

40th

Annual Meeting of the German Association of Isotope Research

from 29th September to 2nd October 2019
at Technische Universität Dresden

Book of Abstracts



**40th Annual Meeting
of the German Association for
Stable Isotope Research**

**from 29th September to 2nd October 2019
at Technische Universität Dresden (TUD)**

Book of Abstracts

Dr.-Ing. Diana Burghardt & Patricia Stock, M.Sc.
Institute of Groundwater Management

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Greetings

In 2019, the German Association of Stable Isotope Research will celebrate their 40th meeting. We are therefore especially happy to welcome you at Technische Universität Dresden!

Technische Universität Dresden (TUD), which was founded in 1828 and obtained the status of a university in 1961, is actually one of the largest universities of technology in Germany. With 18 faculties in five schools, it offers a broad research spectrum with focuses on Health Sciences, Biomedicine & Bioengineering, Information Technology & Microelectronics, Smart Materials & Structures, Energy, Mobility & Environment. Since 2012, TUD has been one of the “Universities of Excellence” in Germany. About 33.000 students are enrolled and about 8.300 employees are working at TUD.

Stable isotope research was established at TUD in 2011. Actually, the Institute of Groundwater Management provides two IRMS systems with focus on hydrological, hydrogeological and hydrochemical research. Since 2016, various investigations of the global carbon cycle have been and continue to be realized at the Institute of Soil Science with an IRMS-system as well as a laser spectrometer.

Dresden, the state capital of Saxony has approximately 541,000 residents. The city stretches out on both sides of the Elbe River at a length of 30 kilometers and is embedded in the foothills of the East Ore Mountains, the Elbe Sandstone Mountains and the Lausitz granite plate. Dresden is not only a city of art and culture, but also an important technology hub.

We wish you a pleasant stay in Dresden and an inspiring meeting at our University.

Rudolf Liedl

Institute of Groundwater
Management

Karsten Kalbitz

Institute of Soil Science,
Chair of Soil Resources and Land Use

Scientific Committee

Prof. Dr. Karsten Kalbitz

TU Dresden, Chair of Soil Resources and Land Use

Prof. Dr. Michael Zech

TU Dresden, Institute for Geography

Prof. Dr. Gerhard Gebauer,

University Bayreuth, Central Laboratory for Isotope Biochemistry
at Bayreuth Center of Ecology and Environmental Research

Prof. Dr. Harald Strauß,

University Münster, Institute for Geology and Paleontology

Prof. Dr. Johannes Barth

University Erlangen- Nürnberg, GeoZentrum Nordbayern, Applied
Geology

Prof. Dr. Nicolas Brüggemann

Forschungszentrum Jülich, Institute of Bio- and Geosciences,
Research Unit Plant-Soil-Atmosphere Exchange Processes

Organization Team at TU Dresden

Dr.-Ing. Diana Burghardt

Patricia Stock, M.Sc.

Nancy Reimann

Doreen Degenhardt

Directions and Location Maps

- public transport in Dresden: <https://m.dvb.de>

- **how to get from TU Dresden/ Dülfersaal to**
 - ... Dormero-Hotel Dresden City/ Conference Dinner**
Kreischauer Str. 2
bus no. 61 direction 'Weißig', from station 'Technische Universität (Fritz-Förster-Platz)' to station 'Wasaplatz', 7 minutes

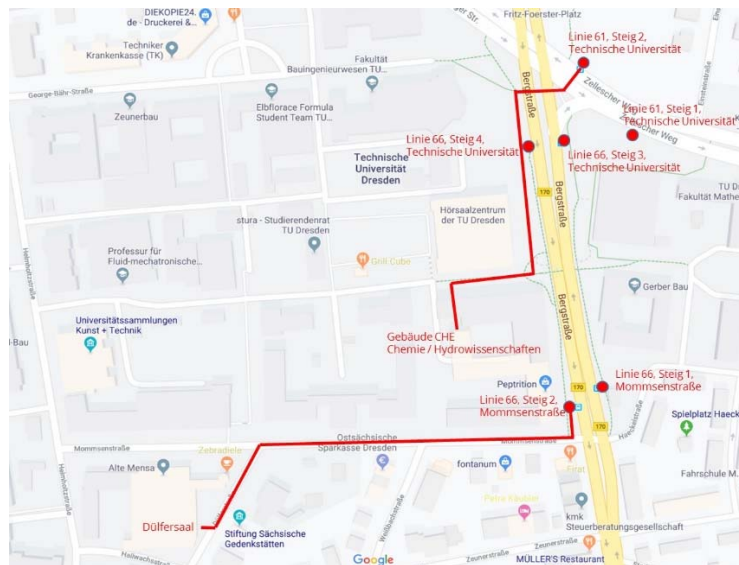
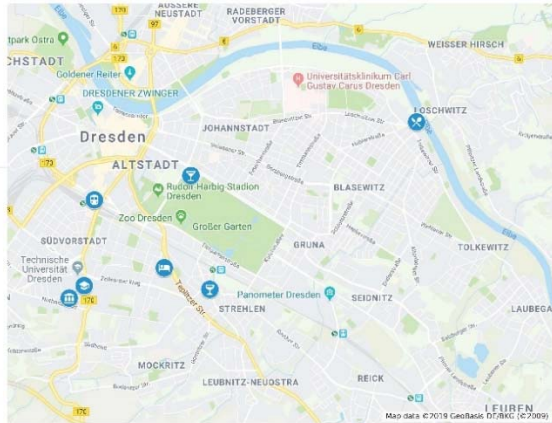
 - ... TU-Gästehaus 'Am Weberplatz',**
Weberplatz 3
bus no. 61 direction 'Weißig', from station 'Technische Universität (Fritz-Förster-Platz)' to station 'Zellescher Weg', 3 minutes and about 10 minutes walkway

 - ... Restaurant e-Vitrum, Gläserne Manufaktur,**
Lennéstr. 1
bus no. 66 direction 'Lockwitz' or 'Nickern' from station Technische Universität (Fritz-Förster-Platz) to station 'Gret-Palucca-Straße', from here with tram no. 10 direction 'Striesen' to station 'Straßburger Platz (Gläserne Manufaktur)', 16 minutes with one change




ASI 2019



Locations


-  DORMERO Hotel
-  Gastehaus "Am Weberplatz"
-  Dölfersaal
-  Gläserne Manufaktur
-  Hauptbahnhof
-  CIE
-  SchillerGarten













List of Participants

Name	Institution
A Ackermann, Annika	ETH Zürich, Isolab Graslandwiss.
Asfaw, Berhane Abirha	Technische Universität Darmstadt, Institute of Applied Geosciences
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Benesch, Marianne	Martin-Luther-Universität Halle-Wittenberg, Bodenbiogeochemie
Beyer, Matthias, Dr.	TU Braunschweig, Institute for Geoecology
Binder, Martin	Technische Universität Dresden, Institut für Grundwasserwirtschaft
 Bindereif, Stefan	University of Bayreuth, BayCEER
 Bittner, Lucas	TU Dresden, Institute of Geography, Landscape Ecology
Blatt, Christina	Deutsche Sporthochschule Köln, Biochemie
Boeckx, Pascal, Prof. Dr.	Ghent University, Isotope Bioscience Laboratory
Bösel, Stefanie	Thermo Fisher Scientific, Unity Lab Service
Böttcher, Michael E., Prof. Dr.	Leibniz Institute for Baltic Sea Research (IOW), Geochemistry & Isotope Biogeochemistry
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S	Scheid, Nicole, Dr.	Bundeskriminalamt Wiesbaden, KT43 – Zentrale Analytik II
	Schierbeek, Henk, Dr.	University of Amsterdam
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	 Schroll, Moritz	University of Heidelberg, Biogeochemistry
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	 Zander, Florian	TU Delft
Z	Zech, Michael, Prof. Dr.	TU Dresden, Institut für Geographie
	Zinsberger, Gerhard	Thermo Fisher Scientific, IOMS Big Biz B

Program Overview

	Sunday, Sep. 29 th	Monday, Sep. 30 th	Tuesday, Oct. 1 st	Wednesday, Oct. 2 nd
9:00 am		Company Presentations and Tutorials 9:00 am to 12:30 pm	Soil and Carbon 9:00 am to 10:45 am	Sediments and Biogeochemistry 9:00 am to 10:30 am
10:00 am				Postersession 10:30 am to 11:00 am
11:00 am			Coffee Break 10:45 am to 11:15 am	Plants 11:00 am to 12:00 pm
12:00 am			Isotope award 2019 11:15 am to 12:15 pm	
		Welcome and Opening 12:30 pm to 1:00 pm	Lunch Break 12:15 pm to 1:15 pm	
1:00 pm		Atmosphere 1:00 pm to 2:30 pm		
2:00 pm			Coffee Break 2:30 pm to 3:00 pm	
3:00 pm		Methods 3:00 pm to 4:30 pm	Soil and Water II 4:00 pm to 5:00 pm	
4:00 pm		Social Event 5:00 pm to 12:00 am		Poster Session/ Lab tour 4:30 pm to 6:00 pm
5:00 pm			Thermo Fisher User Meeting 7:00 pm to 12:00 am	
6:00 pm				
7:00 pm				

Scientific Program

Sunday, 09/29/2019

(Building Chemie/Hydrowissenschaften, Bergstraße 66, CHE183)

14:00 Forum for early career scientists:

14:00 **Welcome**

14:15 Stable isotope signatures of methane released from algae
(**Thomas Klintzsch**, University Heidelberg)

14:45 Isotope analysis on sediment core from Viernheim with
the aim to distinguish calcite and dolomite in terms of
stable carbon and oxygen isotopes (**Wang Feiyu**,
Darmstadt University of Technology)

15:15 BIOMUD - The spatial variability of organic matter degra-
dation in dredged sediments (**Florian Zander**, TU Delft)

15:45 Coffee break

16:00 Establishment and application of ^{15}N - N_2O site preference
analysis for identification of N_2O emission paths from
agricultural soils (**Gesa Schulz**, TU Dresden)

16:30 Preparation and analysis of $\delta^{15}\text{N}$ - NH_4 in water samples
(**Patricia Stock**, TU Dresden)

16:30 Development of a Heatable Precipitation Totalizer
(**Florian Bräuer** et al., TU Dresden)

17:00 Social evening:

Dresden-Loschwitz (Schwebebahn) - walking tour to
Dresden-Blasewitz (Schillergarten, beer garden or
restaurant)

Monday, 09/30/2019

(Building Chemie/Hydrowissenschaften, Bergstraße 66, CHE 183)

9:00 Company presentations and tutorials [p.131]

9:00 ^{13}C and ^{18}O Isotope Effects Resulting from High Pressure CO_2 Cylinder Depletion (**Oliver Schlegel**, Air Liquide) [p.133]

9:15 **T1:** Sample preparation and quality control for IRMS analysis (**Kathrin Reimer**, Elementar Analysensysteme) [p.135]

10:15 Coffee break

10:30 **T2:** Introduction to isotope analysis of water and other liquids (**Oliver Kracht**, Thermo Fisher Scientific) [p.137]

Merits of compound specific isotope analysis and structural identification (**Julian Renpenning**, Thermo Fisher Scientific) [p.137]

Overview of analytical tools in biogeochemistry (**Andreas Hilkert**, Thermo Fisher Scientific) [p.137]

11:30 Lunch break

Monday, 09/30/2019

(Building Mensa, Dölfersaal, Mommsenstraße 13)

12:30 **Welcome and opening** (**Rudolf Liedl**, Institute of Groundwater Management, **Paul Königer**, GASIR-Chair)

13:00 Session 1: Atmosphere
(Chair: **Rudolf Liedl**, TU Dresden)

13:00 **Keynote:** About limitations of the ^{15}N site preference in N_2O for source process attribution (**Nicolas Brüggemann**, Forschungszentrum Jülich) [p.21]

13:30 **P1.1:** The global chloromethane cycle: new insights from triple element stable isotope analysis (**Frank Keppler**, University Heidelberg) [p.23]

13:45 **P1.2:** CH_4 from three widespread marine algal species: release rates, precursor compounds and relevance for the environment (**Th. Klintzsch**, Univ. Heidelberg) [p.25]

14:00 **P1.3:** The carbon stable isotope signature of CH_4 produces by two saprotrophic fungi (**Moritz Schroll**, University Heidelberg) [p.27]

14:15 Coffee break

15:00 Session 2: Methods
(Chair: **Paul Königer**, BGR Hannover)

15:00 **P2.1:** Ten Years of Elementar and IsoPrime: Pioneers in simultaneous CNS isotope ratio analysis (**Simone B. Moos**, Langenselbold) [p.31]

15:15 **P2.2:** Optimizing EA-IRMS: Getting more for less by ultra-high sensitivity (**Oliver Kracht**, Bremen) [p.33]

15:30 **P2.3:** How climate change can help fighting fraudulent declaration of cereal grains (**Stefan Bindereif**, University of Bayreuth) [p.35]

15:45 **P2.4:** Further development of the denitrification method for stable isotopic analysis of N and O in nitrate of natural water samples (**Patricia Stock**, TU Dresden) [p.37]

- 16:00 **P2.5:** N-isotopic composition of NO₃ and NH₄ from aqueous solutions by isotope ratio mass spectrometry (SPIN-MIRMS) (**Jens Dyckmans**, University Göttingen) [p.39]
- 16:15 **P2.6:** Atypical δ¹³C values of urinary norandrosterone in doping control analysis (**Frank Hülsemann**, German Sport University Cologne) [p.41]

16:30 Poster session with snacks

16:30 **lab tours** (limited number of places, registration necessary)

Tuesday, 10/01/2019

(Building Mensa, Dülfersaal, Mommsenstraße 13)

9:00 Session 3: Soil and Carbon (Chair: **Karsten Kalbitz**, TU Dresden)

9:00 **Keynote:** Sulfur Isotopes – Applications in Earth Science (**Harald Strauß**, University Münster) [p.57]

9:30 **P3.1:** Carbon investment of beech (*Fagus sylvatica*) into the rhizosphere to acquire goethite-associated phosphorus (**Bruno Glaser**, Univ. Halle-Wittenberg) [p.47]

9:45 **P3.2:** Experimental approach to monitor DOC-transport and DOC-transformation processes in a series of undisturbed soil samples under controlled physical settings (**Henrik Redweik**, University Hannover) [p.49]

10:00 **P3.3:** Differences in stable isotope signature reflect source and age gradients of organic matter in sediments in the Port of Hamburg (**Florian Zander**, TU Delft) [p.51]

10:15 **P3.4:** Quantification of litter-derived carbon inputs and outputs in different soil depths via isotopic labelling in a forest (**Patrick Wordell-Dietrich**, TU Dresden) [p.53]

10:45 Coffee break

11:15 Award of the isotope prize

12:15 Lunch break

13:15 Session 4: Soil and Water
(Chair: **Diana Burghardt**, TU Dresden)

13:15 **Keynote:** Spatial micro- and nanoanalysis of $^{13}\text{C}/^{12}\text{C}$ abundance in soil (**Eva Lehndorff**, Universität Bayreuth)

13:45 **P4.1:** Snowmelt and rain as groundwater tracers – from the lab to the field (**Martin Binder**, TU Dresden) [p.59]

14:00 **P4.2:** Stable isotopes methods to identify the source of nitrogen in seepage waters of large lysimeters (**Stefan Werisch**, Lysimeter Station BfUL Brandis) [p.61]

