March 2022

Industry Newsletter

Section 3.2
Organic Geochemistry

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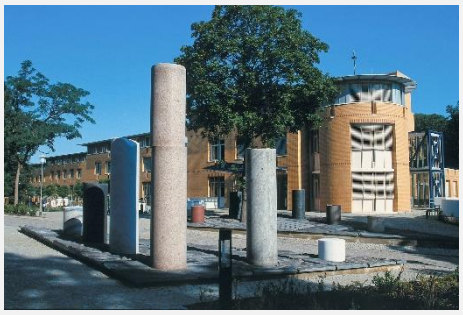

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Welcome to our latest Industry Newsletter, which has returned after a long pause since our former section Head, Brian Horsfield, retired in 2017. Here I would like to take the opportunity to thank Brian as well as Kai Mangelsdorf, who led the section during a transitionary phase, for giving me a smooth start as a new section head.

This newsletter appears in an irregular (but mostly annual) format and serves the purpose of keeping you informed about the activities and achievements of the GFZ organic geochemistry group, in view of opening a two-way avenue for scientific exchange. We would like to tap into your knowledge of latest developments, whereas you can guide our research with your particular needs and interests.

In this context it is important to note that our *Industry Partnership Programme* (IPP) is still active despite the currently challenging transition of the energy world towards renewables. In its next round, it offers a variety of projects that may be initiated with one or with multiple partners, and whose exact workplans will be developed together. Please take a look at the IPP proposal summaries for now and we will send more information in due course.

Today it is my pleasure to provide you with a brief review about our activities during the last years, ongoing efforts, and our vision for the next years.

Our latest publications are listed – please tell us if you would like to receive pdf files of the papers.

I hope you enjoy the read and will be pleased to answer any of your questions.

With best regards,

Christian Hallmann
Head of Section 3.2

The Industry Newsletter is published irregularly by Section 3.2. Please feel free to contact us about issues or topics that may be of interest for you. Comments and suggestions are welcome.

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News

NEW SECTION HEAD

Dear readers, colleagues, friends,

Many new faces have appeared in our section since the last newsletter and I would like to take this opportunity to briefly introduce myself. My name is Christian Hallmann, and I joined the GFZ organic geochemistry group in October 2020.

After studying Geology–Paleontology in Cologne, where I worked on petroleum migration indicators with Lorenz Schwark and Detlev Leythaeuser, I received a PhD from Curtin University in Perth under supervision of Kliti Grice, Ben van Aarssen and Andrew Murray. Research visits to RWTH Aachen (1D basin modeling), Shell E&P (Oman petroleum systems), the University of Newcastle upon Tyne (petroleum biodegradation) and Woodside Energy (Libya petroleum systems) strengthened my petroleum background. Following a postdoc as an Agouron Fellow at MIT, working with Roger Summons on Earth's oldest biomarkers, I became an independent research group leader at the Max-Planck-Institute for Biogeochemistry and worked in parallel as a lecturer at MARUM (University of Bremen), where I taught classes on geobiology and applied petroleum geochemistry.

From a research perspective my interests range from petroleum geochemistry (system analysis, biodegradation, molecular fractionation) via carbon cycle studies (organic preservation, diagenetic rearrangement, global redox, past climates) and a focus on Earth system evolution (paleobiogeochemistry, evolution of primary producers and organismic complexity) to biological questions of lipid biosynthesis and life in the deep subsurface. What combines all of these research lines is a profound questioning of the status quo and the attempt to use novel methods and innovative approaches to answer longstanding questions.

In this regard, my vision for our future research at GFZ is characterized by the desire to push the frontiers of organic geochemistry. Analytically we are exploring the use of high-resolution MS to determine clumped isotopes´ on larger hydrocarbon molecules and intramolecular isotope patterns—a young field with enormous potential. Further we are starting with molecular imaging using MALDI coupled to FT-ICR-MS to reveal minute stratigraphic biomarker anomalies and study mineral-organic interfaces at an unprecedented level. Lastly, we actively work with geneticists to gain an enhanced understanding of how the diagnosticity of particular fossil biomarkers may have changed through Earth history. I invite you to join us on this exciting journey and am looking forward to many fruitful collaborations over the coming years.

Yours sincerely,
Christian Hallmann

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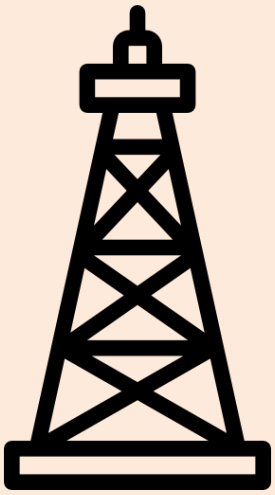
News

NEW IPP PROJECT PROPOSALS

Potential projects are scheduled to start in spring 2023. We here present conceptual 'containers' that can be discussed and adapted according to interests and sample availability. Please contact Hans-Martin Schulz if these are of interest.

