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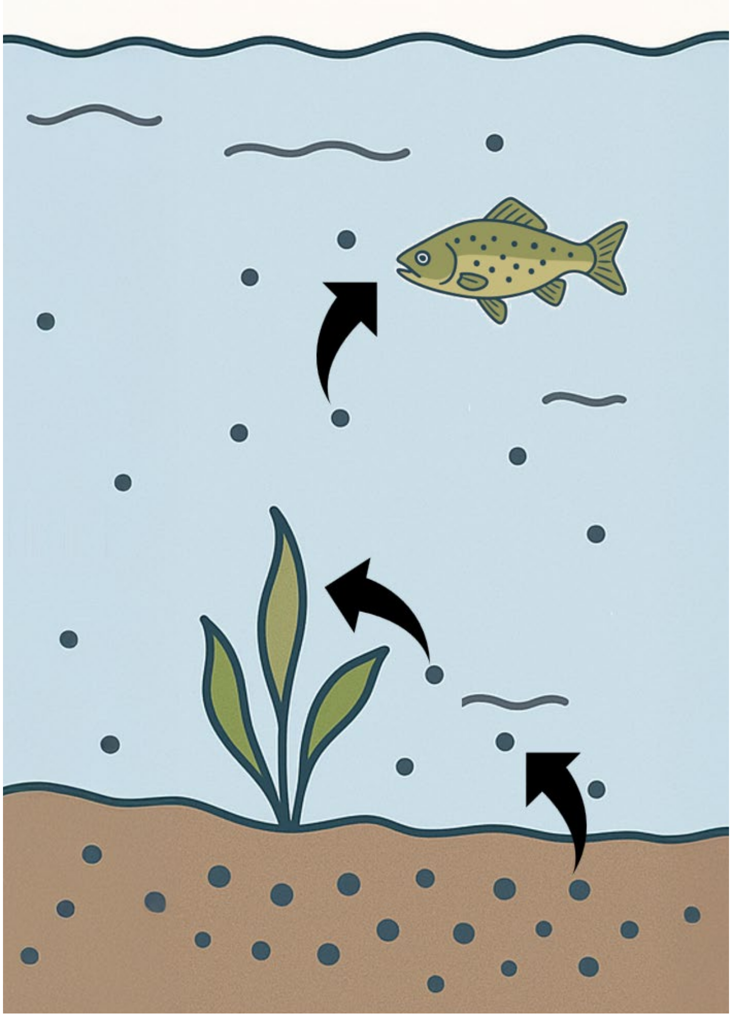

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PROTECTION AGENCY

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# Preface

This report *Mobility, Bioavailability and Toxicity of Sediment Contaminants (MOBILITY)* presents the results of one of the six funded projects within the call Contaminated Sediments from 2020. The research results from this call aim to provide the knowledge base needed for measures and policy instruments regarding risks with and spread of contaminated sediments and hazardous substances from contaminated sediments.

The project has been financed with the environmental research grants from the Swedish Environmental Protection Agency (SEPA) to support the knowledge needs of SEPA and the Swedish Agency for Marine and Water Management.

This report is written by Sofi Jonsson, Alyssa Azaroff, Betty Chaumet, Elena Gorokhova and Anna Sobek at Stockholm University and Stefano Bonaglia at University of Gothenburg.

The authors are responsible for the content of the report.

Stockholm, June 2025

Marie Uhrwing
Department head, Sustainability Department

# Contents

# Summary

Sediments around the world store significant amounts of potentially hazardous chemicals. These chemicals pose a risk to the aquatic environment, as they can be released into the water and transferred to aquatic food webs. Many of the legacy pollutants, including organic compounds such as polychlorinated biphenyls (PCBs) and polycyclic aromatic hydrocarbons (PAHs), and metals such as mercury (Hg), are poorly water soluble and have high affinity for organic matter, which explains why they are found in elevated concentrations in organic carbon-rich sediments. Many chemicals in commerce have similar properties, and it is therefore likely that sediments will continue to be a sink and source of chemicals in the future. To assess sediment contamination, total concentrations of selected chemicals are measured and compared to thresholds such as Sediment Environmental Quality Standards. This approach provides an indication of the potential risk caused by contaminants in the sediment. However, the total sediment concentration of hydrophobic compounds and metals does not provide information on what fraction of the contamination that is available for release to water and biological uptake, as a major part of the contaminant pool in the sediment will be associated to particles. Several factors may further have an impact on the release of contaminants from sediment, including turbidity and particle resuspension, sediment and contaminant properties. In MOBILITY, we applied passive samplers to assess the release of organic contaminants and Hg from sediment, during varying turbid conditions, with the overarching aim to provide tools for more environmentally realistic monitoring of contaminated sediment risk.

We performed three experiments with an artificial sediment which was spiked with PAHs and Hg. PAHs were used as model compounds for Hydrophobic Organic Contaminants (HOCs) commonly occurring in sediment. We quantified the release of contaminants from the sediment using two different types of passive samplers (polyethylene sheets to catch HOCs, and diffusive gradients in thin films (DGT) for mercury). We found that turbidity has an impact on the release of HOCs from sediment, and that conditions with lower turbidity favours release of more polar chemicals through diffusion, while release of more hydrophobic chemicals is favoured at higher turbidity through particle resuspension. Further, we found that passive samplers can be used as a worst-case scenario indicator of biological uptake by the red alga *Ceramium tenuicorne* and toxicity of HOCs released from sediment. For Hg, we demonstrated the release of Hg to be influenced by the sediment grain size. DGT passive samplers were used to assess the bioavailable fraction of inorganic and methylmercury, and we conclude that DGTs should be further evaluated as a tool for assessing the bioavailable fraction of methylmercury in and from sediment. Based on our findings, we provide a number of recommendations for monitoring and assessments of contaminated sediments. These recommendations focus on the use of passive samplers for assessing the bioavailable fraction of the contaminant, on the impact of turbidity on potential contaminant release and how contaminant properties as well as sediment grain size distribution impacts mobility of contaminants in sediment.

# Sammanfattning

Sediment runt om i världen lagrar stora mängder potentiellt skadliga kemikalier, så som olika blandningar av organiska föroreningar och metaller. Dessa kemikalier utgör en risk för miljön, då de kan frigöras till vattnet och sen tas upp av vattenlevande organismer. Typiskt för många av de föroreningar som spreds för flera decennier sen är att de är svårlösliga i vatten och binder starkt till organiskt material. Dessa kemikalier förekommer därför framförallt i sediment som ofta har högt innehåll av organiskt kol. Många av de kemikalier som används i dag har liknande egenskaper, vilket innebär att sediment sannolikt även i framtiden kommer att fungera både som en sänka och en potentiell källa för kemikalier.

För att bedöma risken orsakad av förorenade sediment mäts ofta totalhalten av utvalda ämnen vilka sedan jämförs med tröskelvärden för toxicitet (exempelvis Sediment Environmental Quality Standards). Denna metod ger en indikation på den potentiella risken som föroreningar i sedimentet kan innebära. Dock ger inte totalhalter av hydrofoba ämnen eller metaller någon information om hur stor andel av föroreningarna som faktiskt är tillgänglig för frisättning till vattnet eller för biologiskt upptag, eftersom en stor del av föroreningsmängden är bunden till partiklar i sedimentet. Flera faktorer kan dessutom påverka frisättningen av föroreningar från sediment, däribland grumlighet och partikelresuspension, samt sedimentets och föroreningarnas egenskaper. Inom ramen för projektet MOBILITY har vi använt passiva provtagare för att undersöka frisättning av organiska föroreningar och kvicksilver från sediment under varierande grumlighetsförhållanden. Det övergripande målet är att bidra med verktyg för en mer miljörealistisk övervakning av risker kopplade till förorenade sediment.

Inom projektet genomförde vi ett antal experiment med ett artificiellt sediment som hade laddats med polycykliska aromatiska kolväten (PAH) och kvicksilver. PAH användes som modellföreningar för hydrofoba organiska ämnen (HOC) som ofta förekommer i sediment. För att kvantifiera frisättningen av föroreningar från sedimentet använde vi två olika typer av passiva provtagare: polyetenfilm för att fånga upp HOC samt DGT (diffusive gradients in thin films) för kvicksilver.

Vi fann att grumlighet påverkar frisättningen av HOC från sedimentet. Förhållanden med låg grumlighet gynnade frisättning av mer polära ämnen via diffusion, medan hög grumlighet gynnade frisättning av mer hydrofoba ämnen genom partikelresuspension. Vidare kunde vi visa att passiva provtagare kan användas som indikator för ett worst-case-scenario av biologiskt upptag av HOC i den röda algen Ceramium tenuicorne samt för att indikera toxicitet från ämnen som frisätts från sediment.