14:15 **P4.3:** The role of different water pools on the recovery of the isotopic signal of spike water by cryogenic water extraction (**Jens Dyckmans**, University Göttingen) [p.63]

14:30 **P4.4:** Assessing moisture sources of precipitation using deuterium excess (**Robert van Geldern**, University Nürnberg) [p.65]

14:45 Poster session with coffee & cake

14:45 **lab tours** (limited number of places, registration necessary)

16:00 **P4.5:** Real-time measurements of water isotopes in soils and plants: Status quo and the dream of integrated soil-plant- atmosphere assessment (**Matthias Beyer**, TU Braunschweig) [p.67]

16:15 **P4.6:** Dual-Element isotope analysis of desphenylchloridazon to investigate its environmental fate in a systematic field study – a long-term lysimeter experiment (**Aileen Melsbach**, TU München) [p.69]

16:30 **P4.7:** Sauna, Sweat and Science (**Michael Zech**, TU Dresden) [p.71]

17:00 ASI meeting of members

19:00 Conference dinner, DORMERO Hotel Dresden City

Wednesday, 10/02/2019

(Building Mensa, Dölfersaal, Mommsenstraße 13)

9:00 Session 5: Sediments and Biogeochemistry

(Chair: **Michael Zech**, TU Dresden)

- 9:00 **P5.1:** Isotope biogeochemistry (H, C, O, S) of interstitial fluids from deep sediments of Western Australia (IODP 369) (**Michael E. Böttcher**, IOW Warnemünde) [p.75]
- 9:15 **P5.2:** Dynamics in the isotope biogeochemistry of a SGD-impacted coastal aquifer after a storm event (**Anna-K. Jenner**, IOW Warnemünde) [p.77]
- 9:30 **P5.3:** Application of Sulphate Isotope Analysis in Hydrogeology (**Frank Haubrich**, G.E.O.S. mbH Freiberg) [p.79]
- 9:45 **P5.4:** Carbonate isotope patterns of a 400m deep sediment core in the Cuvelai-Etisha basin, Northern Namibia (**Feiyu Wang**, TU Darmstadt) [p.81]
- 10:00 **P5.5:** Tracking hydrogenase activity with hydrogen stable isotopes (**Michaela Löffler**, UFZ Leipzig) [p.83]
- 10:15 **P5.6:** Revisiting Lake Garba Guracha in the afro-alpine Bale Mountains, Ethiopia – reconstruction of lake level history using $\delta^2\text{H}$ / $\delta^{18}\text{O}$ biomarker analysis [p.85] (**Lukas Bittner**, TU Dresden)

10:30 Poster session with 2nd breakfast

11:00 Session 6: Plants

(Chair: **Michael Zech**, TU Dresden)

- 11:00 **P6.1:** Isotope analyses on charred cereals to identify former soil conditions, cultivation practices and sociological differences (**Frank Schlütz**, Wilhelmshaven) [p.89]
- 11:15 **P6.2:** Towards a holistic approach to study root water uptake: Combining novel in situ and traditional techniques in a tropical dry forest (**Kathrin Kühnhammer**, TU Braunschweig) [p.91]

- 11:30 **P6.2:** Three wood isotopic reference materials for $\delta^2\text{H}$ and $\delta^{13}\text{C}$ measurements of plant methoxy groups
(**Markus Greule**, University Heidelberg) [p.93]
- 11:45 **P6.3:** Do drying and milling procedures influence the stable isotopic composition in wood samples?
(**Jana Ch. Koehne** et al., Grosshahnsdorf) [p.95]

12:00 Conclusion

Abstracts
Session 1: Atmosphere

About the limitations of the ^{15}N site preference in N_2O for source process attribution

NICOLAS BRÜGGEMANN¹

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Most N trace gas studies usually differentiate between nitrification, nitrifier denitrification, “classical” denitrification and fungal denitrification as source processes of N_2O on the basis of stable isotopic information (bulk $\delta^{15}\text{N}$, ^{15}N site preference, $\delta^{18}\text{O}$), but mostly neglect chemical source processes of N_2O , such as reactions of NO_2^- with reduced metal cations, reactions of NO_2^- with soil organic matter (SOM), the comproportionation reaction between NO_2^- and NH_2OH , and the oxidation of NH_2OH by transition metal ions. However, disentangling microbiological from purely chemical N_2O production is impeded by the fact that the chemically formed N_2O is either isotopically undiscernible from N_2O produced during nitrification, or shows an intermediate ^{15}N site preference between that of N_2O from nitrification/fungal denitrification on the one hand, and nitrifier and classical denitrification on the other hand. Results from experiments with live and sterilized soil samples, with artificial soil mixtures and with phenolic lignin decomposition model compounds demonstrate the potential contribution of these abiotic processes to soil N trace gas emissions, but also the limitation of the information gained from the ^{15}N site preference in the N_2O produced. This suggests that new avenues towards unambiguous N_2O source partitioning are needed due to the limited explanatory power of the stable isotopic information.

The global chloromethane cycle: new insights from triple element stable isotope analysis

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Chloromethane (methyl chloride, CH₃Cl) is the most important natural carrier of reactive chlorine to the stratosphere, contributing about 17% to stratospheric ozone depletion. Due to the phase out of anthropogenic emissions of chlorofluorocarbons, chloromethane emissions will largely control future levels of stratospheric chlorine. There is a huge scientific interest in understanding the global chloromethane budget and thus many publications have appeared and addressed the atmospheric history of chloromethane, its concentration and distribution in the atmosphere, the oceanic and terrestrial fluxes, and the mechanisms of production and degradation in nature. A potentially powerful tool in the investigation of sources and sinks and the budgets of atmospheric chloromethane is the use of stable isotope measurements. Stable isotope analysis, when used in combination with chloromethane flux measurements, has the potential to better constrain the atmospheric chloromethane budget. So far isotopic investigations of chloromethane have predominantly focused on stable carbon isotope measurements and stable hydrogen and chlorine isotope measurements have become available only recently. In this presentation recent advances in our understanding of the origin and fate of chloromethane in the environment/ atmosphere with particular emphasis on the applications of stable isotope techniques/ tools including hydrogen, carbon and chlorine will be discussed. Particular focus will be on recent measurements of stable chlorine isotopes of chloromethane associated with the major abiotic and biotic chloromethane sinks in the environment.

Keywords: Methyl chloride, stable hydrogen, carbon and chlorine isotopes, global budget, sinks, sources

Methane from three widespread marine algal species: release rates, precursor compounds, and relevance for the environment

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Despite Methane (CH₄) being an important greenhouse gas that affects radiation balance and consequently the climate on earth, the global CH₄ budget remains ill characterized. The world's oceans are considered to be a source of CH₄ to the atmosphere but it is unclear which marine organisms produce CH₄ and how much they contribute to total net emissions. In particular, the origin of the frequently observed in situ CH₄ production in the ocean mixed layer is of high interest, because oxic CH₄ production has, traditionally, not been regarded as important. Marine algae might contribute to the observed CH₄ oversaturation in oxic waters, but so far direct evidence for CH₄ production by marine algae has only been provided for the coccolithophore *Emiliana huxleyi*. In the present study we investigated, next to *Emiliana huxleyi*, other widespread haptophytes, i.e. *Phaeocystis globosa* and *Chrysochromulina* sp. Our stable isotope data unambiguously demonstrate that all three investigated species produce CH₄ per se. In

cultures that were treated with ^{13}C -labeled hydrogen carbonate ($\text{NaH}^{13}\text{CO}_3$), $\delta^{13}\text{CH}_4$ values increased with incubation time, clearly resulting from the conversion of ^{13}C -hydrogen carbonate to $^{13}\text{CH}_4$. We furthermore identified the algal metabolites dimethyl sulfide (DMS), dimethyl sulfoxide (DMSO) and methionine sulfoxide (MSO), that are ubiquitous in marine surface layers as potential precursors of CH_4 . Based on the addition of $^{13}\text{C}_2$ -DMSO, $^{13}\text{C}_2$ -DMS and ^{13}C -MSO, where only the sulphur-bonded methyl group(s) ($-\text{S}-\text{CH}_3$) were labelled with ^{13}C , it was possible to clearly monitor the occurrence of ^{13}C -enriched CH_4 in cultures of *Emiliana huxleyi*. We propose that CH_4 production could be a common process among marine haptophytes. The metabolic conversion of DMSO, DMS and MSO to CH_4 is different from both the CH_4 formation of "traditional" archaeal methanogenesis, and the methyl phosphonate pathway some bacteria employ in oxic seawater.

The carbon stable isotope signature of methane produced by two saprotrophic fungi

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Methane (CH₄) is the second most important anthropogenic greenhouse gas and plays an important role in atmospheric chemistry. Recent studies have shown that CH₄ production under aerobic conditions occurs in many different organisms and environments including plants, animals, algae and saprotrophic fungi. Saprotrophic fungi play an important role in nutrient recycling in terrestrial ecosystems by their ability to decompose plant litter. Even though the CH₄ production by saprotrophic fungi has been shown, so far, no data for carbon isotope signatures ($\delta^{13}\text{CH}_4$) of the formed CH₄ are available. In this presentation we show the $\delta^{13}\text{CH}_4$ source values of CH₄ emitted by the two saprotrophic fungi *Pleurotus sapidus* and *Laetiporus sulphureus* cultivated on three different substrates (pine wood, grass and corn). The substrates were chosen for their difference in structural components and their distinction in $\delta^{13}\text{C}$ values of their bulk material. Pine wood and grass represent C₃-plants whereas corn belongs to C₄-plants. The $\delta^{13}\text{C}$ values of CH₄ produced by fungi cover a wide range ranging from -40‰ to -69‰ depending on the growth substrate and fungal species. While the CH₄ produced on pine wood shows a similar $\delta^{13}\text{C}$ value for *P. sapidus* and *L. sulphureus*, there are differences in the $\delta^{13}\text{CH}_4$ source values among the two fungal species when the fungi were grown

on grass and on corn, respectively. These findings show that the $\delta^{13}\text{C}$ value of CH_4 emitted by fungi is highly dependent on the metabolized substrate and that its $\delta^{13}\text{CH}_4$ source value can significantly differ from classical biological CH_4 production by methanogenic archaea.

Abstracts
Session 2: Methods

Ten Years of Elementar and IsoPrime: Pioneers in simultaneous CNS isotope ratio analysis

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In 2008 Elementar and IsoPrime (now Elementar UK) joined forces and consolidated their expertise in elemental analyser inlets and stable isotope analysis of organic elements. This unique partnership led to unprecedented technological advances such as the first simultaneous analysis of carbon, nitrogen and sulphur isotope ratios. Here, we briefly review the working principle of Elementar's CNS isotope analysis setup and present key papers using this method. Samples enter the elemental analyser (EA) inlet via an autosampler and a He-purged ball valve, which guarantees blank-free sample introduction. Subsequently, organic sample components are quantitatively converted to a homogenous gas mixture of CO₂, N₂, and SO₂ within a high temperature furnace. CO₂ and SO₂ gases are retained by adsorption columns, while N₂ passes through. Trapped gases can be released individually and in a pulse-like fashion by heating up the respective adsorption column. This technology guarantees complete baseline separation of C, N and S peaks even for extreme elemental ratios without isotopic fractionation and is capable of handling high elemental concentrations (up to 20mg C). Furthermore, it allows for pulse-like injection of each individual sample gas into the isotope ratio mass spectrometer (IRMS), which results in narrower and taller peaks compared to isothermal GC-based systems. Accordingly, we observe an excellent signal to noise ratio and exceptional

instrument sensitivities. For the analysis of substances with a very low S or N content, the sample weight can be increased easily. When the sample weight is increased, the major carbon isotope will reach very high concentrations. To avoid amplifier saturation, our instruments feature a 100V amplifier and a fully automated sample gas dilution system. This EA-IRMS system has been used to determine $\delta^{13}\text{C}$, $\delta^{15}\text{N}$, and $\delta^{34}\text{S}$ values of bone collagen [1], which can assist in the dietary reconstruction of prehistoric man. In this field of research, it is essential that as much information as possible is derived from extremely limited sample amounts. Similarly, ecologists have analysed CNS isotope signatures in single tissue samples via this EA-IRMS system in order to improve their understanding of marine dietary inputs [2].

[1] Elementar Analysensysteme GmbH, 2017, Technical Note

[2] Higgs et al., 2016, Current Biology 26, 3393–3398

Optimizing EA-IRMS: Getting more for less by ultra-high sensitivity

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The Thermo Scientific™ EA IsoLink™ IRMS System has revolutionized EA-IRMS by introducing temperature ramped gas chromatography with a single GC column and a helium management system that reduces cost per analysis. These innovative features open doors to push research boundaries at new levels, especially for the analysis of nitrogen, carbon and sulphur concentrations less than 5µg and on very high C/N and C/S ratio samples (Figure 1), whilst delivering automated routine analysis. In the presentation complete baseline separation is shown with sound background correction and sharp peak shapes for very large (7000µg C) and very small (11µg N and 0.8µg S) analyte amounts. For 5 replicate measurements on wood, $\delta^{13}\text{C} = -24.10 \pm 0.06\text{‰}$; $\delta^{15}\text{N} = 3.20 \pm 0.23\text{‰}$ and $\delta^{34}\text{S} = 5.92 \pm 0.26\text{‰}$. This presentation will focus on the analysis of small concentrations of carbon, nitrogen and sulphur and illustrate with data, how the EA-IRMS utilizes chromatographic principles to routinely increase the sensitivity on NCS measurements and reduce cost per analysis. An example of the gains in sulphur sensitivity will demonstrate measurements on 1mg of bone collagen, where data precision is significantly better than 0.3‰.

Keywords: EA IsoLink; EA-IRMS; sensitivity; wood; collagen

How climate change can help fighting fraudulent declaration of cereal grains

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According to a report by the German Meteorological Service, the year 2018 was one of the driest and warmest since weather records began in 1881. As a result, farmers had to cope with heavy losses in both crop yield and crop quality throughout the country. Such extreme weather events lead to drastic market fluctuations, as they create shortages in high-quality grain supply while simultaneously producing an excess of lower quality grains. To maintain quality parameters like protein content and bulk density, traders are often forced to mix batches from several harvest years, which must be declared. At the same time, more and more customers insist on buying cereal grains from a single harvest year and pay less for mixed batches. Combined with the competitiveness of the market, the risk of mislabelling increases, especially since no method for determination of harvest year is established yet. Isotope-ratio mass spectrometry (IRMS) could be a suitable approach as plant-based products reflect characteristics of their environment and physiology through the stable isotope ratios of the light elements (¹³C/¹²C, ¹⁵N/¹⁴N, ¹⁸O/¹⁶O, ²H/¹H), hence also inter-annual changes in e.g. temperature, amount of precipitation and air humidity (Liu et al., 2015). IRMS is already a well-established approach in wine authenticity testing, in which it helps verifying the vintage year stated on the label (Dinca et al., 2016). To test the feasibility of this method for commercial crops from

Germany, we analysed 406 cereal grain samples (barley: 219, spelt: 187) from the harvest years 2016-2018 for their carbon, nitrogen and oxygen stable isotope data as well as their element concentrations. In addition, we applied near-infrared spectroscopy (NIRS), a technique with various advantages like affordability, rapid measurements, little to no sample preparation and potential to be used online. Special attention was paid during sample selection and data evaluation in order to consider and minimize the variability introduced by factors such as genotype or region. Isolated methods showed clear trends for discrimination between harvest years, especially for the year 2018. Separation of the groups was significantly improved when using combined data sets and multivariate statistical approaches with high correct classification rates. Carbon and oxygen natural isotope abundance were the most important variables included into the model. We are convinced that due to the increased frequency of extreme weather events, this multi-method approach turns out in the future as a valuable and urgently required tool in fighting fraudulent declaration of cereal harvest year.