1. Polars in reservoirs (PoRes)

Due to their polarity, petroleum NSO compounds are strongly affected by partitioning processes between aqueous brines, organic phases and mineral surfaces resulting in their fractionation during migration, reservoir filling and crude oil production. The polar composition of oils thus has a crucial impact on their physical properties such as API gravity, viscosity, wettability and phase/flow behavior. In particular wettability is an important reservoir parameter that is difficult to evaluate and to predict, yet its variation throughout reservoirs significantly affects production and may be steered by lateral and vertical heterogeneities of NSO compounds. Wetting behavior in typical three-phase systems (and the velocity of its changes, e.g. in response to production) depends, amongst others, on the activity of polar surfactants in the organic phase, which are still incompletely understood. It would be desirable if we could make enhanced qualitative projections on wetting and production behavior from the molecular composition of fluids, or even from source rock pyrolysates. The incredibly wide spectrum of polar NSO-moieties in petroleum fluids could never be adequately characterized using traditional GC-MS methods. Using ultra-high-resolution FT-ICR mass spectrometry in addition to conventional petroleum geochemistry we propose to study how heterogeneities in NSO compound compositions from different production horizons of conventional reservoirs can be linked to differences in fluid properties and finally production behavior. This may be paralleled by studying a suite of petroleum fluids in the lab by detailed characterization of their polar inventory, observing correlations to wetting behavior on standardized mineral surfaces by contact angle measurement, and studying molecular adsorption behavior on powdered mineral surfaces. We aim to obtain a better understanding of those components or compound classes that efficiently initiate changes in wettability and affect production efficiency



IPP

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Our Industry Partnership Program (IPP) continues with four new topics that can be worked into proposals, depending on interest and feedback. The projects are envisaged to start in spring 2023 and can be constructed as 3-year PhD projects or 2–3 year postdoctoral projects. The eventual annual cost boils down to the number of consortium partners. We will be in touch soon with a formal invitation to gauge interest in IPP participation and the opportunity to find out more during a video conference-seminar.

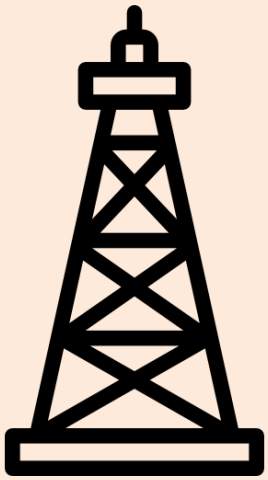
News

2. FT-ICR-MS as an all-in-one tool for petroleum analysis

The molecular-level determination of thermal maturity, biodegradation stage, secondary factors such as water washing, adsorptive and evaporative fractionation, determination of organofacies and source lithofacies, as well as oil-oil and oil-source correlation are still mostly performed on the basis of GC-MS analyses, typically requiring liquid chromatographic cleanup of samples and multiple analytical runs. Petroleomic analysis of whole oils or total lipid extracts using high-resolution FT-ICR-MS carry significant advantages of minimized sample workup and—theoretically—the potential to gain all the aforementioned information in one analysis. Previous IPP projects focusing on thermal maturity parameters and on migration fractionation have yielded successful results in this direction, whereas preliminary facies information on source rock pyrolysates looks highly promising. We here aim to study a large set of oils and source rock extracts in order to systematically evaluate if source rock facies and maturity can be deduced from one-shot analysis of the polar constituents of whole oils.

3. Organo-metal control on petroleum formation and composition

Nickel and vanadium abundances in organic matter have been analyzed for a long time and their ratio has been used as a molecular redox and correlation parameter. However, many more transition metals can be bound into organic complexes and the high catalytic activity that characterizes these metals may have a measurable effect on petroleum generation. Yet exceedingly little is known so far on the metal content, its pattern and effect of petroleum and kerogen. This project aims to generate baseline information on the presence and effect of organo-complexed metals. In parallel to developing preparative methods to isolate kerogen without leaching metals, we will engage in pyrolysis experiments with metal-impregnated kerogen isolates in order to determine the effect of metal type and abundance on source rock kinetics and subtle differences in the composition of resulting fluids. Lastly we may evaluate the utility of metal content and distribution as a correlative tool across a range of thermal maturities. This explorative project will reveal the utility of studying metals in kerogen and oil, with the aim of using this info as a corrective and possibly correlative parameter.



