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H2020-MSCA-ITN-2019
Grant Agreement No: 860497

GMOS-Train

Global Mercury Observation Training Network in Support of the Minamata Convention

Deliverable D7.9

"Training materials from Winter School 3: "Global Hg modelling framework and policy making""

Start date of project: 01.01.2020

Duration: 60 months

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Acronyms and Abbreviations

PROJECT BENEFICIARIES:

AMU	Université d'Aix-Marseille – Mediterranean Institute of Oceanography, France
CNR IIA	Institute of Atmospheric Pollution Research of the Italian National Research Council, Italy
CNRS	Centre National de Recherche Scientifique, France
HEREON	Helmholtz-Zentrum hereon GmbH, Germany
IFREMER	French Research Institute for Exploitation of the Sea, France
IOS	Institute for Environmental Protection and Sensors, Slovenia
JSI	Jožef Stefan Institute, Slovenia
PSA	PS Analytical, United Kingdom – project exit date 1.7.2020
UGA	Université Grenoble Alpes, France
UPPA	Université de Pau et des Pays de l'Adour, France
SU	Stockholm University, Sweden

PROJECT PARNTER ORGANISATIONS:

AMAP	Arctic Monitoring and Assessment Programme, Norway
AUTH	Aristotle University of Thessaloniki, Greece
EEB	European Environmental Bureau, Belgium
Harvard	Harvard University, USA
IPSJS	International Postgraduate School Jožef Stefan, Slovenia
IRD	Institut de Recherche pour le Développement, France
MIT	Massachusetts Institute of Technology, USA
PSA	PS Analytical, United Kingdom – project exit date 1.7.2020
SPRS	Swedish Polar Research Secretariat, Sweden
Tekran	Tekran, Canada
UBL	Université Bretagne Loire, France
UNEP	United Nations Environmental Programme, Switzerland
UPS	Université Paul Sabatier, France
VSL	Dutch National Standard Laboratory, The Netherlands

ESR	Early Stage Researcher
IPR	Intellectual Property Rights

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Executive Summary

In the time from 6th February to 6th March 2023 the GMOS-Train PhD Winter School 3: "Global Hg modelling framework and policy making" was organized by the Helmholtz Centre Hereon and held in Hamburg, Germany. The monthly event consisted of three parts. Part I: Lectures on modelling, Part II: Hands-on Hackathon, and Part III: Lectures on Policy Making.
In total 8 GMOS-Train MSC ITN ESRs participated in person, while the remaining ESRs could participate remotely. In person participation was influenced by visa and travel restrictions and the resignation of ESR12. In summary, the event was a great success and all participating ESRs produced presentable outcomes. In this report, we give an overview of the course, the projects of the individual ESRs, and the results thereof.

Table of Contents

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1. Introduction

As indicated in the name, the Winter School on "Global Hg modelling framework and policy making" has two distinct purposes. First and foremost, the aim was to educate PhDs with an analytical background in basics of the research fields of Informatics, Programming, and Modelling, including hands on training with state-of-the-art numerical modelling methods. Thereby, each ESR was supposed to design and perform a model study related to their work in GMOS-Train. Moreover, the course's policy part was designed to educate ESRs how models can be and are used to answer questions of societal relevance and to inform policy decisions. For this, we invited renowned scientists and representatives of international organizations, which could act as career examples for the early career scientists. In this regard, we put special emphasize on the diversity of speakers. In this report we give a detailed account of the course, its preparation, execution, and results. The course was organized by Dr. Johannes Bieser and Dr. Martin Ramacher from the Helmholtz Centre Hereon, Germany. During the hands-on sessions two PhDs from their junior research group "Multi-Compartment Modelling – from Emissions to Exposure (MCMEE)" were acting as additional tutors for the ESRs. A schedule of the Winter School can be found in Annex A of this Report.

2. Preparation

Preparatory work for the course already began well in advance of the actual event. Most ESRs did initial secondments at Hereon supervised by Dr. Johannes Bieser (Table 1). Besides the presented secondments there were in-person discussions taking place during the annual meeting (2022) in Abisko, Sweden. Moreover, the regular (weekly) WP5 "Multi Media Modelling" online meetings were used for additional discussions with ESRs 1, 13, 14, and 15. With ESR5, there were additional discussions during panel meetings.

#	Month	Duration	Topic
ESR1	M29	4 weeks	Training with the atmospheric model ICON-ART
ESR4	M35	2 weeks	Programming course: Python for beginners
ESR5	M32	4 weeks	Setup of database of incubation experiments and development of methodology
ESR6	M22	1 week	Introduction to FABM model interface
ESR7	M23	5 weeks	Helmholtz Coastal Summer School (4 weeks) and introduction to FABM model interface (1 week)
ESR8	M36	2 days	Remote meeting on box modelling methodologies
ESR13	-	-	PhD located at host institution
ESR14	-	-	PhD located at host institution
ESR15	M29	4 weeks	Training with the atmospheric model ICON-ART

Table 1: List of in-person participants and description of preparatory work.

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2.1 Gender balance

The GMOS-Train MSC ITN commits to actively support underrepresented groups and to female researchers in their career. During the organization of the event, we also actively recruited non-cis-male lecturers where possible. The gender balance of participants was 5 female / 3 male. The gender balance of lecturers was 7 male, 3 female, 1 non-binary. These numbers show, that while traditionally being a male dominated field the gender balance seems to change with age. To commemorate the role of women in the history of computer science, the event was declared under the patronage of Ada Lovelace (1815-1852), the first programmer.

Fig. 1: Ada Lovelace painting at the Hamburg Hackathon

3. Hackathon

3.1 Week I: Lectures on modelling

The first week of the event took place at the Centre for Marine and Atmospheric Sciences (ZMAW). On day one each ESR presented their data and research question to be worked on during the Winter School. The first week had a strong focus on lectures, beginning on Tuesday with basic lectures on informatics, programming, and a general introduction to modelling. In the afternoon, the group visited the nearby German Climate Computing Centre (DKRZ) where the high performance computer (HPV) "levante" is located, on which the participants would eventually work. At DKRZ, Dr. Michael Boettcher and Dr. Anna Fuchs gave lectures on high performance computing. The day ended with a visit of the supercomputer itself (Fig. 2).

Fig. 2: (left) Participants inside the levante HPC and (right) in front of the German Climate Computing Centre.

On Wednesday, lectures focused on applied environmental modelling. Starting with the history of numerical modelling and development of meteorological models over the last century since their first inception by Vilhelm Bjerknes in the early 20th century. Lectures continued to cover major areas of geophysical and biogeochemical modelling. Highlights were presentations by Dr. Oleg Travnikov, a renowned Hg modeller from the UN MSC-east centre and Prof. Dr. Hans von Storch, founder and former Director of Hereon's Institute for Coastal Research (Fig. 3).

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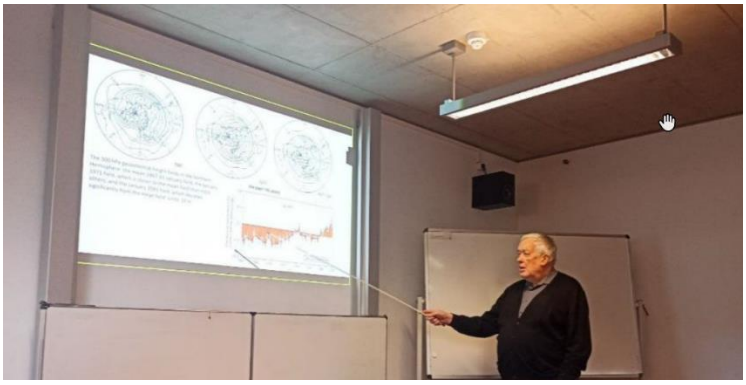

Fig. 3: Prof. Dr. Hans von Storch explaining the Nobel prize winning ideas of Klaus Hasselmann, former Director of the Max-Planck Institute for meteorology.

The final two days of the week were used to define the research question each ESR would work on during the hands-on Hackathon part of the Winter School. Each ESR was asked to produce an expose outlining his/her aim and methodology to reach it (Table 2).

