. The change in surface chemistry and density due to the eco-corona formation may influence the behaviour, fate, bioavailability, and toxicity of the particles. Despite the importance of these altered particle surfaces, most studies so far use only a small set of pristine polymers to investigate fate and transport of particulate plastics. Additionally, the impact(s) of weathering (e.g. hydrolysis, UV photodegradation, mechanical abrasion, biodegradation) on physicochemical properties of plastic is often neglected, which may influence the binding affinity of organic biomolecules towards plastic (Fig. 1). In this context, systematic studies on the sorption between a set of the most environmentally prevalent polymer types (e.g. PE, PP, PET, PS), in their pristine and weathered forms, and a selection of ubiquitous organic biomolecules were performed. Adsorption studies were accomplished in a simulated freshwater environment on polymer coated substrates by exploiting the versatile Quartz Crystal Microbalance (QCM-D) platform. The information obtained about eco-corona affinity towards different plastic types can be employed for further studies regarding the interplay of organic biomolecules and inorganic contaminants with plastics.

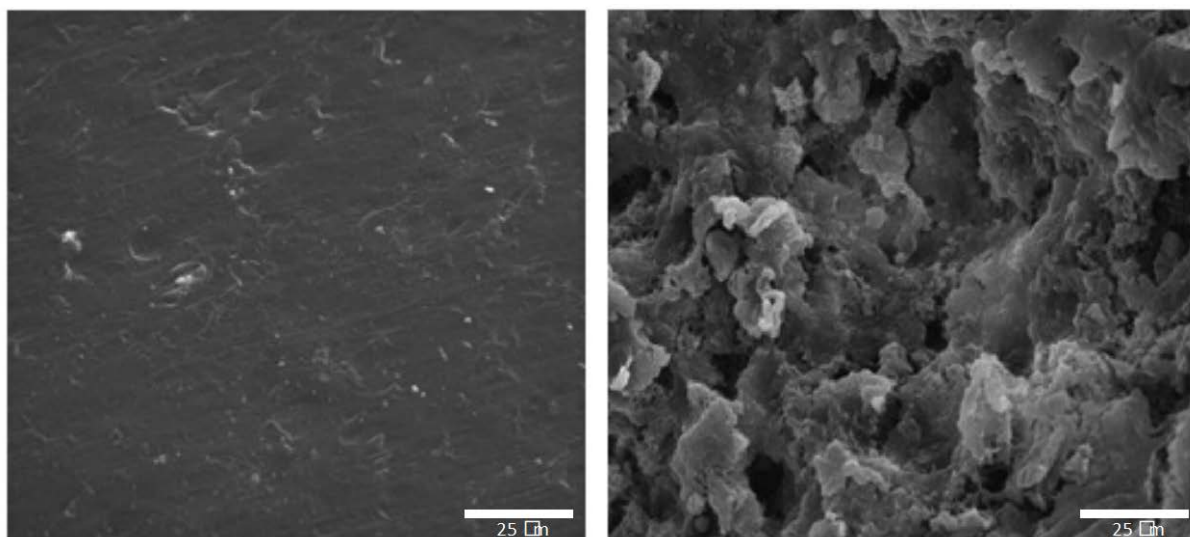


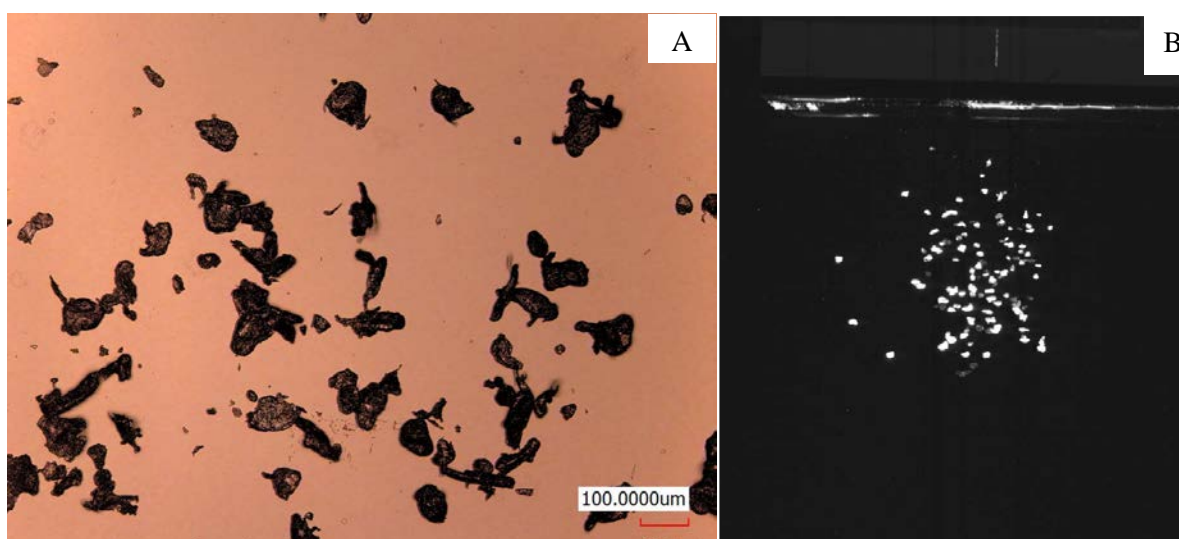
Figure 2: Surface topography image of virgin (left) and weathered (right) PE plastic pellets, by SEM. (Fotopoulou et al. 2014)

## A04 – Settling dynamics of microplastics in freshwater systems

Parrella, Francesco

IBP/Environmental Chemistry/Denise Mitrano's group

To date, there are a limited number of studies which have been conducted to systematically study the processes which drive microplastic fate and transport in the environment. In this project, we aim to improve the knowledge about settling dynamics of plastics and their interactions with solids to assess vertical transport. Freshwater snow, a mixture of organic detritus, algae and natural particles, is responsible for the mass flux of organic matter from the waters' surface to the sediment, and can be a potential vector for microplastics settling through the water column. In this context, we hypothesize that the interactions and aggregation between plastics and freshwater snow will determine their respective fate and transport routes. We will systematically analyze the settling of particles of different densities and morphologies in a plexiglass column, which will be illuminated by a laser to track particles with a camera (Fig 1). We will further assess the distribution of plastic and freshwater snow by sampling water at specific points along the column, using metal-doped microplastic particles which are easier to quantify. The ultimate goal will be to assess if the settling rate changes when plastic and snow are aggregated together, compared to their settling dynamics individually.



*Fig.1: A)Microplastic fragments under 10x magnification optical microscope and B) fragmetns captured by camera during the settling*

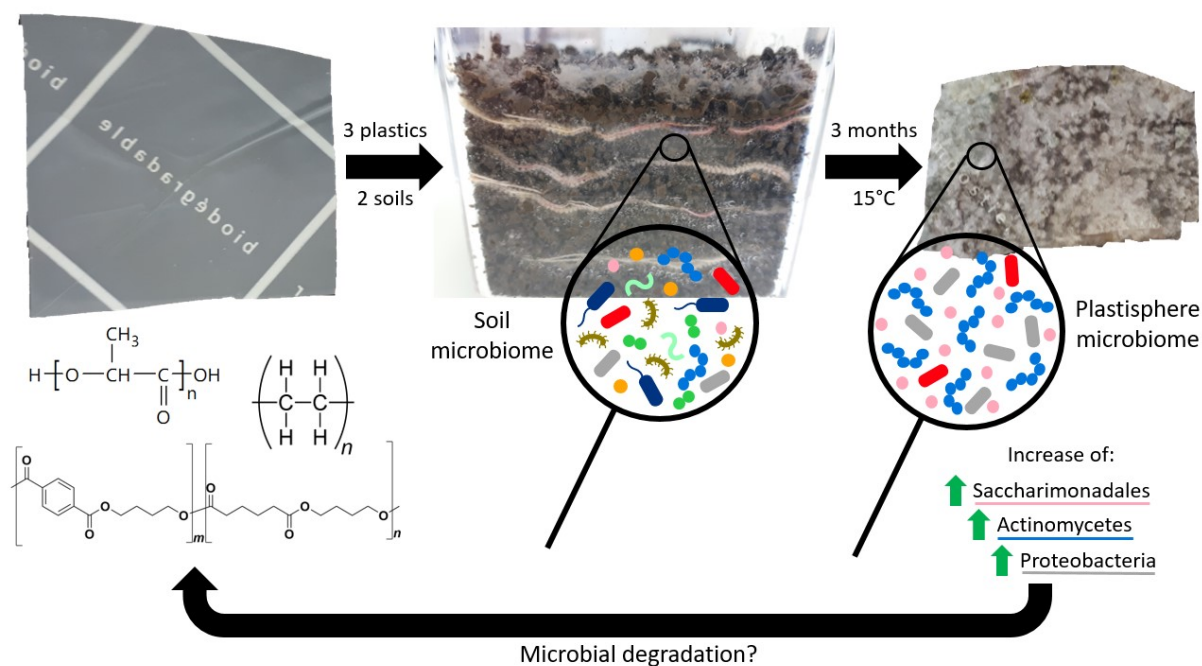
## A05 – Plastic in cold soils selects for a specific plastisphere microbiome

Rüthi, Joel

Forest Soils and Biogeochemistry, Swiss Federal Institute for Forest, Snow and Landscape Research (WSL)

Institute of Biogeochemistry and Pollutant Dynamics, Swiss Federal Institute of Technology, ETH Zürich

Plastic pollution is a global concern threatening inhabitants of numerous ecosystems. While the issue of plastics, and especially microplastics, accumulating in the oceans has drawn a lot of attention, little is known about its fate in terrestrial habitats. Recent studies in Europe have shown that terrestrial plastic litter outweighs the waste ending up in waterbodies and researchers even proved the presence of man-made plastics in pristine regions like Alpine glaciers and the Arctic. Plastics collected from water are regularly shown to bear a microbial community composition different from the surrounding and other inert surfaces. Members of this man-made habitat comprise a wide range of organisms including eukaryotic and prokaryotic taxa, potentially plastic and other pollutants degrading species as well as pathogenic and antibiotic-resistance genes carrying microbes. Here, we aimed to show that the concept of this selective habitat formed on the plastic surface, called the “plastisphere”, also is applicable for the terrestrial cryosphere. By applying metabarcode sequencing of DNA extracted from plastics incubated in Alpine and Arctic soils in a laboratory mesocosm experiment, we found that particularly biodegradable plastics are colonized by a specific microbial community that is distinct from the surrounding bulk soil.



## A06 – Ferrihydrite transformation in flooded rice paddy soils with diffusion limited Fe(II) supply.

Grigg, Andrew R. C.

Soil Chemistry Group, Institute of Biogeochemistry and Pollutant Dynamics

Iron minerals are abundant in soils and may undergo transformation under dynamic redox conditions. Iron<sup>II</sup> can catalyse ferrihydrite (iron oxyhydroxide) transformation to more thermodynamically stable phases. Such mineral transformations can be studied in model systems, but studies in soils face experimental challenges. We introduced ferrihydrite to five contrasting paddy soils using permeable polyethylene terephthalate fabric sachets (approx. 30 × 12 × 3 mm, pore size 51 μm). Mineral transformation was measured after two weeks using X-ray diffraction (bulk) and Raman spectroscopy (spatially resolved, ≥ 1 μm). Lepidocrocite and goethite partially replaced ferrihydrite in bulk samples from redox-active soils. Bulk transformation rates and product composition varied according to the concentrations of key parameters of the soil solution, particularly dissolved Fe<sup>II</sup>. Micro-Raman mapping of mineral sachet cross-sections reveal that sub-millimetre-scale transformation varied from the bulk. Transformation of mineral closer to soil was inhibited, suggesting that chemical species in the porewater inhibited transformation by sorbing to ferrihydrite, whereas lack of transformation in the interior likely reflects diffusion limitation of Fe<sup>II</sup>. Transformed regions contained an inhomogeneous mixture (micrometre scale) of goethite and lepidocrocite. The study demonstrates that contrasting soil conditions and diffusion limitations can impact the rates and pathways of ferrihydrite transformation processes.