Keywords: cereal grains, authentication, harvest year, climate change, NIR, IRMS, chemometrics

Further development of the denitrification method for stable isotopic analysis of nitrogen and oxygen in nitrate of natural water samples

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Due to the growing issue of nitrates in water bodies, the examination of input sources as well as the quantification of nitrate reduction are gaining in importance. Therefore, isotope analysis are helpful tools. A widespread procedure for preparing aqueous samples for subsequent isotope analysis is the denitrifier method, in which nitrate is converted completely into measurable N_2O with the help of *Pseudomonas aureofaciens* bacteria. The aim of the study at hand is the evaluation of the classical denitrifier method, which is based on the study of Sigman et al. (2001), as well as a simplified approach following Zhu et al. (2018) to the application of the method to natural water samples. Various influence factors were tested. In the classical approach an incomplete conversion of the sample nitrate and a high share of extraneous nitrate were detected, which originates from an insufficient induction of the denitrification in the cultivation of the bacteria. This led to defective results. Thus, this procedure has to be discarded for further application. In comparison, it was possible to induce denitrification and convert the sample nitrate free of fractionation using the simplified method. There was no contamination with non-sample nitrate. With the help of the influence factors examined, the simplified method was further optimized. With their high accuracy, the results found testify to the suitability of the procedure. Standard deviations were generally $<0,7\text{‰}$ ($\delta^{18}O$) and $<0,3\text{‰}$ ($\delta^{15}N$). Furthermore, the usability of the method for future research could be proven by means of plausible measurements of the isotopic composition of nitrate from natural water samples.

Keywords: nitrate, $\delta^{18}\text{O}$ and $\delta^{15}\text{N}$, denitrifier method, *pseudomonas aureofaciens*

N-isotopic composition of nitrate and ammonium from aqueous solutions by isotope ratio mass spectrometry (SPIN-MIRMS)

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Analyses of N-isotopic composition of nitrate and ammonium from aqueous solutions are difficult - especially at natural abundance levels. Here we present the SPIN-MIRMS technique that transfers the SPIN-MIMS technique published by Eschenbach et al. (2017) to isotope ratio mass spectrometry. Key advantage of this transfer is the ability to measure isotope composition at natural abundance levels. Performance and caveats of the method will be shown.

Keywords: method developement nitrate ammonium aqueous solution

Atypical $\delta^{13}\text{C}$ values of urinary norandrosterone in doping control analysis

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In routine doping control analysis IRMS has been established to identify an exogenous origin of 19-norandrosterone (NorA) in urine samples. Analysis of the carbon isotope ratio is necessary, as low amounts of urinary NorA might be of endogenous origin. Traces of NorA can be naturally found in human urine samples, with higher concentrations during pregnancy. Additionally, NorA can be formed in urine by in-situ microbial degradation of androsterone. Since 2003 the Cologne laboratory analysed approximately 200 doping control samples with NorA concentrations below 15ng/ml by IRMS. Negative samples show similar $\delta^{13}\text{C}$ values for NorA and the corresponding endogenous reference compounds, whereas NorA originating from pharmaceutical preparations usually show ^{13}C depleted values. However, in 2016 a routine doping control sample did not fit into the usual pattern as it revealed an atypical ^{13}C enriched value for urinary NorA, compared to the corresponding endogenous reference compounds of the athlete. It has been mentioned in literature, that beside endogenous production, traces of urinary NorA may originate from the consumption of offal of intact, non-castrated pigs. In order to check if this could be a potential cause for atypical or even adverse analytical findings in doping control analysis, different excretion studies were conducted. After meals of wild boar offal or meat some volunteers showed urinary NorA with $\delta^{13}\text{C}$ values, which did not correspond to the consumer's endogenous isotopic signature. Further analysis of boar's tissue revealed a high fluctuation of the animal's $\delta^{13}\text{C}$ values over the year. Thus, the consumption of wild boar offal in the hours preceding a doping

control test may result in an atypical or even positive test result, and both athletes as well as anti-doping laboratories and authorities should be aware of this aspect.

Abstracts
Session 3: Soil and Carbon

Compound specific stable isotope analyses and mixing models for sediment source apportionment

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The carbon-13 signal of plant-derived fatty acids is a powerful, complementary tool for soil erosion assessment studies. The ¹³C signal in fatty acids (¹³C-FA) can be used as biomarker to apportion soil sources contributing to sediments in rivers and lakes. Hence, upon determining the ¹³C-FA signal of potential sources and likewise its spatiotemporal signal in sediments in a specific catchment, the proportional distribution of soil sources contributing to the sediment load can be determined with the help of state-of-the-art Bayesian mixing models. In recent years we have improved the method by highlighting and solving a few longstanding caveats. In this presentation we show four crucial conditions (among others) that need to be met to correctly apply ¹³C-FA-based isotopic mixing models for sediment apportionment in eroding catchments: 1) correct choice of fatty acids, 2) use of FA-content-depend mixing models, 3) a deconvolutional modeling approach, and 4) application of a sediment connectivity index as prior information. This will be conceptually explained and demonstrated using data from our study area in Nepal, the Kulekhani catchment.

Carbon investment of beech (*Fagus sylvatica*) into the rhizosphere to acquire goethite-associated phosphorus

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Phosphorus (P) nutrition of European beech (*Fagus sylvatica* L.) forests is deteriorating, indicated by declining leaf P contents. It is known that beech mainly accesses nutrients from the P-rich forest floor, but the majority of P stocks are located in the subsoil associated with goethite and other oxyhydroxides. Therefore, the aim of this work was to study the uptake of inorganic and organic phosphorus from subsoil by beech trees with respect to availability and uptake mechanisms. For this purpose, a mesocosm experiment with beech saplings grown on P-limited subsoil was designed. Phosphorus accumulation was determined by P mass balances. It was further assumed that beech can mobilize P bound to goethite, by means of carbon (C) allocation to the rhizosphere, which was investigated by tracing a stable isotope of carbon (¹³C) after a pulse labelling. Beech saplings were unable to mobilize sufficient quantities of P resulting in low uptake ratios and symptoms of P deficiency. P accumulation was unaffected by goethite. Inorganic P supply significantly increased C allocation into roots accompanied by slight increases in P accumulation. Root growth and internal P redistribution from stem to leaves were identified as a unanimous mechanisms adopted by beech saplings under P deficiency.

Keywords: Soil Rhizosphere ¹³C labelling PLFA

Experimental approach to monitor DOC-transport and DOC-transformation processes in a series of undisturbed soil samples under controlled physical settings

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Subsoils are considered to be an important C sink regarding their storage capacity of more than 50% of the global soil organic carbon (SOC). However, the specific processes regulating C sequestration in forest subsoils like C-transformation, -sorption and -exchange with organic components already sorbed at solid surfaces remain still unclear when realistic environmental conditions are considered. A new experimental laboratory design is introduced to analyze and quantify carbon turnover processes in top and subsoils. A column experiment setup with undisturbed soil samples embedded into two gas sealed chambers allows on time evaluation of soil respiration and carbon turnover processes in simulated realistic conditions (water flux rate, moisture content, temperature, DOC concentration). This experimental setup carries the newly developed flow cell (FC) concept by Krueger and Bachmann (2017) into a fully controlled atmospheric mesocosm, allowing mutually the analysis of C enrichment in the gaseous phase or in the effluent during percolation with dissolved organic carbon (DOC), as well as the analysis of surface properties and processes on the 2-D undisturbed soil sample. Correspondingly, ¹³C-labelled DOC is used to locate C enrichment in the solid, liquid, and gaseous phase by mass spectrometry. In two different experimental arrangements we combine topsoil and subsoil FC in a serial flow and a parallel flow setup: In the serial flow setup ¹³C labelled DOC percolates both FC respectively their layer of excavation, simulating DOC flow through a soil profile. In the parallel flow

setup ^{13}C labelled DOC percolates the FC individually, allowing us to evaluate sorption and transport rates for different soil profile depths. This supports us to control and monitor C mass balance in the system. Furthermore, the undisturbed FC permits the analysis of preferential flow paths and their effect on C sequestration and transport in combination with CT- scans and hyperspectral imaging as well as the location of microbial hotspots and their contribution to C respiration by enzyme mapping. (Krueger & Bachmann, 2017) Krueger, J., & Bachmann, J. (2017). New Field Sampling Method to Analyze Spatial Distribution of Small-Scale Soil Particle Surface Properties and Processes in Intact Soil. *Vadose Zone Journal*, 16(11), 0. <https://doi.org/10.2136/vzj2017.06.0116>

Keywords: Carbon, mass-balance, subsoil, small-scale heterogeneity

Differences in stable isotope signature reflect source and age gradients of organic matter in sediments in the Port of Hamburg

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The project BIOMUD (www.mudnet.eu) investigates the decomposition of sediment organic matter (SOM) in the Port of Hamburg. It is hypothesized that SOM physicochemical properties and degradability follow a toposequence along the investigated spatial stretch of about 30 river kilometres and a chronosequence within the sediment depth profile at any one location. Sediment is currently sampled every four to eight weeks at nine hotspots of sedimentation within the Port of Hamburg using a 1m sediment corer operated from aboard a port survey vessel. Subsequent analyses comprise (1) Aerobic and anaerobic decomposition of SOM (2) Density fractionation, including analysis of TOC, TN, $\delta^{13}\text{C}$ in fractions and bulk material (3) Chemical dissolved organic carbon fractions (4) Microbial biomass and community composition, concentration of DNA, extrapolymeric substances and lipids (5) Standard analytical solids and pore water physical and chemical parameters. A clear gradient of increased upstream organic matter degradability and decreased degradability at downstream locations was found. The share of SOM in the easily accessible light density fraction (not bound in organo-mineral complexes) was higher upstream, whereas further downstream, the heavy fraction dominated. These gradients were accompanied by a shift in $\delta^{13}\text{C}$ signature with less negative values (^{13}C enrichment) downstream and more negative values upstream. The $\delta^{13}\text{C}$ gradient (range of 2 ‰ VPDB) is assumed to signify different SOM sources with upstream locations receiving suspended and sediment-bound organic matter from the Elbe catchment while downstream

organic matter enters the system from the North Sea and the tidal marshes as a result of tidal pumping. The hypothesized age gradient at individual locations was supported by decreased lability and therefore increased stabilization of SOM with depth. This gradient was also reflected by an enrichment in ^{13}C in deeper layers at some, but not all locations. Differences in $\delta^{13}\text{C}$ values ranged between 0.05 to 0.5‰ and were therefore significantly smaller than observed for the spatial gradient. $\delta^{13}\text{C}$ signature was expected to increase with depth due to preferred consumption of ^{12}C . The depth and hence age-related enrichment in ^{13}C was less probably detectable due to the highly dynamic hydro-morphological conditions (variable flow rate, tide, dredging), leading to variability in input SOM, thereby confounding depth gradients that would be visible if they reflected an age gradient of exactly the same original material.

Quantification of litter-derived carbon inputs and outputs in different soil depths via isotopic labelling in a forest

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Soils contain the largest carbon pool of the global terrestrial carbon (C) cycle and can act as a source or sink for CO₂. More than 50% of the carbon stocks are stored in subsoils below 30cm. The low C content and high mean residence time of C in subsoils indicate that that subsoils may have the potential to sequester additional C on the long-term and counteract increasing anthropogenic CO₂ emissions. In order to assess the potential of subsoils to store additional C, there is an urgent need to determine C inputs and outputs in different soil depths in dependence on soil and environmental conditions. This will also increase the knowledge of factors controlling C turnover and stabilisation processes in whole soil. The use of stable isotopes in soil science is a widespread method to distinguish between C sources and follow different C pathways in the soil. In a field labelling experiment in a beech forest in NW Germany, the natural leaf litter was replaced by a ¹³C enriched (1880‰) leaf litter at an area of 6.5m² with three field replicates. To quantify the amounts of litter-derived C inputs

and outputs in the whole soil we monitored and sampled CO₂ in the soil atmosphere and seepage water in different soil depths (up to 150cm) over a period of two years. We also measured soil respiration at the surface to determine C losses to the atmosphere. Two years after labelling soil cores were taken to determine the amount of retained labelled ¹³C in different soil depths, i.e. the portion of fresh litter-derived C in the soil. The contribution of litter-derived C in all samples was determined by isotope ratio mass spectrometry. Over two year around 35% of the initial leaf litter was mineralised at the surface. Isotopic data showed that in average only 1.2% of litter-derived C was retained in the mineral soil. Whereby, most of the label was found in the first 20cm of the soil profile. Further the amount of litter-derived C in seepage water decreased strongly with soil depth. This indicates that fresh C input from litter via seepage water accounts only for a small proportion of total C inputs into subsoil horizons over a short time scale of two years.

Abstracts
Session 4: Soil and Water

Sulfur Isotopes – Applications in Earth Sciences

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Stable sulfur isotopes applied towards research objectives in earth sciences date back to the late 1940s/early 1950s. Already early on, a substantial variability of samples were analyzed, ranging from igneous to sedimentary rocks and from ancient to modern as well as including extraterrestrial materials. Key objectives in sulfur isotope studies have always been source and/or process identification, both inorganic as well as microbially mediated, with wider implications for characterizing Earth System evolution. Aside from basic research, sulfur isotopes have successfully been utilized in environmental geochemistry, tracing the anthropogenic impact on terrestrial and aquatic environments.

This presentation will illustrate a broad portfolio of sulfur isotope applications in Earth Sciences, both from basic as well as applied research and on a variety of spatial and temporal scales.

**Snowmelt and rain as applied groundwater tracers –
From the lab to the field**

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In hydrogeological science as well as in consulting, tracer tests are routinely used to reveal the transport characteristics of aquifers. Hereby, the value of any tracer test strongly depends on many factors, including the aquifer characteristics and the experimental design. Even more important, most tracer substances are subject to a variety of physical and chemical detrimental impacts eventually leading to a non-conservative transport behavior of the tracer and, therefore, biasing the test outcome. This, in turn, may lead to misinterpretations. In this context, this study assesses the applicability of liquid precipitation, i.e., rain and snowmelt as employable groundwater tracers in order to provide a cost-effective and almost conservatively transported multi-tracer solution, exploiting the naturally occurring ²H and ¹⁸O offsets of these waters relative to typical groundwaters. The investigation included three essential steps and was related to a fluvial groundwater test site located in Pirna-Copitz, Saxony, Germany. First, three natural precipitation waters typical for the region, specifically one snowmelt and two rain waters, were injected into a laboratory-scale sand column and traced via stable isotope analysis. Their migration behavior was compared to that of widely used groundwater tracers, specifically to the saline tracer substances sodium chloride

and potassium bromide as well as to the fluorescent dye uranine. Second, the amount of precipitation water required for a tracer test on real field scale was estimated for three selected injection approaches using a series of 2-D numerical groundwater flow and transport model simulations. Finally, a small field-scale push-pull tracer experiment with approx. 1m³ of snowmelt was successfully conducted at the mentioned field site, monitoring both the ²H and ¹⁸O signals as well as the electrical conductivity. The captured data was then evaluated via a ²H-¹⁸O-plot and by a 3-D numerical flow and transport model. The study showed that collected precipitation waters such as snowmelt and rain are generally suitable as injection waters in artificial tracer tests. However, the preferred areas of application are test scenarios with short travel distances and short overall duration (e.g., a push-pull tracer test).