För kvicksilver visade vi att sedimentets kornstorleksfördelning påverkar frisättningen. DGT-provtagare användes för att mäta den biotillgängliga fraktionen av oorganiskt kvicksilver och metylkvicksilver. Vi drar slutsatsen att DGT-tekniken bör utvärderas vidare som verktyg för att bedöma den biotillgängliga fraktionen av metylkvicksilver i och från sediment.

Baserat på våra resultat lämnar vi ett antal rekommendationer för övervakning och bedömning av förorenade sediment. Rekommendationerna fokuserar på användning av passiva provtagare för att uppskatta den biotillgängliga fraktionen av föroreningar, på grumlighetens betydelse för potentiell frisättning av föroreningar samt på hur ämnesspecifika egenskaper och sedimentets kornstorleksfördelning påverkar mobiliteten hos föroreningar i sediment.

# 1. Introduction

## 1.1 Background

### 1.1.1 Contaminated Sediments in Sweden

In the late 19th and early 20th centuries, Sweden experienced rapid industrial growth resulting in both economic growth and modernization of the Swedish society. Natural resources such as wood and ore were transformed into goods in the wood and metal industries. For logistical reasons, many of these industries were located along the coastline or near inland waters. Hazardous chemicals released from the industries reached nearby waters and as a consequence, coastal and inland sediments store high amounts of chemicals emitted from the industries. With reduced primary emissions from industry, contaminated sediments turn into secondary sources of hazardous chemicals, posing risks to both humans and the environment. To reach national and international development and environmental goals, including *A Non-Toxic Environment* (Swedish environmental goal) and *Life Below Water* (United Nations 14th sustainable development goal), some of these contaminated sites will need to be remediated. Sediment remediation is, however, a costly process and prioritizing sites is important. In this project, we focus on the mobility, bioavailability and toxicity of Hydrophobic Organic Compounds (HOCs) and mercury (Hg) in contaminated sediments.

Hydrophobic Organic Compounds are a class of hazardous chemicals with low solubility in water and high affinity for organic matter in e.g. sediment and tissues of aquatic organisms. Many legacy contaminants are HOCs, such as polycyclic aromatic hydrocarbons (PAHs). PAHs frequently contaminate sediments, many of them bioaccumulate and cause adverse effects on the environment such as growth reduction, DNA damage or narcosis on aquatic organisms (Behera et al., 2018; Oliveira dos Anjos et al., 2023). In Sweden, historical industrial activities, particularly around sawmills, have been significant sources of PAHs, as creosote, a pesticide used as a wood preservative, contains a significant amount of these contaminants and was extensively used particularly from the mid-1900s, and banned in 2003. Chemical use and emissions increase over time (Persson et al., 2022), with a doubling of production in less than 20 years. More than 350 000 chemicals are currently placed on the global market (Wang et al., 2020).

Mercury is a naturally occurring element that cycles in the environment in different chemical forms, each with its own properties. In its elemental form ($Hg^0$), Hg is a volatile substance, allowing for atmospheric transport and resulting in global spread. In terrestrial and aquatic systems, however, Hg is primarily present in its oxidized inorganic form ($Hg^{II}$). A small fraction of this $Hg^{II}$ (up to a few %) in soils, sediments and natural waters gets methylated by microbes to methylmercury (MeHg). MeHg is a highly toxic form of Hg which bioaccumulates in aquatic food webs to levels of concern for both human and wildlife health. The chlor-alkali and pulp and paper industries are two major contributors to the severe contamination of sediments in Swedish waters. High concentrations of Hg in sediment does not, however, necessarily results in proportional high concentrations of MeHg (Hsu-Kim et al., 2018). The reason for this is that the methylation of Hg is controlled by the microbial activity and the chemical speciation of Hg in both the solid and aqueous phase. In addition, MeHg produced may be converted back to iHg through both biotic and abotic pathways. The multiple pathways linking the legacy of iHg stored in contaminated sediments to high levels of MeHg exposure introduce further layers of complexity in assessing the risks of Hg-contaminated sediments.

### 1.1.2 Remobilization of Sediment Contaminants

Many contaminants, including HOCs and Hg, accumulate in sediments as they are hydrophobic and have a strong affinity to particles. These properties also contribute to the long-term retention of HOCs in sediments, ultimately leading to burial in deeper sediment layers. However, these contaminants may still pose ecological risks if they are remobilized from sediment into the water column, transferred to pelagic and benthic organisms and subsequently bioaccumulated.

Contaminants are released from sediment into the water column primarily through diffusion and sediment resuspension. Diffusion is driven by concentration gradients between the sediment pore water and the water above. While diffusion is typically a slow process, sediment resuspension may result in the rapid release of larger amounts of contaminants. Wind, as well as human activities such as dredging, trawling, or dragging of fish gear along the seafloor and marine traffic, are some of the processes that may result in sediment resuspension. For the resuspended particles, the equilibrium of the contaminant between the solid and aqueous phases shifts, potentially resulting in contaminant desorption into the water phase, since the concentration of contaminants in the water column typically is lower than in sediment pore waters. To what degree different contaminants desorb and become available for biological uptake is dependent on both the properties of the contaminants and the properties of the resuspended particles. Particle size, organic carbon content and characteristics influence the sediment sorption capacity of organic and inorganic contaminants (Badin et al., 2008; Nybom et al., 2021), and thus also to what extent contaminants are released from sediment to water (Mustajärvi et al., 2019) and how bioavailable they are (Kreitinger et al., 2007). **Current risk assessment procedures, however, do not account for the variability in the risk of contaminant remobilization potential across sites with different contaminant mixtures and sediment properties.** These assessments are instead based on comparing total sediment contaminant concentrations ($C_{tot}$) with $C_{tot}$-based sediment quality criteria (SQC). Hence, current procedures contrast to the general agreement in the research community that the freely dissolved concentration ($C_{free}$) best predicts bioavailability, mobility, and toxicity of particle reactive contaminants (Cornelissen et al., 2005; Greenberg et al., 2014; Lydy et al., 2014a; Mayer et al., 2014). To be bioaccumulated by an aquatic organism, a substance must be bioavailable, meaning freely dissolved in the water ($C_{free}$) (EN ISO 17402) to then be able to cross the organisms' biological membranes (Semple et al., 2004). As described in the following section (1.1.3), passive samplers can be employed to assess $C_{free}$ for contaminants where direct measurement of $C_{free}$ is challenging.

### 1.1.3 Passive Samplers

A passive sampler is designed to absorb analytes from the environment over an extended period (Figure 1). Only the freely dissolved fraction of the compound ($C_{free}$)

will diffuse from the surrounding environment (e.g. water, sediment, air, biota) to the passive sampler, not the total concentration of analytes in the medium ($C_{tot}$) (Lydy et al., 2014b).

Passive samplers work in two different ways: they are either kinetic or equilibrium-based (Figure 1). In the kinetic regime, analytes accumulate progressively, and the time-weighted average concentration is calculated based on the collected mass of contaminant, exposure duration, and sampling rate. In the equilibrium regime, after an initial kinetic phase, the system eventually stabilizes, achieving a thermodynamic equilibrium between the surrounding medium and the passive sampler. The freely dissolved concentration ($C_{free}$) is calculated from the determined concentration of the contaminant in the passive sampler and the partition coefficient between the surrounding medium and the passive sampler if the system has reached equilibrium, and if not, the time to reach equilibrium is included in the calculation (Vrana et al., 2005). The time required to reach equilibrium varies by sampler type, with larger surface areas increasing uptake.

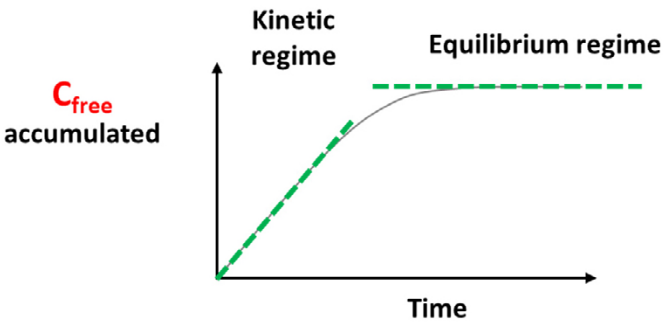

Figure 1. Schematic representation of the kinetics of analyte accumulation in a passive sampler.

There are many different types of passive samplers and their applicability depend on the type of target substances. For HOCs, samplers such as semi-permeable membrane devices (SPMDs) have commonly been employed (Kot-Wasik et al., 2007; Namieśnik et al., 2005; Vrana et al., 2014). Currently, various polymers, including silicones and polyethylene, are often employed for sampling of non-polar compounds like PAHs and PCBs (Charrasse et al., 2014; Lydy et al., 2014b). These devices accumulate the contaminants over time until an equilibrium is reached (equilibrium regime, Figure 1).