#	Research question	Model	Development
ESR1	What are drivers of interhemispheric Hg transport?	Atmospheric chemistry transport model ICON-ART	Implementation of special tracer species into ICON-ART and setup of source-receptor relationships.
ESR4	What role do hydrothermal vent emissions play in the natural Hg cycle?	Marine circulation model ICON-O (Korn et al. 2022)	Development of an comprehensive emission inventory for hydrothermal vent Hg emissions.
ESR5	What mechanisms are able to reproduce observed Hg dynamics/kinetics? Can reaction rates for marine Hg species be determined additively from selective incubation experiments?	1D ocean column model with Hg chemistry module GOTM-MERCY (Bieser et al., 2023)	Development of a generalized ODE optimization model and definition and testing of chemical mechanisms. Implementation of new reaction rates into MERCY.
ESR6	What mechanisms are able to reproduce dynamics of observed Hg partitioning between dissolved and particulate phase?	1D ocean column model with Hg chemistry module GOTM-MERCY (Amptmeijer et al., 2023)	Development of a generalized ODE optimization model and definition and testing of partitioning mechanisms. Implementation of new partitioning rates into MERCY.
ESR7	What role does terrestrial organic matter play for marine Hg cycling?	Biogeochemical marine Hg model MECOSMO (Bieser and Schrum, 2016)	Implementation of riverine organic matter input fields into MECOSMO. Sensitivity analysis on log(kd) values.
ESR8	What effect does our changing climate have on Hg in Arctic permafrost?	Box modelling approach	Development of a conceptual box model for Hg cycling in Arctic permafrost.
ESR13	Do feeding strategies impact Hg accumulation in marine biota?	1D ocean column model with Hg chemistry module GOTM-MERCY (Bieser et al., 2023) (Amptmeijer et al., 2023)	Implementation of different feeding strategies for macro benthos species. Model sensitivity analysis.
ESR14	Can we deduce marine Hg emissions from long-term datasets?	Mathematical approach	Employment of backward trajectories and mathematical tools to extract the marine signal.

Table 2: ESR work plan. Models: List of in-person participants and description of preparatory work.

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3.2 Week II: Literature research, data curation, and method development

At the beginning of the second week, the group switched location. The hands-on Hackathon event was located on the 3rd floor of the 4WALLS co-working space. There, the 8 ESRs together with the 2 organizers and 2 PhDs acting as tutors set up computer work places. Additionally, a social room, and a silent room for meetings or quite work was available (Fig. 4).

The first Hackathon week was dedicated to literature research, curation of data, and method development. Notably, an ordinary differential equation (ODE) optimization tools (ESR5 & ESR6) and the hydrothermal vent emission model (ESR4) was programmed in python during this week. ESR1 implemented advanced tracer capabilities into ICON-ART, overcoming limitations preventing the planned model study.

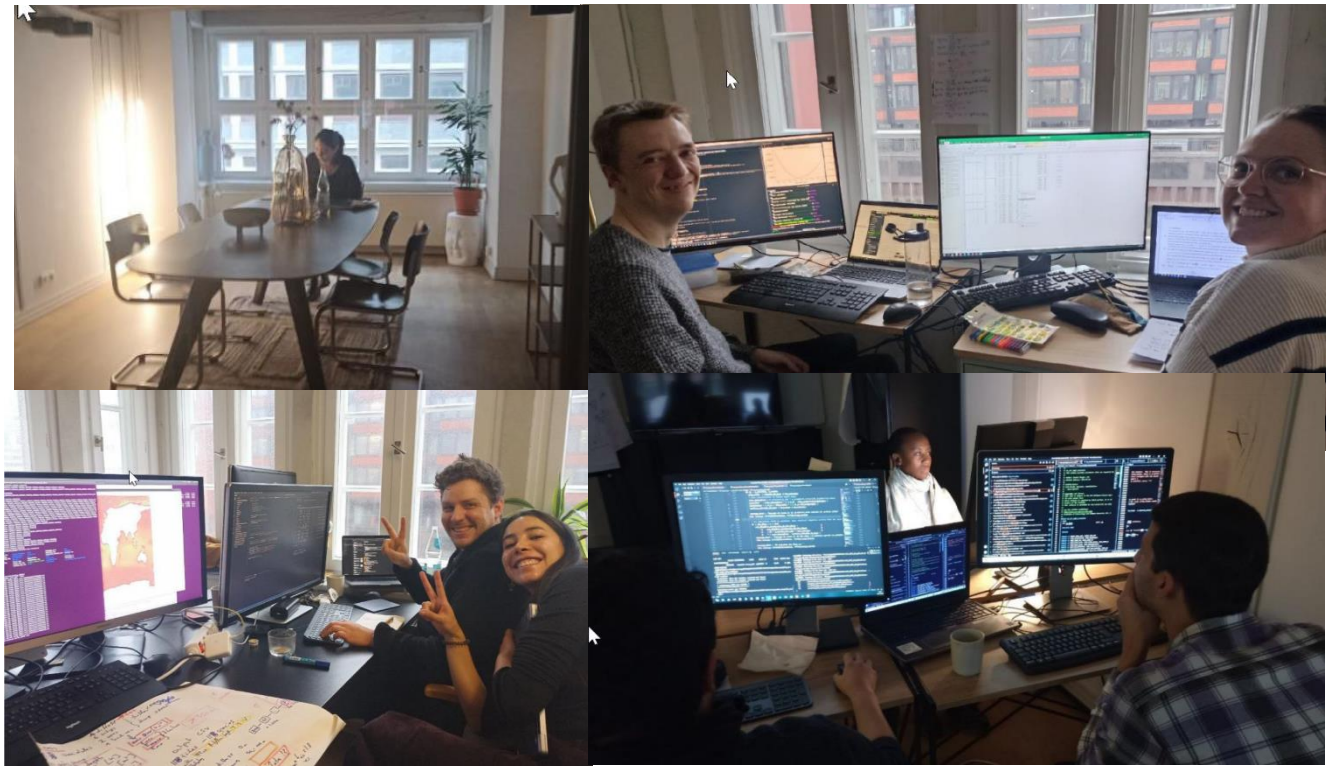

Fig. 4: Hackathon co-working space in Hamburg

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3.3 Week III: Hands-on modelling – Proof of concept

The third week was dedicated to the actual modelling work. Completing a scientific modelling study within a few weeks is obviously not feasible. Due to the meticulous planning in the year ahead of the event, we were able to finish most the methodological work up to this point. Our aim was to apply these methods (e.g. datasets, emission inventories) to generate a realistic proof of concept (PoC). On the basis of these PoC works we were able to show the feasibility of the individual ESRs projects and each ESR model study has the potential to become a stand-alone peer-reviewed publication or, at least, a chapter in a Dissertation. Which studies eventually will lead to publications cannot be predicted at this point but one month after the event, projects are still actively worked on.

3.4 Week IV: Visualization and preparation for the GMOS-Train annual meeting

In the final week, the first days were used to finalize work, that had not been finished in the previous week. On Wednesday, we left the co-working space. On this day, Helen Angot from the University of Grenoble, France gave a lecture on "How to successfully combine analytical research with state-of-the-art modelling.". Helen is a renowned yet still young researcher. Her work focuses heavily on mercury and the young researchers of the GMOS-Train MSC ITN could learn how to proceed with a science career after the PhD. Moreover, Helen is one of the few examples of a researcher using both analytical and numerical methods for her research.
On Thursday, the group visited the Helmholtz Zentrum Hereon, which is located outside Hamburg in the city of Geesthacht. There, ESR finalized their posters for presentation at the annual GMOS-Train meeting the following week. Moreover, they had the chance to present the outcome of their work to Prof. Dr. Corinna Schrum, Director of the Institute for Modelling and System Analysis (Fig. 5).

Fig. 5: Visit at the Helmholtz Zentrum Hereon.

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4. Lectures on policy support

On Monday, 6th March, lectures on policy support were held, again at ZMAW where the GMOS-Train MSC ITN annual meeting would commence the day thereafter. The event featured speakers focusing on how research in general and models in particular can be used to inform decision makers and support questions of global societal concern. The aim was to broaden the scope of GMOS-Train and show ESRs other global environmental issues where their training in the GMOS-Train MSC ITN could be of use. Topics were:

- Persistent Organic Pollutants (POPs) under the UN Stockholm Convention
- Climate Engineering, chances and dangers of anthropogenic actions on the climate system
- Lecture on the upcoming Effectiveness Evaluation of the UN Minamata Convention on Mercury

Especially noteworthy is the presentation on the UN Minamata Convention Effectiveness Evaluation by Manoela Pessoa De Miranda from the UN Environment Programme (UNEP) in Geneve, Switzerland.

Finally, the event ended with a lecture on how to write a Marie Sklodowska-Curie individual fellowship proposal. This way the ESRs were directly trained in how to acquire their own research funding for those who wish to continue pursuing a career as an independent researcher.

5. Presentation at the annual meeting

Each ESR presented their research question and results of the Winter School Hackathon in a 15min presentation. Moreover, posters were shown publicly over the course of the GMOS-Train MSC ITN annual meeting (Fig. 6). The presented posters with the Proof of Concept results for each ESR project will be published alongside this report.

Fig. 6: Winter School / Hackathon results poster presentations at the GMOS-Train MSC ITN annual meeting.