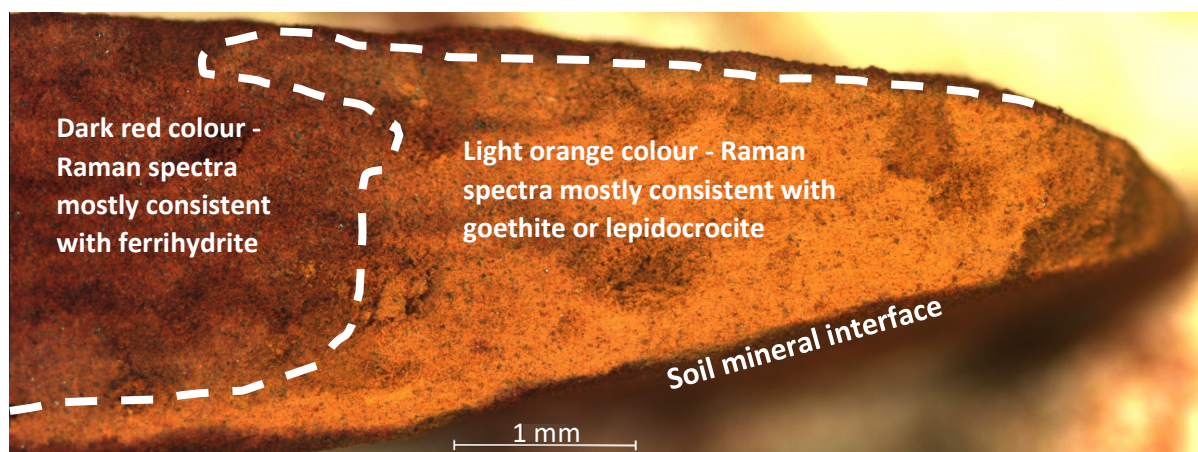


Figure 1. Microscope image of a partial cross-section of transformed mineral.



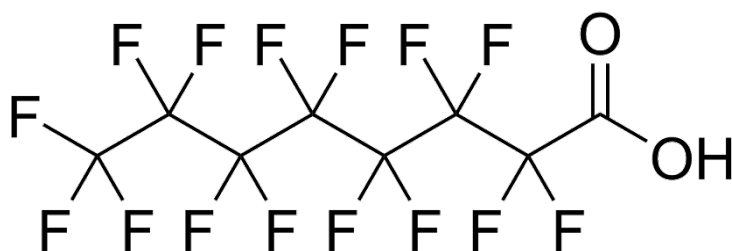
## A07 – Alternatives to PFAS and the regulation of very persistent substances

London, Rachel

Environmental Chemistry / Institute for Biogeochemistry and Pollutant Dynamics / D-USYS

Some members of a persistent group of chemicals known as per- and polyfluoroalkyl substances (PFAS) are damaging to human health and the environment. There have been calls from around the world to regulate PFAS, most recently in the 2020 EU *Chemicals Strategy for Sustainability*, part of the European Green Deal. However, many PFASs perform functions in a wide range of uses in many types of products for consumer and professional use. The aim of the first part of this project is to investigate if the goal of these uses can be achieved without PFAS, whilst minimising detrimental impacts on human health and the environment.

The European effort to control PFAS has also shown the weaknesses in current legislation when trying to protect citizens and the environment from very persistent chemicals. The second part of this project will try to develop methodologies for hazard and risk assessment and investigate possible grouping strategies to streamline the regulation of very persistent substances.



The best known PFAS – Perfluorooctanoic acid (PFOA)

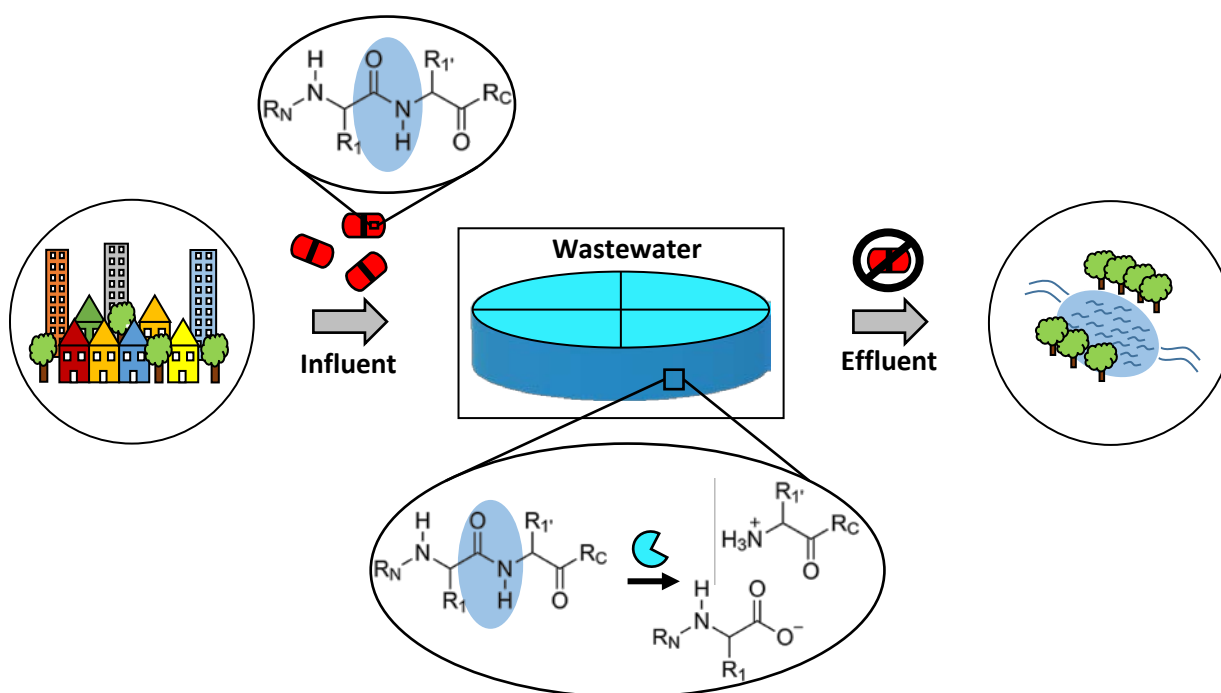


## A08 – Exploring the potential of wastewater enzymes to biotransform peptide-based antibiotics

Wichmann, Natalie

EAWAG – Department Environmental Microbiology

Substantial amounts of antibiotics enter wastewater and are – if not completely removed during wastewater treatment – released into aquatic environments downstream of wastewater treatment plants (WWTPs). It is expected that the presence of antibiotics in wastewater and natural environments contributes to the emergence and propagation of antibiotic resistance. Antibiotics that are rapidly inactivated by extracellular enzymes present in wastewater could be one solution to this problem. Antimicrobial peptides (AMPs) are particularly promising because of their specificity for target pathogens and because they might be susceptible to inactivation by peptidases in wastewater. The aim of my PhD project is to assess the potential of extracellular wastewater peptidases for the biotransformation of AMPs. In this contribution, we will present initial results from activity measurements of peptidases sampled from different stages of biological wastewater treatment, which revealed promising activity of extracellular peptidases in influents of WWTPs. Investigating the specificity of these peptidases on a set of model peptides, we detected peptide bonds that are prone to hydrolysis by extracellular wastewater peptidases. The goal of our future work is to identify the responsible enzymes and to assess their potential to inactivate peptide-based antibiotics in wastewater.



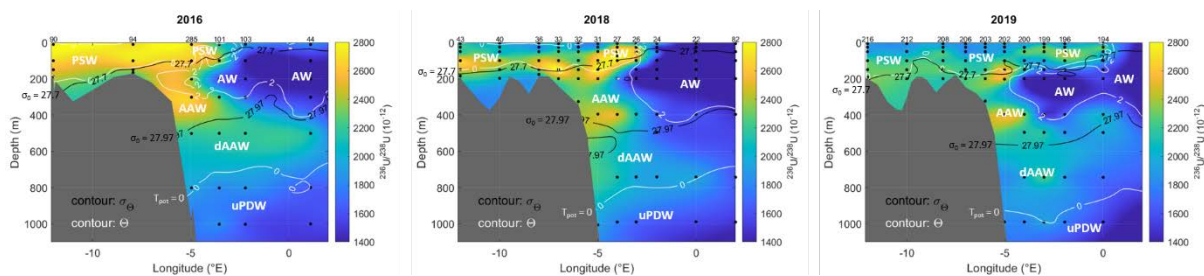
## A09 – Annual variability of the long-lived anthropogenic radionuclide $^{236}\text{U}$ in the Fram Strait

Wefing, Anne-Marie

Inorganic Environmental Geochemistry

Anthropogenic chemical tracers are powerful tools to study pathways, water mass provenance and mixing processes in the ocean. Releases of the long-lived anthropogenic radionuclides I-129 and U-236 from European nuclear reprocessing plants label Atlantic Water entering the Arctic Ocean with a distinct signal that can be used to track pathways and timescales of Atlantic Water circulation in the Arctic Ocean and Fram Strait. Apart from their application as transient tracers, the difference in anthropogenic radionuclide concentrations between Atlantic- and Pacific-origin water provides an instrument to distinguish the interface between both water masses.

Here we present a time-series of U-236 (and some I-129) data across the Fram Strait, collected in 2016, 2018, and 2019. While the overall spatial distribution of U-236 was similar among the three sampling years, significant differences were observed in the upper water column of the EGC, especially between 2016 and 2018. This study is the first attempt to investigate the potential of U-236, in combination with I-129, as water mass composition tracers in the East Greenland Current.

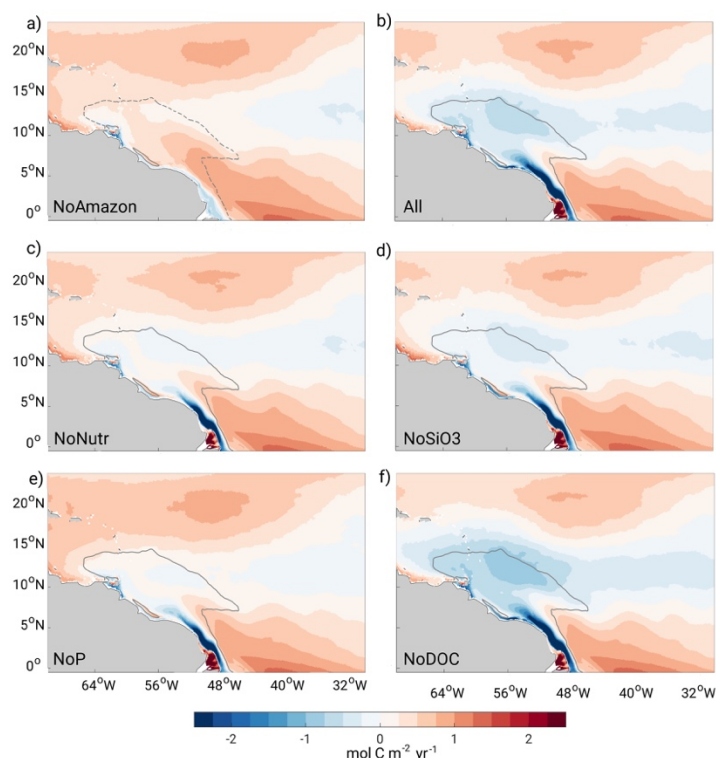


## A10 – The imprint of the Amazon River on the marine carbon cycling

Louchard, Domitille

Department of Environmental Systems Science / Environmental Physics (UP Group)

The Amazon River greatly modifies the physical and chemical properties of the ocean up to 3000 km away from its mouth, reversing the typical CO<sub>2</sub> outgassing of the Western Tropical Atlantic (WTA). The exact quantification of this plume-related carbon sink is still disputed. To unravel the complex interplay between physical and biogeochemical processes that leads to this unique effect of the Amazon, we set up a modeling experiment using an eddy-resolving configuration of a regional model (ROMS) that incorporates a full biogeochemical/ecological module. We ran a set of different simulations to isolate the effect of the riverine inputs. While the relative contribution of each process varies significantly in space and time, the enhancement of the biological pump is progressively the dominant control of the surface pCO<sub>2</sub> as the plume moves off-shore. The strength of this biological pump is associated with a unique group of symbiotic diatom-diazotroph assemblages that sustains a diatom-dominated phytoplankton community, fueling carbon sequestration in the otherwise oligotrophic tropical waters.