Keywords: deuterium, oxygen-18, precipitation, laboratory experiment, field experiment

Stable isotope methods to identify the source of nitrogen in seepage waters of large lysimeters

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The lysimeter station Brandis provides observations of water and solute fluxes under agricultural land use since 1981. Besides quantification of the individual fluxes, understanding and evaluation of current agricultural management strategies is one of the primary goals of these long term observations. The main instruments are 3m high, weighable lysimeters containing 8 different soil types, which provide a perfect basis for the quantification of groundwater recharge and the associated nitrogen loading associated with conventional agricultural management. Substantial efforts in regulation and assessment of fertilizer needs have been undertaken since the early nineties, to reduce nitrogen fertilization excess in order to protect groundwater resources from pollution. Despite these efforts and success in reduction of fertilization excess, the seepage water analysis reveals an increasing level of nitrate concentration in groundwater recharge in a broad range of soil types, putting the often assumed direct relationship between fertilization excess and seepage water concentrations into question. The long time observations in Brandis provide various indications that the soil nitrogen pool, and mobilization and immobilization from this pool, might be the major controller of nitrogen fate. Further evidence, that the nitrogen in groundwater originates almost exclusively from the soil organic nitrogen pool, was provided by tracer experiments with ¹⁸O and ¹⁵N on two soils. This contribution employs state of the art $\delta^{15}\text{N}$ methods to all

investigated soils in the lysimeter station Brandis. Analysis of soil and seepage water samples highlight the substantial role of the soil organic nitrogen pool on nitrogen dynamics and recharge concentrations in all relevant soils. Furthermore, the results hold an explanation why the current regulation efforts have not led to the desired results. Thus, the combination of large scale lysimeter investigation and stable isotope methods are excellent tools to gain understanding of the governing processes and nitrogen sources to allow the development of effective reduction strategies.

Keywords: nitrogen, groundwater recharge, lysimeter, soil organic nitrogen

The role of different water pools on the recovery of the isotopic signal of spike water by cryogenic water extraction

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The effects that alter the isotopic composition of water added to soil samples that have been oven-dried previously are not fully understood. To clarify the role of fractionation and (water) exchange for spike recovery, oven-dried clay-rich soil was repeatedly rewetted with two waters of strongly differing isotopic composition. This approach allowed to determine the amount and the isotopic composition of soil-bound water that exchanges with spike water after rewetting. The results show that the isotopic difference between extractable (mobile) water and non-extractable (soil bound) water explains the isotopic effects observed in spike water experiments. This difference however, can also lead to a considerable isotopic offset between extractable and total soil water.

Keywords: cryogenic water extraction, hydrology method validation

Assessing moisture sources of precipitation using deuterium excess

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Air moisture of oceanic origin can be subject to long-range transport and could contribute to precipitation at distant places. With ongoing climate change the relationship between water vapour sources and sinks is under constant evolution and plays an important role for water budget assessments. This study analysed monthly integrated and event-based precipitation samples from two field sites in the Western Pamir Mountains (Tajikistan) for stable isotope compositions of oxygen and hydrogen of water. The aim was to investigate water vapour sources and, in particular, to evaluate contributions of water vapour from the Mediterranean region. The latter has been often postulated as a potential moisture source region for Central Asia. Deuterium excess values (d), that serve as a fingerprint of moisture origin, were below 13 permil in monthly integrated samples, for most of the year. This indicates a smaller contribution of high Mediterranean moisture (about 20 permil) to the Western Pamir Mountains than originally expected. A maximum d value of 19 permil was observed in March, which is not in agreement with the common observation of increased

Mediterranean contribution during winter (DJF). A Lagrangian backward trajectory model (HYSPLIT) was applied to infer the general air mass origin for sampled precipitation events. A maximum contribution of 'western' moisture of 40% was also detected in March, while 40%–60% of moisture that contributed to precipitation events in winter was transported by trajectories that originated from the Northern Indian Ocean.

Keywords: deuterium excess, Mediterranean, moisture sources, Western Pamir, atmospheric vapour transport

Real-time measurements of water isotopes in soils and plants: Status quo and the dream of integrated soil-plant-atmosphere assessments

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The number of ecohydrological studies employing water stable isotopes is increasing constantly due to technological and methodological advances. These further enable researchers from a broad scientific background to incorporate water-isotope based methods into their research. Contemporaneously, an ongoing debate on the analysis and interpretation of water isotopes from plant and soil samples was initiated. Several isotope effects are currently not fully understood, but essential for many investigations at the soil-vegetation-atmosphere interfaces (e.g. the determination of root water uptake depths). Controversy exists on i) extraction methods for soil and plant water and methodological artifacts potentially introduced by them; ii) the pools of water measured with those methods and iii) spatiotemporal issues of water stable isotope research in ecohydrology. Real-time (or: on-line, in situ) methods have been proposed as an innovative and necessary way to approach the abovementioned issues. They are required to disentangle isotope effects and take them into account when studying soil-plant-atmosphere interaction with water stable isotopes. Herein, we review the current status of in situ developments for measuring water stable isotopes in soils and plants (transpiration & xylem), point out current issues and highlight potential as well as needs for future research. Intensified efforts on field-deployable methods are urgently required. We further find that, based on recent advances, the widely used assumption that the isotopic composition of tree xylem represents an

unaltered mixture of all potential water sources does not necessarily hold true under all conditions. It is crucial to incorporate all relevant isotope effects into source water studies. Consequently, we propose and demonstrate an integrated methodology for measuring both soil and plant water isotopes in situ when carrying out studies at the soil-vegetation-atmosphere interface.

Keywords: water isotopes, in situ, ecohydrology, source water

Dual-Element Isotope Analysis of Desphenylchloridazon to Investigate its Environmental Fate in a Systematic Field Study - A Long-Term Lysimeter Experiment

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Desphenylchloridazon (DPC), the main metabolite of the herbicide chloridazon (CLZ), is more water soluble and persistent than CLZ and is frequently detected in water bodies at concentrations exceeding 10 µg/L. When assessing DPC transformation in the environment, results can be non-conclusive if based on concentration analysis alone, because estimates may be confounded by simultaneous DPC formation from CLZ. This study investigated the fate of DPC by combining concentration-based methods with complementary compound-specific stable isotope analysis (CSIA) of ¹³C/¹²C and ¹⁵N/¹⁴N. In addition, DPC formation and transformation processes were experimentally deconvolved in a dedicated lysimeter study considering three scenarios. First, direct surface application of DPC enabled to study its degradation separately, in the absence of CLZ. Here, CSIA provided evidence of two distinct DPC transformation processes, one resulting in significant changes only in ¹³C/¹²C, and another one involving changes in both ¹³C/¹²C and ¹⁵N/¹⁴N ratios. Second, surface application of CLZ mimicked a realistic field scenario and showed that during DPC formation,

carbon isotope ratios of DPC were depleted in ^{13}C relative to CLZ, while nitrogen isotope ratios remained constant. Finally, CLZ injection at 40cm depth simulated preferential flow and demonstrated the importance of the topsoil to retain DPC. Hence, by the combination of a dedicated lysimeter study with CSIA as a new, complementary method, we obtained insight that was superior to classical concentration studies enabling a better evaluation of DPC transformation in the field.

Keywords: CSIA, DPC, GC-IRMS, LC-IRMS, Lysimeter

Sauna, Sweat and Science

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Inspired by a previous 'Sauna, Sweat and Science' study (Zech et al., 2015, *Isotopes in Environmental and Health Studies* 51(3), 439-447) and for curiosity and enthusiasm for stable isotope and sauna research we aimed at answering the question 'do we sweat (isotopically) what we drink'? We therefore pulse-labelled 5 test persons in a sauna experiment with beverages that were ²H-enriched at about +25,600‰. Sweat samples were collected during 6 sauna rounds and the hydrogen isotopic composition $\delta^2\text{H}_{\text{sweat}}$ was determined using an isotope ratio mass spectrometer. Before pulse labelling, $\delta^2\text{H}_{\text{sweat}}$ – reflecting by approximation body water – ranged from -32 to -22‰. This is ~35‰ enriched compared to usual mid-European drinking water and can be explained with hydrogen-bearing food as well as with respiratory loss of ²H-depleted vapour. The absence of a clearly detectable ²H pulse in sweat after pulse labelling and $\delta^2\text{H}_{\text{sweat}}$ results of $\leq +250$ ‰ due to a fast ²H equilibration with body water are moreover a clearly negative answer to our research question also in a short-term consideration. Given that the recovery of the tracer based on an isotope mass balance calculation is clearly below 100%, we finally answer the question 'where did the rest of the tracer go?'

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Zech M, Benesch M, Hepp J, Polifka S, Glaser B. resubmitted. Sauna, Sweat and Science II - Do we sweat what we drink? *Isotopes in Environmental and Health Studies*, resubmitted.

Keywords: Sauna; tracer; isotope pulse labelling; deuterium; body water; perspiration; sweat; urine; isotope mass balance

Abstracts
Session 5: Sediments and Biogeochemistry

P 5.1 in Session 5/ Sediments and Biogeochemistry:

Isotope biogeochemistry (H, C, O, S) of interstitial fluids from deep sediments off Western Australia (IODP Leg 369)

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Interstitial waters extracted from long sediment cores retrieved during expedition 369 (Sites U1513-U1516) of the International Ocean Drilling Program (IODP) were analysed for the stable water isotopic (H and O isotopes) composition to constrain hydrographic changes in this region prior to modern time and possible changes due to water-rock interaction. Dissolved inorganic carbon (C isotopes), sulfate (S and O isotopes), and sulfide (S isotopes) were analyzed to characterize, in concert with concentration measurements, diagenetic microbial processes in the benthic coupled carbon-sulfur cycles. The measurements demonstrate substantial downcore variations in both water isotope ratios covering overall dynamics of more than 4‰ ($\delta^{18}\text{O}$) and 10‰ ($\delta^2\text{H}$). The C isotope composition between -14.8 and +4.8‰ indicates both, mineralization of organic matter and water carbonate rock interactions. Net microbial sulfate reduction with depth was observed at all sites, but sulfate was not found to be consumed completely, within the investigated core lengths. Whereas associated sulfur isotope fractionation is characteristic for medium range fractionation factors, the oxygen isotope composition provides evidence for a much more complex story of sulfur diagenesis at the investigated sites: At Site U1516, the oxygen isotope composition of dissolved

sulfate is equilibrated with pore water, although sulfate concentrations remain above 20mM. This indicates an intense re-oxidative sulfur cycle. At Site U1513, on the other hand, the oxygen isotope composition remains out of isotope exchange equilibrium although sulfate concentrations fall below 20mM.

Keywords: Stable isotopes, water, sulfate, dissolved inorganic carbon, deep marine biosphere, IODP, Western Australia

Dynamics in the isotope biogeochemistry of a SGD-impacted coastal aquifer after a storm event

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The interface of land and sea is of particular interest regarding the exchange of elements, like nutrients, carbon and sulfur. Submarine groundwater discharge (SGD) is an important pathway for element exchange from the terrestrial to the marine environment and vice versa. The discharging water can not only consist of fresh ground water but also of a considerable proportion of recirculated often brackish seawater. Here, we followed the water and element exchange and associated biogeochemical transformation processes in front of a rewetted peatland at the southern Baltic Sea. Vertical pore water profiles were retrieved via up to 5m long multi-port pore water samplers on a seasonal base. An extraordinary storm event in early 2019 not only led to the partial flooding of an associated coastal peatland with brackish water but also pushed Baltic Sea water into the coastal aquifers allowing to investigate the time-dependent return to previous subterrestrial 'normal' conditions via SGD-induced freshening. Weekly sampling was carried out to follow the changes after the storm event in the sediments in front of a coastal peatland. Here we present new results of the pre- and after storm event pore water profiles. A focus was set on the investigation of tracers for concentration gradients of major and redox-sensitive trace elements, nutrients and the stable isotope composition (H, C, S, O) of water, dissolved inorganic carbon (DIC) and sulfate to understand the mixing processes and superimposing biogeochemical transformation

reactions. We found evidence for a strong control of the bottom-pore water exchange by lithology and a high activity of dissimilatory sulfate-reducing microorganisms in the coastal sediments leading to the accumulation of substantial DIC superimposed by corrosion of sedimentary carbonates.

Acknowledgement: This study is supported by the DFG research training group Baltic TRANSCOAST and the Leibniz IOW.

Application of Sulphate Isotope Analysis in Hydrogeology

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In hydrogeology sulphate concentrations are often used in addition to other ionic concentrations to compare water bodies. If the sulphate concentration in receiving water changes or exceeds legal thresholds, usually nothing can be said about the possible (additional) sources of sulfur. The ^{34}S - ^{18}O signatures in the sulfate represent a fingerprint which allows determination of these sulphate sources. By having an appropriate database available, sulfur sources can be identified and environmental changes detected (for example, effects of redox changes). However, this requires a solid database. Basic data on the $^{34}\text{S}/^{18}\text{O}$ signatures was obtained by using sulfates and sulfides. As a result, atmospheric precipitation, unaffected receiving waters in the catchment area of the rivers Flöha, Zschopau and Zwickauer Mulde and the main sulphide ores of the Ore Mountains were determined as background values in the area of the Ore Mountains. Finally, follow-up applications for the provenance analysis of mining waters, thermal waters and landfill water are shown and examples of the origin of salt efflorescence in Saxon Switzerland and in residential buildings in Freiberg are presented.

Keywords: Stable Isotope, ^{34}S , ^{18}O , sulfate, sulfide, groundwater, receiving water

Carbonate isotope patterns of a 400m deep sediment core in the Cuvelai-Etосha basin, Northern Namibia

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From the late Cretaceous throughout the Tertiary, the Cuvelai-Etосha basin in Northern Namibia has been an area for sediment accumulation (Miller 1997). A core drilling (well WW203302) with a length of 400m reaches through the entire Andoni formation and into the Olukonda formation of the upper Kalahari sequence. The sediments were deposited into the basin by local rivers and lakes of shallow, standing water, which were regularly drying up (Miller 2016). During cycles of a humid and arid shifting climate, both conditions promote carbonate precipitation. Oxygen isotope composition is mainly dominated by meteoric water which $\delta^{18}\text{O}$ values correlates with mean temperature conditions and influences the $\delta^{18}\text{O}$ value of carbonate precipitates near the surface (Dworkin 2005). On the other side, $\delta^{13}\text{C}$ of carbonate reflects the stable carbon isotope composition of CO_2 (Cerling 1993). Because carbonate appears nearly over the entire core, this work investigates carbonate isotopes as a climate proxy to estimate trends regarding to temperature and vegetation transition in North Namibia. Samples were collected every meter from the sediment core, sieved, milled, and analyzed as bulk carbonate. Despite core loss or carbonate free sections, 296 samples in total were measured in triplicates for stable isotope values using a Thermo Scientific Delta V Advantage IRMS connected with a Gas Bench II. $\delta^{18}\text{O}$ values show a decreasing trend from past to present with increasing fluctuation. $\delta^{13}\text{C}$ values

basically decrease until the depth of around 75m, after slightly increasing to -3.5‰ and decreasing to the previous level, a sudden rise is observed at the depth of around 30m. $\delta^{18}\text{O}$ and $\delta^{13}\text{C}$ curves are linked to paleoclimate events according to lead/uranium age dating results from the same core. An age of about 60Ma was assigned at the depth of 400m, which possibly relates to the Late Paleocene. A sudden rise of $\delta^{13}\text{C}$ values may reflect a transition from C_3 plant to C_4 plants. Although trends of $\delta^{18}\text{O}$ values correspond to that of global temperature, and an increase of $\delta^{13}\text{C}$ values may reflect C_3/C_4 transition, components of bulk carbonate still need to be distinguished based on the lithology log while pedogenic carbonate is desired as a proxy for paleoclimate interpretation.