IPP

We gratefully acknowledge funding that comes from the participating industry members. Co-operation with these companies also allows access to valuable samples and geological data for our research.

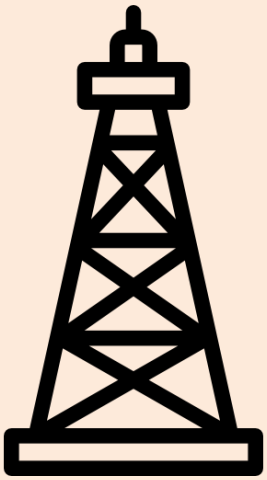
If the listed topics are of potential interest to you, or if you would be interested after modification, possibly with specific highlights or particular questions, please contact Hans-Martin Schulz and we will be happy to discuss your interests, needs and possible cooperation framework.

News

4. Clumped isotopes in petroleum

The stable carbon or hydrogen isotope analysis of individual molecules has become common practice in organic geochemistry. What is rarely studied is the isotope anatomy of molecules: the majority namely does not contain any heavy isotopes. On the contrary, molecules that are substituted with two heavy isotopes (e.g. 2x ^{13}C, 2x D or ^{13}CD), so-called 'clumped' isotopologues, are rare but may carry valuable information on the formation conditions of a molecule under thermodynamic equilibrium. For example, a clumped methane thermometer is well established by now. Although we broadly understand the range of thermal maturity under which compounds are released from the kerogen by cracking, obtaining a temperature range per compound could yield very valuable information on basin dynamics (e.g. fast vs. slow subsidence), petroleum mixing and secondary cracking. Thus far, clumped isotope analysis is mostly studied on gases and volatiles, and represents a very young, yet fast growing field.

Using ultra-high-resolution Orbitrap mass spectrometry present at GFZ, we can separate clumped isotope mass peaks, allowing us to determine clumping in whole molecules and molecular fragments, as long as we can isolate and ionize the analytes. In this project we aim to explore stable carbon isotope clumping in larger petroleum hydrocarbons, in order to evaluate the utility of this parameter. The project will initially focus on alkanes and polyaromatics in non–source rock extracts of differing maturity (to avoid expulsion effects), alkanes in petroleum samples, and alkanes generated by pyrolysis experiments from authentic precursor standards and from kerogen under different temperatures and with different matrices. Analytes will be isolated using preparative HPLC and GC, followed by Orbitrap-based stable isotope analysis. We anticipate the results to form the basis for the potential development of a new parameter informative about physical conditions of petroleum generation and cracking.



IPP

Also note that we may be able to accommodate different topics or project-studies on individual petroleum systems and that service-analysis is possible if woven into a (even small) project.

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IMOG

The first fully-virtual **International Meeting on Organic Geochemistry (IMOG)** took place in September 2021. Our section was present with eight talks given, including three plenary talks*, and several poster presentations and session chairs.

IMOG talks

Hoshino, Y., Nettersheim, B., Hallmann, C., Vinnichenko, G., Brocks, J., Gaucher, E. (2021): 2-METHYLHOPANES AS UNIQUE CYANOBACTERIAL BIOMARKERS BEFORE 1.2 BILLION YEARS AGO.

*Ismail, S., Vieth-Hillebrand, A., Pötz, S., Noah, M., Mangelsdorf, K. (2021): DECIPHERING THE INPUT FROM FOSSIL AND RECENT ORGANIC CARBON TO SOILS IN RECULTIVATION SITES IN LUSATIA, GERMANY.

Lopes Martins, L., Schulz, H.-M., Noah, M., Pötz, S., Portugal Severiano Ribeiro, H. J., Feitosa da Cruz, G. (2021): NEW PALEOENVIRONMENTAL PROXIES FOR THE PERMIAN IRATI BLACK SHALES BASED ON ACIDIC O1 AND O2 COMPOUNDS ASSESSED BY FT-ICR-MS.

*Mahlstedt, N., Noah, M., Horsfield, B. (2021): ASSESSING SOURCE ROCK ORGANOFACIES USING THE FT-ICR MS AMENABLE NSO-COMPOUNDS INVENTORY OF PYROLYSATES

Mangelsdorf, K., Adler, K., Liu, Q., Kämpf, H., Bussert, B., Plessen, B., Schulz, H.-M., Lipus, D., Krauze, P., Horn, F., Wagner, D., Alawi, M. (2021): DEEP MICROBIAL SIGNATURES IN TERTIARY SEDIMENTS OF THE HARTOUŠOV CO2 MOFETTE SYSTEM, NW BOHEMIA -

*Pötz, S., Liu, Y., Vieth-Hillebrand, A., Yang, S., Magnall, J. M., Gleeson, S. A., Schulz, H.-M. (2021): THE KUPFERSCHIEFER IN SPREMBERG, EAST GERMANY: SIGNALS OF ORGANIC MATTER ALTERATION FROM HYDROGEN ISOTOPES AND NSO COMPOUNDS.