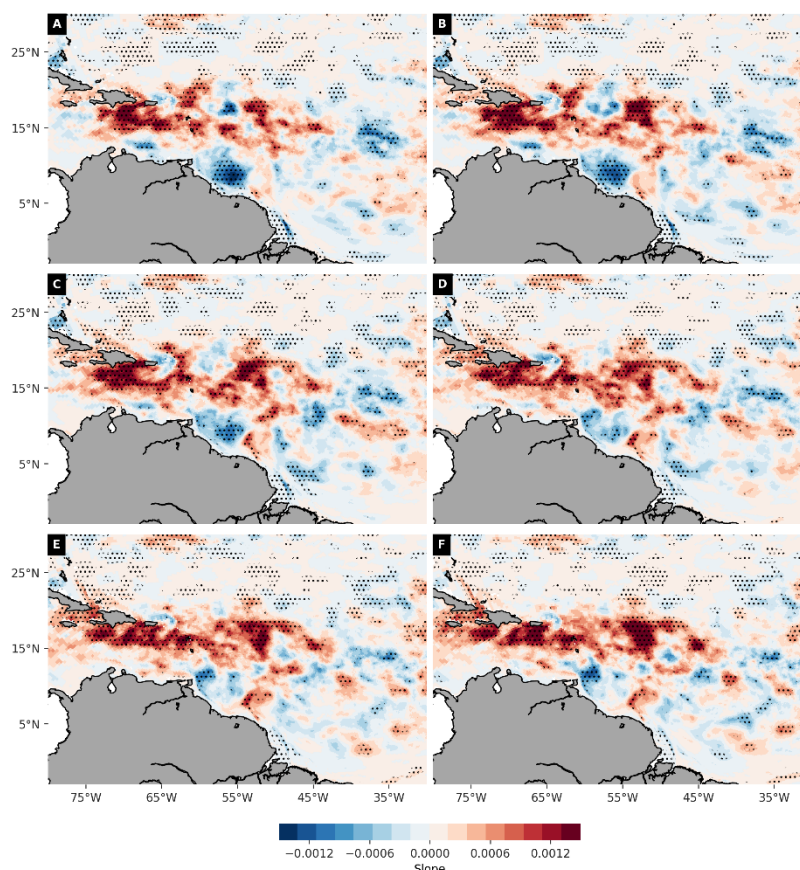
*Annual average air-sea CO<sub>2</sub> fluxes in different simulations: (a) a simulation without the Amazon River, (b) a baseline simulation, (c) a simulation where the Amazon does not deliver nutrients, (d) a simulation where the Amazon does not deliver SiO<sub>3</sub>, (e) a simulation where the Amazon does not deliver phosphorus and (f) a simulation where the Amazon does not deliver Dissolved Organic Carbon. The red colors correspond to an outgassing of CO<sub>2</sub> to the atmosphere, the blue colors correspond to an uptake of CO<sub>2</sub> by the ocean. The grey line locates the average position of the river plume.*

## A11 – The interannual variability of marine N<sub>2</sub> fixation in the Western tropical Atlantic

Härri, Jana

IBP/Master student

Marine nitrogen fixation replenishes the surface ocean with “new” nitrogen, maintaining ocean productivity. In the Atlantic, the majority of the N<sub>2</sub> fixation occurs in the (sub)tropics, particularly in the Western tropical Atlantic (WTA) owing to nutrient input by the Amazon River. On interannual timescales, the runoff and its associated nutrient input vary, which is speculated to impact the N<sub>2</sub> fixation. To unravel the N<sub>2</sub> fixation variability attributed to the discharge variability, we use a biogeochemical model (ROMS-BEC), which we force with two discharge scenarios, one including and the other excluding interannual discharge variability. We show that discharge-attributed N<sub>2</sub> fixation anomalies amount to ~40% of the total interannual N<sub>2</sub> fixation variability between 1983 and 2015. Generally, elevated nutrient input enhances diazotrophy and vice versa, but an inverse response exists upstream of the plume owing to high competition. The El Niño-Southern Oscillation and Atlantic Meridional Mode, which are the main drivers of discharge variability, also impact the N<sub>2</sub> fixation by modulating ocean circulation. We demonstrate that discharge and climate variability are the main drivers of N<sub>2</sub> fixation variability in the WTA. This variability in the N<sub>2</sub> fixation rate can have a substantial impact on the nitrogen and carbon cycle.



Slopes in  $\mu\text{Mol N m}^{-2} \text{d}^{-1}$  per  $\text{m}^3/\text{s}$  estimated by the linear regressions fitted with the discharge anomalies as the explanatory variable and depth-integrated N<sub>2</sub> fixation rate differences between the two simulations as the independent variable. Areas where the linear regression is significant on the 0.95 level are indicated by dots. Different time lags of zero to five months are shown (A-F), the difference in the depth-integrated N<sub>2</sub> fixation rate lagging the discharge anomalies.



## A12 – Singlet oxygen production in aqueous organic aerosols: seasonality and predicting molecular markers

Bogler, Sophie

Institute for Biogeochemistry and Pollutant Dynamics/ETH Zurich

Singlet oxygen ( $^1\text{O}_2$ ) is a reactive oxygen species that has gained attention as a competitive oxidant in the atmosphere. Despite  $^1\text{O}_2$ 's capability of affecting the lifetime of many organic atmospheric components, its spatiotemporal distribution in aqueous organic aerosols is currently unknown. We hypothesized that biomass burning organic aerosols emitted during winter lead to higher  $^1\text{O}_2$  production compared to summer. The winter aerosols likely contain more chromophores, a prerequisite for  $^1\text{O}_2$  formation. Therefore, we investigated the  $^1\text{O}_2$  production ability of organic aerosols sampled on PM10 filters throughout 2013 in Frauenfeld and San Vittore, Switzerland. We extracted the water-soluble organic components and quantified the  $^1\text{O}_2$  steady-state concentration and quantum yield. Thus far our results show a range between  $0.38 - 6.05 \times 10^{-13} \text{ M}$  for  $^1\text{O}_2$  steady-state concentrations (Figure) and quantum yields up to  $2.1 \pm 0.5 \%$ . More importantly, the filters analysed indeed show a strong seasonal trend, with increased  $^1\text{O}_2$  production in winter compared to summer. To extend this analysis, we are currently correlating these results with molecular markers based on mass spectrometry data available from previous filter analysis. Finding these correlations will enable the prediction of  $^1\text{O}_2$  sensitizing abilities of organic material present in the aerosols both qualitatively and quantitatively.

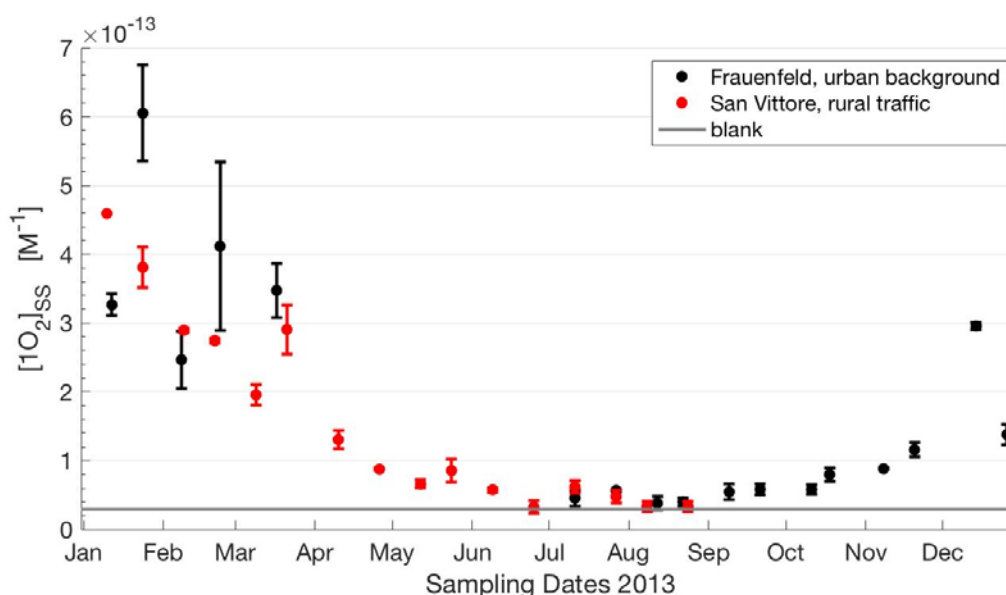


Figure: Results from on-going filter analysis showing  $^1\text{O}_2$  steady-state concentrations produced by water-soluble organic component extracted from PM10 filters, which were sampled 2013 in Frauenfeld and San Vittore.



### A13 – Salts affect the ice nucleating ability of macromolecules beyond freezing point depression

Went, Jon

Department of Environmental Systems Science

Cloud properties and lifetimes represent large uncertainties in climate predictions. Notably, ice formation in mixed-phase clouds can form from ice nucleating macromolecules (INMs). Sea spray aerosols can be an influential population of INMs in pristine ocean air, yet salt is known to cause a freezing point depression (FPD) thereby complicating the analysis. FPD corrections assume translatable ice nucleation abilities with and without salt. In this study, we tested the hypothesis that the ice nucleating ability of INMs is affected beyond the FPD correction. Using our Freezing Ice Nuclei Counter (FINC), we quantified eight INMs (namely taurine, isethionate, xylose, mannitol, glucose, dextran, laminarin and xanthan) in pure water and in artificial sea water, known to be exudates of microorganisms in the sea surface microlayer, at temperatures relevant to mixed-phase clouds (e.g. 50% activated fraction above  $-23^{\circ}\text{C}$  at 10mM concentration). Six INMs lost their freezing activity in sea water compared to pure water, even after FPD correction. Based on our results, we hypothesize that sea salt inhibits the ice activity of INMs beyond a FPD correction. This effect influences our understanding of how INMs nucleate ice and how sea-surface microlayer samples should be treated with care.