Protocols on how to use passive samplers for assessments of $C_{free}$ of organic compounds are more established than those for metals. A major reason for this is that most metals, unlike many HOCs, can be measured from collected water without *in situ* preconcentration. Metals, including Hg, however, exist in various chemical and oxidation states, each differing in their capacity to bioaccumulate. $C_{free}$ of metals may therefore not reflect the bioavailable fraction of the chemical as it does for organic contaminants. By resembling a biological membrane, passive samplers may be used to assess the bioavailable fraction of metals in sediments and waters. The most common passive sampler for metals is the diffusive gradients in thin films (DGT), which may, for example, be used for monitoring metals and other ions by binding dissolved metals as they diffuse through a gel layer and work in the kinetic regime (Figure 1; Gao et al., (2014), Davison & Zhang, (1994, 2012)). Passive samplers previously tested for mercury are further discussed below (3.3.2).

### 1.1.4 Chemical activity

Traditional methods for sediment risk assessment based on total contaminant concentrations can be misleading because they do not reflect how bioavailability or toxicity vary across different types of sediments. The freely dissolved concentration ($C_{free}$) reflects the fraction of the compound that is available for biological uptake or toxic effects, but concentrations of individual compounds cannot be added up to achieve the toxicity of the mixture. Chemical activity is an alternative measure which is additive and can be calculated for a mixture of chemicals.

Chemical activity of a chemical in a matrix mirrors the potential of the compound to transfer between compartments, such as sediment, water, and organisms (Schwarzenbach et al., 2017), and is therefore relevant in environmental risk assessments.

Chemical activity ($a$) is calculated as:

$a = C_{free} / S$

where $C_{free}$ is the freely dissolved concentration in water, and S is the compound's subcooled solubility. $C_{free}$ is estimated as:

$C_{free} = C_{matrix} / K$

where $C_{matrix}$ is the contaminant concentration in a specific material (e.g., biota, sediment, or passive sampler), and K is the partitioning coefficient, which describes how the compound distributes between the matrix and water.

Ranging from 0 to 1, higher chemical activity values indicate greater saturation of the chemical in the particular matrix and an increased likelihood of movement to another matrix. Hence, the chemical activity of a chemical in an environmental matrix offers a measure of the contaminant mobility and risk. As chemical activities of individual compounds are additive, the total activity of a mixture can be estimated by summing the activities of individual compounds. This makes it especially useful for assessing the toxicity of complex pollutant mixtures, including PAHs and other HOCs (Gobas et al., 2018) and to compare contamination across sites from a regulatory perspective.

## 1.2 Aim of MOBILITY

The overarching goal of MOBILITY was to generate knowledge that can help improve risk assessment and monitoring procedures of contaminated sediment including assessments of release and spread of sediment contaminants.

More specifically, the research conducted within MOBILITY aimed to

i) Evaluate how sediment resuspension, sediment and contaminant characteristics impact release of HOCs and Hg from sediment to water, and how this can be captured by passive samplers (Experient I and II).

ii) Evaluate how passive samplers can be used to assess bioavailability and bioaccumulation potential of contaminants released from sediment and to establish links between the passive sampler uptake of these contaminants and their biological effects (Experiment III).

iii) Demonstrate the applicability of passive samplers for assessment and monitoring of contaminated sediment, and develop recommendations on how to integrate the use of passive samplers in risk assessments and monitoring of contaminated sediments (Experiment I–III, literature review and test with natural sediments).

# 2. Material and Methods

Contaminated sediments contain complex mixtures of contaminants, as a result of past and ongoing anthropogenic activities. PAHs were chosen as model substances for HOCs because they are affordable and easy to handle and analyse in the laboratory, and they are highly relevant to the Baltic Sea, where previous studies have shown that they dominate the total chemical activity, making them key contributors to overall contamination and risk (Josefsson, 2023). In MOBILITY, four PAHs were used as model compounds; acenaphthene ("ACE"), phenanthrene ("PHE"), fluorene ("Flu"), and fluoranthene ("FluO"). These four compounds cover a range in hydrophobicity and solubility from log $K_{OW}$ 3.9 to 5.2 and from 0.1 to 4 mg $L^{-1}$, respectively. Their range of hydrophobicity fit the uptake range of the polyethylene passive sampler, without being too hydrophobic to be resuspended in the water column. The chemical activity of each compound was calculated in order to determine the chemical activity of the whole mixture. In addition to these HOCs, Hg in the form of MeHg was used.

The main experimental studies included in the MOBILITY project were carried out using a custom-designed resuspension system containing artificial sediments spiked with our model PAHs and MeHg. The artificial sediments were prepared from coarse sand, quartz sand, kaolin and peat following modified OECD n°218 guidelines (OECD, 2004) and spiked as further described in Appendix 1. In the two first experiments, the role of turbidity, sediment particle size distribution, and contaminant hydrophobicity for the release of contaminants from sediment was tested. In the third experiment, biological uptake and toxicity of contaminants released from sediment were tested.

A key component in this project was to use well-established passive samplers and methods to assess $C_{free}$, and how $C_{free}$ is affected by sediment characteristics, and its impact on mobility, re-contamination, bioavailability and toxicity. Polyethylene (PE) sheets, commonly used for hydrophobic HOCs, were used for the four model PAHs included. As the scientific basis for using passive samplers for Hg is not as strong as it is for organic pollutants, a literature review was conducted. Based on this review, commercially available DGT samplers were used for total-Hg (THg) and MeHg in Experiment III. In addition, we also applied these DGT samplers to sediment slurries collected within the Swedish EPA-funded project *Formation and spread of methylmercury – the weak link in risk assessment of mercury-contaminated sediments* (2020–2024, led by Erik Björn, Umeå University). Combining data from the two projects allowed us to evaluate potential linkages between the amount of $Hg^{II}$ and MeHg concentrated on the passive sampler, HgII and MeHg determined in sediment pore water by direct measurements, Hg speciation in the pore water and Hg methylation rates.

## 2.1 Passive samplers for Hg – literature review

A literature review was conducted (Bachler's thesis by Embla Lindholm, Appendix 2) aiming to identify suitable passive samplers for Hg that could be used in MOBILITY and for risk assessment of Hg-contaminated sediments (Table 1). There were no specific geographical boundaries for the research area, but the research was limited to aquatic environments and the use of passive samplers for quantification of dissolved Hg and/or Hg bioavailability. No in-depth review was conducted on methods to prepare or analyze passive samplers.

**Table 1. Methodology for the literature review.**

| Variable | Input (source or criteria) |
|---|---|
| Databases | PubMed, Stockholm University Library, Google Scholar, Taylor, and Francis Online, EBSCO |
| Keywords | Mercury, methylmercury, passive samplers, aquatic, and passive sampling |
| Criteria | Only peer-reviewed original research articles and reviews were included. |
| Timespan | 2012–2022[1)] |

1) Some articles published prior to 2012 were included if these were frequently referred to in the selected literature (2012–2022) and contributed with additional data not covered in the more recent literature.

## 2.2 Resuspension Experiments

### 2.2.1 Resuspension System

The resuspension system consisted of columns where sediment resuspension was mechanically simulated with the help of rotating rods. The columns were made from polycarbonate pipes (inner diameter of 46 mm, height of 300 mm) and were sealed at the bottom using rubber plugs (Figure 2a). Polycarbonate material was chosen for its low sorption capacity with the 4 studied PAHs, which makes it an inert material that does not interfere in the experiment. During the experiments, the columns were placed in a circular stand that held 20 columns per stand (Figure 2b). In the center of the stands, a motor (Nidec Brushed Geared DC Geared Motor, 66 rpm, Nidec) and a disk with magnets (Eclipse Neodymium Magnet 52 kg, Width 40 mm) were mounted (Figure 2c). In each column, magnetic rods were mounted using discs with a diameter adapted to the inner diameter of the pipes so that the height of the magnetic rods could be adjusted. The rotation of the magnetic rods was driven by the rotating disk with magnets around which the columns were placed. The rotational speed of the magnetic rods was adjusted by the motor's speed and the number of magnets on the rotating disk. The position of the columns (distance to the magnets), the number and strength of the magnets used, as well as the speed of the rotating disk, were tested to achieve the most even resuspension possible.

All experiments were done using artificial sediments spiked with HOCs and/or Hg and artificial brackish seawater (the sediment preparation protocol is given in the Appendix 1 and was prepared to reflect a typical sediment from the Baltic Sea). The same sediment composition was used for all experiments to ensure consistency. While natural sediment can be assumed to better represent natural conditions, artificial sediment has the advantage of allowing one parameter, such as particle size distribution, to be altered while keeping other parameters, such as organic carbon content, constant. About 100 g of sediment was added to the cores, followed by 350–400 mL of brackish water, slowly poured to avoid sediment resuspension. The cores were left in a thermoregulated room at 10 °C (in the dark for stabilisation for 2 to 9 days before initiating the experiments.