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7. Appendix A: Schedule

GMOS-Train winter school on modelling

6th – 8th February, 2023

&

modelling workshop/hackathon

9th February – 3rd March, 2023

Day 1, Monday, 6th February 2023 – Part I: Introduction and state of PhD projects

9:00 – 9:30	*Introduction: Lecture and workshop aims, plan for the upcoming weeks, organization* ***(J. Bieser & M. Ramacher, hereon)***
9:30 – 10:30	*ESR presentations, á 30min: what can your PhD project gain from modelling?*
10:30 – 11:00	***Coffee break***
11:00 – 12:00	*ESR presentations, á 30min: what can your PhD project gain from modelling?*
12:00 – 13:00	*Discussion*
13:00 – 14:30	***Lunch break***
14:30 – 15:30	*ESR presentations, á 30min: what can your PhD project gain from modelling?*
15:30 – 16:00	***Coffee break***
16:00 – 17:00	*ESR presentations, á 30min: what can your PhD project gain from modelling?*
17:00 – 18:00	*Discussion*

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Day 2, Tuesday, 7th February 2023 – Part II: Introduction to numerical modelling

zoom link: https://us06web.zoom.us/j/83355400939?pwd=WXhBT0MwZ3JqQ1hhRTdndDRUcDVhQT09

09:00 – 10:30	*Introduction to Informatics & programming I*	***(J. Bieser, hereon)***
10:30 – 11:00	***Coffee break***	
11:00 – 12:30	*Introduction to Informatics & programming II*	***(J. Bieser, hereon)***
12:30 – 14:00	***Lunch break***	

Excursion to the DKRZ German Climate Computing Centre (Room 034 + Supercomputer visit)

14:00 – 15:00	*DKRZ lecture 1: High performance computing*	***(A. Fuchs, DKRZ)***
15:00 – 16:00	*Visiting DKRZ supercomputer levante*	***(M. Böttinger, DKRZ)***
16:00 – 17:00	*DKRZ lecture 2: Visualization & outreach*	***(M. Böttinger, DKRZ)***

Day 3, Wednesday, 8th February, 2023 – Part III: Introduction to numerical modelling

zoom link: https://us06web.zoom.us/j/87685263076?pwd=MUZ6TXl0dy92d2ordCs2MTZhU0dHZz09

9:00 – 10:00	*Development and limitations of weather forecasting - A modelling perspective*	***(M. Quante, hereon)***
10:00 – 11:00	*Introduction to hydrodynamic and physical ocean modelling*	***(K. Logemann, hereon)***
11:00 – 11:30	***Coffee break***	
11:30 – 12:30	*Chemistry in numerical models*	***(V. Matthias, hereon)***
12.30 – 13.30	*State of the art and applications of contemporary mercury models*	***(O. Travnikov, JSI)***
13:30 – 14:30	***Lunch break***	
14:30 – 15:30	*Ernst Hasselmann lecture*	***(Hans v. Storch, Hamburg University)***
15:30 – 16:00	***Coffee break***	
16:00 – 17:00	*How to interpret model output (impulse + discussion)*	***(Hans v. Storch, Hamburg University)***

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Day 4, Thursday, 9th February, 2023 - PhD project workshops to prep. modelling workshop

09:00 – 10:30	*Workshop: Hackathon preparation*
11:00 – 11:30	***Coffee break***
11:30 – 12:30	*Workshop: Hackathon preparation*
12:30 – 14:00	***Lunch break***
14:00 – 15:30	*Workshop: Hackathon preparation*
15:30 – 16:00	***Coffee break***
16:00 – 17:30	*Workshop: Hackathon preparation*

Day 5, Friday, 10th February, 2023 - PhD project workshops to prep. modelling workshop

09:00 – 10:30	*Workshop: Hackathon preparation*
11:00 – 11:30	***Coffee break***
11:30 – 12:30	*Workshop: Hackathon preparation*
12:30 – 14:00	***Lunch break***
14:00 – 15:30	*Workshop: Hackathon preparation*
15:30 – 16:00	***Coffee break***
16:00 – 17:30	*Workshop: Hackathon preparation*

The lecture week will be followed by a 3-week hackathon where ESRs will get hands on lessons and practical knowledge in various modelling techniques. Based on their previous work in GMOS-Train and preparations during earlier secondments at Hereon selected ESRs will work on combining observational results with model studies.

Locations:

Modelling winter school:

Mon 6th Feb - 10th Feb: ZMAW room 133, Centre for Atmospheric and Marine Sciences, Bundesstraße 53, 20146 Hamburg 1st floor

Hackaton / modelling workshops:

Mon 13th Feb - 4th Mar: 4Walls, Deichstraße 47, 3rd floor, 20459 Hamburg

GMOS-Train annual meeting:

Mon 6th Mar - 8th Mar: ZMAW room 022/023, Centre for Atmospheric and Marine Sciences Bundesstraße 53, 20146 Hamburg 1st floor

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Day 1, Monday 6th March 2023

Morning session: Science to policy

9:00 – 9:15	Introduction (*Local organizer, GMOS-Train Coordinator*)
9:15 – 10:15	*Markus Quante (HEREON)* "Climate Engineering: Chances and Risks"
10:15 – 10:45	*Ralf Ebinghaus (HEREON)* "POPs and Stockholm convention"
10:45 – 11:00	*Coffee break*
11:00 – 12:00	*Manoela Pessoa De Miranda (UN environment programme)* "Effectiveness evaluation of the Minamata Convention – update"
12:00 – 12:30	*Nicola Pirrone (CNR)* "EO data, technologies and models as basis of co-designed mitigation strategies to support environmental policy"
12:30 - 13:30	*Lunch Break*

Afternoon session: Project proposal writing. Part 1. MCSA IF writing

13:30 – 17:30	*Dr. Stojan Sorčan (NCP)* "Introduction to project writing according to the MSCA Individual fellowship scheme"
18:00	*Reception*

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Appendix B: ESR Posters

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GMOS TRAIN winter school on numerical modelling 2023

www.gmos-train.eu

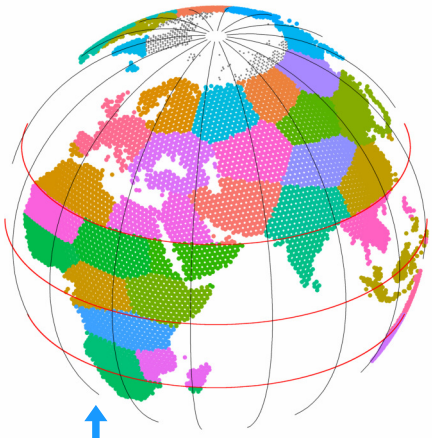
Alkuin Maximilian Koenig --- Université Grenoble Alpes --- alkuin-maximilian.koenig@univ-grenoble-alpes.fr

Where does stuff go? Where does stuff come from?

... estimating global source-receptor-relationships.

Motivation

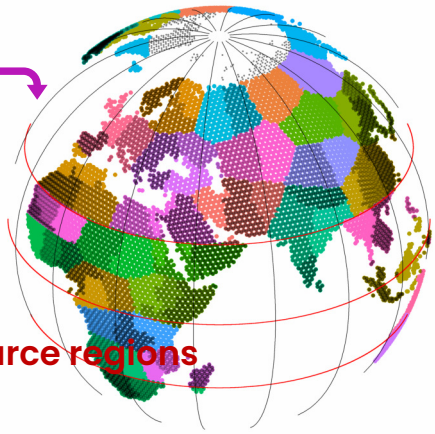
Atmospheric pollutants with a lifetime exceeding several months, such as atmospheric mercury, enter global circulation and can affect regions far from their point of emission. Here we aim to develop a global source-receptor-relationship data product that can be multiplied by an emission inventory to quantify the global dispersion of different atmospheric pollutants.



Methodology

A. **Model:** We use the state-of-the-art numerical weather prediction model ICON-Atmosphere. Instead of a rectangular grid, it uses a triangular grid, which allows for more uniform coverage of the earth and avoids the "pole singularity". This model can be very efficiently computed on a supercomputer.

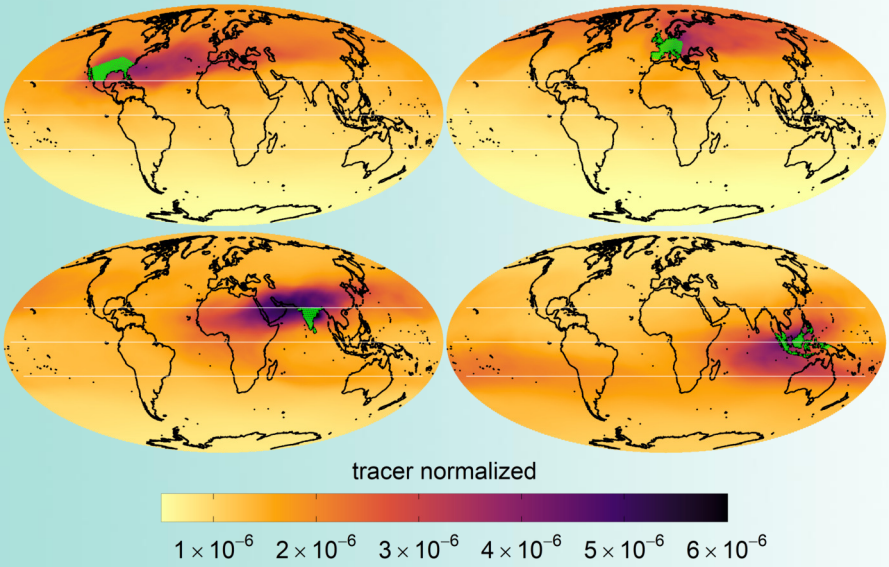
B. **Source regions:** We defined source regions in a two-step clustering approach. We first clustered together gridpoints based on their geographical closeness into ~~46 major regions. We then subdivided~~, based on population density, each of the 46 regions into 1 - 3 parts, giving 111 unique source regions.