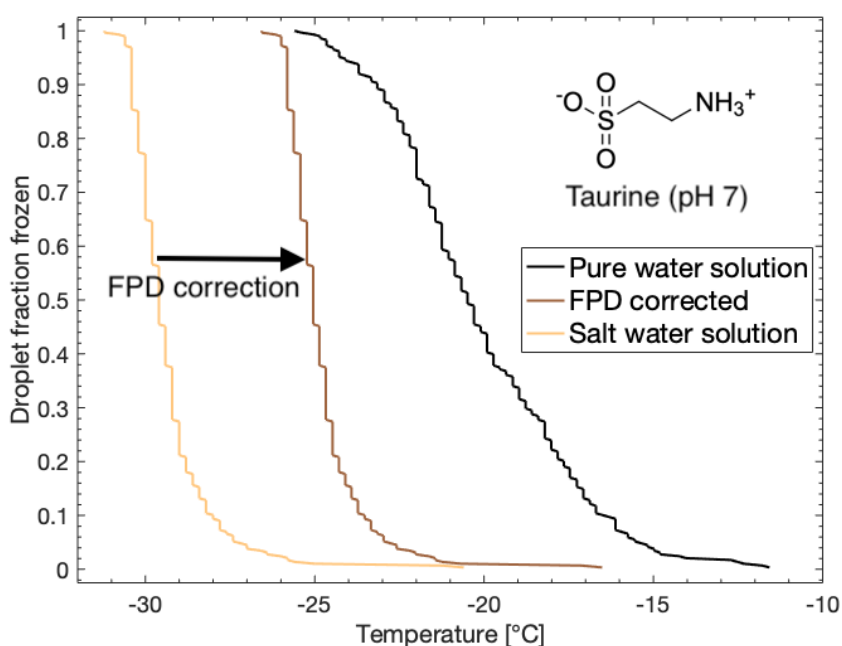


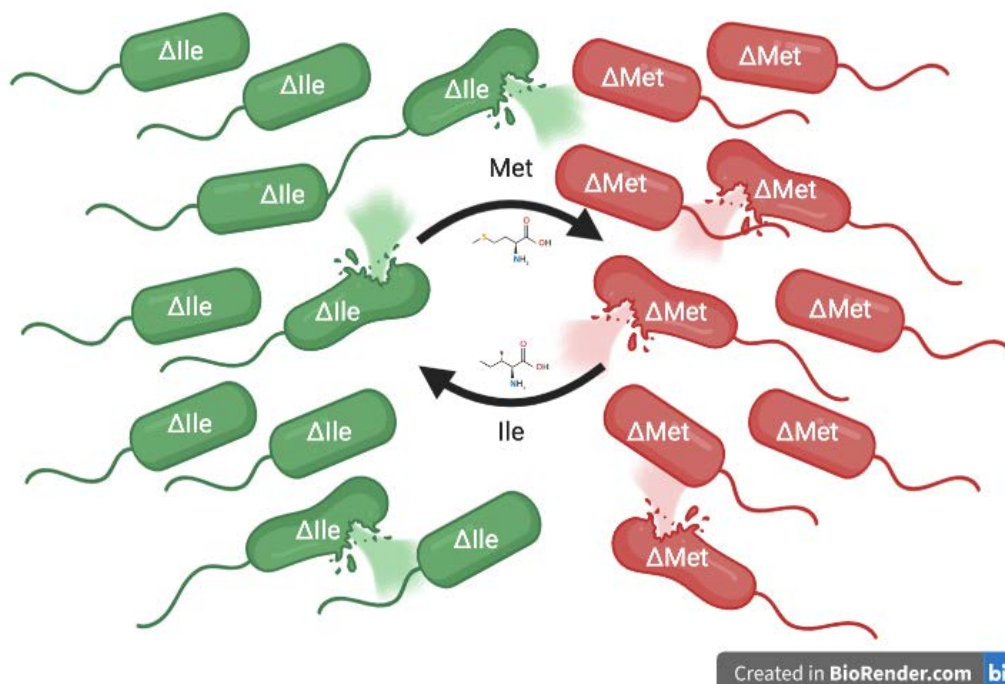
Figure 3: A comparison of the frozen fraction of taurine, structure shown in the upper right corner, in a pure water solution and a salt water solution before and after freezing point depression correction.

## A14 – The role of the Lambda prophage in a cross-feeding microbial community

Fara, Emanuele

Institute of Biogeochemistry and Pollutant Dynamics / Eawag

Viruses are present in every environment of the Earth's surface. Traditionally, viruses have been considered as just parasitic entities eager to infect and hijack their hosts to replicate. However, recent insights have suggested that viruses may play a crucial role in many aspects of life, from biogeochemical cycles to host-microbiota dynamics. One of the most well-known viruses is the Lambda bacteriophage, a virus that infects the common bacterium *Escherichia coli*. Although the mechanism of Lambda infection is somewhat understood at the molecular level, we still have little perception about the effect of its induction in a cross-feeding microbial community. I aim to fill this knowledge gap by studying the function of the Lambda prophage in a community composed of two amino acid auxotrophs derived from *E. coli*. This type of synthetic consortium resembles a more complex community that can be found in natural environments. The two strains need to cooperate if they want to grow in a minimal medium without the supplement of the needed amino acids. By using a temperature-sensitive Lambda phage, I intend to study the effect of prophage induction in this community, thus shedding light on the metabolic interactions between the two strains at the single-cell level.



Cross-feeding microbial community composed of two amino acid auxotrophs: isoleucine knock-out ( $\Delta\text{Ile}$ , in green) and methionine knock-out ( $\Delta\text{Met}$ , in red). This community can grow in a minimal medium without any amino acid because they share nutrients by cross-feeding ( $\Delta\text{Ile}$  produces methionine that can be used by  $\Delta\text{Met}$ , and the latter produced isoleucine that can be used by the former). The presence of a temperature-sensitive phage would allow me to study how prophage induction, and eventual cell lysis, can influence the metabolic interactions between the two bacterial strains. The hypothesis is that a small fraction of cell lysis may help the community to share nutrients and start growing earlier than when there is no or too much lysis.

## A15 – Mn<sup>2+</sup> and Mg<sup>2+</sup> incorporation in the ferrous phosphate mineral vivianite

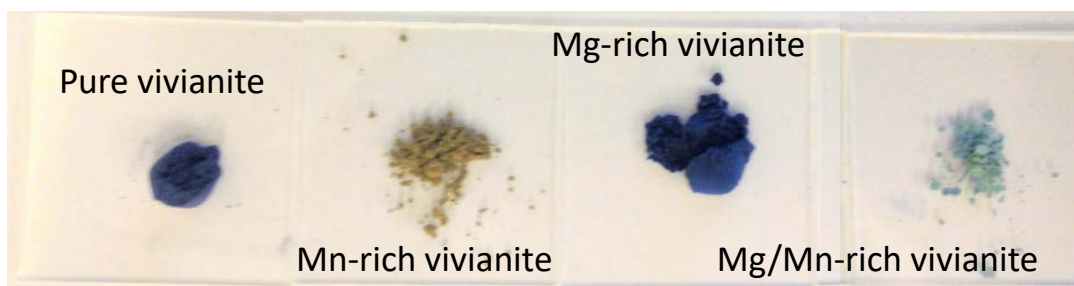
Kubeneck, L. Joëlle

Soil Chemistry Group, Institute of Biogeochemistry and Pollutant Dynamics

Phosphorus (P) is an important nutrient for primary producers in aquatic ecosystems but excessive concentrations can lead to eutrophication. The chemical form in which P is associated in soils and sediments determines its bioavailability. Under reducing, non-sulfidic conditions, the ferrous phosphate mineral vivianite can be a major P burial phase in coastal sediments. Depending on the surrounding geochemical conditions, ferrous iron (Fe<sup>2+</sup>) in vivianite may be substituted by other divalent cations such as magnesium (Mg<sup>2+</sup>) and manganese (Mn<sup>2+</sup>). Substitution of Fe<sup>2+</sup> could influence vivianite's mineralogical characteristics, with implications for mineral reactivity and thus P and iron cycling in coastal sediments.

We studied the incorporation of Mn<sup>2+</sup> and Mg<sup>2+</sup> into vivianite in aqueous coprecipitation experiments at pH 7 with varying ionic strength, resembling an estuarine gradient. Changes in mineralogy with different degrees of Mn<sup>2+</sup>/Mg<sup>2+</sup> substitution were studied with X-ray powder diffraction, Mössbauer spectroscopy and total elemental dissolution.

Our results show that up to 50% of Fe<sup>2+</sup> can be substituted in the vivianite structure, resulting in smaller crystal sizes. Furthermore, increases in ionic strength led to a decrease in Mg<sup>2+</sup> substitution. Overall, we will discuss the factors impacting Mn<sup>2+</sup> and Mg<sup>2+</sup> incorporation into vivianite and how incorporation changes mineral characteristics.

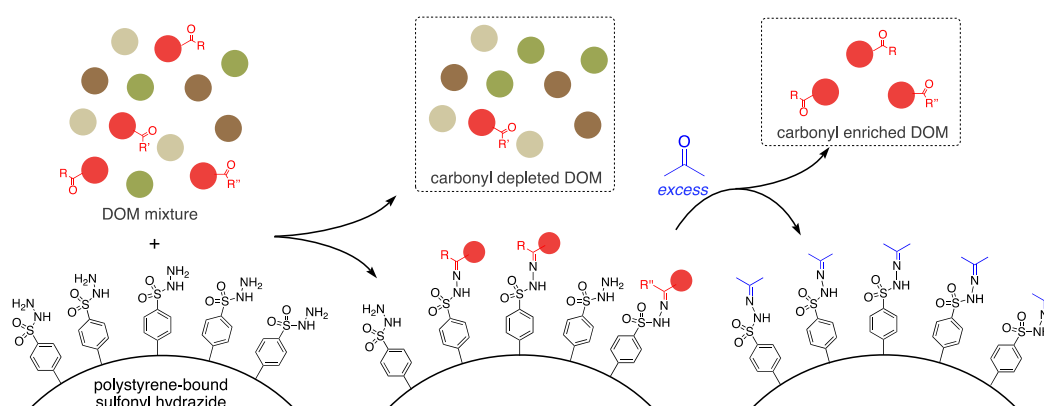


## A16 – Assessing the contribution of ketones to DOM photochemistry through selective chemical trapping

Amacha, Maya

Environmental Chemistry

Chromophoric dissolved organic matter (CDOM) is the light absorbing fraction of dissolved organic matter present in aquatic systems. CDOM undergoes photoexcitation to form triplet CDOM ( $^3\text{CDOM}^*$ ) when water is exposed to light.  $^3\text{CDOM}^*$  plays a vital role in the oxidation of anthropogenic contaminants that are discharged into water bodies. However, the fact that  $^3\text{CDOM}^*$  is a complex mixture poses a real challenge towards its understanding and characterization. The aim of this work is to gain a deeper insight into the composition and reactivity of the major chemical species that represent the oxidative properties of CDOM. This will be achieved first by isolating the carbonyl-containing fraction, an important fraction of  $^3\text{CDOM}^*$  that is thought to be central to CDOM photochemistry, using solid-supported hydrazine. This will lead to the development of an optimized method to separate the carbonyl-containing fraction, which will be shown on the poster. The second part of the project will cover the photochemical characterization of both the carbonyl-depleted and -enriched fractions of CDOM, and their ability to form other reactive intermediates ( $\text{OH}^\bullet$ ,  $\text{H}_2\text{O}_2$ , etc.).



Carbonyl catch-and-release concept, trapping ketones as hydrazones using polymer-bound toluenesulfonyl hydrazide, and release of the ketones by hydrazone exchange with acetone.

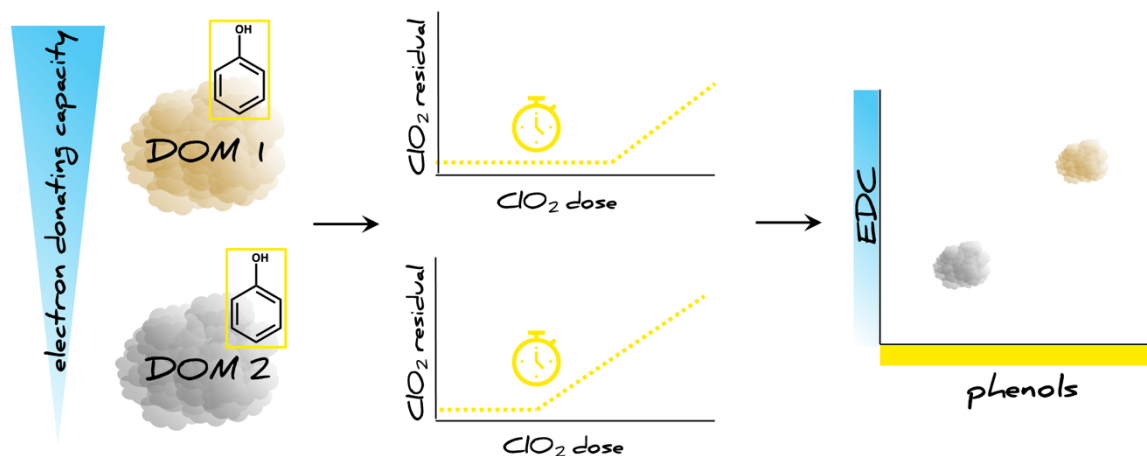
## A17 – Quantification of Oxidant-Reactive Carbonous Sites in Dissolved Organic Matter

Houska, Joanna

Eawag/EPFL

The application of ozone for disinfection or abatement of micropollutants during treatment of drinking water and wastewater is accompanied by ozone reactions with matrix components such as dissolved organic matter (DOM). For a better prediction of the efficiency of the oxidation processes and the formation of ensuing products, knowledge about concentrations of reactive DOM sites is essential. Our proposed method is based on the assumption, that oxidants such as ozone, chlorine dioxide or chlorine are selective towards electron-rich moieties in DOM, which is reflected in distinct kinetic behavior.