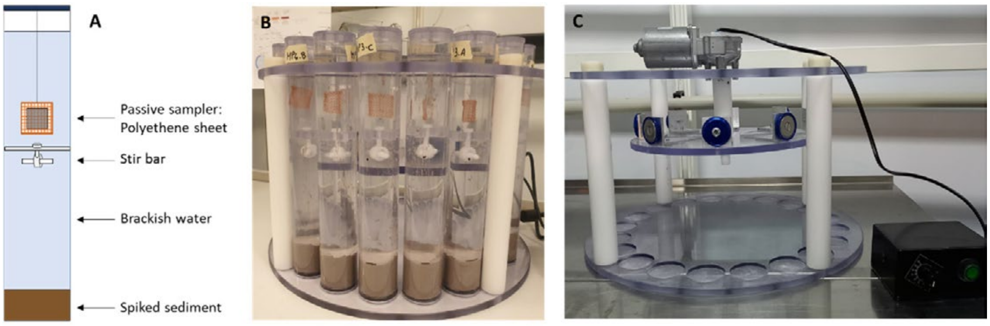

Figure 2. Illustration of a resuspension core (A), photos of one of the experimental sets with (B) and without (C) the resuspension cores. Figure adopted from Chaumet et al., (2025).

## 2.2.2 Passive Samplers

For the PAHs, a 35 µm polyethylene (PE) sheet was used as passive sampler (Figure 3A). The passive samplers were employed in the resuspension cores wrapped in a copper net to prevent biofilm growth (Figure 3B and C). For Hg, a DGT sampler was selected (LSNB-AP, DGT® Research, Figure 3D) as it is commercially available and there is existing research supporting its use to monitor Hg bioavailability. The sampler (diameter 31.4 mm) is composed of a filter polyethersulphone membrane (thickness: 0.14 mm), an agarose diffusive gel (thickness: 0.8 mm) and a binding layer of 3-mercaptopropyl-functionalized silica gel to preconcentrate divalent Hg ($Hg^{2+}$) and MeHg (Figure 3E).

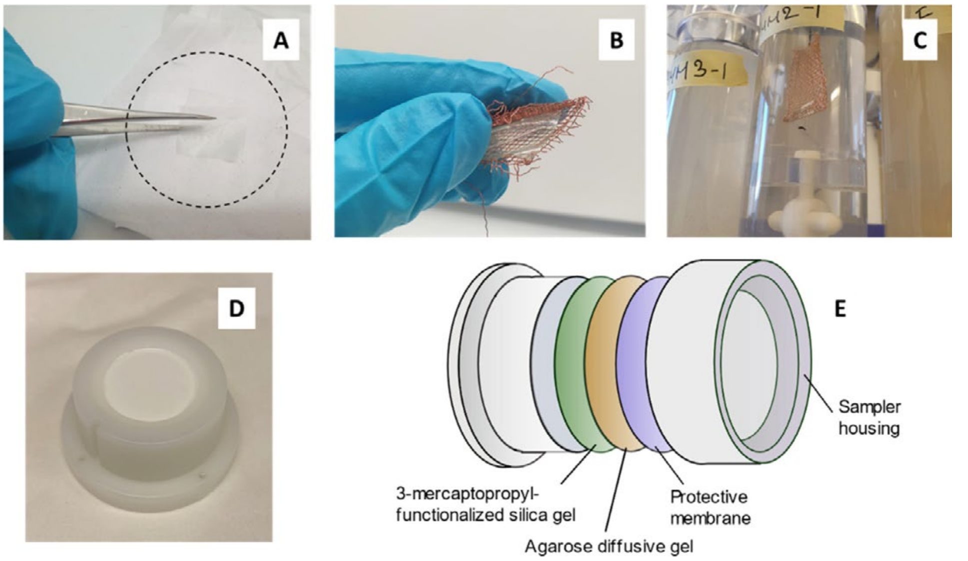

Figure 3. Photo of polyethylene film (A), polyethylene film inside the cupper net (B), polyethylene film placed in a resuspension core (C) and DGT sampler (D). Illustration of the construction of DGT sampler (E). Photo and illustration: Betty Chaumet and Sofi Jonsson.

### 2.2.3 Influence of Turbidity and Hydrophobicity on PAH Release (Experiment I)

To test the influence of hydrophobicity on the PAH release from sediment to water, artificial sediments with a final concentration of 3 mg $kg^{-1}$ dry weight of the four model PAHs were prepared. Four different treatments were applied in which the stirring speed was adjusted to create different regimes of sediment perturbation (n = 3 per treatment, (low: continuous stirring at speeds of 6 cm $s^{-1}$, medium: 13 cm $s^{-1}$, high: 18 cm $s^{-1}$ and pulse: pulse treatment at 18 cm $s^{-1}$ for 30 minutes twice a day). Passive sampler and sediment for extraction and quantification of model PAHs were collected after 2, 3 and 4 weeks of experiment. Further information on the experimental setup is provided in Chaumet et al., (2025). The resulting turbidity in the four different treatments is shown in Figure 4. For the two lower resuspension levels, the treatment resulted in relatively stable turbidity during the course of the experiment. For the treatments *high* and *pulse*, the turbidity initially increased and thereafter decreased to reach similar turbidity levels as the other two treatments. Possible explanations for the lower turbidity observed in the second half of the experiment may be redistribution of the sediment and formation of biofilms which would lead to aggregation of the particles in the sediment.

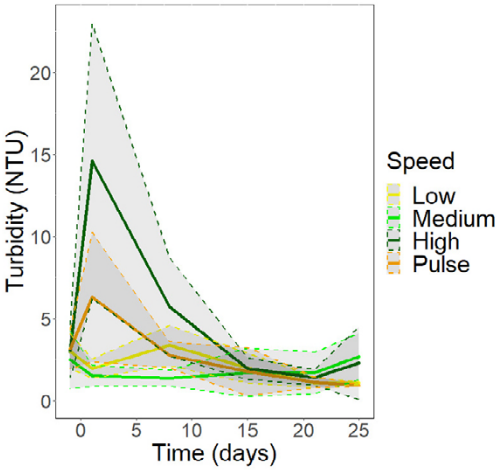

Figure 4. Turbidity during the course of Experiment I at the different stirring speeds applied. Figure adopted from Chaumet et al., (2025).

### 2.2.4 Influence of sediment grain size on the Release of PAHs and MeHg from sediment (Experiment II)

To test the influence of sediment grain size distribution on the release of contaminants from sediment to water, sediments with varying silt and clay content were prepared, resulting in particles smaller than 63 µm ranging from 43 % to 72 % (Figure 5). In addition to the four model PAHs at a final concentration of 3 mg $kg^{-1}$, MeHg was added to a final concentration of 5 µg $kg^{-1}$. The material used to prepare the sediments contained ~10 ng $g^{-1}$ of THg and 0.16 ng $g^{-1}$ of MeHg. At the start and end of the experiment we detected 3.9 ± 0.38 and 4.1 ± 0.46 ng MeHg $g^{-1}$, respectively, which correspond to around 40 % of THg as MeHg after sediment spiking. The resuspension cores were prepared in triplicates for each type of sediment together with 3 blanks (sediment with no contaminants added). Water was sampled before initiating resuspension as well as during the experiment for quantification of dissolved Hg. Each time water was sampled it was replaced with brackish water (in total < 10 % of the total water volume was replaced during the experiment). The experiment was conducted over two weeks at 10 °C in the dark. After two weeks of exposure passive samplers and sediment were collected for quantification of PAHs and Hg. In all treatments, the DOC content increased and turbidity decreased during the course of the experiment (Figure 5B).

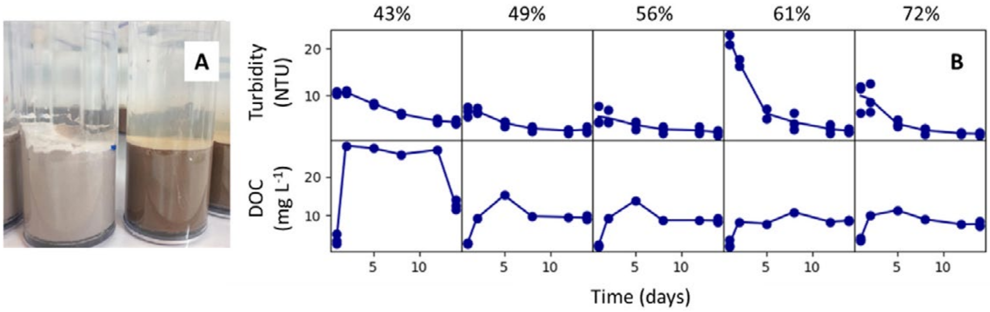

Figure 5. Photo of two of the prepared sediments for Experiment II with 43 % (left core) and 72 % (right core) of particles < 63 µm (A). Turbidity and DOC concentration observed during Experiment II for the sediments with contrasting sediment grain size distribution (43 to 72 % of particles < 63 µm) (B). Dots represent individual datapoints and solid line shows the average values. Photo: Betty Chaumet.