Sakai, L., Pudenzi, M. A., do Nascimento, C. A., Schulz, H.-M., da Cruz, G., Lopes Martins, L. (2021): SIGNIFICANCE OF ACIDIC POLAR SPECIES ASSESSED BY FT-ICR MS TO REVEAL GEOCHEMICAL INFORMATION OF OILS FROM THE SERGIPE-ALAGOAS BASIN.

Schulz, H.-M., Krüger, D., Wagner, D., Yang, S., Schovsgo, N. H., Noah, M., Panova, E. (2021): ORGANIC MATTER OCCURRENCE AND ALTERATION IN THE URANIUM-RICH ALUM SHALE FORMATION: IMPLICATIONS FOR MICROBIAL ACTIVITY.

EAGE

Parallel to—and as an integrated part of—IMOG the first fully-virtual **3rd EAGE Workshop on Petroleum Geochemistry in the Middle East** also took place in September 2021. GFZ's Hans-Martin Schulz acted as co-chair in the Technical Committee.

New professorship

Hans-Martin Schulz was appointed visiting professor at Changsha University (China) in 2021.

Hans-Martin Schulz

More news here:
https://www.gfz-potsdam.de/en/section/organic-geochemistry/overview/

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News

CHANGES, COMINGS AND GOINGS

Brian Horsfield, former head of our section, retired in 2017. Since then he has remained active as a scientific advisor to GFZ and continues his work as CEO of GeoS4, a GFZ spin-off. The recently concluded IPP projects concerning polar compounds in fluid inclusions as geochemical tracers (PIFI), the development of a rapid MSSV method for releasing bound biomarkers (QBB), and utilising NSO-compounds for assessing migration- and production-related fractionations (P'Move) were conceived by him, and run jointly by GFZ and GEOS4. New joint ventures are in the development stage.

Brian Horsfield

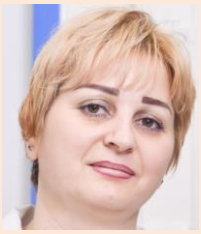
Yosuke Hoshino, PhD in Geobiology at Macquarie University (Sydney), worked as PostDoc at the Georgia Institute of Technology and Georgia State University (Atlanta, USA), Max Planck Institute for Biogeochemistry (Bremen, Germany), and as Opt-device engineer at Shimadzu Corporation (Kyoto, Japan). His research focus at GFZ will be the combination of geochemical lipid biomarker analyses and molecular analyses of associated biosynthesis pathways to resurrect ancient biochemistry in the geological context and elucidate the evolution of life at a molecular level.

Yosuke Hoshino

Maxime Julien studied biochemistry and received his PhD in Analytical Chemistry from the CEISAM Laboratory (University of Nantes, France) in 2015, and worked since last year as a Postdoc at the Tokyo Institute of Technology. Maxime joined our group in 2021, and is a specialist on the ^{13}C position-specific isotope analysis (PSIA) of organic compounds. His work at GFZ will focus on isotope signatures in modern and ancient ecosystems, and the development of a new PSIA technic using high-resolution magnetic resonance Mass Spectrometry (MR-MS) to study fossil lipids extracted from rocks to unravel their biological origin and to reconstruct the metabolic evolution over the course of Earth history.

Maxime Julien

Shirin Ismail completed her PhD thesis in 2011 (Sedimentology and Petroleum Potential of the Late Cretaceous Shiranish Formation in the Euphrates Graben, Syria), and worked as a lecturer at Aleppo University. Since 2019 she is a PostDoc in our section, funded by the Philipp Schwartz initiative of the Alexander von Humboldt foundation. Her research topic is “Using ultrahigh resolution mass spectrometry to decipher the input from different organic carbon pools to the soil organic matter in opencast mining reclamation sites: A case study from Lusatia”.



Shirin Ismail

Nicolaj Mahlstedt is a long-standing senior guest scientist at GFZ. His current research combines classical pyrolysis approaches with FT-ICR MS to unravel the common structural entities traversing kerogen, polar compound and hydrocarbon compositions. He leads GEOS4’s activities concerning the compositional kinetic modelling of primary and secondary petroleum-forming reactions, and utilising FT-ICR MS as a facies and fractionation tracer tool in shale resource plays. He was the principal investigator of the IPP P'Move sub-project P'Move-unconventionals.