In this study, we quantified phenolic sites with chlorine dioxide ( $\text{ClO}_2$ ) by oxidative titration. The quantification was successful for several DOM isolates and two secondary clarifier wastewater samples and a clear linear relationship to the electron donating capacity (EDC) was observed. Further evaluation of the formation of inorganic  $\text{ClO}_2$ -byproducts and changes due to a novel molecular tagging for phenols revealed a better understanding of DOM characteristics. Chlorination combined with EDC indicated that the arrangement of hydroxy groups is crucial and the potential of  $\beta$ -diketones to the quantified sites deserves further investigation. Overall, oxidative titrations provide a novel and promising tool to quantify oxidant-reactive sites in complex mixtures such as DOM.



*Oxidative titration of phenols in complex matrices by chlorine dioxide*





## **A18 – Interbacterial Killing in the Oceans**

Stubbusch, Astrid

EAWAG & ETHZ

Over the last decades, the study of microbial communities allowed for the discovery of diverse and ubiquitous microbial interactions, which remained unnoticed in previous study of microbes in monocultures. Despite the appreciated diversity and ubiquity of interbacterial interactions, we lack a quantitative understanding of their impact on microbial communities and microbial functions. In my PhD project I focus on contact-dependent mechanisms of interbacterial antagonism. In recent years, several mechanisms of contact-dependent bacterial antagonism were found that require cell-to-cell contact to export antibacterial ‘effector’ proteins (usually via ‘secretion systems’) to harm or kill neighbouring cells. In my PhD project, I strive to understand the extent and impact of bacterial lysis by interbacterial antagonism. It is an open question what ecological role and implications contact-dependent interbacterial lysis may exert on the ocean, where particles of organic matter are remineralized by densely attached microbes. To address this question, I use transcriptomic data from simple artificial communities as well as marine (meta)genomic and metatranscriptomic data. The goal of this research is to increase our understanding of the prevalence, importance, and implications of bacterial antagonism in the ocean.

## B01 – Marine heatwave detection in the global ocean

Wong, Meng Cheng Joel

IBP/UP

Marine Heatwave (MHW) events in the oceans have recently received more attention in scientific studies due to its expected increase in frequency and intensity. This increase is commonly attributed human-induced climate change, and can have far reaching effects on various biological systems. Since MHWs impact each organism differently, methods to detect them depend greatly on the temperature thresholds tolerable by such organisms. There is thus no standard way of defining a MHW event. In this work, a recently published MHW detection method with some variations is applied to a hindcast simulation of the global ocean. This simulation is the Community Earth System Model (CESM) with a daily temporal resolution, a nominal 1° horizontal grid resolution, and a depth interval of 10m up to 155m. This detection and set of results are a first step towards investigating MHW events at higher resolution in the Southern Ocean, with a focus on particular ectothermal organisms. It will eventually be of interest to examine the impact of MHWs on their population size and migration.

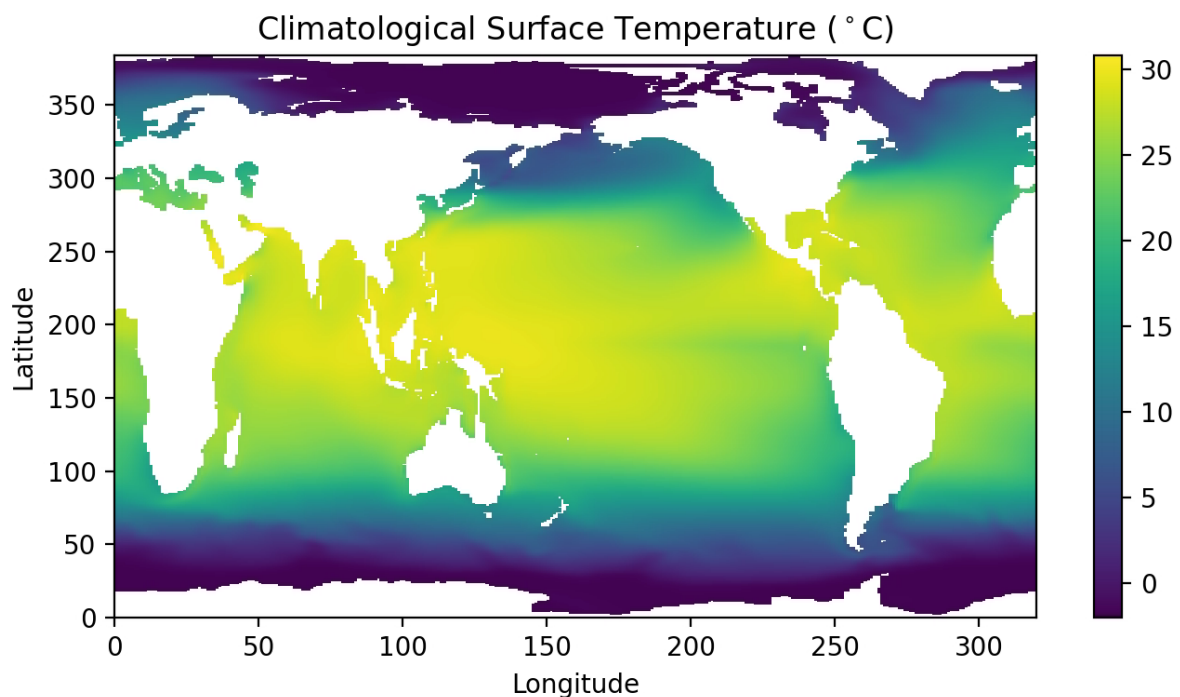


Figure: Global surface temperature on 30<sup>th</sup> June of a climatology created from 41 years of daily CESM temperature data. The climatology is used to investigate the intensity of the detected MHW events.

## B02 – Biodegradation of polyester mulch films: comparison between model systems and agricultural fields

Cerri, Mattia (collaboration with Arn Silvan)

D-USYS, UChem

Modern agriculture heavily relies on the use of plastic mulches to increase crop yields while lowering the consumption of water and herbicides. However, the use of products based on non-biodegradable plastics - like polyethylene - leads to the accumulation of persistent film fragments in fields, with long-term negative consequences for their productivity. A possible strategy to avoid accumulation is to employ biodegradable mulch films designed to be degraded *in situ* by soil microorganisms. While such products are already available on the market, the legal framework to certify their biodegradability relies on laboratory incubations only. Yet, the factors determining the rate of biodegradation under actual field conditions remain poorly understood. To identify the key polymer properties and soil characteristics governing mulch film biodegradation in agricultural soils, we will perform long-term incubations of commercial products under different conditions, and quantify the amount of degraded polymer over time. We will replicate the setup at different scales – laboratory, greenhouse mesocosms and fields.



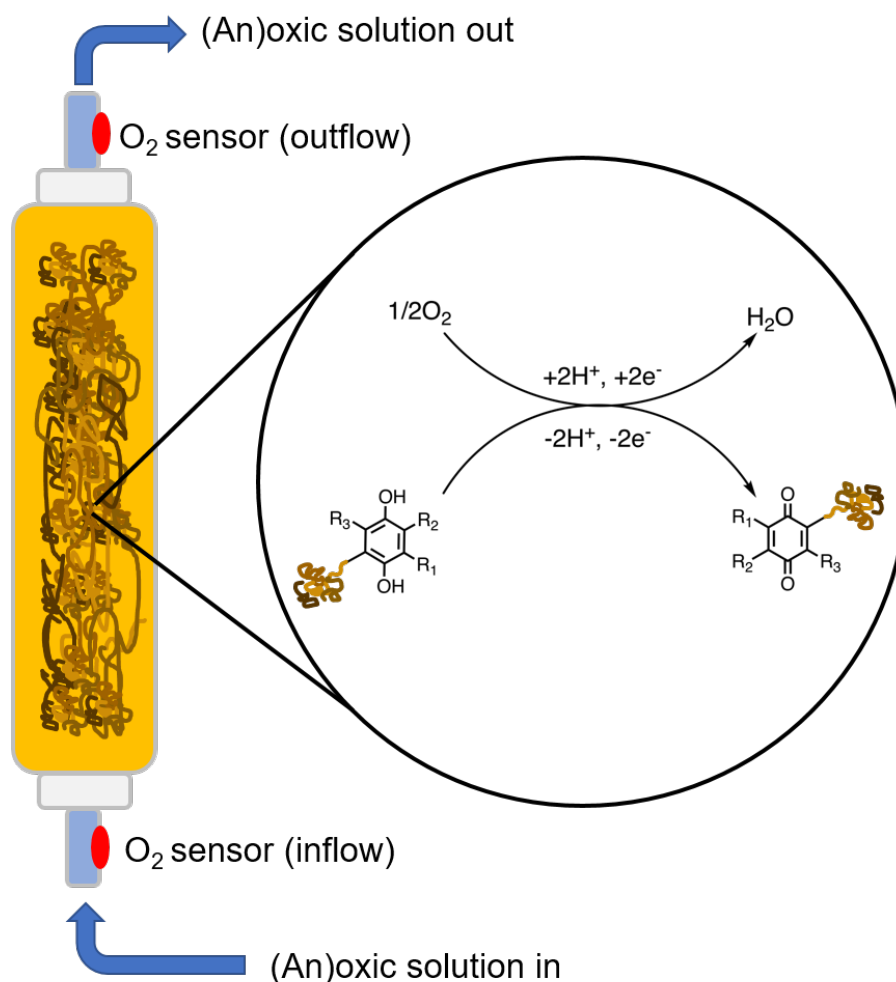
Figure 4 - In house built mesocosms for the greenhouse incubations

### B03 – Electron donating capacity of particulate organic matter from ombrotrophic bogs

Obradović, Nikola

IBP

Due to the anoxic conditions and nutrient scarcity, it is expected that methanogenesis prevails as the main organic matter decomposition pathway in ombrotrophic bog systems. Previous research has shown that these systems release less CH<sub>4</sub> than expected, pointing towards other terminal electron acceptor (TEA) in the microbial metabolic pathways. Our working hypothesis is that peat particulate organic matter (POM) acts as a reversible TEA. This will hold true if the reduced peat POM gets reoxidized during water-table drawdown. In this work, we have quantified the electron donating capacity (EDC) of peat POM with respect to the most important natural oxidant, O<sub>2</sub>, using column breakthrough experiments with fluorescent oxygen sensor-spot technology. Our results show high intra- and inter-peat variability and indicate both a correlation with POM decomposition state and a presence of sites with varying reaction kinetics in the peat POM. Furthermore, the obtained EDC values allow for a better understanding of the potential amounts of CH<sub>4</sub> that could be stored as reducing equivalents in POM.



## B04 – Ultratrace level speciation of Se, As and S in atmospheric deposition

Breuninger, Esther

Inorganic Environmental Geochemistry,  
Institute of Biogeochemistry and Pollutant Dynamics, ETH Zurich  
Swiss Federal Institute of Aquatic Science & Technology, EAWAG Dübendorf

The atmosphere is an important reservoir for the essential elements selenium (Se) and sulfur (S) as well as for the toxic element arsenic (As). Atmospheric wet and dry deposition are sources of these elements to agricultural soils and terrestrial food chains. The fate of atmospheric deposition in surface environments strongly depends on the deposited chemical forms (speciation). However, the drivers controlling Se and As speciation in atmospheric deposition (e.g. atmospheric sources and processes) remain poorly understood. Previous studies have mostly reported total elemental concentrations and/or speciation data with large unidentified fractions. The generally low Se and As concentrations in atmospheric samples (sub-ng·L<sup>-1</sup> in precipitation) require ultrasensitive methods. In this study, we optimized pre-concentration and different liquid chromatography methods coupled to ICP-MS/MS to determine Se, As and S speciation in atmospheric samples. We applied these methods on precipitation, cloud water and aerosol samples collected during Sept-Oct 2019 at Pic du Midi Observatory (French Pyrenees; 2877 m.a.s.l.). This high altitude site enables the investigation of long-range elemental transport from both marine and continental sources. New information on precipitation chemistry in combination with meteorological data will give new insights into atmospheric sources and processes controlling Se and As speciation in atmospheric deposition.