## 2.2.5 Biological uptake and effects of contaminants released from sediment (Experiment III)

The filamentous red alga *Ceramium tenuicorne* was used as a model organism to determine the applicability of passive samplers as indicators for biological uptake of contaminants released from sediment. This species is common in the Baltic Sea soft bottoms, inhabiting areas with low salinity, down to 2–3 PSU. These habitats are characterized by their proximity to the shore and can be occasionally turbid, which influences the alga's growth and distribution patterns (Rinne and Kostamo, 2022). The brackish water strain used in the present study originates from the area located about 100 km south of Stockholm; it was isolated in 1995 by Dr. Britta Eklund at Stockholm University. This strain has been used to develop and standardize bioassays for sediment toxicity testing (Eklund, 2017; Eklund et al., 2010, 2016).

The algae were cultivated in natural, filtered (< 20 µm) autoclaved brackish water with a salinity of 6.8 ± 0.1 ‰. The water was enriched with nutrients (nitrate, phosphate), vitamins and trace elements following the guidelines of Bruno and Eklund (2003) to provide optimum growth rates. The female clones were grown in sterilized polystyrene Petri dishes at 22 ± 1 °C with a light intensity of 35±5 µmol $m^{-2}$ s and a light/dark regime of 14:10. Top branches were transferred to a new medium weekly to ensure a constant supply of actively growing algae.

Sediments were prepared as presented for experiment I, and spiked at a concentration of 100 mg $g^{-1}$ dry weight for each PAH. Such high concentrations were chosen to ensure measurable bioaccumulation in biota and thus enhance the detection of transfer mechanisms. However, these concentrations were carefully selected to remain within levels observed in contaminated environments, maintaining ecological relevance (Niehus et al., 2018). Two stirring treatments were applied (6 and 18 cm $s^{-1}$) in order to generate a gradient of PAH concentrations in the water column. The experiment was run for 7 days at 21 °C with a dark/light alternation of 10:14. At the end of the experiment, passive samplers, *C. tenuicorne*, water and sediment samples were collected for quantification of PAHs and total Hg, MeHg, and ancillary parameters. Physiological responses to the exposure were assessed by examining changes in pigment composition (Chl *a*, Chl *c*, and carotenoids), photosystem II performance, total antioxidant capacity, and algal stoichiometry measured as carbon: nitrogen ratio in *C. tenuicorne*.

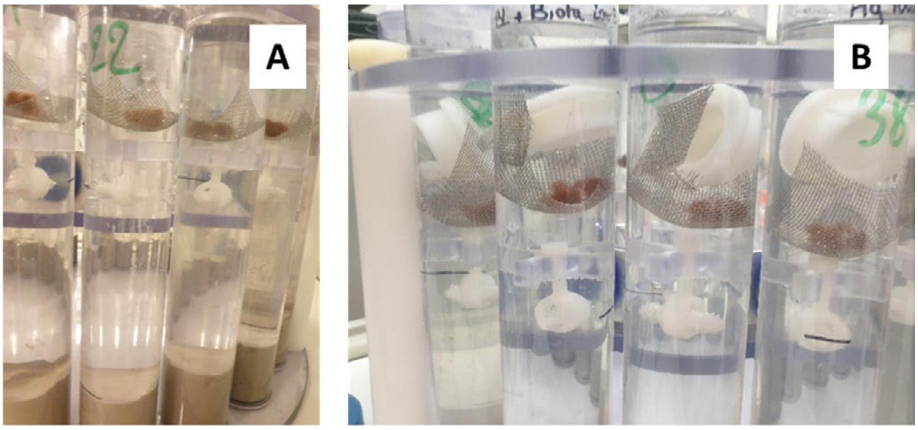

Figure 6. Picture of A) the cores mounted with the *C. tenuicorne*, and B) after the addition of the passive samplers.

## 2.3 Application of passive samplers for Hg in contaminated sediments

In 2024, contaminated sediments were collected from 25 sites in the Baltic Sea within the Swedish EPA-funded project led by Erik Björn, Umeå University. We received sediment slurries from these 25 sites and employed two DGT samplers to each slurry for quantification of THg (sum of $Hg^{II}$ and MeHg) and MeHg. At Umeå university, potential methylation rates (km $d^{-1}$), and concentrations of THg and MeHg in the porewater and solid phase (using direct measurement techniques) were determined. In addition, they modelled the chemical speciation of Hg in the dissolved phase.

## 2.4 Quantification of PAHs, Hg, biofilm and ancillary parameters

PAHs were extracted and preconcentrated from the passive samplers, sediment and *C. tenuicorne*, and then quantified by GC-MS. Total Hg and methylmercury was extracted and preconcentrated from water, sediment and *C. tenuicorne* and quantified using GC coupled to CVAAFS or ICP-MS. Biofilm formation was evaluated by quantifying the DNA concentration from biofilm collected from the polyethylene films (passive sampler for the organic compounds). Ancillary parameters monitored included dissolved oxygen, conductivity, pH, turbidity, dissolved organic carbon (DOC), total carbon and nitrogen in sediments and particle size distribution.

## 2.5 Statistical Analysis

Statistical analysis was performed to determine the impact of turbidity, the substances' hydrophobicity, the sediment PSD, and DOC on contaminant released after sediment resuspension. Generalised linear models (GLM) were established to estimate the release of contaminants based on the previously listed parameters or to estimate the potential contaminant uptake in the biota based on the uptake in the passive sampler. The GLM analysis was performed using R software (R version 4.3.1 2023-06-16) and the package "DHARMa". To identify the specific turbidity and log $K_{OW}$ values at which these factors influenced the PAHs release, a combination of GLM analysis and the Johnson-Neyman procedure was applied.

# 3. Results and Discussion

## 3.1 Release of Organic Contaminants

### 3.1.1 Impact of Hydrophobicity

The hydrophobicity of organic contaminants influences the partitioning of the contaminant between organic carbon-rich particles and surrounding media. Contaminant hydrophobicity thereby also impacts the risk of contaminant release from sediment to water via diffusion or after sediment resuspension. In MOBILITY, we analysed the release of model compounds (PAHs) with log $K_{OW}$ ranging from 3.9 to 5.2 (acenaphthene ("ACE"), phenanthrene ("PHE"), fluorene ("Flu"), and fluoranthene ("FluO")), in three different resuspension experiments. Figure 7 illustrates the distribution of each PAH between the passive sampler and sediment (Log ($a_{PS}$ / $a_{sed}$)) in the three experiments (A–C). In all of the experiments, there was a significant correlation between the PAH hydrophobicity (log $K_{OW}$) and release from sediment (Log ($a_{PS}$ / $a_{sed}$)), with lower release observed for the more hydrophobic compounds (i.e., compounds with a higher log $K_{OW}$). This trend is expected, as the more hydrophobic compounds more strongly partition to sediment organic matter, which lowers the partitioning to the dissolved phase ($C_{free}$).

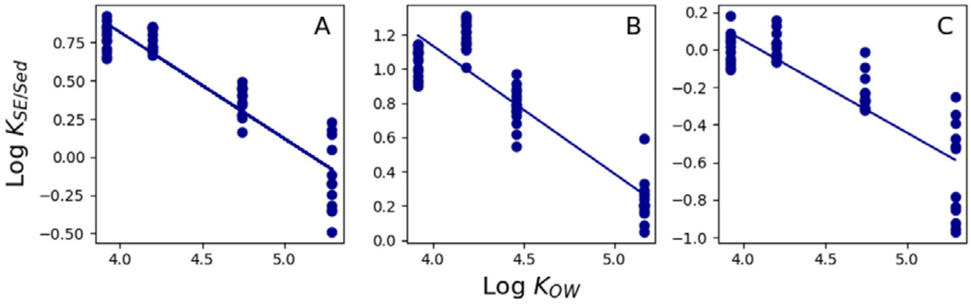

Figure 7. Relationship between PAH hydrophobicity and release from sediment to water (expressed as Log ($a_{PS}$ / $a_{sed}$)) in experiment I (A, Chaumet et al., 2025), II (B) and III (C).

### 3.1.2 Impact of Turbidity

Turbidity, commonly quantified in Nephelometric Turbidity Units (NTU), is a measure of the haziness of the water. Under typical conditions, turbidity in the Baltic Sea ranges from 0.5 to 2 NTU, but during strong resuspension events, it can increase tenfold due to the resuspension of surface sediments (Kyryliuk & Kratzer, 2019; Rasmus et al., 2015). In experiment I, we aimed to create different turbidites by altering the stirring speed.