Nicolaj Mahlstedt

News

CHANGES, COMINGS AND GOINGS

Mareike Noah Biogeochemical completed her PhD thesis in 2017 ("Process studies on oil sand tailings used for land reclamation in Alberta, Canada") and will start working again on a re-entry post. Her main focus will be on calibrating FT-ICR-MS data into quantitative results.

Mareike Noah

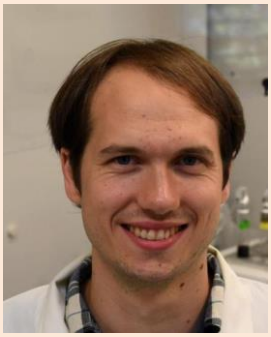
Arne Leider received his PhD from the University of Bremen in 2012. Since then, he worked as a PostDoc in the Organic Paleobiogeochemistry group, affiliated with the Max Planck Institute for Biogeochemistry (Jena). His topic was tracing the co-evolution of life and depositional environments during the Precambrian era by evaluating contamination risks, as well as the detection and preservation potential of biomarkers in organic-poor sedimentary rocks as old as 3.4 billion years. He joined our section in 2021, and focuses on the thermal stability of ironhydroxide-Dissolved Organic Matter (DOM) complexes to investigate their potential role for the atmospheric oxygen balance of early Earth. This work is funded by the German Science Foundation within the framework of SPP 1833: Building a Habitable Earth.

Arne Leider

Ilya Bobrovskiy received his PhD from ANU Research School of Earth Sciences in Canberra (Australia), where he worked with Jochen Brocks on the fossilization of soft bodied organisms and on fossil lipids in individual preserved fossils of the Ediacara biota. After a PostDoc at CalTech, he received a fellowship from the Branco-Weiss foundation, with which he joined our section. At GFZ, he will continue to work on the evolution of animals and algae and focus on compound-specific and position-specific stable carbon isotope analysis in fossil lipid biomarkers.

Ilya Bobrovskiy

Benjamin Nettersheim received his PhD from the Australian National University in Canberra. Under the guidance of Prof. Brocks, he analysed world's oldest biomarkers in the framework of CSIRO's 'Organic Geochemistry of Mineral Systems Cluster'. He then joined the Max Planck Institute for Biogeochemistry as an Agouron Fellow. As an independent postdoc in the Hinrichs Lab at the University of Bremen, he works on the mass spectral imaging of geological samples using laser-desorption-ionisation coupled to ultra-high-resolution FT-ICR-MS and teaches classes in molecular geobiology and applied petroleum geochemistry. As a GFZ guest scientist and future staff, he enhances our mass spectral imaging expertise.



Benjamin Nettersheim

GFZ Helmholtz Centre Potsdam

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STUDENT NEWS

A number of PhD students have finished their PhD thesis, and left the group:

- Nana Mu, now scientist at the China University of Geosciences in Beijing,
- Yaling Zhu, now scientist at the School of Earth Sciences at the Yangtze University in Hubei (China),
- Janina Richter, Helmholtz Open Science Office
- Shengyu Yang is working as associate professor at the China University of Petroleum in Qingdao,
- Yuanjia Han became a full professor of petroleum geochemistry at the China University of Geosciences in Wuhan,
- S. Hossein Hosseini joined the Department of Geoscience at the University of Calgary (Canada) as Postdoctoral Associate,
- Ricardo Ruiz Monroy joined a consultant company in Bogota (Colombia),
- Volker Ziegs became employee at the Hanseatisches Umwelt-Kontor GmbH (Lübeck, Germany), and
- Sascha Kuske moved to GuD Geotechnik und Dynamik Consult GmbH (Potsdam).

Current PhD students are:

- Huiwen Yue,
- Karsten Adler,
- Alessio Leins,
- Roman Feal, and
- Mostafa Nasr Monged.

Details about current PhD projects can be found here:

https://www.gfz-potsdam.de/en/section/organic-geochemistry/projects/

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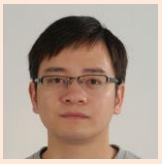
News


Nana Mu


Yaling Zhu


Shengyu Yang


Yuanjia Han


Janine Richter


Sascha Kuske


Ricardo R. Monroy


Karsten Adler

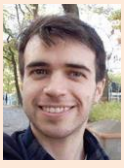

Volker Ziegs


Hossein Hosseini


Huiwen Yue


Mostafa Monged


Alessio Leins


Roman Feal

Helmholtz research

THE HELMHOLTZ RESEARCH APPROACH

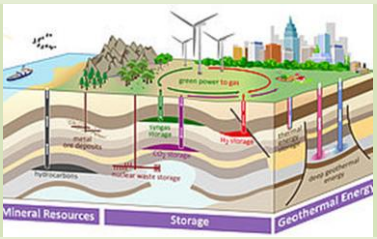
As a member of the Helmhotz Association, GFZ is commited to working within the framework of an overarching Helmholtz Research Programme "Changing Earth - Sustaining our Future" which spans the period 2021–2027.