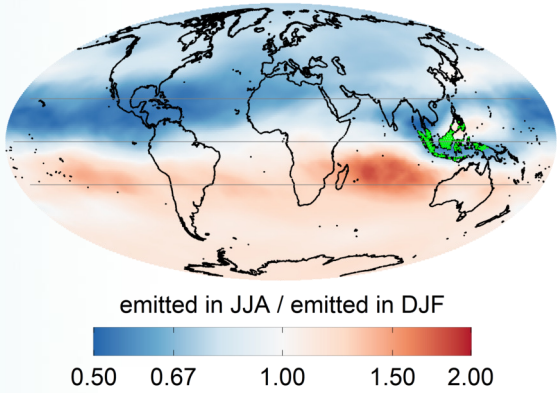
C. **Tracer emission:** We emitted for each source region a 3-month pulse of a passive tracer with a lifetime of 6 months. We then computed its global dispersion for 18 months. We repeated the procedure for 4 different seasons: December – February (DJF), March - May (MAM), June – August (JJA), and September – November (SON).

Preliminary results: Dispersion of emissions from selected source regions

Pressure level: 300 hPa; emitted season: June - August (JJA)



Seasonality of tracer dispersion (300 hPa)



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Linking Oceanic hydrothermal Vent Emissions to Hg baseline levels

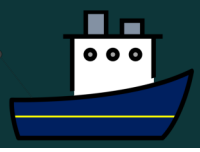
LOVE-Hg

The problem

It is thought that anthropogenic activities have increased mercury (Hg) concentrations in the ocean, although the magnitude of this increase is still being debated. The common approach to assess this increase is by quantifying historic anthropogenic emissions and then estimating the natural levels of mercury in the ocean. This approach is challenging due to a lack of data.

The approach

As geogenic Hg is the only natural source of Hg to the ocean (atmospheric deposition, riverine inputs, and submarine groundwater discharge are secondary Hg sources that recycle natural and anthropogenic Hg to the ocean) we quantify how much Hg would be in the ocean if just hydrothermal vents release Hg to the ocean.

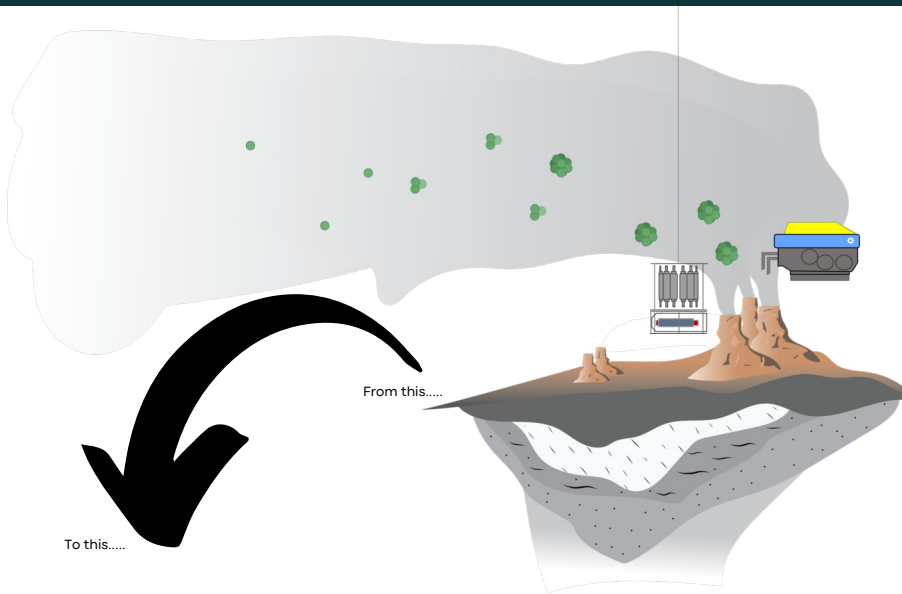


The goal

To provide for the first time a view of the natural mercury baseline of the pre-historic ocean by quantifying the natural fluxes of mercury into the ocean...

...then add current anthropogenic fluxes to:

1. Quantify the natural and anthropogenic mercury in the ocean today.
2. Estimate how much time it will take to reduce mercury levels in the ocean to baseline levels under restrictive policies.



Work in progress!

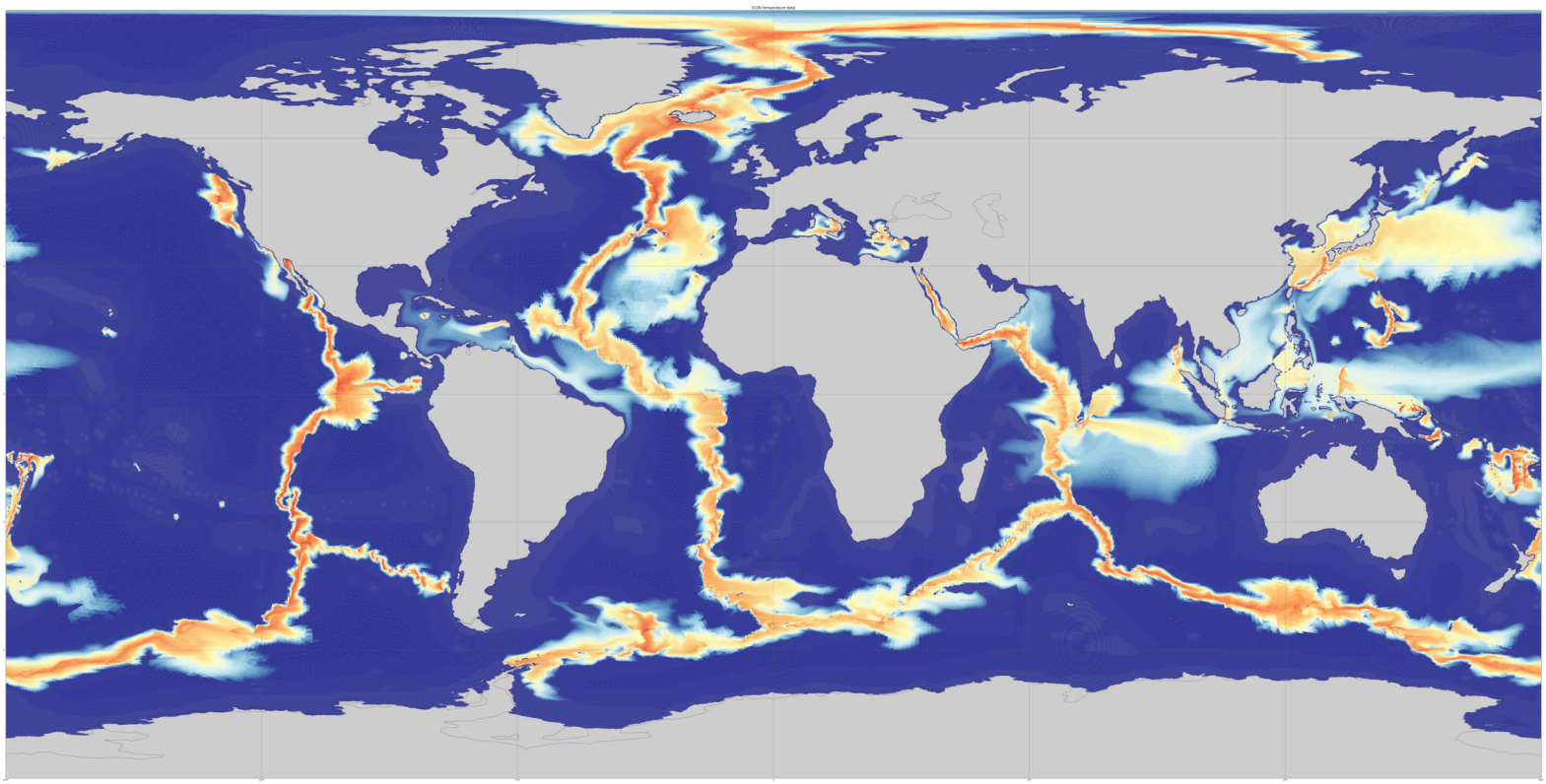


Fig 1. Global map showing hydrothermal vents' Hg emissions. Darker colors indicate higher concentrations.

More details?