In Figure 8, the concentration of the released PAHs is presented as a function of turbidity. For the most hydrophobic compound (FluO), a higher $C_{free}$ was observed in systems with turbidity exceeding 6 NTU after two weeks of resuspension. In contrast, a lower $C_{free}$ was observed for the least hydrophobic PAH (ACE). These results suggest that resuspension may affect the release of organic compounds differently based on their hydrophobicity, as released from sediment by compounds of varying hydrophobicity likely is dominated by different processes. During calmer conditions (NTU < 2.8) diffusion leads to a greater release of compounds with lower log $K_{OW}$ values (< 4). Enhanced PAH diffusion during calmer conditions has also previously been shown (Belles et al., 2016). During sediment resuspension events, i.e., at higher turbidity, resuspension and subsequent desorption of contaminants from the resuspended particles lead to an enhanced release of more hydrophobic compounds (e.g., FluO, log $K_{OW}$ > 4). For contaminants with log $K_{OW}$ between 4.1 and 4.5, our experiment suggests that turbidity has a minor effect on the amounts released from the sediment.

In our experiment, the highest turbidity measured was 8.31 NTU after two weeks of exposure. Hence, although passive samplers are known to integrate contamination over time, including extreme events such as floods which usually bring peaks of contamination (Bernard et al., 2022; Godlewska et al., 2020), further research is needed to understand release from sediment and uptake capacity of passive samplers at high turbidity events. The results from Experiment I are further described in Chaumet et al., (2025).

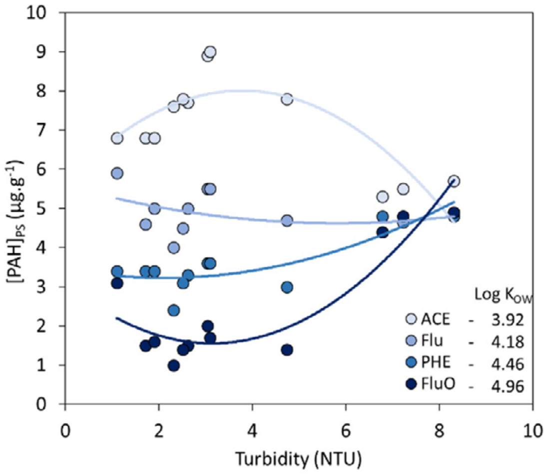

Figure 8. PAH (acenaphthene (“ACE”), phenanthrene (“PHE”), fluorene (“Flu”), and fluoranthene (“FluO”)) release from sediment to water as a function of turbidity, in Experiment I. Figure reprinted from Chaumet et al., (2025).

### 3.1.3 Impact of Sediment Composition

In addition to the turbulence, sediment resuspension may also depend on sediment composition. Factors such as organic matter content and grain size influence both the sediment’s binding capacity and its physical structure, which together affect release potential of contaminants from sediment through diffusion and determine how easily the sediment is resuspended. In experiment II, we tested the role of sediment composition by altering the contribution of fine particles (< 63 µm) in the tested sediments between 43 and 72 % (TOC of 2.2 %). The contribution of particles in sediments with a size smaller than 63 µm is commonly referred to as the fine fraction of the sediments and is used as a proxy for the content of silt and clay. In the Baltic Sea sediments, the fine fraction of surface sediments varies greatly geographically (from 0 to 100 %) due to the sorting of particles according to size as they are transported from the rivers to off-shore areas (Leipe et al., 2017).

We observed higher DOC in the water in the coarsest sediment treatment, and higher turbidity in the beginning of the experiment for the sediment with the fine fraction of 61 % (Figure 5). For the remaining sediments, no large differences in turbidity or DOC were observed between the different treatments. The higher diffusion of DOC in the coarsest sediment treatment may be caused by increased diffusion from the sediment due to a more porous sediment structure. The non-linear effect of sediment grain size observed on the turbidity may be due to multiple processes involved: DOC diffusion, sediment resuspension and vertical redistribution of different sediment size fractions at the top of the sediment.

There were no statistical differences between the release of PAHs between the sediments with different fine particle contribution, with the exception for a lower release of ACE from the 61 % fine particle sediment (Figure 9). That higher release of DOC from the coarsest sediment tested (Figure 4) was observed, while a proportional increase in release of PAHs was not found, suggest that DOC more easily diffuses from the sediment than PAHs do. The lower release of ACE in sediment with a sediment fine fraction of 61 %, where also higher turbidity was observed (Figure 4), further indicates that sediment properties may have an effect on contaminant release. In the field, larger variability of sediment properties can be expected than what was covered with the artificial sediments included in this experiment.

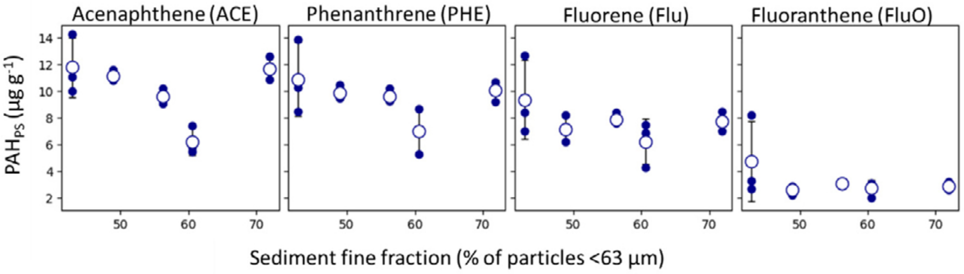

Figure 9. PAH release from sediment measured as $C_{free}$ using PE samplers (Experiment II) for the different sediments with varying proportion of fine particles. Blue filled circles show the datapoints, white circles show the average and error bars the standard deviation.

### 3.1.4 Implications for HOC monitoring and contaminant assessment

We used the linear relationship observed between PAH hydrophobicity and release (Experiment I; Figure 7) to estimate the hypothetical contaminant mixture release from measured contaminant concentrations in Baltic Sea sediments (data from the Effect Screening Study 2.0, Gorokhova et al., (2023)) at two turbidity scenarios (> 2.7 and < 2.7 NTU, respectively). The Effect Screening Study 2.0 included 15 PAHs with log $K_{OW}$ ranging from 3.4 to 7.4 and these 15 PAHs contributed with 84 % to 100 % of the total load of contaminants (expressed as chemical activity, *a*) of 86 monitored organic contaminants in the sediment samples. Based on the PAH chemical activity measured in the sediments, we estimated their potential release in the water under the two turbidity scenarios. Figure 10 shows the composition of the PAH mixture in the sediment and in the released fraction for the two most contrasting Baltic Sea sites. The results provide a theoretical example of how turbidity and compound hydrophobicity can influence the risk associated with contaminated sediments.

At station *N26*, the contribution of naphthalene (log $K_{OW}$ = 3.41) was about 19 % in the sediment. When the two turbidity scenarios were applied, its contribution increased up to 87 % and 76 % in the released fraction at low and high turbidity, respectively. At station *Bråviken8*, the relative contribution of naphtalene was 1.3 % in the sediment, but 20–46 % in the released fraction under the low and high turbidity scenario, respectively. In contrast, indeno[1,2,3-cd]pyrene, which was the most hydrophobic compound included in the assessment (log $K_{OW}$ of 7.09), contributed to 20 % of total the mixture in the sediments but did not exceed 2 % relative contribution in the released fraction at the different tested turbidities. These results highlight the importance of considering the type of chemical mixtures in contaminated sediments when assessing the risk of contaminant remobilization. The modelled release of the PAH mixture from these two sediments further demonstrate that the mixture of contaminants present may control the risk effect of high turbidity events. Here, the high fraction of less hydrophobic PAHs at station *N26* resulted in increased mobilization at turbidities exceeding 2.75 NTU, while the opposite was observed for *Bråviken 8*.

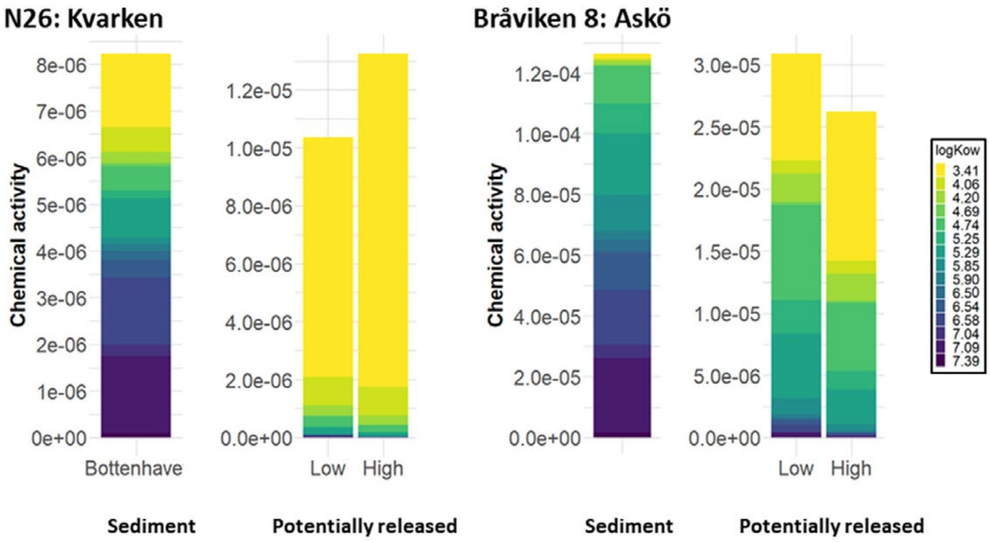

Figure 10. Chemical activity of a PAH mixture in sediment and hypothetical contaminant mixtures release (potentially released)at low (< 2.7 NTU) and high (> 2.7 NTU) turbidity, at two of the sites investigated using data from Experiment I and sediment data from the Effect Screening Study 2.0, Gorokhova et al., (2023). Figure adopted from Chaumet et al., (2025).