Tracking hydrogenase activity with hydrogen stable isotopes

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A hydrogen-based renewable power system requires storage of hydrogen (H₂) in underground reservoirs. The potential oxidation of H₂ in such reservoirs by lithoautotrophic microorganisms is an important but less studied aspect. Our long-term goal is to develop a stable isotope tool based on changes in the $\delta^2\text{H}$ signature of H₂ during oxidation by hydrogenases to detect and monitor potential biological losses during underground storage. Most microorganisms are equipped with at least one hydrogenase. Hydrogenases are a diverse class of enzymes catalyzing the reversible cleavage of molecular H₂ into two electrons and two protons. During H₂-consumption, a subsequent superimposing isotope exchange with water takes place quasi-simultaneously, resulting in an inverse isotope effect. We questioned whether the exchange reaction can occur independently from the H₂ cleavage reaction. For this, H₂ oxidation of cell suspensions of the sulphate-reducing model organism *Desulfovibrio vulgaris* Miyazaki was inhibited by the addition of sodium molybdate, circumventing electron flow to the final electron acceptor sulphate. Although H₂ was not consumed, $\delta^2\text{H}$ values changed to isotope equilibrium with water, demonstrating that the exchange reaction still proceeds in the absence of the H₂ cleavage reaction. Our study shows that the isotope exchange is directly linked to the enzyme's activity and can be tracked with a GC-IRMS setup with a precision of $\delta^2\text{H} = 0.7 \pm 0.4\text{‰}$

Revisiting Lake Garba Guracha in the afro-alpine Bale Mountains, Ethiopia – reconstruction of lake level history using $\delta^2\text{H}/\delta^{18}\text{O}$ biomarker analyses

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Our knowledge about East African paleoclimate history is largely based on marine and paleolimnological records. Accordingly, more humid climatic conditions such as the African Humid Period (AHP) are usually associated with summer insolation-driven increased monsoonal precipitation. In order to contribute to the paleoclimate reconstruction of the afro-alpine Bale Mountains, Ethiopia, within the DFG Research Unit 2358 'The Mountain Exile Hypothesis: How humans benefited from and re-shaped African high-altitude ecosystems during Quaternary climate changes' we revisited Lake Garba Guracha. The latter contains sediments representing a continuous, high altitude (3950m asl) Late Glacial – Holocene archive (Tiercelin et al., 2008; Umer et al., 2007). Results from organic geochemical and XRF analyses document that minerogenic input dominated during the Late Glacial and organic matter input increased considerably only from 11 cal. ka BP on. We investigated sugar and lipid biomarkers as well as their compound-specific stable oxygen and hydrogen isotopic composition ($\delta^{18}\text{O}_{\text{sugar}}$ and $\delta^2\text{H}_{\text{n-alkane}}$) to infer past hydrological patterns. The

coupling of $\delta^2\text{H}_{\text{alkane}}$ with $\delta^{18}\text{O}_{\text{sugar}}$ allows establishing a deuterium excess record (Hepp et al., 2019; Zech et al., 2013) that can be interpreted in terms of lake water evaporation. We thus evidence virtually permanent lake overflow occurred from about 10 to 8 cal. ka BP and during the Little Ice Age, whereas the period from about 8 to 5 cal. yr BP experienced strongest at least seasonal lake evaporation. A newly established fire record from the Garba Gura-cha lake supports our isotope climate reconstruction. Accordingly, lake level lowstands coincide with charcoal maxima. Additionally, we present new sedimentary data and mean annual temperature brGDGTs results indicating a Younger Dryas cold event in East African high altitude ecosystem.

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Abstracts
Session 6: Plants

Isotope analyses on charred cereals to identify former soil conditions, cultivation practices and sociological differences

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Isotopes in plants can reflect to a certain degree the soil conditions in their growing area. When plants get charred this information is archived in the remains. In Archaeobotany, stable isotopes therefore can be used to reconstruct growing conditions and cultivation practices like water availability ($\delta^{13}\text{C}$) and nutrient supply ($\delta^{15}\text{N}$) in the past. For that, charred remains of cultivated plants are cleaned from adhesions and their isotope signature is measured. We analysed a set of over 1000 charred kernels of the two early domesticated wheats Emmer (*Triticum dicoccum*) and Einkorn (*Triticum monococcum*) found during the excavation of the early Bronze Age settlement Fidvár near Vráble (ca. 2000 – 1600 BC) in the Danubian Hills of SW Slovakia. By that, it was possible to identify social differences between households (based on soil quality of fields) in the settlement as well as changes over time. The data suggest that the overall less common cultivated Einkorn seems to reach higher portions in the harvest under wetter conditions. Probably Einkorn was intentionally cultivated on wetter sites and/or as an admixture in Emmer fields to secure yields in years of higher precipitation. It seems questionable to which degree the relative high $\delta^{14}\text{N}$ values indicate manuring or reflect the naturally high fertility of the loess soils in the area.

Towards a holistic approach to study root water uptake: Combining novel in situ and traditional techniques in a tropical dry forest

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On land surfaces, plant transpiration is the largest flux returning water to the atmosphere and therefore plays a critical role in the water cycle. Through their roots, trees can access deep soil water or groundwater and hereby maintain their water supply during dry periods. However, the amount of transpired water is poorly quantified in hydrology and the contribution of different water sources, e.g. different soil depths, and parts of the root system, i.e. lateral and tap roots, is insufficiently understood. One reason is the complexity of interacting factors that also result in high temporal and spatial variability.

To investigate short term dynamics of root water uptake depth we used novel in situ techniques to determine the water stable isotope composition of soil and tree xylem water in a tropical dry forest in the northwest of Costa Rica. With simultaneous sap flow measurements, this allowed us to connect, for the first time in high time resolution, information on plant source water depths with the velocity and amount of water transported in conductive tree xylem. To disentangle the contribution of deep and shallow root system, root xylem was investigated next to stem xylem water. Additionally, we collected data on factors driving root water

uptake, i.e. soil physical (soil moisture, matric potential), plant physiological parameters (water potential, leaf area index) and climate conditions. With this holistic setup, we followed the dynamic changes in the water uptake of two tree species (*Swietenia macrophylla* and *Sideroxylon capiri*) during the dry season 2019 and in response to multiple irrigation events with both tap and artificially $\delta^2\text{H}$ enriched water.

For determining water stable isotope composition in tree xylem in situ, we applied the new borehole equilibration method in a challenging field environment. This, on one hand provided new insights into possibilities and constraints of this method as well as potential pitfalls. On the other hand, for the first time, information on both amount and source of root water uptake in high time resolution can be compared to disentangle mechanisms behind root water uptake dynamics and take a closer look at contrasting species-specific water uptake strategies.

Keywords: ecohydrology, field experiment, in situ methods, root water uptake, tropical dry forest, water stable isotopes

Three wood isotopic reference materials for $\delta^2\text{H}$ and $\delta^{13}\text{C}$ measurements of plant methoxy groups

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$\delta^2\text{H}$ and $\delta^{13}\text{C}$ values of methoxy groups (OCH_3) of plant organic matter have large potential for applications in biogeochemical, atmospheric and food research. So far, normalization of measurements to isotope- δ scales of stable hydrogen and carbon isotopes of plant methoxy groups are hampered by the lack of proper reference materials. Recently, to fill this lack we have recommended two methyl sulfate salts (HUBG_1 and HUBG_2) to be applied as methoxy reference materials. Nevertheless, both methyl sulfate salts have $\delta^2\text{H}_{\text{OCH}_3}$ values in a quite narrow range (HUBG_1 : $-144.5 \pm 1.2\text{mUr}$; HUBG_2 : $-102.0 \pm 1.3\text{mUr}$) and thus have their limitations to be applied for correction of $\delta^2\text{H}_{\text{OCH}_3}$ values of plant methoxy groups that often show $\delta^2\text{H}_{\text{OCH}_3}$ values in the range of -150mUr to -300mUr . Thus, there is the need to extend the isotopic range covered by reference materials especially for $\delta^2\text{H}$ measurements. We now have determined three wood samples of different geographical origins to be applied as reference materials for measurements of $\delta^2\text{H}$ and $\delta^{13}\text{C}$ methoxy group values. In a first step tree slices (amount of 2-10 kg) were homogenized and stored in 2L glass flasks (2-8 batches each). In a second step methoxy groups of homogenized wood sub-samples were quantitatively extracted as iodomethane (according to the Zeisel reaction) and subsequently purified and sealed into borosilicate glass break-seals. Finally, the extracted iodomethane was calibrated against

international reference substances by EA-IRMS. The calibrated $\delta^2\text{H}$ and $\delta^{13}\text{C}$ methoxy group values of the three wood materials obtained by EA-IRMS are $-272.9 \pm 1.5\text{mUr}$ and $-29.40 \pm 0.13\text{mUr}$ (HUGB₃); $-239.1 \pm 1.4\text{mUr}$ and $-30.17 \pm 0.13\text{mUr}$ (HUGB₄) and $-191.7 \pm 0.8\text{mUr}$ and $-29.77 \pm 0.13\text{mUr}$ (HUGB₅), respectively. To ensure the homogeneity and the comparability of the different batches of each wood species sub-samples from each flask were analyzed for both $\delta^{13}\text{C}_{\text{OCH}_3}$ and $\delta^2\text{H}_{\text{OCH}_3}$ values. We suggest that all three wood materials can be applied as reference materials for normalization of isotope measurements of hydrogen and carbon of plant methoxy groups and are ideally suited for long term usage, long-term data management and for inter-laboratory comparison.

Do drying and milling procedures influence the stable isotopic composition in wood samples?

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Illegal logging, especially of tropical woods becomes more and more a problem all around the globe. Hence the need for analytical methods to proof wood provenance increases. At the moment tracking wood provenance is mainly done by paper or electronic documentation which can easily be manipulated. In this study, we aim to get information on timber origin by combining analysis results of C, N, S, O and H isotope signatures in bulk wood. To be effective for provenance tracing, the method used has to be fast, easy to handle and low in cost. To examine if sample preparation influences the isotopic composition of bulk wood samples several tests were performed. Different drying methods (Freeze drying, drying cabinet) as well as different drying duration and temperatures were tested. Additionally, the sample homogenisation by milling was tested. Different mills and milling equipment were examined concerning their suitability to produce homogeneous, fine wood meal. This was rather tempting as different particle sizes were still present in very thoroughly milled samples. Therefore, we analysed these fine and coarse wood powder fractions to check for differences in isotopic composition. We chose three different tropical hardwood species for this first approach. The species are *Lophira alata* (Bongossi) from Cameroon, *Dipteryx micrantha* (Brazilian Teak) from Peru and *Hymenaea* spp. (Jatoba) from Brazil. Wood shavings were collected at three different sites in each country, transferred to Germany and processed here. The first results will be presented.

Keywords: Bulk Wood, Sample Preparation, Wood Provenance, Timber Origin, Drying, Milling, IRMS

Abstracts of Posters

Poster [1]

Method optimization for the determination of total organic carbon, total nitrogen, $\delta^{13}\text{C}$ and $\delta^{15}\text{N}$ in carbonate-containing soils

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The quantification of total organic carbon (TOC), total nitrogen (TN) as well as the determination of the stable isotope composition ($\delta^{13}\text{C}$ and $\delta^{15}\text{N}$) in soils are important proxies to follow the fate of organic matter (OM) in (paleo)ecological studies. However, carbonate-containing soils impede such measurements in Elemental Analysis- Isotope ratio mass spectrometry (EA-IRMS) due to the presence of inorganic C. Therefore, a pre-treatment for decarbonisation is needed. Different methods for decarbonisation of carbonate-containing soils were discussed in literature, but still there is an ongoing discussion about the most suitable method for EA-IRMS measurements. Our study compares well-known acidification methods using (i) HCl with different concentrations and forms of application (fumigation: 32% HCl, 37% HCl; in situ acidification: 3% HCl, 16% HCl), (ii) different analytical vessels (glass, silver capsules), (iii) a single temperature-based combustion method and (iv) the inclusion of additional treatment steps. In this study we aimed at determining an optimized method, which provides the most accurate and precise results with a minimum of practical constraints (e.g. reactor exhaustion, sample loss, or laboratory work). Therefore, six different soil samples from Amsdorf, Germany (Calcaric Regosol) were chosen and spiked with 10% CaCO_3 and 10% MgCO_3 , respectively. Pure SiO_2 was included as control and treated similarly. The samples were measured in three-fold repetition using a Euro EA (EuroVector, Hekatech, Germany) coupled to an IRMS (Thermo Fisher, Germany). Among

all tested methods, fumigation of the soil with 32% HCl for 8 h and direct acidification with 3% HCl showed the most accurate and precise results for TOC and $\delta^{13}\text{C}$, respectively. In contrast, fumigation with 37% HCl or the direct acidification with 16% HCl alter these values possibly by decomposing labile organic compounds. The direct combustion of TOC in soil at 550 °C is easy to set up and includes a minimum of laboratory work and no harming chemicals which could damage e.g. the reactor. However, it did not provide accurate TOC or $\delta^{13}\text{C}$ values in our study. In general, all methods under investigation showed that TN and $\delta^{15}\text{N}$ should be measured separately on untreated samples whenever possible.

Keywords: Decarbonatization, Elemental Analysis- Isotope ratio mass spectrometry, TOC, TN, $\delta^{13}\text{C}$, $\delta^{15}\text{N}$

Poster [2]

A closer look Part II: The Nitrogen blank in elemental analyser/isotope ratio mass spectrometry

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One important limitation for the precise measurement of minute amounts of N in solid samples by elemental analyser/isotope ratio mass spectrometry (EA/IRMS) is the accurate determination and/or minimization of the analyser blank value. Here we present more insights towards more precise measurements of minute amounts of N in solid samples.

Poster [3]

Application of N₂O isotopes for N₂ flux determination. Validation with ¹⁵N gas flux method.

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In the process of soil denitrification N₂O is partially reduced to N₂. The quantification of N₂ flux is difficult due to the high atmospheric background. To estimate this flux under field conditions only the ¹⁵N gas flux method is available, but it is very expensive, laborious, and applicable with a low temporal and spatial variability. Based on the isotope effects associated with N₂O reduction to N₂ the so-called N₂O isotopocule method should theoretically provide an alternative tool for N₂ flux quantification. However, application of this method is problematic due to possible variations in isotopic fractionation factors and isotopic signatures of produced N₂O, resulting in large uncertainties.

Here we present the comparison of results obtained from N₂O isotopocule method and from ¹⁵N gas flux method. Both approaches have been applied in parallel in laboratory and field studies. For interpretation of the N₂O isotope results the mapping approaches (SP-δ¹⁸O and SP-δ¹⁵N) were applied. From ¹⁵N traced results we obtained independent information on the origin of N₂O and the magnitude of the N₂ flux based on laboratory and field studies with three parallel treatments at natural abundance, ¹⁵N nitrate and ¹⁵N ammonium labelling.