The model is a combination of the previously reported models PB2002[1], the linear regression of vent field frequency to spreading rate[2], hydrothermal fluid fluxes calculated from the isotopic mass balance of thallium in the ocean crust[3], and mercury data.

References

[1] Bird, P. An updated digital model of plate boundaries. Geochem Geophys Geosystems **4**, (2003).
[2] Beaulieu, S. E., Baker, E. T. & German, C. R. Where are the undiscovered hydrothermal vents on oceanic spreading ridges? Deep Sea Res Part Ii Top Stud Oceanogr **121**, 202–212 (2015).
[3] Nielsen, S. G. et al. Hydrothermal fluid fluxes calculated from the isotopic mass balance of thallium in the ocean crust. Earth Planet Sc Lett **251**, 120–133 (2006).

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement no. 860497.

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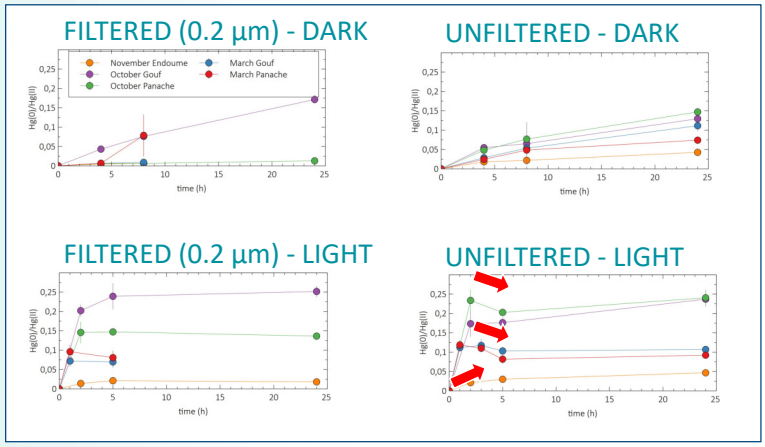
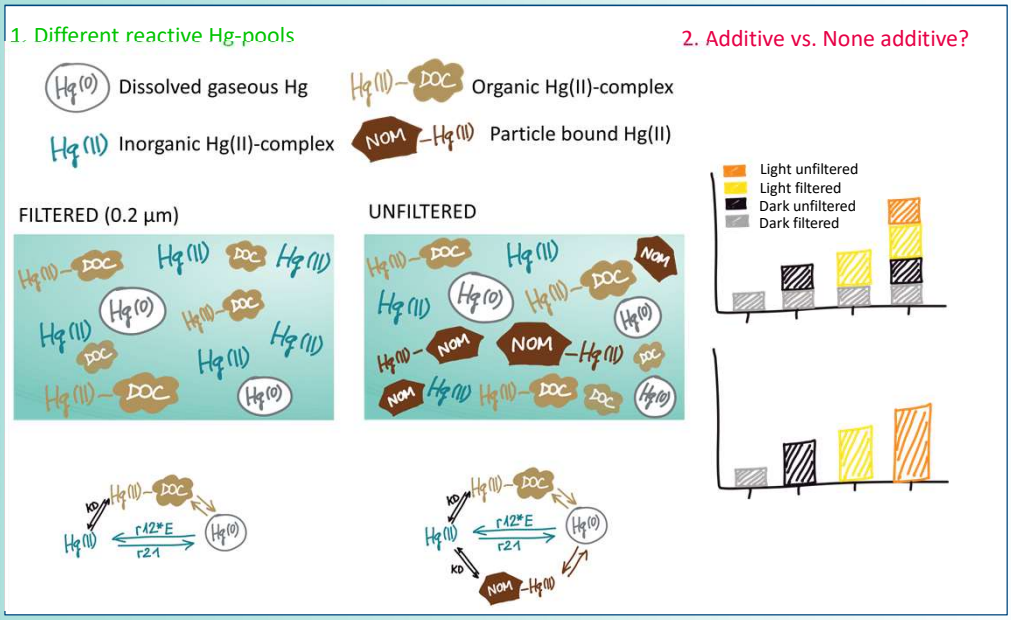
Computational Rate Approximation Program CRAP

Alina Kleindienst, University of Pau, a.kleindienst@univ-pau.fr
Pascal Simon, HEREON, pascal.simon@hereon.de

How to fit rate constants to experimental data for dissolved gaseous mercury (Hg) production for distinct waters/trends?

Incubation experiments were conducted to quantify the reduction of Hg(II) to Hg(0) in different coastal surface waters under distinct conditions. Two trends were observed for experiments conducted under natural light conditions. For estuarine influenced coastal waters in the Bay of Biscay (Atlantic, Panache and Gouf) for two seasons, a fast sharp increase was followed by a slight decrease in Hg(0) concentrations. Such "overshoot" was not observed for the experiment conducted on coastal water in the Mediterranean Sea (Endoume).



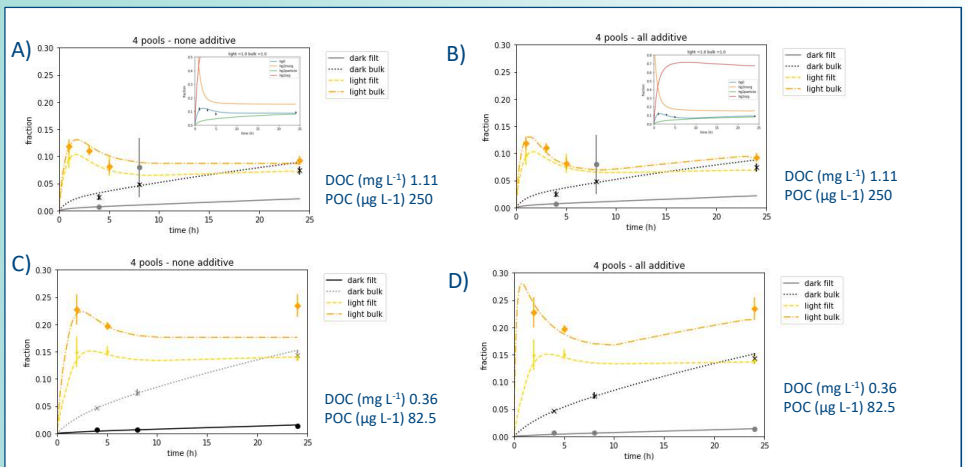


The CRAP

We developed a model with 4 Hg-pools: dissolved gaseous Hg, inorganic Hg(II), organically bound Hg(II), and particle-bound Hg(II). Rate constants between inorganic Hg(II) and organically bound and particle-bound Hg are defined by the partitioning coefficient (KD) and the half-life of the reaction. We hypothesize that the overshoot is the result of a competing reaction that constrains the Hg pools available for reduction. The CRAP model gives us the possibility to easily test conditions & hypothesis:

- Different reactive Hg pools participating in the reaction
- Different equilibria governing the back reaction
- Are reactions additive or not?

Preliminary Results



Panache March	Dark filtered s^{-1} $T^{n}C^{-1}$	Dark bulk s^{-1} $T^{n}C^{-1}$	Light filtered s^{-1} m^2 W^{-1}	Light bulk s^{-1} m^2 W^{-1}
A) r12 – none additive	7.8e-08	4e-07	8e-08	1e-07
R^2	0.82	1.58	0.10	0.77
Equilibrium	1	0.5	3	2
B) r12 - additive	7.8e-08	3.3e-07	8e-08	4e-08
R^2	0.82	1.61	0.11	0.63
Equilibrium	1	0.5	3	2

Panache October	Dark filtered s^{-1} $T^{n}C^{-1}$	Dark bulk s^{-1} $T^{n}C^{-1}$	Light filtered s^{-1} m^2 W^{-1}	Light bulk s^{-1} m^2 W^{-1}
C) r12 – none additive	2.2e-08	2.8e-07	9.9e-08	2.2e-07
R^2	5.89	0.38	0.23	2.68
Equilibrium	1	0.5	3	2
D) r12 - additive	2.2e-08	2.6e-07	9.9e-08	9.9e-07
R^2	5.89	0.32	0.28	1.09
Equilibrium	1	0.5	3	2

!! Overshoot reproducible with competing reactions at different rates

!! Reproducible Equilibrium concentrations in Late Spring (March) and Late Fall (October) with distinct DOC/POC pool sizes

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement no. 860497.

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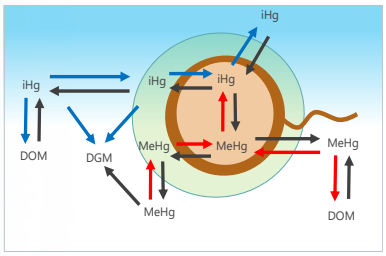
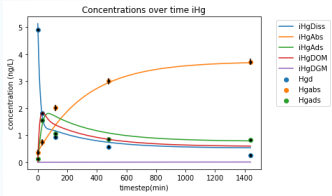
Isabel Garcia-Arevalo -- IFREMER/ CCEM -- igarciaa@ifremer.fr

Mercury species uptake and partition kinetics' ODE numerical integration model

At which rate Hg species are taken up by living particles?