## 3.2 Release of Mercury

In addition to the four model PAHs, we studied the release of Hg added as MeHg in Experiment II. We observed a negative trend between the concentration of Hg in the dissolved phase and the particle size distribution, suggesting higher mobilization of Hg with coarser sediments (Figure 11A). This trend was not observed for MeHg, where no significant correlations were found (Figure 11B). Additionally, the concentration of MeHg in the water decreased, while the concentration of THg increased over the course of the experiment. For THg, a close correlation was found between the concentration in the dissolved phase and DOC (Figure 11C), aligning with a large body of research that demonstrates a strong correlation between DOC and Hg in natural waters. It remains unclear why MeHg does not follow the same trend. One possible explanation may be the different sources of THg and MeHg in the sediment: while > 90 % of the MeHg observed at the end of the experiment in the sediment originated from MeHg which was added to the artificial sediment, THg primarily originated from the artificial sediment itself (> 70 %). Although the MeHg was pre-equilibrated with the peat for two days before the experiment, it is possible that some of the iHg that was already present in the material used had occupied weaker binding sites in the sediment, and thus more easily diffused from the sediment to the water column. Demethylation of MeHg in the water may also have contributed to the lack of an observed treatment effect for MeHg, as well as explain the lower concentrations observed at the end of the experiment than in the beginning. Although MeHg is the form of Hg which bioaccumulates to concentrations of concern, iHg (the main fraction of THg) released from the sediments may be methylated e.g. in the gut of invertebrates, and thus be incorporated in the aquatic food web.

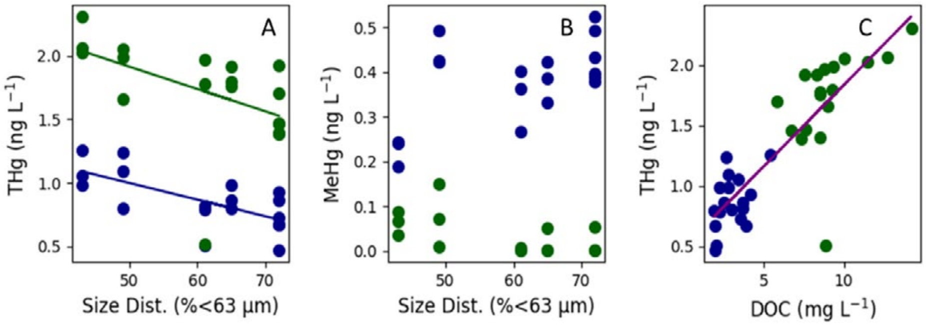

Figure 11. Concentration of THg (ng $L^{-1}$) and MeHg (ng $L^{-1}$) as a function of sediment grain size distribution (% particles < 63 µm; A and B, respectively) and concentration of THg (ng $L^{-1}$) as a function of DOC content (mg $L^{-1}$; C). Data presented was collected at the start and at the end of the experiment (blue and green data points and regression line, respectively).

## 3.3 Use of Passive Samplers

### 3.3.1 Passive samplers for HOCs

Experiment III demonstrates that chemical activity in the *C. tenuicorne* correlates with chemical activity in the passive sampler (Figure 12A), suggesting that polyethylene (PE) passive samplers could be effective for estimating PAH accumulation in biota. The linear relationship observed in Figure 12 has a regression coefficient below 1. In theory, at equilibrium, all the compartments should present the same chemical activity (Gobas et al., 2018) which is not the case here as $a_{PS}$ is higher than $a_{Biota}$. We assumed that the biota did not reach equilibrium, potentially due to the limited duration of exposure (7 days), which may have been insufficient for complete equilibration. For unicellular phytoplankton, an exposure time of 72 hours is enough for the four PAHs tested in MOIBILITY to reach equilibrium with water (Oliveira dos Anjos et al., 2023, 2024), but *C. tenuicorne* has a more complex structure and may require longer for equilibrium to be reached. Even though the uptake of PAHs in *C. tenuicorne* did not reach equilibrium, the correlation with the chemical activity in the passive sampler makes the passive sampler a possible indicator of a worst-case exposure scenario for biota.

The physiological responses in *C. tenuicorne* were assessed by examining photosynthesis inhibition (Figure 12B) as a function of the total contaminant load in the biota, which was assessed in two ways: i) as the load quantified in the *C. tenuicorne,* and ii) calculated from $C_{free}$ determined from the passive samplers. The theoretical load in the biota was recalculated based on the relationship between the uptake in the passive sampler and the bioaccumulation in the biota (Figure 12A). The dose-response curve provided an effective chemical activity ($Ea_{50}$) of 0.01 for both approaches used to assess the chemical activity exposure level, thus supporting PS as a good proxy for biota bioaccumulation of HOCs released from sediment. The observed inhibition occurred through inhibition of the photosynthesis II system, and indirectly by negatively affecting the photosynthesizing pigments. Beyond photosynthesis inhibition, PAH exposure reduced the nutritional quality of the algae by altering its elemental stoichiometry (reduced carbon and hydrogen content, and lowered carbon to nitrogen ratio), which could have downstream effects on aquatic organisms that rely on algae as a food source, as well as higher-level consumers. Together, these results suggest that the passive samplers are not only suitable for assessing the bioavailable fraction, but may also be used as an indicator of biological effects.

It should be noted that the results obtained from this project are not directly applicable on environmental conditions as experimental conditions are controlled and less variable than natural systems. The artificial sediment prepared in this project had the same composition for all the experiments for comparison purposes, and any effects caused by variability across sediment types or biological activity in the sediments are not captured.

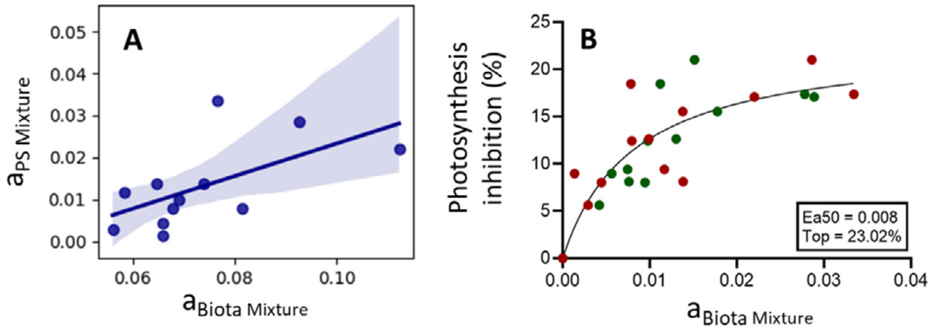

Figure 12. (A) Comparison of the load of the PAH mixture (expressed as chemical activity) in the passive sampler ($a_{PS\ Mixture}$) with the load in *C. tenuicorne* ($a_{Biota\ Mixture}$) with individual data points representing measured data and the shaded grey area indicating the 95 % confidence interval. (B) Photosynthesis inhibition (%) as a function of the PAH load ($a_{Biota}$) calculated from PAH load in the passive samplers (red) and observed in the *C. tenuicorne* (green).

## 3.3.2 Passive samplers for Mercury

To select a suitable passive sampler for Hg, a literature review was conducted (Degree project by Embla Lindblom, full project included as Appendix 2). Four different types of passive samplers were identified, Simple Polymer Films, Polymer Inclusion Membranes (PIMs), Chemcatcher®, and Diffusion Gradient Thin films (DGTs). Taking advantage of Hg's strong affinity to reduced sulphur, most of the tested passive samplers were based on modified polymers containing sulphur ligands. Among the four types of passive samplers identified in the literature, DGTs have received the most scientific attention. Several studies have also demonstrated a positive correlation between the amount of Hg (or MeHg) observed on DTGs deployed in sediments and in water and the amounts of Hg accumulated in lower trophic levels (Gade et al., 2024). For instance, Clarisse et al., (2012), demonstrated a strong correlation between the concentrations of Hg accumulated in DGT (with similar binding resin as the one used in our study) and in the clam *Macoma baltica* ($r^2 = 0.89$) in experimental systems across a salinity range of 10 to 30 ‰ and in systems with and without dissolved organic matter. Efforts have also been made to correlate the fraction of iHg enriched on DGTs with Hg methylation rates in sediments (Ndu et al., 2018). Although DGTs in this case were successful in estimating the fraction of iHg available for methylation, they do not necessarily provide insight into net Hg methylation in different systems, as this also depends on the composition and activity of the microbial community. In a recent review of the use of DGTs to measure Hg bioavailability, it was concluded that while there is a growing support for usefulness of DGTs, there are still a lot of open questions which remain to be addressed, including how nm sized particles may alter the DGTs and thus affect the DGT performance (Gade et al., 2024). In addition, standard protocols for the application of Hg-DGTs for monitoring needs to be developed.