The various studies yielded varying results regarding the agreement between both approaches. Here we discuss which conditions are most suitable for a robust outcome of the N₂O isotopocule method. It appears that soil moisture is one of the key factors controlling the magnitude of fluxes. Under reduced oxygen conditions when we can expect that denitrification is the prevailing process, the method provides adequate results. However, when we deal with lower fluxes and when N₂O is emitted via several pathways, the interpretation of results is not straightforward. Further developments are ongoing to interpret N₂O isotopocule data with the aim to derive N₂ fluxes.

Poster [4]

Using the N₂O isotopocule mapping approach to improve our understanding of N₂O source processes from field studies

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Until now, data about N₂O production pathways and N₂O reduction to N₂ from field studies are very limited, even though understanding of N₂O processes and identification of sources are needed in order to devise mitigation options. A promising tool to address this is the combination of stable isotope analyses of soil-emitted N₂O ($\delta^{18}\text{O}_{\text{N}_2\text{O}}$ and $\delta^{15}\text{N}^{\text{SP}}_{\text{N}_2\text{O}}$, i.e. the intramolecular distribution of ¹⁵N within the linear N₂O molecule) and an enhanced approach for data interpretation (isotopocule mapping approach, Lewicka-Szczebak et al. (2017)). The isotopocule mapping approach (plotting $\delta^{18}\text{O}_{\text{N}_2\text{O}}$ vs. $\delta^{15}\text{N}^{\text{SP}}_{\text{N}_2\text{O}}$) allows to simultaneously estimate the magnitude of N₂O reduction to N₂ and the origin of the N₂O, i.e. the fraction of N₂O emitted from the bacterial denitrification pathway or fungal denitrification and/or nitrification. This approach is based on the comparison of measured isotopic values with isotopic 'endmember areas' for the N₂O

produced from different sources reported in the literature. Two main scenarios with different assumptions for N_2O produced were calculated: N_2O is reduced to N_2 before residual N_2O is mixed with N_2O of various sources and vice versa. Isotopocule data from field studies about varying techniques (chemical and mechanical conversion) of grassland conversion to maize cropping on four different soil sites with varying soil texture (sandy to clayey) in the north-western part of Germany were analysed. The isotopic composition of soil-emitted N_2O largely coincided with the range of values typical for production by bacterial denitrification and variable N_2O reduction to N_2 . The isotopocule mapping approach indicated a different impact of N_2O reduction on isotopic composition of soil-emitted N_2O depended on the soil type. N_2O reduction was very variable, partially very high resulting in large N_2 fluxes. However, future attempts with larger test datasets and reliable endmember values are needed to reduce uncertainty of the mapping approach. References: Lewicka-Szczebak, D., Augustin, J., Gieseemann, A. and Well, R. (2017) Quantifying N_2O reduction to N_2 based on N_2O isotopocules – validation with independent methods (helium incubation and ^{15}N gas flux method). *Biogeosciences* 14(3), 711-732.

Poster [5]

Dynamics in the isotope hydrobiogeochemistry in a coastal peatland and associated surface waters at the southern Baltic Sea

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In the present study the temporal and spatial dynamics in the isotope hydrobiogeochemical composition of surface water in a

rewetting coastal peatland was investigated during different hydrological conditions. The peatland is located at the southern Baltic Sea and is under impact by rare storm-induced flooding events. The temporal changes in salinity and element concentrations have substantial consequences for the biogeochemical processes taking place in the organic-rich soils that are further reflected by the composition of peatland surface waters. Using a multi-isotope (H, C, O, S) tracer approach in combination with redox-sensitive trace elements and nutrients, the aim of this study was the characterization of water mixing processes and sinks, sources and transformations in associated biogeochemical element cycles as reflected by the composition of connected surface waters of the southern Baltic Sea. After a strong storm event in winter 2019 a large surface area of the peatland was flooded by brackish Baltic Sea surface water enhancing the salinity in the surface waters. The input from brackish seawater modified the stock of electron acceptors to foster microbial sulfate reduction. The peatland is draining via surface water flow into the Warnow river estuary and via submarine ground water flow directly into sediments of the coastal Baltic Sea. Therefore, seasonal sampling was also carried out in the Warnow river since year 2017. The upper part of the Warnow river reflects changes in seasonal meteorological and hydrological conditions in the catchment area that is under multiple anthropogenic impacts. The estuarine part of the Warnow river is further impacted by temporal mixing with Baltic Sea water. Acknowledgement: This study is supported by the DFG research training group Baltic TRANSCOAST, DAAD, and the Leibniz IOW.

Poster [6]

Reconstruction of environmental and human history based on pedological and geoarchaeological investigations of the Mesolithic site Ullafelsen, Fotschertal, next to Innsbruck, Austria

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The archaeology of high mountain regions attracts much attention since the discovery of the copper age mummy called "Ötzi" in the Ötztal Alps in 1991. Results of former archaeological research projects show that mesolithic hunter-gatherers lived in alpine regions since the beginning of the Holocene, 11700 years ago (CORNELISSEN & REITMAIER 2016). Amongst others, the mesolithic site Ullafelsen and surroundings represent a very important archaeological reference site in the Fotschertal (Stubai Alps) (SCHÄFER 2011). Many archaeological artifacts were found at different places in the Fotschertal, which provides evidence for the presence and the way of living of our ancestors. The "mesolithic project Ullafelsen" includes different scientific disciplines ranging from high mountain archaeology over geology, geomorphology, soil science, sedimentology, petrography to palaeobotany (SCHÄFER 2014). By applying pedological, biogeochemical and geoarchaeological analytic tools, we aim at addressing the following research questions: (i) Which vegetation dominated before, during and after the settlement by humans at the mesolithic site Ullafelsen and surroundings, (ii) which climate conditions prevailed before, during and after the settlement by

humans at the Ullafelsen and (iii) how intensive was the environment altered due to the settlement by humans at the Ullafelsen and surroundings. These research questions are addressed using different biomarker and stable isotope analyses. Biomarkers for the reconstruction of vegetation are n-alkanes and sugars, whereas the isotopic compositions $\delta^{18}\text{O}_{\text{sugars}}$ and $\delta^2\text{H}_{\text{n-alkanes}}$ are used for climate reconstruction (ZECH et al. 2011). Black carbon and sterols/stanols (faecal biomarkers) as well as phosphorus and $\delta^{15}\text{N}$ are interrogated as proxies for human history. Samples from archaeological and non-archaeological soil profiles from the Ullafelsen as well as bog samples from two different sites in the Fotschertal were taken. First results show a high total n-alkane concentration in the topsoils of the archaeological soil profiles, whereas no n-alkanes could be detected in buried humus-enriched subsoils. We propose that these soil horizons are influenced by podsolization and can be categorized pedogenetically as Bh-horizons. Former fireplaces on the Ullafelsen were detected using a small corer along a grid sampling scheme and the ratio of carbon to nitrogen (C/N) as charcoal proxy. Results of the coupling $\delta^{18}\text{O}_{\text{sugars}}$ and $\delta^2\text{H}_{\text{n-alkanes}}$ as well as n-alkane ratios indicate a vegetation change between trees and grasses/shrubs at the bog location of the "Potsdamer Hütte Moor".

Multidimensional stable isotope fingerprinting as a tool to identify the origin of the organophosphorus pesticide chlorpyrifos

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Chlorpyrifos belongs to the group of organophosphorus pesticides (OPs) which are a diverse family of insecticides in use since the 1940s. It acts on the nervous system of insects by inhibiting the acetylcholinesterase and it is one of the most widely used organophosphate pesticides in agriculture. Chlorpyrifos is considered moderately hazardous to humans by the World Health Organization. The continuous and excessive use of chlorpyrifos paired with its toxicity and persistence in nature has led to significant environmental contaminations. As they have repeatedly been detected in soils, sediments, waterbodies, as well as within food and drinking water, public concerns are increasing. Thus, tools are needed to understand sources, reactive transport pathways and sinks of chlorpyrifos in the environment. Multi-dimensional stable isotope fingerprinting is a valuable method for the characterization of the provenance of chemicals as the isotopic profile reflects the isotopic composition of raw materials, synthetic pathways and purification processes. To evaluate this approach, pure batches and commercial formulations of chlorpyrifos were collected from more than 30 manufactures in India, China and Germany. These were isotopically characterized using Elemental Analyzer – Isotope Ratio Mass Spectrometry (EA-IRMS) for analyzing the $\delta^{13}\text{C}$, $\delta^2\text{H}$, $\delta^{18}\text{O}$ and $\delta^{15}\text{N}$ isotopic composition and Gas Chromatography – Multiple Collector – Inductively Coupled Plasma Mass Spectrometry (GC-MC-ICPMS) for determining the $\delta^{37}\text{Cl}$ isotopic signature. The isotopic composition of analyzed

chlorpyrifos samples varied for $\delta^{13}\text{C}$ from -31.9 to -24.1‰, for $\delta^2\text{H}$ from -271 to -157‰, for $\delta^{18}\text{O}$ from -0.9 to 24.6‰, for $\delta^{15}\text{N}$ from -3.4 to -0.1‰ and for $\delta^{37}\text{Cl}$ from -1.3 to 3.1‰. Taking the typical uncertainties of 0.5‰ for $\delta^{13}\text{C}$, 5.0‰ for $\delta^2\text{H}$, 0.5‰ for $\delta^{18}\text{O}$, 0.3‰ for $\delta^{15}\text{N}$ and 0.3‰ for $\delta^{37}\text{Cl}$ into account the combination of different isotopic signatures gives a unique fingerprint to track sources in the environment. Thus, this study highlights the potential of multidimensional stable isotope profiling to identify sources, and provides an isotopic database of chlorpyrifos that might improve the tracing of origin, transport pathways and the environmental fate.

Poster [8]

Dual C-Cl isotope fractionation pattern during reductive degradation of chloroform (CHCl_3): implication to managed aquifer recharge as sustainable storage solution for desalinated water (MAR-DSW) in Menashe recharge basin, Israel.

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In Israel, excess desalinated water is stored in a carbonate coastal aquifer. During the storage, residual chlorine in the desalinated water may react with natural organic matter and form toxic disinfection by-products (DBPs), like trihalomethanes (THMs). Chloroform (CHCl_3) has been detected as a main contaminant of interest at the site and surrounding production wells. In order to ensure managed aquifer recharge as a storage solution for desalinated water in the basin, it is important to understand the

mechanisms of the formation and degradation of such DBPs with the use of compound-specific stable isotope analysis (CSIA) method. In this work, the degradation of chloroform (CHCl_3) was investigated to derive carbon and chlorine isotope enrichment factors in a batch experiment in the laboratory as a part of the Israel-German joint research "Aquifer recharge as sustainable storage solution for desalinated water (MAR-DSW)". A 100ml of deionized water spiked with 30mg/l chloroform in a reactor was saturated with hydrogen, which serves as an electron donor. Degradation starts by adding 0.25g/l palladium as palladium-on-alumina ($\text{Pd}/\text{Al}_2\text{O}_3$, 10% wt.) to catalyze the reaction. Samples were taken at specified intervals from a sampling port designed at the bottom of the reactor, which is closed with a plunger from the top so that no headspace was created both as samples were taken out and during the entire experimental period. During the reductive hydrodechlorination, the change in chlorine isotope ratios of CHCl_3 was determined using a gas-chromatograph-mass spectrometer online connected to a purge and trap system (P&T-GC/MS). This simple online method was developed and optimized at TU Darmstadt. The carbon isotope values were determined using GC-C-IRMS (Delta V Advantage, Thermo Scientific). The stable isotope data can potentially be used as a tool to discriminate the source, path and fate of the compound of interest so as to foresee the feasibility of medium and long term use of managed aquifer recharge as a storage solution.

Keywords: compound-specific stable isotope, chloroform, managed aquifer recharge, desalinated water

Poster [9]

Development of a Heatable Precipitation Totalizer

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Stable isotope and tritium analysis of water samples can contribute to investigations of groundwater residence times as well as identification of different water sources. But it requires reliable and long time series of local precipitation isotope data as input or background values. An online available IAEA/GNIP precipitation sampling guide (V2.02, September 2014) recommended the use of precipitation totalizers with a paraffin oil layer or, alternatively with a dip-in tube for pressure equilibration according to Groening et al (2012) as evaporation protection measures. However, the sampling of precipitation at sub-zero temperature is not taken into account in this guide where sublimation or drifting of collected snow may cause a falsification of analyzed isotope values. For the above reason, we focused on the development and construction of a new precipitation totalizer which will allow the collection of representative snow samples without $\delta^{18}\text{O}$ -/ $\delta^2\text{H}$ fractionation due to sublimation. Additionally, the monthly sampling volume will be at least 1L for an additional tritium sample collection. During the winter term 2019/2020, prototypes of the new precipitation totalizer should be tested under field conditions in cooperation with the Federal Institute of Hydrology at some of the German surface water measuring stations.

Keywords: precipitation totalizers

A data analysis of long-term GNIP data sets with respect to climate change

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Stable isotopes of oxygen and hydrogen are routinely used to assess movement of water between compartments of the water cycle. One of the most widely used concepts is the Global Meteoric Water Line (GMWL). When first introduced by Craig in 1961, it established the average empirical relation between hydrogen and oxygen isotopes in natural waters on the basis of around 400 samples. A linear relationship of $\delta^2\text{H} = 8 \times \delta^{18}\text{O} + 10\text{‰}$ was derived and is being used by many studies e.g. to compare local water samples to the global relation, or to determine the isotope composition of source water from evaporated water bodies. An update of the equation (Rozanski et al., 1993) resulted in a minor change of slope and intercept from a significantly increased dataset, the Global Network of Isotopes in Precipitation (GNIP) of the International Atomic Energy Agency (IAEA) and the World Meteorological Organization (WMO). GNIP has collected isotope data in precipitation from the last 60 years. We reevaluated its isotope data with a focus on the temporal evolution of global average isotope values and GMWL parameters. Because most isotope processes are ultimately temperature controlled, an interesting question is if the global temperature increase due to climate change is mirrored also in the global isotope data. Additionally, the changes of GMWL slope and intercept over time derived from present data may set limitations as to which paleoclimatic settings allow the use of the standard Craig's GMWL values. We will present first results of this analysis.

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Poster [11]

Using stable isotopes for the quantification of water fluxes via preferential flow pathways in forest soils

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In the last decade, many studies have demonstrated the applicability of stable water isotopes to understand the dynamics and interactions of the water cycle within the soil-plant-atmosphere continuum. However, besides the increasing understanding of soil water dynamics, the magnitude and dynamics of water fluxes through preferential flow pathways are still not very clear. We present the results of an experiment, which aimed to determine the contribution of preferential flow in forest soils to nutrient export. At three forest sites in Germany, we installed zero tension lysimeters in three depths in six replications. The lysimeters were filled with coarse material to prevent flow from the soil matrix and promote flow from preferential pathways. All experimental plots were irrigated with water of known isotopic composition at three times after covering for four weeks to simulate a dry period. During and after irrigation, water samples were continuously taken from the lysimeters to determine isotopic (¹⁸O, ²H) and chemical composition, and to quantify water fluxes. The preliminary results indicate that the water from the lysimeters differs in the isotopic composition from the water used for

irrigation mainly at the beginning of the sampling. However, over the course of the experiments the isotopic composition from lysimeters and irrigation water became more similar. In the paper we discuss the suitability of the use of isotopic analysis in our proposed experimental setup to quantify water fluxes via preferential flow pathways in forest soils.