Figure 5: Field sampling at Pic du Midi Observatory

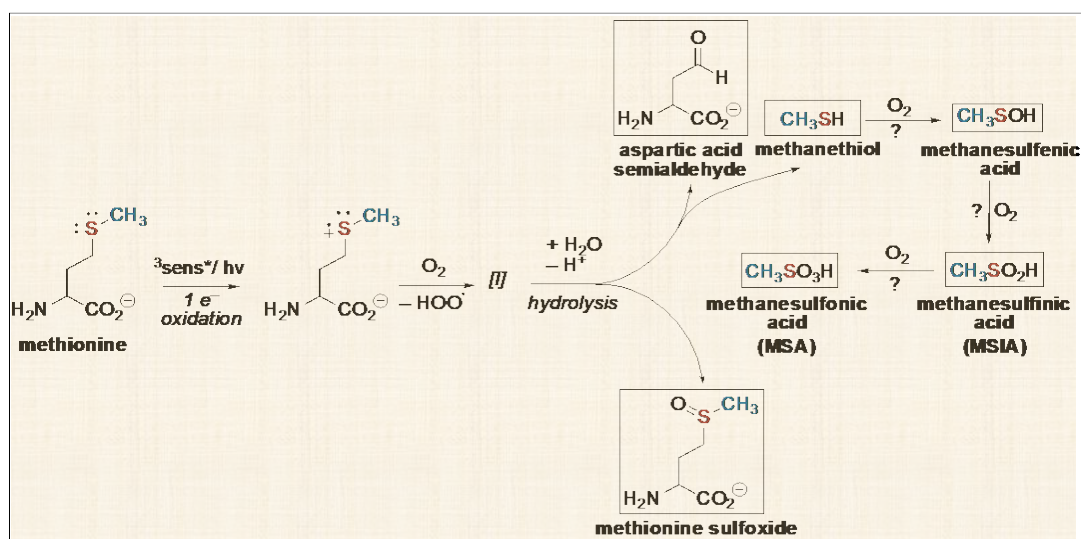


## B05 – Investigating the mechanism of methane sulfonic acid formation from photosensitized degradation of Methionine

Naim Sahar

Institute of Biogeochemistry and Pollutant Dynamics /Environmental Chemistry Group

Methane sulfonic acid (MSA) is the simplest form of photochemically stable alkyl sulfonic acids. It plays a significant role in marine aerosol formation and contributes to the sulfur cycle dynamics. Recent findings in the McNeill's research group suggest the production of MSA during the exposure of dissolved organic matter (DOM) to light, implying the importance of solar photochemical processes in the fate of dissolved organic sulfur (DOS). Among a pool of different model compounds, only methyl thioethers produce MSA during photolysis. Yet, the process of the photoproduction of MSA from DOS in aquatic systems remains unclear. Here, we select Methionine as an environmentally relevant methyl thioether model compound, and demonstrate its photosensitized degradation pathway toward MSA formation. Steady-state photolysis experiments on methionine in the presence of a sensitizer confirmed the gradual formation of MSA over the time of light exposure by IC analysis. Other methionine photoproducts were observed by HPLC/FLD analysis, including Methionine sulfoxide, a well-known methionine oxidation product, in addition to four other newly identified methionine photoproducts. A plausible mechanism was proposed after examining all confirmed photoproducts. Understanding MSA formation is crucial to help us fill in the gaps in our knowledge about the sulfur biogeochemical cycle.



A proposed mechanism for the formation of methanesulfonic acid from methionine degradation under photosensitization induced by triplet excited sensitizers

## B06 – From data science to mechanistic modelling to gain knowledge about community assembly

Chollet Ramampiandra, Emma

EAWAG

The climate and environmental crisis raise many new challenges, including the need to better understand ecosystems with a focus on reducing human impact on them. Based on this issue, we will carry out the project outlined here to improve our understanding of community assembly and develop a comprehensive process-based model for predicting occurrence of taxa. First, we will apply different model types to the same significant macroinvertebrate biomonitoring data set. The models will be machine learning algorithms, statistical models, and a mechanistic model. They differ in their use of prior knowledge, interpretability, computational power, and amount of data needed for calibration. We will therefore compare their quality of fit and predictive performance, and carefully account for uncertainty at each step, to learn about the most important influence factors. Using the acquired knowledge, we will then develop a model that is as simple and efficient as possible, considers the most important mechanisms, and is optimized for prediction. As a last step, we will run model simulations to identify macroinvertebrates metrics that are sensitive to future environmental changes. This will hopefully bring new insights for predicting community assembly that will inform the management of aquatic ecosystems in response to future environmental changes.

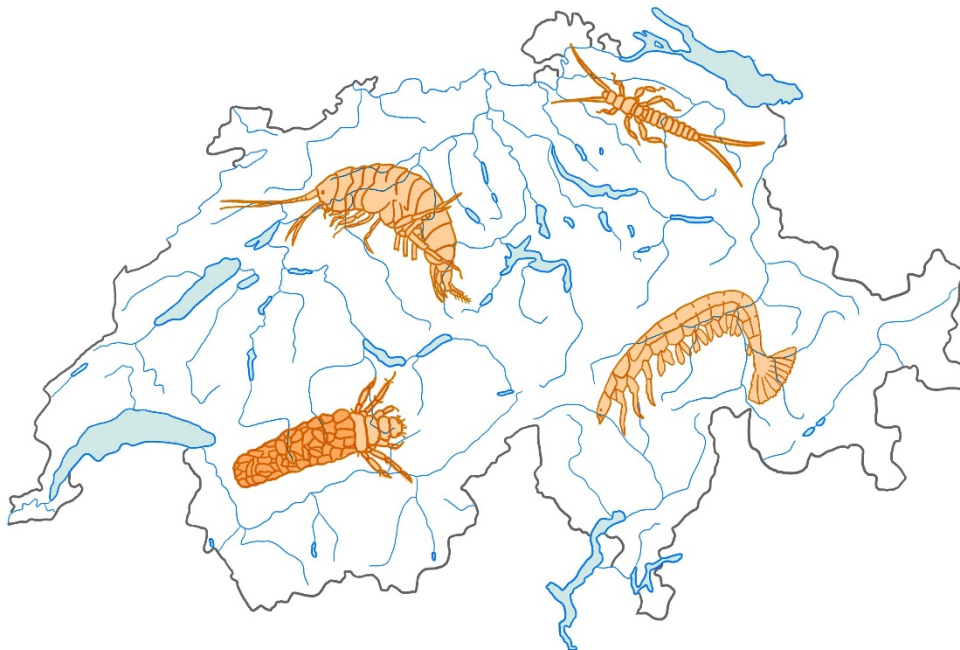


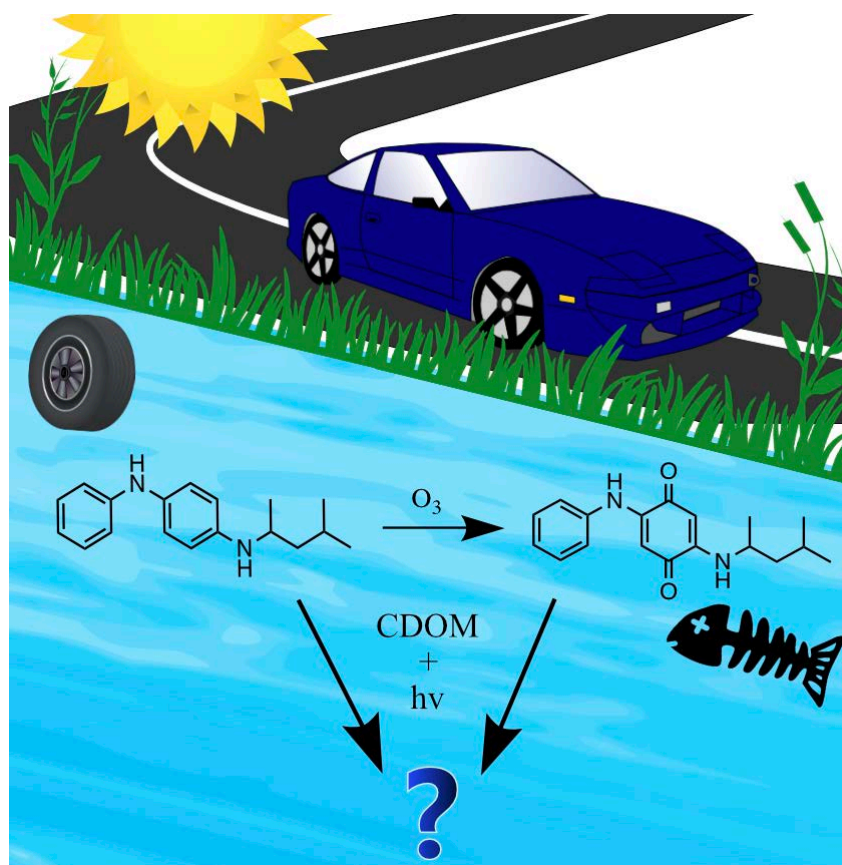
Illustration of freshwater stream macroinvertebrates in Swiss rivers

## B07 – Photochemical Reactivity of Phenylenediamines and the Toxic Degradation Product Causing Fish Kills

Platt, Katie

D-USYS PhD Student

Mass fish kills of Coho salmon have been occurring in northwestern USA since the 1980s without a causal explanation. A recent 2020 study has finally pinpointed the source of the toxic effects to a degradation product of the ubiquitous tire rubber antidegradant, N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine (6PPD). This compound transforms upon ozonation to 6PPD quinone which is a highly toxic and previously unknown transformation product. The transport and reactivity of 6PPD and similar phenylenediamines requires study to better understand their fate in the environment. This project will determine the aquatic photochemical reactivity of 6PPD and 6PPD quinone, via both direct photolysis and indirect photolysis through excited triplet state chromophoric dissolved organic matter ( $^3\text{CDOM}^*$ ) and other photochemically produced reactive intermediates. The relative contributions of the compounds' reactivity with  $^3\text{CDOM}^*$ ,  $^1\text{O}_2$ ,  $^{\bullet}\text{OH}$ , and  $\text{H}_2\text{O}_2$  will be studied using both steady state photolysis and time resolved laser spectroscopy techniques. Additionally, the conversion rate of 6PPD to 6PPD quinone will be investigated to help approximate the prevalence of this toxicant in waterways. The research plan and initial experimental insights of the project will be discussed.



**B08 – Formation and transformation of iron(III) and calcium precipitates:  
Consequences for phosphate trapping**

Nenonen, Ville

Department of Water Resources and Drinking Water, Eawag

The cycling of phosphorus in terrestrial and aquatic systems is tightly coupled to the redox-cycling of iron (Fe). The oxidation of dissolved Fe(II) in natural waters leads to the precipitation of amorphous to poorly crystalline Fe(III)-solids that can bind phosphorus as phosphate (P) and other nutrients as well as toxic compounds. The formation of Fe(III)-precipitates by the oxidation of dissolved Fe(II) in natural waters is strongly affected by solutes (Ca, P, Si, dissolved organic matter) that interfere with Fe(III) precipitation and polymerization, and thereby also affect P binding. Consequently, there is a need for a mechanistic understanding of relevant Fe (and Ca) phase formation and transformation processes and their effects on P. This project specifically focuses on two aspects: (I) Effects of organic ligands on the structure, colloidal properties and P uptake of fresh Fe oxidation products, and (II) structural transformation of fresh Fe(III)-precipitates during aging and effect on P retention. This mechanistic project forms part of the EU training network P-TRAP (<https://h2020-p-trap.eu/>) aimed at developing Fe-based methods to trap diffuse P release from soils and sediments into surface waters.