- **The uptake of dissolved MeHg by phytoplankton is the initial entry of Hg accumulation in the aquatic food webs.**
- **For management and mitigation strategies that promote human and wildlife health it is important to understand the role of these living particles in MeHg dynamics in the marine environment.**
- **Hg partitioning and speciation rates between dissolved and particulate phases are one of the major uncertainties in ocean Hg bioaccumulation models and play a major role for a better understanding of the fate of Hg currently in the ocean.**





Diss>>DOM	0.034
Diss>>Ads	0.0097
Ads>>Abs	0.0031
Diss>>Abs	0.00255
Abs>>Diss	0.00018
Abs>>Ads	0.00078
Diss>>DGM	$9*10^{-6}$

Proof of concept - model description

1. Define rates for Hg transfer between compartments.

When $K_D = \frac{[Hg]p_1}{[Hg]d_1}$ at eq $\sim \frac{r_{pd}}{r_{dp}}$; $r_{pd} = r_{dp} * K_D * POC$ or $r_{dp} = r_{pd} * \frac{1}{K_D * POC}$

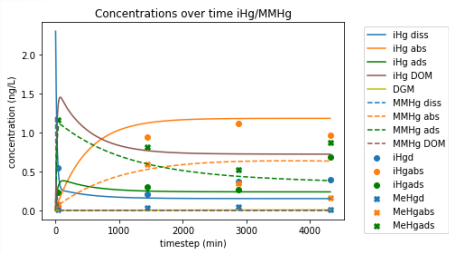
When $\frac{d[Hg]p}{dt} = 0$; $r_{dp} = r_{pd} * \frac{[Hg]p_1}{[Hg]d_1}$

When $\frac{d[Hg]p}{dt} = r_{pd} * [Hg]p + r_{dp} * [Hg]d$; $\frac{d[Hg]p}{dt} = r_{dp} * [Hg]d + 0$; $r_{dp} = \frac{d[Hg]p}{dt}$

2. Establish assumptions. $r_{dDOM} = \frac{\ln(2)}{\tau}$ then $r_{DOMd} = r_{dDOM} * K_D * DOC$

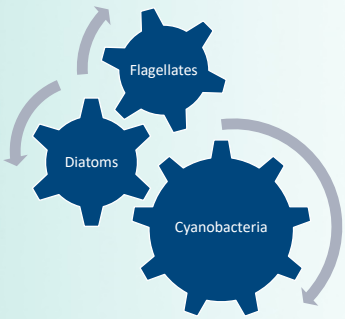
3. Obtain best fit rates based on lowest MSE.

DOM>>Diss
DOM>>Abs
DOM>>Ads
$\} \; r \in [r_1; r_2] | MSE_{min}$

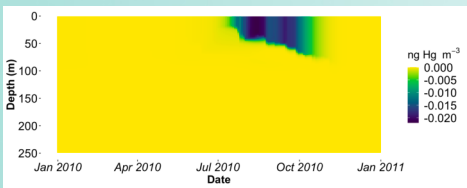


1D model parameterization

Adaptation of uptake and release rates, refined in previous step, to mgC based on surface to volume ratio of three principal groups of phytoplankton.

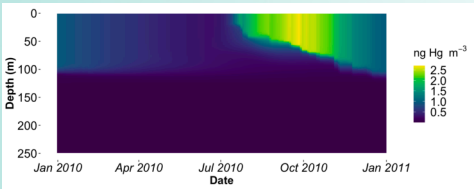


Implications of Hg transfer in the Baltic ocean:



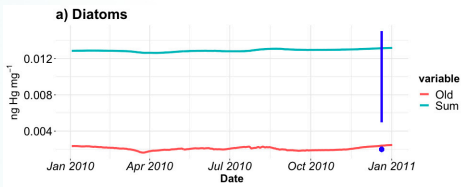
Decrease of MeHg in meso zooplankton

Increase of MeHg in fish

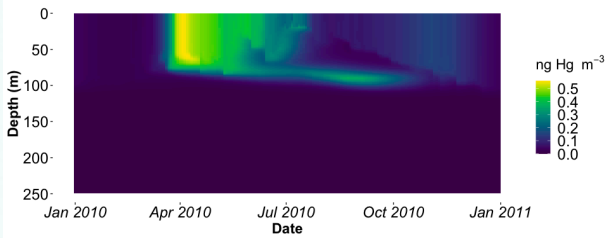


Preliminary results

Comparison of measurements with model output with parameters taken from literature and new parameters.



Increase of MeHg in diatoms from model output with new parameters.



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Stockholm University

Helmholtz-Zentrum hereon

The fate of terrestrial mercury and methylmercury in the Baltic Sea

Baltic Sea Characteristics

| shallow semi-enclosed sea | riverine inputs of 440 km³ per year | approximately 85 million people living in the catchment area | leading to intense pollution (Norbäck Ivarsson et al., 2019)

Motivation

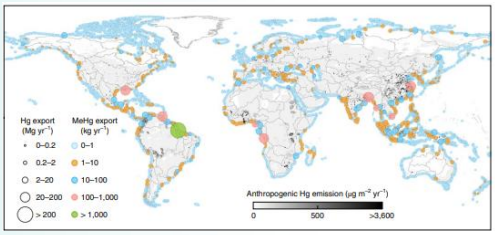


Figure 1: "Rivers as the largest source of mercury to coastal oceans worldwide" (Liu et al., 2021)

Concept

Combine riverine runoff data (GRDC), MeHg & HgII riverine export (Liu et al., 2021) & TOC export (Baltic Sea Centre) for the MERCY study area; adjust the log K for HgII and MeHg binding to organic matter.

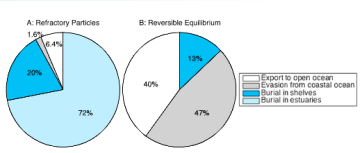
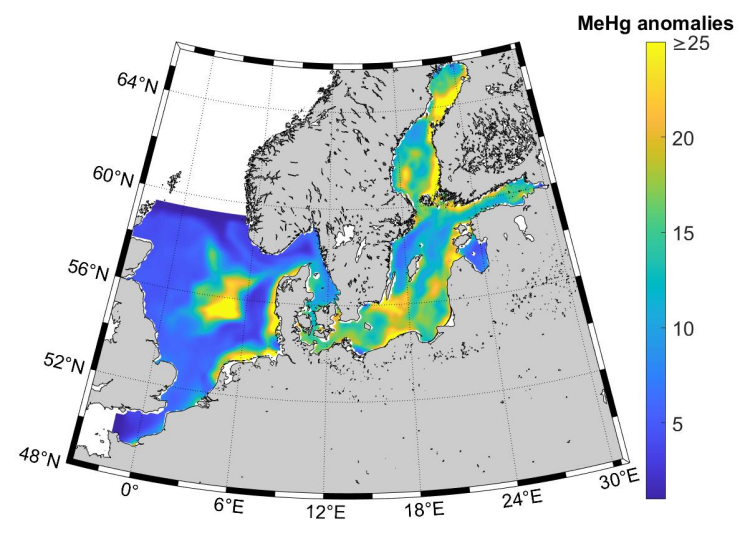


Figure 2: Fate of riverine Hg strongly dependent on parameterization of the binding to terrestrial OM (Zhang et al., 2015)

Table 1: logK values used in the different scenarios

Species	Labile original	Humic original	Labile updated	Humic updates
MMHg DOC	6	N/A	17.16	17.5
MMHg POC	5.9	N/A	16.87	17.21
HgII DOC	6.6	N/A	17.68	18.03
HgII POC	6.4	N/A	17.14	17.48

Results



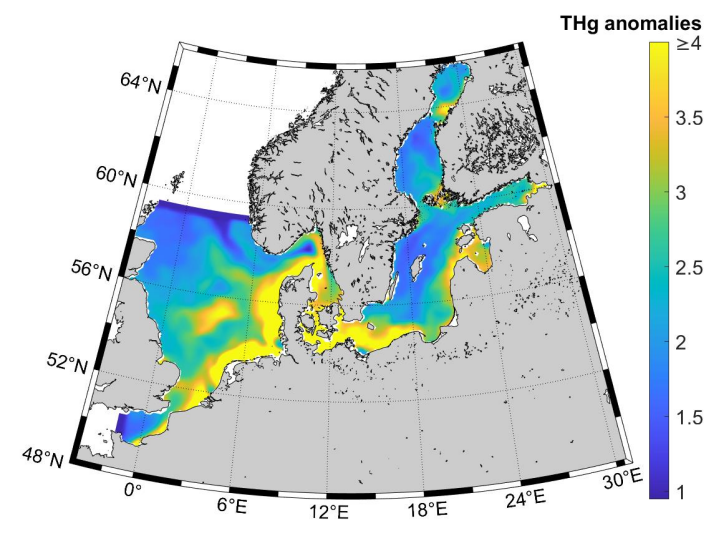


Figure 3: Relative differences in MeHg (left) and THg (right) using different logK values for organic matter (OM). In the original model, no terrestrial OM binds Hg and MeHg. In these plots, we used new logK values (see table 1) for humic (terrestrial) and labile (marine) OM and devided the values for THg and MeHg in surface water on one day in 2003 using our new parameterization by the values from the old parameterization.