Keywords: stable water isotopes, preferential flow, water fluxes

Poster [12]

Spatiotemporal variability of stable isotopes in an unconsolidated sedimentary aquifer (Fuhrberger Feld, Germany)

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Stable isotopes variability (²H-H₂O, ¹⁸O-H₂O, ¹³C-TIC, ¹⁵N-NO₃) in soil- and groundwater allow investigating processes such as solute transport, water movement, evaporation and groundwater recharge. The "Fuhrberger Feld" (52°34'44"N, 9°51'18"E) is a well-characterized hydrogeological site in Northern Germany [1-3], partially because it provides groundwater for the drinking water supply of Hannover and its suburbs (up to 85.000m³/day). In March and April 2019, a sampling campaign was conducted and more than 300 water samples were collected from multi-level observation wells and analyzed for hydrochemistry and stable isotopes at the laboratories of BGR (Picarro L2120-i CRD, Thermo Scientific Delta V Advantage connected with TCEA and EA Flash 2000). The stable isotope results are compared with values from earlier campaign conducted from August to October 2012 and in 2015 [2]. The results indicate a variability of water isotopes in the upper aquifer and rather constant values in the lower part of the aquifer in most of the multi-level sites. These patterns reflect direct infiltration of precipitation and groundwater recharge depending on vegetation and agriculture.

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Keywords: Stable isotopes Fuhrberger Feld

Poster [13]

Spatial and temporal isotopic characterisation ($^2\text{H}/^1\text{H}$ and $^{18}\text{O}/^{16}\text{O}$) of modern day precipitation in the Bale Mountains, Ethiopia, and isotope incorporation into plant biomarkers

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East Africa is an underrepresented region in respect of monitoring stable isotopic composition of precipitation. Moreover, Ethiopia is characterized by a well-known regional anomaly with strikingly positive isotope values. For our study in the Bale Mountains, Ethiopia, we collected precipitation samples from ten weather stations located along an altitudinal transect ranging from 1304 to 4375m a.s.l. The $\delta^{18}\text{O}_{\text{prec}}$ and $\delta^2\text{H}_{\text{prec}}$ values vary from -8.7‰ to +3.7‰ and -38.2‰ to +28.6‰, respectively. The local meteoric water line is characterised by a lower slope, a higher intercept and more positive d-excess values ($\delta^2\text{H} = 5.2 * \delta^{18}\text{O} + 14.9$) than the global meteoric water line. Both altitude and amount of precipitation correlate with our isotope results. The $\delta^{18}\text{O}_{\text{prec}}$ and $\delta^2\text{H}_{\text{prec}}$ values show seasonal patterns reflecting rainy versus dry season. More enriched isotope values prevailed shortly after the end of the dry season. By contrast, the most negative isotope values coincide with high precipitation amounts recorded in May, August and September. HYSPLIT trajectory studies reveal that during the dry season water vapor originates from the Gulf of Aden and the Arabian Sea, whereas during the wet season, water vapor originates primarily from the Southern Indian Ocean. This finding challenges the traditional amount effect interpretation of isotope records from East Africa and points to a hitherto likely underestimated source effect instead. Finally, preliminary results of compound-specific stable isotope analyses will be presented showing that the isotope signal of precipitation is incorporated into plant-derived lipid and sugar biomarkers to a variable degree depending on the type of vegetation.

Keywords: East Africa, local meteoric water line, $\delta^2\text{H}_{\text{prec}}$, $\delta^{18}\text{O}_{\text{prec}}$, amount effect, altitude effect, trajectories, biomarkers

A microcontroller-based automatic rain sampler for stable isotope studies

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The stable isotopes ^{18}O and ^2H are popular tracers in hydrology and other disciplines and many applications require data on the isotopic composition of precipitation. While automatic collectors offer a convenient way to gather corresponding samples, most commercial devices are costly and do not reduce post-sampling evaporation and the associated isotope fractionation sufficiently. Hence, we have developed a microcontroller-based collector enabling timer-actuated integral rain sampling, with time intervals ranging from minutes to weeks. The low-cost device is robust, oil-free, and customizable. Aiming at a quasi-evaporation-free collector, we harness the concept of a Tube-dip-in-water collector with pressure equilibration tube (Gröning et al., 2012), which has been successfully tested under hot and arid conditions (Michelsen et al., 2018). To evaluate the collector, a 6-months evaporation experiment with pre-filled bottles in a lab oven (diurnal temperature regime, 21-31°C) was performed. Small evaporative mass losses (<1%) and negligible isotopic shifts suggest that even multi-week field deployments in warm climates are feasible. We thus believe that our sampler represents a useful addition to the isotope hydrologist's toolbox.

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Hydraulic redistribution of water by silver fir – a Deuterium labelling experiment under controlled conditions

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Drought-susceptible European beech is projected to be severely affected by climate change. Mixtures of beech with silver fir have been proposed to increase the resilience of these forests. Under drought conditions, beech could hypothetically benefit from lifted water only accessible by deep-rooting silver fir by the mechanism known as “hydraulic redistribution”. Until now, this widespread assumption has not been proven for silver fir, which inspired us to shed light into the water dynamics taking place in silver fir-beech mixed stands. For this, we conducted a split-root experiment in plant-soil mesocosms with beech and fir seedlings (approx. 3 years old) separated in polyvinylchlorid compartments and the only connection generated by a redirected fir root leading into the beech compartment. A soil water potential gradient was established between the fir and beech compartment: After exposing the mesocosms to drought until a soil volumetric water content of 4 - 16% was reached, we applied deuterium labelled water ($\delta^2\text{H} = +6000\text{‰}$) only to the bottom soil zone of the fir compartment. Beech compartments were rewetted with tap water after 2 months in order to eliminate the gradient in water potential in the fir and beech compartment and therefore the conditions required for hydraulic redistribution. We measured $\delta^2\text{H}$ of soil water vapour in the beech compartment at specific intervals during the following 10 weeks by sampling soil air via semipermeable tubes in real-time

using a Picarro cavity ringdown spectrometer. Our results showed a maximum isotopic enrichment in $\delta^2\text{H}$ of approx. 300‰ on average, whereas the isotopic composition of sample air in control boxes (two without labelling and one without trees) stayed at atmospheric levels around -100‰ during the entire measurement period. After rewetting of beech compartments, sample air $\delta^2\text{H}$ dropped to approx. 100‰ and stayed at this level until the end of the experiment. These data suggest that water was redistributed by the redirected fir root as triggered by the gradient in soil water potential. In conclusion, we were able to prove in this mechanistic study that hydraulic redistribution by silver fir exists. For future studies, it remains to quantify the use of redistributed water by beech trees, and to prove the relevance of this effect for adult trees under field conditions.

Keywords: hydraulic redistribution, fir, split-root experiment, deuterium labelling

Poster [16]

Searching for mycoheterotrophy among leafy and leafless *Neottia* species from Japan and Taiwan: A multi-element stable isotope approach

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At least 235 orchid species in 43 genera are leafless and rely on fungi as their C and N source (Merckx, 2013). These mycoheterotrophic plants display much higher ^{13}C and ^2H abundances in their tissues than surrounding autotrophic C_3 plants (Gebauer and

Meyer, 2003; Gebauer et al., 2016). An interesting genus where achlorophyllous leafless plants, next to leafless plants with a green stem and also potentially autotrophic leafy species are found, is the genus *Neottia* (Orchidaceae) (Yagame et al., 2016). The leafless species with a green stem could thereby display a transition state in the evolution to achlorophyllous full mycoheterotrophic plants, but the stable isotope abundances of those Asiatic species of the genus *Neottia* remained up to date unknown. Hence, we here investigated the C, N and H stable isotope patterns of two leafy (*Neottia makinoana*, *Neottia puberula* var. *maculata*), two leafless species with a green stem (*Neottia furusei*, *Neottia listeroides*) and two leafless achlorophyllous *Neottia* species (*Neottia inagakii*, *Neottia acuminata*) from Japan and Taiwan. Relative C and N isotope natural abundances were measured in dual element analysis mode with an elemental analyser coupled to a continuous flow isotope ratio mass spectrometer via an open-split interface. The relative isotope abundances of H and O were measured using thermal conversion through pyrolysis coupled to a continuous flow isotope ratio mass spectrometer via an open-split interface. Isotope abundances showed statistically significant enrichment in all leafless *Neottia* species in ^{13}C and ^{15}N , whereas the *Neottia* species with green stems, were even more enriched than the achlorophyllous species. No enrichment in ^{13}C and ^{15}N was detectable in the leafy *Neottia* species. The ^2H isotope abundances confirmed the findings of the C and N measurements regarding the leafless *Neottia* species but also revealed an enrichment in ^2H in the two leafy *Neottia* species. Despite the green stem, the two investigated species, at least in the sampled habitat, seem to be full mycoheterotrophic plants, displaying an obviously far advanced transition state to the full mycoheterotrophic achlorophyllous *Neottia* species. Furthermore, we were able to verify a partial C gain from fungi of the two leafy *Neottia* species *N. makinoana* and *N. puberula* var. *maculata*, due to an enrichment in ^2H .

Poster [17]

Determination of sources of water uptake by hybrid Poplar plantations (*Populus* spp.) under different groundwater accessibility using stable isotopes analysis

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Aim Understanding the plant-water-soil relationship in sites under Short Rotation Coppices (SRC) Poplar plantations is necessary for water resources management. This includes the understanding of water movement within the unsaturated zone and water uptake by the trees. We investigate the sources for water uptake by SRC hybrid Poplar trees on sites under different groundwater accessibility and root morphology. **Methods** To determine the sources for water uptake by Poplar trees, measurements of the isotopic composition from precipitation, soil water, xylem-water and groundwater are proposed. Additionally, drought simulations will be performed ensuring to include the trees where the sensors for measurement of root sapflow have been installed. Effectiveness of the simulation will be evaluated using TDRs already installed in the soil profiles. Sprinkler experiments with water of known isotopic composition, at different depths to determine the role of groundwater and soil water in plant water uptake are considered and will be performed in two sites with fluctuating and far groundwater accessibility. For extraction of the aliquots from soil and xylem water, field-collected samples will be tested using the centrifuge method. Water stable isotope composition will be evaluated using Isotope Ratio Mass Spectrometry (IRMS).

Poster [18]

Do the elusive 'dark septate fungal root endophytes' have an influence on the ^{15}N stable isotope abundance of plants?

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Introduction/Aim: Plant roots are colonized by a great variety of fungi, for instance, the highly investigated mycorrhizal fungi and the elusive (dark) septate endophytes (DSE). The mycorrhizal symbiosis was multiple times reported as beneficial for the plant as well as the mycorrhizal fungi with both being involved in a vivid bi-directional nutrient transfer, while very little is known about the function of DSE. These fungi have been reported for 100 plant families often co-existing with mycorrhizal fungi, however, the DSE manage to colonize plant families generally considered as 'non-mycorrhizal' (e.g. Caryophyllaceae, Cyperaceae, Juncaceae, Onagraceae). The plant tissue ^{15}N abundance is suggested to be closely correlated with the presence and type of mycorrhizas, which was disclosed in nitrogen-nutrient limited conditions. Possibly, the respective fungi provide nutrients originating from a different nitrogen-nutrient source ('ecological niche'). We questioned, if we could disclose a specific ^{15}N -pattern for plants colonized by DSE-only due to DSE-specific abilities to acquire nitrogen-nutrients inaccessible for most mycorrhizal fungi? Materials and Methods: Plant species colonized by DSE-only (Caryophyllaceae, Cyperaceae) and neighbouring non-mycorrhizal as well as mycorrhizal plant species as references were sampled in NE-Bavaria. Fungal colonization was checked by staining approaches. After measuring the $\delta^{13}\text{C}$ and $\delta^{15}\text{N}$ stable isotope natural abundance (EA-IRMS) the isotope data were normalized to enrichment factors ϵ which disclose the relative difference between the target (DSE-only) and reference plants. Results: The nitrogen stable

isotope enrichment $\delta^{15}\text{N}$ was significantly higher in most investigated plant species solely colonised by DSE, while mostly no significance was found in $\delta^{13}\text{C}$ when comparing DSE-colonized plants with reference plants. Discussion: Our results fit the pattern of plant species considered as 'non-mycorrhizal' being more ^{15}N -enriched than mycorrhizal plants [1]. However, for the first time, we address here the question whether this ^{15}N -pattern of 'non-mycorrhizal' plants is also based on a fungal effect, namely by dark septate endophytes. DSE are known to be capable of utilizing organic detrital nutrients and thus, may transfer those to 'non-mycorrhizal' plants. We conclude that DSE could provide a distinct nitrogen-nutrient source for the plant, thereby changing its ^{15}N pattern which consequently differs from mycorrhizal plant species' ^{15}N abundance. This study not only provides further support for suggestions that plants' ^{15}N abundance is largely influenced by their fungal partner [1], but also adds one puzzle stone to the function of the elusive DSE.

Reference: [1] Craine et al. (2009). *New Phytol.*, 183(4), 980-992.

Keywords: Mycorrhizal vs. 'non-mycorrhizal' plants, dark septate endophytes, Caryophyllaceae, Cyperaceae

Poster [19]

Multi-element stable isotope natural abundance in 13 arbuscular mycorrhizal mycoheterotrophic plant species of different taxonomic groups and wide geographic origin

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Fully mycoheterotrophic (MH) plants not only obtain soil nutrients from fungal sources, as usual in mycorrhizal associations, but also

carbon (C) that ultimately derives from interconnected, photosynthetically active plants. Retracement of element flows by analysis of natural stable isotope abundances has been extensively deployed for mycoheterotrophs associated to mycorrhizal fungi of different types. Studies revealed ^{13}C and ^{15}N enrichments as well as high nitrogen (N) concentrations in most MH plants compared to autotrophic reference plants. In this context, only five MH species from just two plant families engaging in arbuscular mycorrhiza, the most dominant mycorrhizal type, have been studied yet. In the present study, one orchid species associated with saprotrophic fungi and 13 fully MH plants of five families associated with arbuscular mycorrhizal (AM) fungi have been sampled together with autotrophic reference plants and soil in the tropics and the temperate zone of the southern hemisphere. Analyses of $\delta^{13}\text{C}$, $\delta^{15}\text{N}$, $\delta^2\text{H}$, $\delta^{18}\text{O}$ and N concentrations were conducted, and DNA of reference plants and fungal hosts were sequenced. We found significant ^{13}C enrichments in most MH species, trending to be low in *Thismia* sampled in the temperate zone, and ^{15}N enrichments in several MH species except for *Gentianaceae* which exhibited the same N isotopic composition as autotrophic plants. Mycoheterotrophs associated with *Rhizophagus irregularis* fungi were stronger enriched in ^{15}N , while associations with *Non-Rhizophagus Glomeraceae* led to higher ^{13}C enrichments. The N concentrations in MH plants were significantly higher than in green plants. Despite *Thismia hillii*, mycoheterotrophs were also enriched in ^2H . A unique $\delta^2\text{H}$ and $\delta^{18}\text{O}$ pattern as observed for *T. hillii* was previously found for plants following a unique transpiration pattern, like hemiparasites. In conclusion, ^{13}C enrichments of $5.1 \pm 2.2\text{‰}$ can generally be attributed to AM mycoheterotrophs, while they are not compulsorily characterised by ^{15}N enrichments. The differences between isotopic compositions of MH plants most likely result from family-specific physiological characteristics and the type of fungal hosts.