## B09 – Revision of the eMLR(C\*) Method to Determine the Oceanic Uptake of Anthropogenic CO<sub>2</sub> in the 2010s

Zhu, Donghe

Institute for Atmospheric and Climate Science

The ocean serves as a significant carbon sink, absorbing roughly one third of anthropogenic CO<sub>2</sub> emissions, which largely mitigates climate warming. Different approaches have been brought up in order to better estimate the oceanic carbon sink. Among the observation-based approaches, estimates of the storage of anthropogenic carbon (C<sub>ant</sub>) in the ocean interior rely on sparse ship-based observations. Clement and Gruber (2018) introduced an extended multiple linear regression (eMLR) method applied to the tracer C\* which successfully retrieved changes in C<sub>ant</sub> between 1994 - 2007 with small bias on both global and basin scales. Since the last application of this method, almost a decade of additional observations were made available through the Global Ocean Data Analysis Project (GLODAP). Aiming at a quantification of changes in C<sub>ant</sub> throughout the post-2010 era, we reprogrammed the eMLR(C\*) method in R and performed sensitivity tests with synthetic data sampled from a hindcast run of a global ocean biogeochemical model (GOBM), which allows us to compare reconstructed changes of C<sub>ant</sub> with the model “truth”. The main goal of this effort is to adjust the parameterizations of the eMLR(C\*) approach and further improve the accuracy and robustness of this method for the specific data coverage of the post-2010 era.

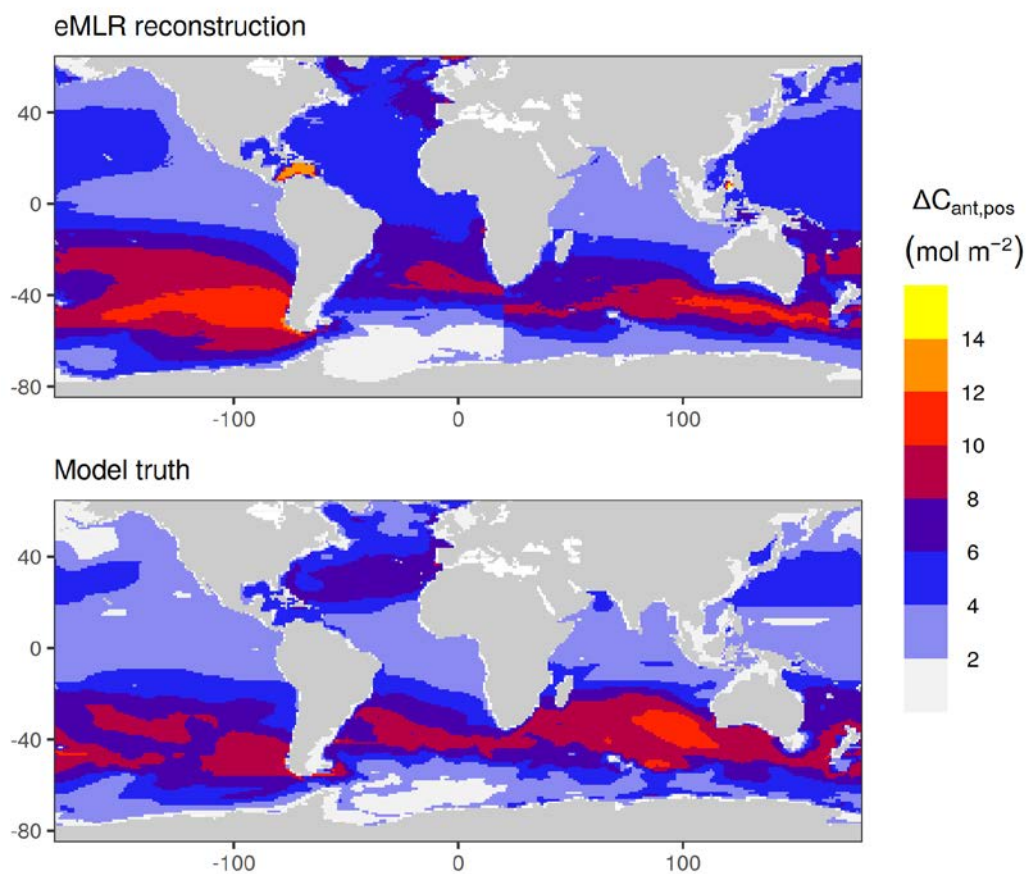


Figure 1: Column inventory map for the changes in anthropogenic CO<sub>2</sub> comparing the eras 2000-2012 to 2012-2019.



**B10 – Deep Sea MnammoX: Could it be and how can we see it?**

Bakker, Lena

IBP/ Master student in the environmental microbiology group

Oligotrophic deep sea sediments are some of the largest habitats on earth and the microbial community structure and the performed functions there are still very much understudied. In this project abyssal sediment gravity cores retrieved from the Gloria Fault between the Azores and the Madeira Torres rise on the Meteor Cruise M162 are analyzed. The community composition was investigated with qPCR and barcode sequencing revealing an interesting community difference between oxic and anoxic layers. Additionally interesting Mn and N species geochemical profiles were seen that could be indicative of anoxic oxidation of ammonium with Mn. This process has been proposed to sustain life but has not yet been seen in nature, and the goal of the next step of the project is to show the MnammoX in incubation experiments. Therefore the sediment samples are incubated with isotopically labeled ammonium and  $Mn^{4+}$  and the isotopic composition of the  $N_2$  gas in the headspace is analyzed to trace the fate of the nitrogen in the ammonium. Possibly enrichment of the organisms and rate determinations will be performed following this.



Overview of the proposed process investigated in this project, the most important educts on the left and the possible products on the right



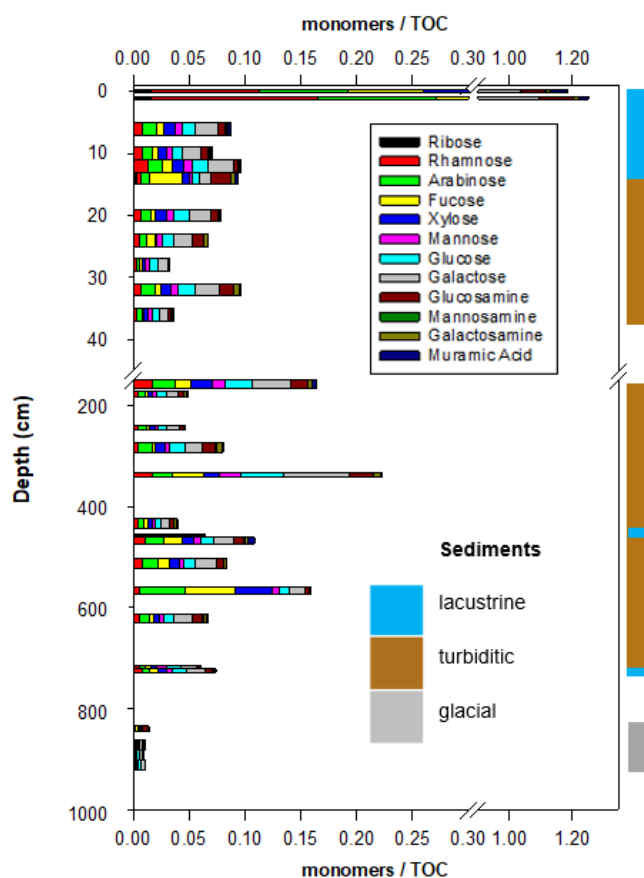


## B12 – What controls the fate of carbohydrates in lake sediments?

Gajendra, Niroshan

Institute of Biogeochemistry and Pollutant Dynamics/ Environmental Microbiology

Carbohydrates account for a major fraction of the global sedimentary organic carbon budget. Yet, carbohydrate compositions and the factors that determine the long-term preservation of carbohydrates in sediments are poorly constrained. Using a novel sequential extraction method, we investigate the distribution and composition of carbohydrates along a Quaternary sedimentary sequence of Lake Cadagno that is characterized by distinct layers of autochthonous lacustrine, turbiditic, and/or terrestrial organic matter. Accordingly, carbohydrates represent most total organic carbon (TOC) at the lake floor. But they drop to values around 10 % of TOC within the top 10 cm, implying intense and selective degradation of carbohydrates within the first 200 years after deposition. In all sediment layers, carbohydrate monomers are dominated by the neutral sugars galactose and glucose. Besides, reflecting the differences in organic carbon sources, there are higher proportions of amino sugars in glacial sediments, and of fucose, arabinose, and xylose in turbiditic deposits. These suggested shifts in carbohydrate sources are further assessed by pyrolysis-GC/MS. This study provides new insights into carbohydrate pool sizes and compositions in lake sediments and improves the current understanding of the controls on carbohydrate preservation and degradation in the vast global sedimentary carbon sink.



### B13 – Toxicokinetics of pesticides in Gammarus under field conditions: Different to laboratory data?

Lauper, Benedikt

Eawag, UChem

Bioaccumulation and biotransformation of organic micropollutants in aquatic organisms have been investigated in laboratory experiments extensively. For several micropollutants (MPs), however, the measured internal concentrations in *Gammarus* spp. in field trials exceeded the predictions based on the laboratory data, sometimes by multiple orders of magnitude. These exceedences were mainly observed for pesticides, especially neonicotinoid insecticides and azole fungicides.

In this work, we tested the impact of both dietary uptake and aqueous exposure dynamics on the toxicokinetics of pesticides in aquatic invertebrates with a field trial using caged *Gammarus* spp. deployed in a small Swiss stream known for receiving high pesticide loads. Using a fully automated mobile LC-ESI-HRMS/MS system, the aqueous concentrations of 77 micropollutants were measured at high temporal resolution (20 min for 1 month). The data from this caging study were then employed to model exposure pathways of pesticides into gammarids, with a hypothesis that several routes of exposure can contribute to the overall bioaccumulation. The internal concentration of gammarids was modelled using a one-compartment toxicokinetic model with parameters taken from literature. Different exposure scenarios were explored and compared to the body burden measured in caged gammarids.

Using laboratory toxicokinetic data systematic underestimation of internal concentration was observed.

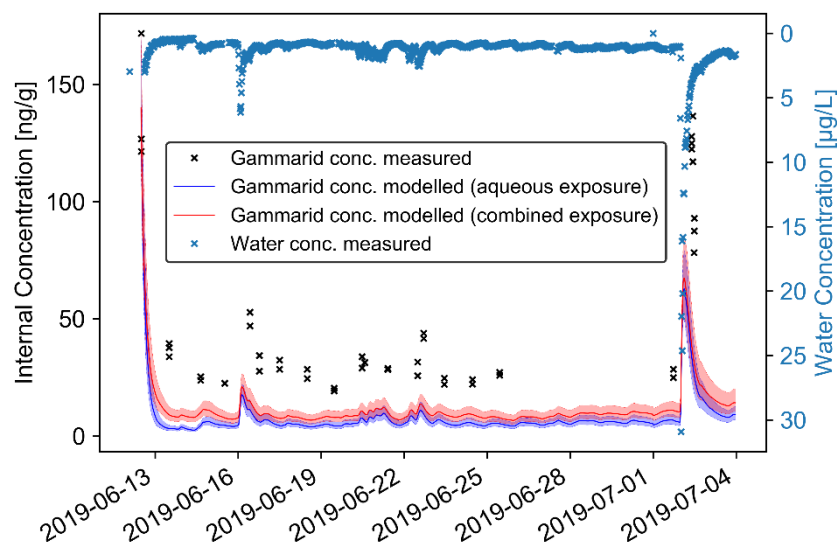


Figure 6: Predicted internal concentration of fluopyram using a single compartment toxicokinetics model. Different exposure scenarios were explored to determine the primary exposure pathway of pesticides in gammarids. The measured water concentration used in the model (blue crosses) is plotted with inverse y-axis to avoid overlap.