References

M. Liu, Q. Zhang, T. Maavara, S. Liu, X. Wang and P. A. Raymond, Rivers as the largest source of mercury to coastal oceans worldwide, Nat. Geosci., , DOI:10.1038/s41561-021-00793-2.

Norbäck Ivarsson, L., Andrén, T., Moros, M., Andersen, T. J., Lönn, M. and Andrén, E.: Baltic sea coastal eutrophication in a thousand year perspective, Front. Environ. Sci., 7(JUN), doi:10.3389/fenvs.2019.00088, 2019.

Zhang, Y., Jacob, D. J., Dutkiewicz, S., Amos, H. M., Long, M. S., & Sunderland, E. M. (2015). Biogeochemical drivers of the fate of riverine mercury discharged to the global and Arctic oceans. Global Biogeochemical Cycles, 29(6), 854–864. https://doi.org/10.1002/2015GB005124.

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Charlotte Haugk, Department of Environmental Science, Stockholm University,
Charlotte.haguk@aces.su.se

Transport and Speciation of Hg following Permafrost Thaw

Permafrost thaw gradient and Hg mobility

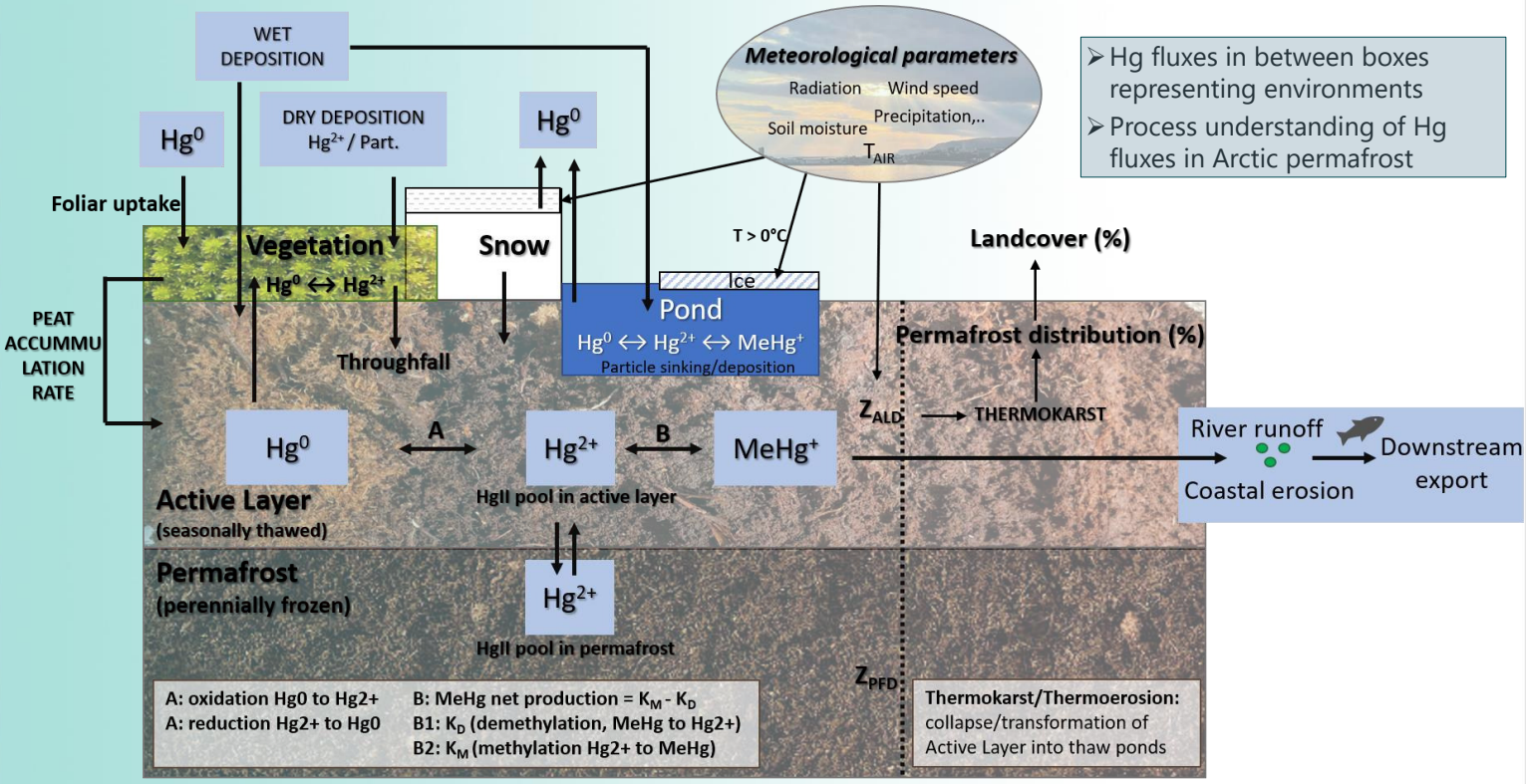
Peat plateau (permafrost)

Collapse fen (permafrost)

Fen (no permafrost)

https://www.grida.no/resources/13358

Conceptual Box Model



- Hg fluxes in between boxes representing environments
- Process understanding of Hg fluxes in Arctic permafrost

Outlook: Future Scenarios

- ✓ Parameterization
- ✓ Identify variables to describe processes around PF thaw/Hg speciation
- ⏲ Apply **Climate change scenarios** – IPCC projections
- ⏲ Active Layer deepening -Thermoerosion increases - change of landcover distribution – change in Hg reactions within environmental compartments (uptake/reemission,..)
- ⏲ Include **Hydrological model** with groundwater flow & runoff output (Ground Ice %, SOC, Soil moisture, Slope, ...)

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement no. 860497.

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The effect of the ecosystem in Hg cycling

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2 IFREMER, RBE/BE- LBCM, BP 21105, 44311 Nantes Cedex 3, France

Introduction

Mercury (Hg) speciation and bioaccumulation in coastal seas is an essential link between Hg pollution and methylmercury (CH3Hg$^+$) exposure in humans. Yet, the dynamics and interactions between the ecosystem and marine Hg cycling are still poorly understood. We designed a bioaccumulation model to investigate the role of the ecosystem in marine Hg cycling and run it in a shallow highly productive shallow Southern North Sea setup. We model the accumulation of Hg^{2+} and CH_3Hg^+ and run it with and without bioaccumulation, biogenic reduction and the partitioning to dissolved and organic carbon (DOC/POC).

Interaction:	Bioaccumulation	Biogenic reduction	Partitioning
Cause	• Uptake by organisms • Modelledfor CH_3Hg^+ and Hg^+	• Hg^{2+} reduced to Hg^0	• DOC/POC bounds Hg^{2+}, CH^3Hg and HgS
Relevance	• Prevents evaporation and Hg chemistry	• Hg^{2+} bioaccumulated • Hg^0 is volatile	• Prevents evaporation and Hg chemistry • Sinking POC transports Hg • POC can sediment

Comparison to observations

There is good agreement with existing observations for dissolved Hg and CH_3Hg^+ and their accumulation in phyto- and zooplankton (Fig. 1).

Bioaccumulated total Hg

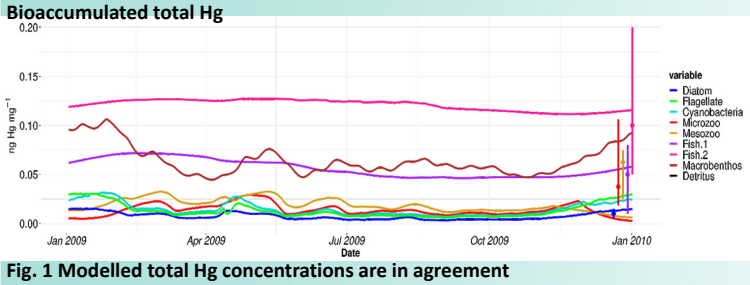

Fig. 1 Modelled total Hg concentrations are in agreement with observations

The effect of the ecosystem

Figure 2 shows the relative increase in total and methylmercury caused by the ecosystem by dividing the total and organic mercury with and without an ecosystem. There is up to 30% more total mercury and up to 1000% more present in our simulation with an ecosystem. The increase is largest during spring and smallest during autumn.