In this context, GFZ is engaged in the Research Field "Earth & Environment" in which seven Helmholtz centres have joined forces. Here, one of our two research foci is (Topic 8) "Georesources for the Energy Transition and a High-Tech Society", which is coordinated by GFZ. This topic will address one of the most fundamental challenges facing society: securing the future supply of energy and raw materials needed to sustain our 21st century infrastructure, to enable the transition from fossil and nuclear energy to renewables. In doing so, the aim is to achieve the targeted reduction of CO_2 emissions and also to support a growing circular economy. During this transition, geoscience solutions to sustainable energy, raw materials supply, and subsurface storage of waste will be required, with a growing emphasis on the deep subsurface.

Our section will contribute to the following research foci:

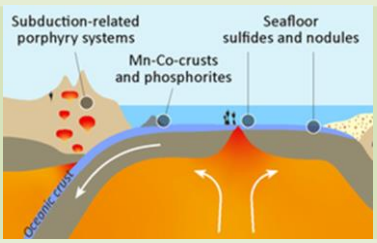
8.1. Geoenergy

- Geothermal energy
- Subsurface storage of energy products (e.g., heat, synthetic gas, Hydrogen)
- A cleaner, more efficient use of carbon resources



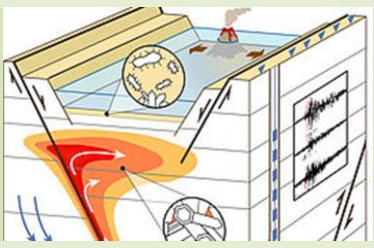
8.2 Raw materials

- Constraining the key processes that form high value massive sulfide deposits in sedimentary basins
- Designing new observational, experimental and simulation platforms to assess the coupled thermal, hydraulic, mechanical, chemical, and biological controls on resources



8.1. Integrating Geoenergy and Mineral Systems

- Developing new system models that integrate coupling, feedback and cascading effects into conventional THMC models of fluid flow, reactive transport and permeability evolution.
- This includes studying the role of organic-inorganic and microbial interactions, which can be particularly important for the formation of mineral and energy resources in sedimentary basins, and for developing strategies for energy production and storage potential.



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Helmholtz research

Research snapshot 8.1 Geoenergy

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Reflect

(Redefining geothermal fluid properties at extreme conditions to optimize future geothermal energy extraction)

The efficiency of geothermal exploitation depends heavily on the behavior of the fluids that transfer heat from the subsurface to the power plant, which is determined by their chemical and physical properties. Regarding the chemical properties, there are still few data on the occurrence of organic compounds in geothermal fluids. As part of the REFLECT project, several fluids from different geothermal sites (mainly Europe) were sampled to characterize DOM. The aim of this work is the interpretation of the data with respect to various site parameters such as reservoir formation, temperature, and depth. A better understanding of the origin of organic compounds in geothermal sites and their impact on geothermal fluid physical and chemical properties might contribute to future studies aimed at optimizing geothermal energy extraction.

Alessio Leins
(PhD student, Reflect project)

Research snapshot 8.2 Raw materials

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Rock-fluid-microbe interactions

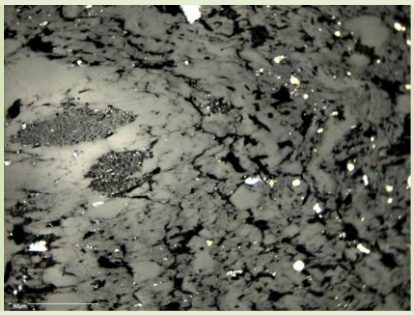
Complex interactions take place in the geological underground. These interactions are part of interrelated networks of processes, and the participating compounds are the rock matrix, aqueous fluids, organic solids and liquids, and –moreover- microbes.
Currently, two topics fall under this research direction:

Uranium-OM-fluid- microbe interactions

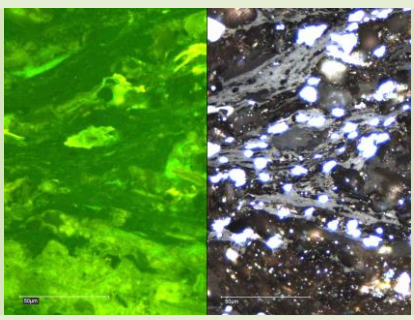
The influence of α-particles released from the decay of ^{238}U on the composition and petroleum potential was heavily studied in the Cambro-Ordovician Alum Shale from Northern Europe. Curently, we are investigating the remaining potential for microbial domains and whether there is potential for microbial gas formation.