Keywords: mycoheterotrophy, arbuscular mycorrhiza, ^{13}C , ^{15}N , ^2H , ^{18}O , carbon and nutrient cycling

Short-term cycling of carbon at a Sphagnum farming site during the extreme summer of 2018

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Using drained peatlands for agriculture causes the release of large amounts of carbon dioxide (CO₂) into the atmosphere. Paludiculture, in contrast, aims at the production of biomass under wet and peat preserving conditions and could combine ecological and economic goals in formerly drained peatlands. The cultivation of peat mosses (Sphagnum) as a horticultural substrate is currently tested in a former peat extraction area northwestern Germany. The site is characterized by 70cm of strongly decomposed "black" peat and is, after two years, almost completely covered by Sphagnum mosses (mainly Sphagnum papillosum LINDB.) with scattered Molinia caerulea (L.), Eriophorum angustifolium HONCK. and Erica tetralix (L.). Measuring greenhouse gas emissions revealed that these sites could quickly become carbon-neutral or even a sink of atmospheric carbon dioxide (CO₂) under optimal conditions, i.e. high groundwater levels, a low interference initial growth phase and average climatic conditions. Passive warming of air and soil temperatures by Open Top Chambers (OTC) slightly decreased CO₂ uptake. However, it remains unclear how much of the sequestered CO₂ is stored in the medium term in which compartment and how much carbon is quickly released back into the atmosphere. Therefore, we conducted a pulse labelling experiment with enriched carbon dioxide (¹³CO₂, 99.9 at%). The isotopic signatures of emitted CO₂ and methane (CH₄), vascular and bryophyte biomass, soil microbial biomass as well as dissolved gases (CO₂ and CH₄) and dissolved organic carbon (DOC) in 10cm and 30cm depths were measured before label addition and 1, 2, 3, 5, 7, 10, 14, 21, and 140 days thereafter. The tracer experiment took place during the dry and hot summer 2018, when,

despite all management efforts, groundwater levels fell below optimum condition for peatland species. Tracer uptake was thus generally low, but uptake by Sphagnum mosses was particularly small compared to the uptake by vascular plants. The concentration of labelled carbon in plant tissue and ecosystem respiration decreased from an early peak to nearly pre-labelling values after 21 days, but was still slightly enriched after 140 days. The amount of tracer in DOC was negligible. However, the signatures of dissolved CO₂ in 10cm depth peaked shortly after the peaks in plant biomass, the peak in 30cm depth was shifted and smaller. OTCs seemed to have no significant effect on carbon partitioning and residence time, possibly because conditions were already extreme during the experiment.

Keywords: peatlands, paludiculture, ¹³CO₂, pulse labelling

Poster [21]

Application of a quick one-step method for the production of fatty acid methyl esters from rape seed for compound-specific isotope carbon and hydrogen analysis

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To develop a fingerprinting approach for investigation of the geographical origin of oil plants, compound-specific stable isotope analysis (CSIA) of carbon and hydrogen ($\delta^{13}\text{C}$, $\delta^2\text{H}$) of individual fatty acids of several hundred rapeseeds are to be analyzed with GC-C-IRMS in the present research. For GC separation, fatty acids in rapeseed oil first need to be converted to fatty acid methyl esters (FAMES). The conventional method for the preparation of FAMES involves multiple steps, i.e. oil extraction, saponification, transmethylation prior to the instrumental analysis. Moreover,

during the multiple chemical conversion steps, isotope fractionation may occur in each step, which could influence the precision of CSIA of carbon and hydrogen of FAMES. In this study, we applied and modified the one-step method for sample preparation by Garcés et al., which was developed for the purpose of the determination of fatty acid composition of plant oil. First, a mixture of methanol, toluene, 2,2-Dimethoxypropane (DMP) and Sulfuric acid is prepared. Rapeseed is added to the mixture with heptane in a 20mL glass reactor, where the digestion of seeds, lipid trans-methylation, FAMES production and extraction take place simultaneously. After a certain reaction time, the upper phase of heptane/toluene, in which FAMES will be enriched, is taken and analyzed directly in GC-C-IRMS. Experimental conditions including reaction time and sample amount were varied to optimize the one-step method. The precision and accuracy of the one-step method were evaluated with regard to the stable isotope ratios of carbon and hydrogen of different FAMES ($\delta^{13}\text{C}$, $\delta^2\text{H}$ of C16:0, C18:1, C18:2, C18:3, C20:0, C20:1 FAMES etc.) derived from rapeseed oil. The lipid content, fatty acid profile as well as the $\delta^{13}\text{C}$ of C16:0 FAMES in reaction time 60, 90 and 120min have no significant difference, showing that the reaction has completed before 60min. The precision of the one-step method for $\delta^{13}\text{C}$ of C16:0 FAME was 0.28‰ (SD of the GC-C-IRMS is ca. 0.2‰ for C16:0), when the FAMES were produced in three different batches under the same conditions with a reaction time 120min. Our results show that the one-step method enables a quick production of FAMES from rapeseed for isotope fingerprint analysis with high precision.

Keywords: fatty acid methyl esters of rapeseed; compound-specific stable isotope analysis; one-step method; trans-methylation; extraction

Stress and recovery dynamics: Effects of drought and heat waves on carbon metabolism and allocation patterns in Scots pine

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Plant physiological processes are closely coupled to climate, especially by the cycling of carbon (C) and water between plant, soil and atmosphere. Extreme droughts and heat waves are expected to alter carbon allocation and storage, which could result in impaired tree functioning lasting beyond the extreme event. However, models often lack reliable input to make predictions about the resilience of our forests in the face of climate change. The aim of this study was to investigate hydraulic properties, C cycling and storage of Scots pine saplings in response to heat-drought scenarios and subsequent recovery. For this, we used single tree cuvettes (n=18) allowing us to continuously measure above- and belowground gas exchange, ¹³CO₂ effluxes and stem increment in response to gradually intensifying heat or heat-drought stress (min. leaf water potential of - 2.8MPa) and compare the results to a control treatment. Two days after stress release, we applied a 45% ¹³CO₂ pulse-label to trace the newly assimilated C during a 3-week recovery phase. We continuously sampled plant tissues to determine turnover times of recently assimilated C in the different organs and compounds. Whereas net photosynthesis (Anet) declined to ~60% of control values in heat stressed trees, it was almost suppressed in heat-drought treated trees. After stress

release, Anet recovered quickly, reaching 115% and 90% of control values, respectively. This was reflected in stem growth dynamics, where we found heat-treated trees to have larger stem increment rates than control trees, whereas heat-drought trees had persistently lower growth rates post-stress. The ^{13}C -label was detected first in root respiration of previously heat stressed trees (~5h after the start of labeling), then in control trees (~5-6h) and at last in previously heat-drought stressed trees (~11h), indicating generally slower C translocation in the latter. This was supported by a longer retention time of ^{13}C in needles of the heat-drought stressed trees throughout the 3-weeks recovery period. The slower turnover of C in this treatment indicates ongoing repair processes, whereas heat stress alone (max. 40°C needle temperature) apparently did not result in a persistent damage of trees, but rather in a compensation of stress-induced reductions in C uptake and stem growth.

Keywords: *Pinus sylvestris*, pulse-labeling, ^{13}C , carbon cycling, recovery

Poster [23]

Stable isotope determination in natural water: International Atomic Energy Agency Inter-Comparison Study “WICO”

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Every process involving water, from photosynthesis to seawater evaporation, has a characteristic isotope fractionation ratio, indicating how much it favors heavier or lighter isotopes of oxygen and hydrogen. Thus, measurements of these ratios reveal much about the history and source of natural water samples. Additionally, in many life- and geo-sciences studies, known

amounts of these stable isotopes are actively introduced as labels to track water through various pathways and biological processes. The Isotope Hydrology Laboratory of the International Atomic Energy Agency (IAEA) organized a water isotope inter-comparison for international laboratory performance assessment of stable isotope determination ($\delta^{18}\text{O}$ and $\delta^2\text{H}$) in natural water with various technologies. We hereby present and analyze the results obtained with a new generation of laser infrared analyzers, based on Off-Axis Integrated Cavity Output Spectroscopy (OA-ICOS).

Eight unknown water samples were measured by an OA-ICOS isotopic water analyzer. The samples represented a wide array of challenging cases, including contaminated, depleted, enriched, and salinized waters. The assigned isotope values for the samples were determined by IAEA by consensus of four dual-inlet isotope-ratio mass spectrometry international reference laboratories. The OA-ICOS $\delta^{18}\text{O}$ and $\delta^2\text{H}$ readings were within 0.06 ‰ and 0.6 ‰ of the assigned values of the standard water samples, respectively, and within the convoluted uncertainties of the measured and assigned values. The optional depleted, enriched, and salinized water $\delta^{18}\text{O}$ and $\delta^2\text{H}$ OA-ICOS measurements were within 0.05 ‰ and 1.2 ‰ of the assigned values, respectively, and well within the uncertainty of the assigned values.

The work also highlights the benefits of an integrated spectral identification module that flagged a methanol-contaminated water sample. The isotope reading was corrected and the measurements of $\delta^{18}\text{O}$ and $\delta^2\text{H}$ were within 0.26 ‰ and 0.3 ‰ of the uncontaminated values, respectively, despite the high level of contamination and without any pretreatment.

Company Presentations and Tutorials

Company Presentation 1

^{13}C and ^{18}O Isotope Effects Resulting from High Pressure CO_2 Cylinder Depletion

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An equilibrium isotope fractionation in the liquid-vapor system of CO_2 for C and O isotopes is well established (i.e. Grootes, et al., 1969, Z. Physik 221). C isotopes tend to be enriched in ^{13}C in the vapor phase and O isotopes tend to be depleted in ^{18}O . This observation has particular relevance in contemporary stable isotope laboratory practices due mainly to the advent of Continuous Flow-Isotope Ratio Mass Spectrometry (CF-IRMS). For ^{13}C and ^{18}O measurements, CF-IRMS relies almost exclusively on incorporating a high pressure cylinder of CO_2 as a calibrated internal reference gas. If this reference gas contains a liquid phase, the laboratory's ability to produce reliable isotope data will be dependent on whether the isotopic composition of the CO_2 changes during cylinder depletion. Intuitively, one may presume that as the liquid CO_2 within that cylinder decreases, the vapor produced from that liquid will change isotopically to reflect known isotopic fractionation between those phases. This work quantifies the isotopic effect for ^{13}C and ^{18}O as a function of CO_2 cylinder depletion. CO_2 vapor samples from a cylinder that contains both liquid and vapor phases will be taken regularly and measured for both ^{13}C and ^{18}O . CO_2 will be depleted during sequential sampling and resulting cylinder contents monitored gravimetrically. Observed isotopic effects (fractionation) of the vapor from the depleted CO_2 cylinder will be reflected in the ^{13}C and ^{18}O composition of that vapor. Thus the last remaining liquid within the cylinder will likely show the largest isotope effects in both ^{13}C and ^{18}O in the CO_2 liquid-vapor system. These data will be useful for CF-IRMS researchers that rely on high pressure cylinders for CO_2 reference gas.

Keywords: CO_2 , fractionation, liquid-vapor, depletion, enrichment

Tutorial 1 / Elementar Analysensysteme GmbH

Sample preparation and quality control for IRMS analysis

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Sample preparation and standardization is essential for all analytical work and therefore also for stable isotope work. The measuring errors don't only come from the instruments but also from all the steps before. General tips and tricks in sample preparation, analyzing and referencing strategies will be shown. Software utilities integrated in ionOS® and ArDB support the user with all their quality control tasks. Within ionOS all calculations (drift and blank corrections, multi-point calibration) can be performed on all datasets. ArDB performs quality control statistics calculations using the Shewart Tests which allows consistent testing of all data sets. One significant advantage of utilising ArDB for creating a database of analytical results as well as performing instrument quality control is to be able to validate the results of new/unknown samples in ArDB. By being able to scrutinize internal and external QC results alongside sample data allows the analyst to ensure that only robust data is used for the on-going research themes that they are pursuing.

Keywords: sample preparation, EA-IRMS, GC-IRMS, ionOS, ArDB

Tutorial 2/ Thermo Fisher Scientific GmbH

T 2.1 Introduction to isotope analysis of water and other liquids

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T 2.2 Merits of compound specific isotope analysis and structural identification

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T 2.3 Overview of analytical tools in biogeochemistry

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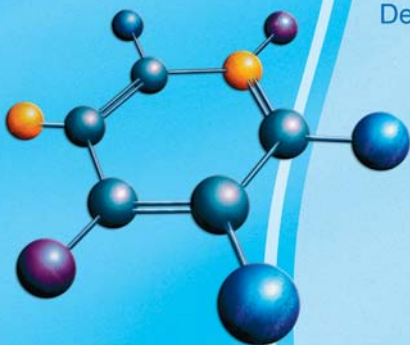
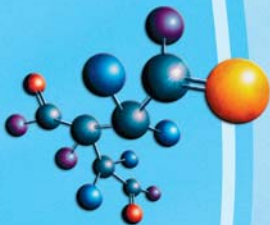
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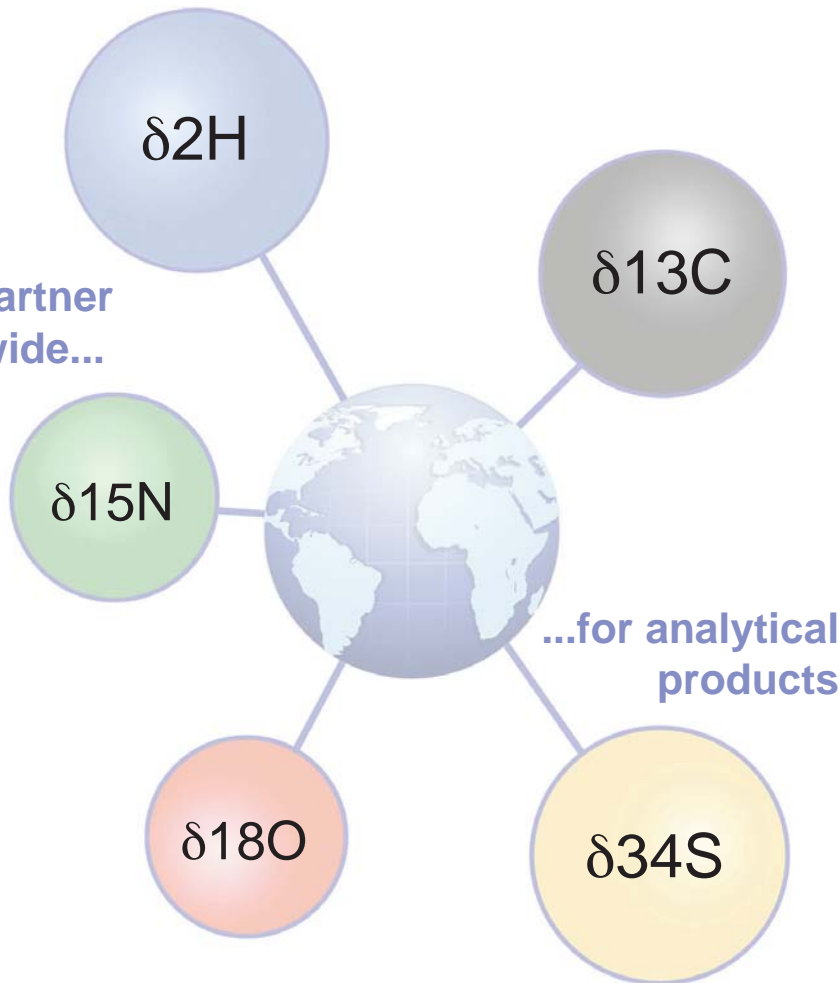
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