Total Hg **Organic Hg**

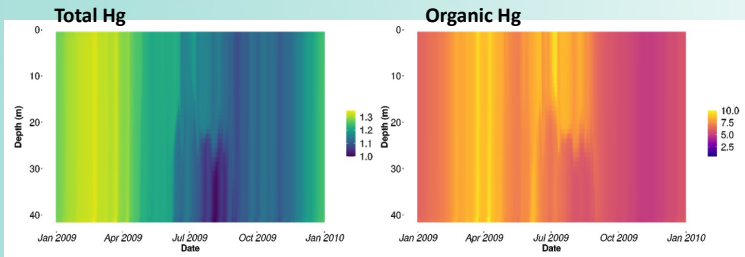

Fig. 2 The relative difference between our simulations $\frac{With\ ecosytem}{Without\ ecosytem}$ interactions.

Drivers of the variation

In figure 3 the most important ecosystem interactions have been plotted that drive the difference in total and organic Hg. Total Hg is mostly influenced by the partitioning to DOC/POC, as this increases water column Hg by decreasing evaporation. A second important driver is biogenic reduction. This in terms increases the evaporation of Hg. Organic mercury is mostly increased due to the direct effect of bioaccumulation. Bioaccumulation of CH_3Hg^+ prevents (photo)degradation making it more stable which leads to a higher build-up.

Total Hg **Organic Hg**

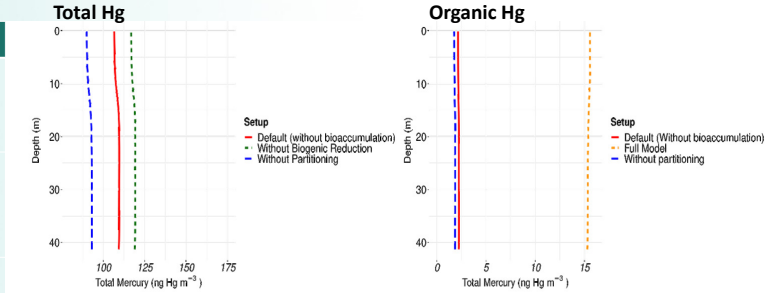

Fig. 3 The effect of different ecosystem interaction on (organic) Hg.

Conclusion

In the Southern North Sea setup total water column Hg is increased by DOC and POC while decreased by cyanobacteria. CH3Hg+ is increased by bioaccumulation due to a reduction in (photo)degradation. Thus it can be concluded that ***the ecosystem has an important role in mercury cycling.***

Discussion

Literature shows that DOC/POC reduce bioaccumulation as partitioning and bioaccumulation compete for Hg[(1)] and cyanobacteria can increase bioaccumulation due to their large surface-to-volume ratio[(2)]. This means that both cyanobacteria and DOC/POC can increase or decrease bioaccumulation and more research is needed to determine under which circumstances which effect dominate.

Additionally, the measuring of mercury in low trophic organisms does not receive the same recommendation for sampling Hg in air, water and seafood from the UNEP[(3)]. We show that the ecosystem plays a role in Hg cycling and we would recommend that this model gap is filled with models where measurements are unavailable.

References

1) Pickhardt, Paul C. and Nicholas S. Fisher (Jan. 2007). "Accumulation of inorganic and methylmercury by freshwater phytoplankton in two contrasting water bodies". In: Environmental Science and Technology 41.1, pp. 125–131.
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3) Conference of the Parties to the Minamata Convention on Mercury Fourth meeting (2021). "Guidance on monitoring of mercury and mercury compounds to support evaluation of the effectiveness of the Minamata Convention ". In: UNEP.

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Analysis of long-term datasets to investigate ocean-atmosphere exchange of Hg

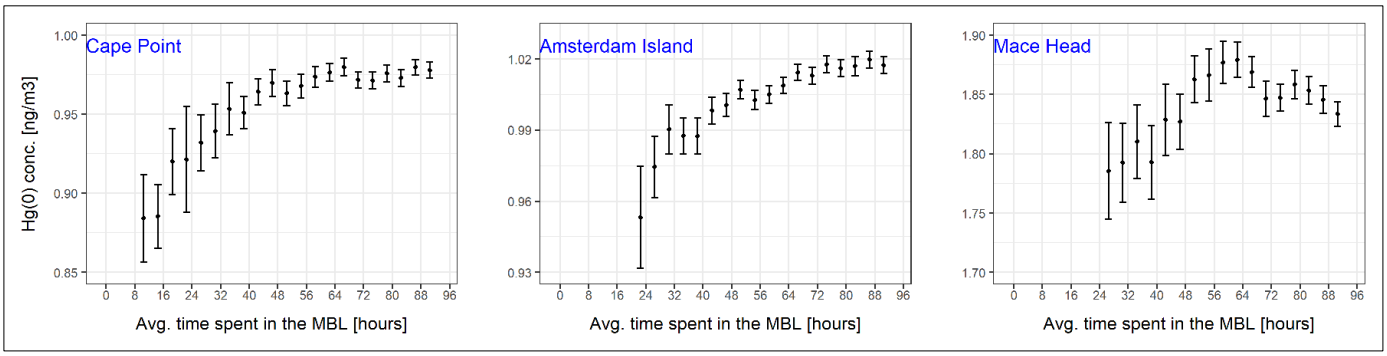
Application of trajectory analyses to gain insight into ocean-atmosphere exchange

Cycling of mercury (Hg) in the atmosphere provides arguably the most important pathway by which the toxic pollutant distributes throughout the globe. Net evasion of elemental Hg from the ocean represents the largest single flux of Hg into the atmosphere[1]. Despite this, the dynamics of Hg air-sea exchange are still not fully understood. Here, we combine long-term observations of atmospheric gaseous elemental atmospheric (Hg(0)), from 3 coastal stations with air mass back trajectories to gain insight into ocean-atmosphere exchange.

Trajectory analysis

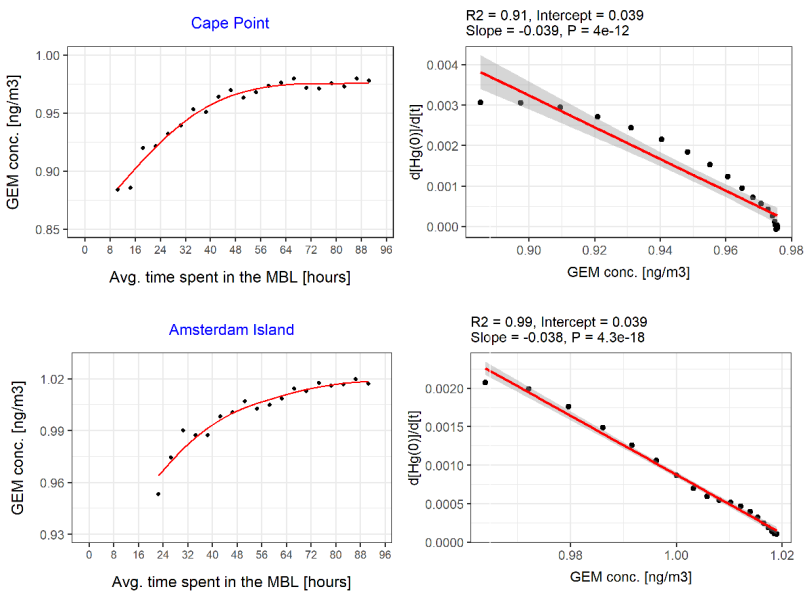
We calculated 96-hour air mass back trajectory for each Hg(0) data point using HYSPLIT. Trajectory segments were then assigned as either within the marine boundary layer, (ii) above the MBL, within the planetary boundary layer (PBL) or the above PBL.

Preliminary results I



- **Marine signal observed: increased Hg(0) concentrations with increased time air masses spent over the MBL before arriving at the sites.**
- **Equilibrium in atmospheric Hg(0) concentration also clearly observed at Cape Point and Amsterdam Island.**

Prelim. results II: Estimation of surface ocean elemental Hg concentration



$$\mathbf{Flux} = \mathbf{k} * [\mathbf{C_{air}} - \mathbf{HC_{aq}}]$$

k is the rate constant
C_{air} is the atmos. Hg(0) conc.
C_{aq} is the surface ocean dissol. gaseous Hg conc.

at equilibrium

$$\mathbf{C_{aq}} = \frac{\mathbf{C_{air}}}{\mathbf{H}}$$

H is Henry's law constant given by[2]:

$$\mathbf{H} = \exp\left(\frac{-2404.3}{\mathbf{T}}\right) + 6.92$$

T is temperature (in K)

Station	Cape Point	Amsterdam Island
Temperature (K)	288.15	288.15
H	0.24	0.24
C(air)	0.98	1.02
C(aq)	4.08	4.25

Next steps...

- **Estimate ocean evasion flux from the datasets presented above**

References

[1]Global Mercury Assessment, 2018. United Nations Environment Programme.

[2]Andersson, M.E., Gårdfeldt, K., Wängberg, I. and Strömberg, D., 2008. Determination of Henry's law constant for elemental mercury. *Chemosphere*, *73*(4), pp.587-592.