OM-fluid- microbe interactions as controls of metallogenesis of Upper Permian Kupferschiefer

Up to now, the processes how metals were enriched are a matter of debate, and also how metal zonations were caused. Here, new conceptual approaches are being tested ranging from hydrogeochemical modelling over microbiological fingerprinting.



Reflected light image of an uranium-rich Alum Shale sample.



UV (left) and reflected light image (right) of Kupferschiefer.

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Research highlights

Solid H_2S at low temperature

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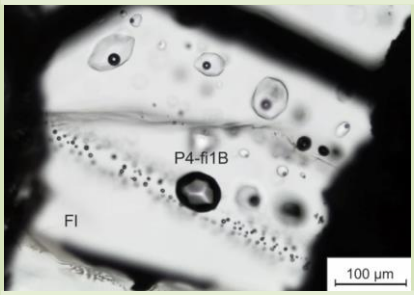
C–O–H–N–S-bearing fluids are known as one of the most challenging geochemical systems due to scarcity of available experimental data. H_2S-rich fluid systems were recognized in a wide array of world-class mineral deposits and hydrocarbon reservoirs. Here low-temperature ($T \geq -192$ °C) phase transitions observed in natural CH_4–H_2S–CO_2–N_2–H_2O fluid inclusions is described, which are modeled as closed thermodynamic systems and thus serve as natural micro-laboratories representative of the C–O–H–N–S system. For the first time, we document solid–solid H_2S ($\alpha \leftrightarrow \beta \leftrightarrow \gamma$) transitions, complex clathrates and structural transformations of solid state H_2S in natural inclusion gas mixtures. The new data on Raman spectroscopic features and a complete sequence of phase transition temperatures in the gas mixtures contribute to scientific advancements in fluid geochemistry. Enhanced understanding of the phase equilibria in the C–O–H–N–S system is a prerequisite for conscientious estimation of P-T-V-X properties, necessary to model the geologic evolution of hydrocarbon and mineral systems.

Sośnicka, M., Lüders, V. Phase transitions in natural C-O-H-N-S fluid inclusions – implications for gas mixtures and the behavior of solid H2S at low temperatures. Nature Communications 12, 6975 (2021).



H_2S–CO_2– Microphotograph of analyzed CH4–H2S–CO2–N2–H2O fluid inclusions in FIA1 and FIA2 hosted in fluorite (FI).

Lithofacies controls NSO composition

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Lithofacies influences the composition of NSO (nitrogen-, sulfur- and oxygen- containing) compounds in unconventional petroleum systems, and has been investigated using examples of biogenic carbonate-rich Niobrara Shale, biogenic quartz-rich Barnett Shale and detrital clay-rich Posidonia Shale. The chosen sample sets all contain Type II marine kerogen in the peak–late oil window. Solvent extracts were analyzed using Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR-MS), combined with atmospheric pressure photoionization in positive ion mode ((+)-APPI) and electrospray ionization in negative ion mode ((−)-ESI). Covering source and reservoir units, the results study furthermore enables tracing the impact of lithofacies on primary petroleum migration within the Niobrara and Barnett shales.

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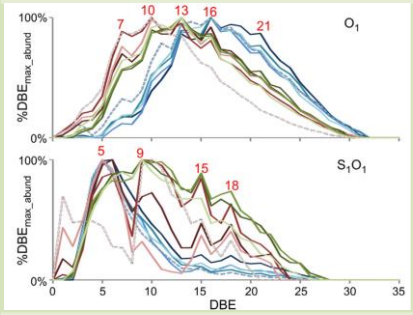

DBE distributions of (+)-APPI ionizable O1 and S1O1 classes, normalized to the most abundant DBE class (DBE_{max_abund}) in each compound class.

March 2022

GFZ Helmholtz Centre Potsdam

Industry Newsletter February 2022
Section 3.2 Organic Geochemistry

Just finalized

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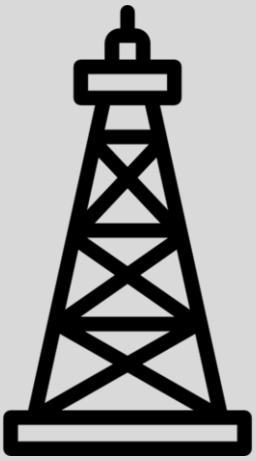
Industry partnership programme (IPP) projects

We developed two new analytical methods within projects funded by our IPP programme. The first one allows the analysis of NSO-compounds in oil-bearing fluid inclusions applying the FT-ICR-MS technique. This method provides insights into thousands of compounds not accessible before and can give, for instance, valuable information on reservoir charge, leakage histories and compositional changes during oil migration processes. The second method is a pyrolysis procedure based on the Micro Scale Sealed Vessel (MSSV)-technique using a mix of a catalyst and hydrogen-donor. This method enables the analysis of biomarkers bound to the kerogen matrix from small sample amounts and can provide crucial information on petroleum properties when the original oil phase is deteriorated by e.g. contamination and biodegradation. Furthermore, we investigated the properties and petroleum generation kinetics of source rocks in the South Yellow Sea Basin offshore eastern China.