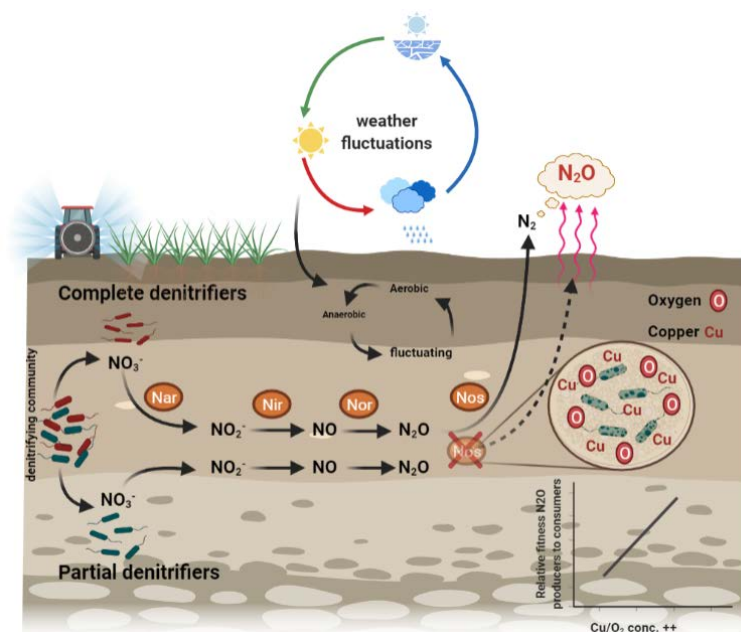


## B14 – A Synthetic Ecology Approach to Elucidate the Causes of Microbial Nitrous Oxide Release during Denitrification

Almoammar, Hassan

Department of Environmental Microbiology, Institute of Biogeochemistry and Pollutant Dynamics,

Nitrous oxide (N<sub>2</sub>O) is a powerful atmospheric greenhouse gas and contributes towards the destruction of the ozone layer. Microbial denitrification is a major source of N<sub>2</sub>O from both terrestrial and aquatic systems. My goal is to identify the environmental conditions when partial denitrifiers that produce N<sub>2</sub>O as an end-product have a selective advantage over complete denitrifiers, and thus when nitrous oxide is likely to be released to the environment. To address this, I use a synthetic ecology approach where I assemble communities from isolates. This provides me with a strong model system, minimizes confounding factors, and helps establish causality. In essence, using synthetic ecology to understand the properties and dynamics of microbial communities can provide a foundation for understanding complex natural microbial communities. I use *P. stutzeri* as a model organism because different strains within this species display variance in their denitrification capabilities. My project emphasizes the importance of detailed causal knowledge, where small differences in environmental conditions could lead to large changes in microbial community dynamics and N<sub>2</sub>O production. Eventually, I hope this project will help us predict in which environments N<sub>2</sub>O is likely to be released or consumed, thus improving our knowledge of a critically important greenhouse gas.



How do factors affect the oxide during

denitrification?

environmental release of nitrous microbial



## B15 – Insights from mapping noble gases in the Danube Delta

Maier, Marie-Sophie

Eawag SURF

Europe's second largest river delta, the Danube Delta, is a mosaic of aquatic environments such as large river branches, small channels and shallow lakes. Nutrient inputs from the main river, abundant macrophytes in the lakes and lateral influx of water from adjacent wetlands add to the spatial heterogeneity. Consequently, the delta exhibits large concentration ranges in CO<sub>2</sub> and CH<sub>4</sub> with distinct hot spots in small channels. To shed light on the processes that lead to these patterns, we measured dissolved He, O<sub>2</sub>, Ar and N<sub>2</sub> using a membrane-inlet mass spectrometer (MIMS) installed on a houseboat. Helium saturations as low as 60% indicated that ebullition occurred frequently in the lakes of the delta, which also decreased N<sub>2</sub> and Ar concentrations. Comparing O<sub>2</sub> with Ar, which has similar solubility properties, suggests that O<sub>2</sub> production from macrophytes could cause the ebullition and reduces O<sub>2</sub> concentrations in the lakes by about 1-2mg/L. Interestingly, CO<sub>2</sub> and CH<sub>4</sub> hotspot sites receiving lateral water inflow from the wetland showed elevated He saturations and oversaturation in both N<sub>2</sub> and Ar, which indicates the formation of excess air in the reed bed.

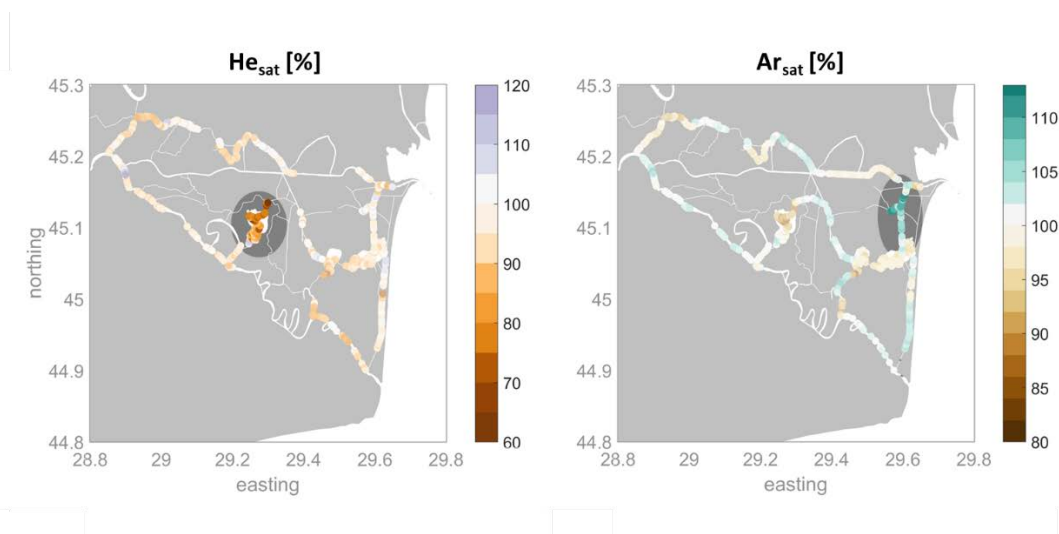


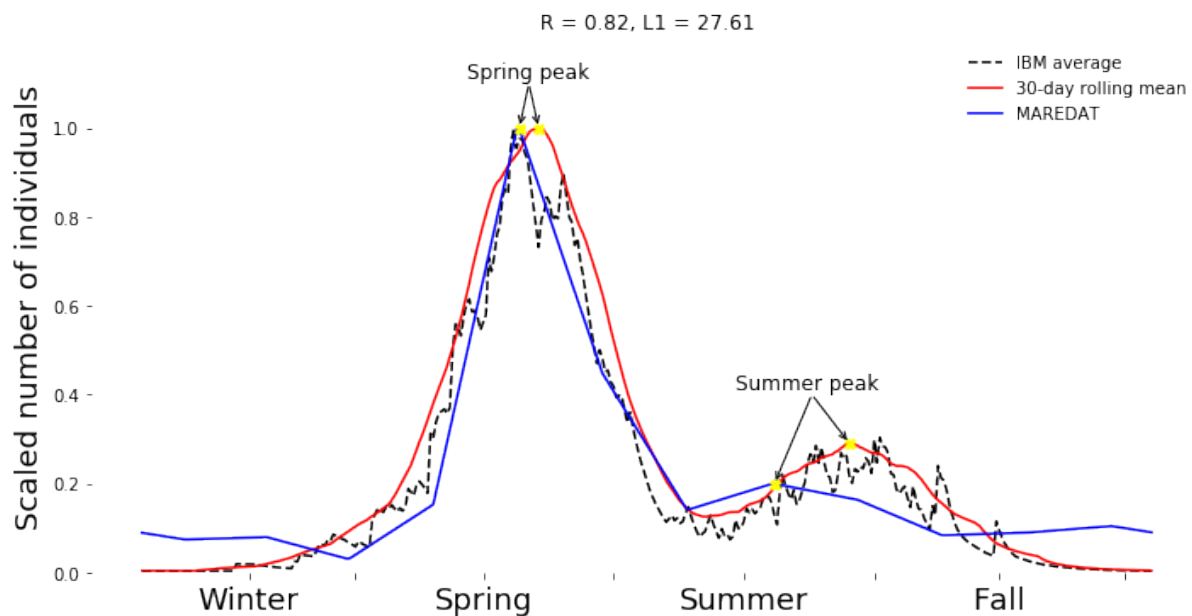
Figure 1: Saturation of He (left) and Ar (right) in different waterscapes of the Danube Delta. The location of lakes Uzlina and Isak are highlighted on the left, which is where we see strongest He undersaturation, while the area corresponding the CO<sub>2</sub> hotspot is highlighted on the right, where Ar and N<sub>2</sub> were oversaturated.

## B16 – Individual-based modelling of shelled pteropods

Hofmann Elizondo, Urs

D-USYS Environmental Physics

Shelled pteropods are cosmopolitan, free-swimming organisms of biogeochemical and commercial importance. They are widely used as sentinel species for the overall response of marine ecosystems to environmental stressors associated with climate change and changes in ocean chemistry. In-situ observations of individual pteropods have shown widespread shell dissolution caused by changes in ocean chemistry. However, the effects of climate change on a population level remain elusive. This is in part due to the missing spatio-temporal characterization of the response of pteropods to environmental stressors, and the difficulty to take into account the life history and life cycle of pteropods. In this study, we implement a shelled pteropod Individual-Based Model (IBM) as a possible approach to resolve these limitations, i.e. we simulate a pteropod populations as a set of discrete individuals over several generations. The model provides the life stage composition of a pteropod population throughout a year, highlighting periods when younger and more susceptible life stages are most abundant.

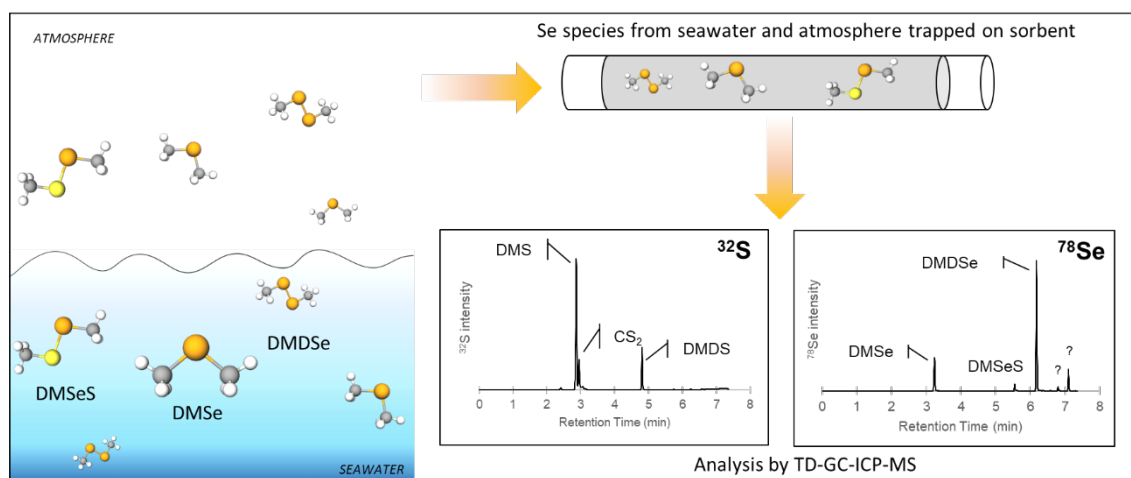


## B17 – TD-GC-ICP-MS as novel analytical method to study marine Se and S emissions

Le Bras, Zoé

IBP – Inorganic Environmental Geochemistry

Selenium (Se) is an essential trace element for many organisms, including humans. The atmosphere is an important reservoir of Se, in which yearly around 13 000 – 19 000 tons Se are cycled. Atmospheric Se, which is deposited to land and ocean surfaces via wet and dry depositions, functions as a source of this essential micronutrient to food chains and ecosystems. Marine biogenic emissions represent around 30-50 % of atmospheric Se and are dominated by volatile methylated species, i.e. dimethyl selenide (DMSe), dimethyl diselenide (DMDSe) and dimethyl selenyl sulphide (DMSeS), present in (sub)surface seawater in pmol.L<sup>-1</sup> to fmol.L<sup>-1</sup> levels. The distribution of these volatile organic Se species and their mechanisms of formation remain poorly understood due to the lack of sensitive and high throughput analytical methods for trapping and analysis of Se species. Here we present a thermal desorption unit coupled with gas chromatography inductively coupled plasma mass spectrometry (TD-GC-ICP-MS) as a highly sensitive and selective analytical method to analyze volatile Se and S species at ultra-trace levels (fM-pM). Our preliminary results show that application of gas trapping during marine research cruises, followed by TD-GC-ICP-MS analyses, give new insights into marine biogeochemical Se cycling and air-sea emissions.





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