IPP

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IRTG StRATEGY

(International Research and Training School Surface processes, Tectonics and Georesources: The Andean foreland basin of Argentina)

Part-1: Organic geochemical characterization of the Yacoraite Formation (NW-Argentina)-paleoenvironment and petroleum potential/ PhD thesis by Ricardo Ruiz (2021)
The Yacoraite Fm. (Maastricht-Danian; Cretaceous Salta Rift Basin, NW Argentina) was deposited under changing conditions (from marine, lacustrine to hypersaline), and has a potential to generate mainly low-sulfur oils. Taking into account data from bulk kinetics enabled basin modelling scenarios for the calculation of the various transformation ratios and PVT properties.

Part-2: Quantification of Central Andes growth and erosion in relation to sedimentation in the Neuquén and Colorado basins - a source-to-sink approach/ Ongoing PhD project by Roman Feal
The aim of the project is to study the evolution of the Neuquén and Colorado basins using properties of Late Cretaceous sediments deposited adjacent to the orogenic belt during the deformation.

Conceptually, a geochronological study utilizing U-Pb dating of detrital zircons and a provenance analysis of synorogenic strata shall be carried out. The results shall be integrated in a regional tectonic model to better understand the Andean Orogeny at this latitude.

DFG

March 2022

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Industry Newsletter February 2022
Section 3.2 Organic Geochemistry

Our instrumentation

Thermovaporisation-(GC-MS)
Analysis of volatile hydrocarbons in source rocks, bitumens & crude oil
Whole oil characterization

Source Rock Analyzer
Kinetic studies

Elemental analyses
Determination of CHNS in solid samples

Pyrolysis-(GC-FID./ GC-MS)
Open and closed system (MSSV) pyrolysis
Pyrolysis-GC-IRMS
Thermodesorption and-Pyrolysis

Extraction
Soxhlet extraction
Ultrasonic extraction
Flow-blending extraction
Accelerated Solvent Extraction (ASE)

Preparative liquid Chromatography
Medium Pressure Liquid Chromatography (MPLC)
Heterocompound-Medium Pressure Liquid Chromatography (HMPLC)
Prep High Performance Liquid Chromatography (HPLC)

Gas Chromatography (GC)
Flame Ionization Detector (FID)
Headspace-Sampler (HS)

Gas Chromatography-Mass Spectrometry (GCMS)
Electron Impact Ionization (EI)
Chemical Ionization (CI)
TOF High Resolution Mass Spectrometry (HRMS)
QqQ Mass Spectrometry-Mass Spectrometry (MS-MS)

Analytical Liquid Chromatography
Liquid Chromatography Organic Carbon Detection (LC-OCD)
Normal & reversed phase HPLC-MS
Electrospray Ionization (ESI)
Atmospheric Pressure Chemical Ionization (APCI)
Orbitrap High Resolution Mass Spectrometry (HRMS)
QqQ Mass Spectrometry-Mass Spectrometry (MS-MS)

Isotope Ratio Monitoring-Gas Chromatography-Mass Spectrometry (IRM-MS)
Compound-specific carbon and hydrogen isotope analysis
Liquid chromatography and gas chromatography interfaced

Fourier transformation ion cyclotron resonance mass spectrometry (FT-ICR-MS)
Ultrahigh resolution mass spectrometry (UHRMS), Direct infusion using electrospray ionization (ESI), Atmospheric pressure photoionization (APPI) Atmospheric pressure chemical ionization (APCI)
Crude oils, bitumen, rock/sediment extracts, asphaltenes, water samples

Ion Chromatography
Organic acids in water samples

Infrared Microthermometric Equipment
Fluid inclusion analysis

Organic Petrology
Maceral analysis
Vitrinite reflectance

Analytical capabilities

Analytical equipment

Our analytical chemistry laboratory is furnished with state-of-the-art equipment and is constantly being modernized to support the increasing demand for high-resolution geochemical analyses. Please contact us if you wish to have more details regarding certain applications.

Basin Modeling

Modeling Tools:

- Petromod 3d
- EarthVision
- Kinetics 2005
- Petrel
- PVTsim
- Feflow

BugLab during a cruise in the Barents Sea (Image GFZ)

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