Given the scientific support for using DGTs to monitor bioavailable $Hg^{II}$ and MeHg fractions, and the availability of commercial samplers designed for preconcentration of $Hg^{II}$ and MeHg (Figure 3C–D), DGTs were selected for the experiments performed within MOBILITY. We tested the DGTs both in Experiment III and in the sediment slurries collected from 25 contaminated sites in the Baltic Sea. Data analysis for both studies are ongoing, but evaluation of the data from Experiment III suggests that we were not able to establish a statistically significant relationship between the concentration of MeHg on the DGT and in the *C. tenuicorne*. It is important to note that our dataset is relatively limited (n = 6) and that the MeHg range observed in the *C. tenuicorne* was quite narrow, ranging from 160 to 280 ng MeHg (as Hg) g (dry weight)$^{-1}$. Thus, the lack of a relationship in our test does not necessarily contradict earlier studies where a relationship between DGT and biota MeHg levels has been established.

Deploying DGTs in the sediment collected from contaminated sites in the Baltic Sea allowed us to evaluate potential relationships between the amount of iHg and MeHg caught on the DGT, with the chemical speciation and concentration of Hg in the dissolved phase and potential Hg methylation rates of different (data provided by Umeå University). While we observed a positive correlation between the THg concentrations calculated from the Hg retained on the DGTs and the dissolved concentration of THg measured by direct methods, this was only true when looking at the complete dataset including the two sites with THg exceeding 10 ng $L^{-1}$ (Figure 13A). At THg concentrations below 10 ng Hg $L^{-1}$, the amount of Hg on the DGTs correlated positively with DOC and negatively with sulfide concentrations (Figure 13B–C). Both DOC and sulfide strongly influence the chemical speciation of Hg in the dissolved phase, no correlation was, however, found between the THg on the DGT and the concentration of the dominant iHg complexes in the dissolved phase ($HgS_2^{2-}$, $HgSH^-$, $Hg(SH)_2$). When comparing the concentration of iHg (iHg = THg – MeHg) determined using the DGTs and potential Hg methylation rates, no correlations was observed. These results strengthen earlier work concluding that although passive samplers may be used to determine the fraction of Hg available for biotic methylation, this alone is not enough to assess Hg methylation among contaminated sediment systems, as differences in microbial activity and community composition are not accounted for (Ndu et al., 2018).

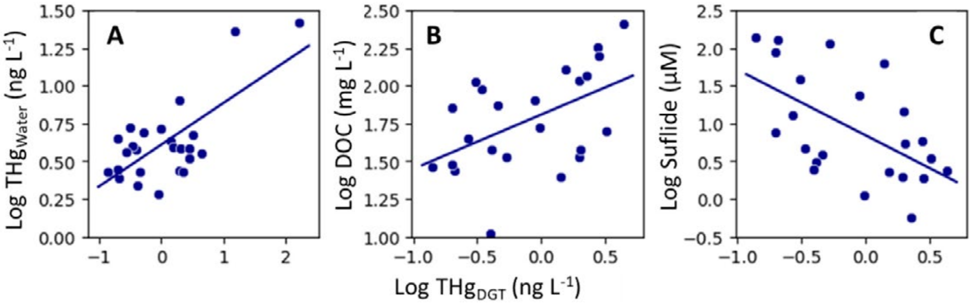

Figure 13. Concentration of total Hg (THg) in the water calculated from Hg in DGT samplers (Log $THg_{DGT}$) as a function of the THg (Log $THg_{Water}$, A). $THg_{DGT}$ (excluding values above 10 ng $L^{-1}$) as a function of dissolved organic carbon (Log DOM, B) and sulfide (Log Sulfide, C) in the pore water. Blue lines show the linear regression model ($p < 0.05$).

# 4. Conclusions

Based on the experimental work and literature review conducted, we draw the following conclusions.

- Turbidity impacts the release of HOCs from contaminated sediments, with lower turbidity favoring the release of more polar chemicals and higher turbidity favoring the release of less polar chemicals.
- Variability in sediment grain size affects the release of DOC and contaminants, influencing bioavailability and the subsequent interpretation of contamination levels and risks.
- Passive samplers can be used as a worst-case scenario indicator of biological uptake and potential effects of HOCs in *Ceramium tenuicorne*.
- There is scientific support for the use of passive samplers (DGTs) for assessing the bioavailability of methylmercury, further studies are needed to further examine how these passive samplers perform under different environmental conditions.
- While passive samplers may be used to assess the availability of inorganic Hg for Hg methylation organisms, it does not provide valuable insight into the net methylation potential of contaminated sediments.

# 5. Recommendations

Based on the "MOBILITY" project findings, these are recommendations for using passive samplers to monitor HOCs and Hg under varying turbidities caused by sediment resuspension. These recommendations aim to improve the utility of passive samplers in capturing real-time contaminant mobility under variable environmental conditions, with particular focus on resuspension, to support effective monitoring and risk assessment.

- Incorporate passive samplers in regulatory assessments.
    - Passive samplers can be used to measure freely dissolved concentrations ($C_{free}$) for both HOCs and MeHg, as $C_{free}$ provides a more accurate prediction of contaminant mobility and bioavailability compared to total sediment concentrations ($C_{tot}$). For HOCs, PS can also be used to predict toxicity in *C. tenuicorne*.
    - Explore how existing Standard Operating Procedures (SOPs) for deploying and analyzing passive samplers (U.S. EPA/SERDP/ESTCP, 2017) can be used under different water turbulence/turbidity conditions to ensure consistent data across different environmental contexts and enhance comparability of monitoring data across sites and time periods.
- Consider variations in turbidity in survey/monitoring protocols as an indicator for use in contaminated sediment risk assessments.
    - For example, tailor contaminant assessment in sediment in its current form (i.e., single chemical concentrations normalized to sediment mass) to capture possible variations in the contaminant release under different turbulence levels. In particular, our results suggest that scenarios for substantial effects of turbidity on the observed concentrations of dissolved PAHs include lower turbidity (< 3 NTU) in combination with high contribution of low log $K_{ow}$ (< 4.1) compounds, and high turbidity (> 3 NTU) in combination with high log $K_{ow}$ (> 4.5) compounds. In these scenarios, the higher turbidity (e.g., during storms, runoff events, or human activities like dredging) enhances the release of PAHs with log $K_{OW}$ > 4.5 through resuspension and desorption mechanisms, whereas the low log $K_{OW}$ PAHs (< 4.1) are more readily released at the low turbidities through diffusive mechanisms. Therefore, joint assessment of contaminant concentrations in sediment and turbidity levels and sources in the bottom layers can improve the risk assessment of contaminants released in the water phase as exemplified by our analysis of the data originated from the Effect Screening Study (section 3.1.4).
    - Similarly, in field studies, variations in turbidity can lead to fluctuations in HOC uptake by passive samplers when monitoring $C_{free}$ in the water column (Figure 8). Therefore, turbidity measurements taken alongside passive sampler deployment at monitoring sites can help explain variability in the $C_{free}$ data in the water phase.
    - To obtain the worst-case assessment scenarios for HOCs using passive samplers, the frequency and timing of measurements should target periods with alternative resuspension regimes depending on the HOCs of interest and/or locations. For instance, sediments contaminated by highly hydrophobic

    and toxic chemicals, such as dioxins and furans, should be monitored during high-turbidity periods as these conditions facilitate the contaminant release. By contrast, low-hydrophobicity PAHs, such as naphthalene, acenaphthene, and fluorene, are the most likely to remain in the water column following an oil spill, and measuring them is most appropriate under low-resuspension conditions when the relative influence of contaminant binding to particles is lower. Finally, increasing the frequency of passive sampler deployments in areas prone to episodic turbidity (e.g., coastal regions with frequent wind-induced sediment disturbances) and prolonged periods of calm conditions can capture close to maximal and minimal values of the contaminant release; thus, providing an average risk profile for ecosystems impacted by these fluctuations.
  - Validate the influence of turbidity and hydrophobicity on contaminant release by conducting further validation studies across a broader range of compound properties in both mesocosm and field settings to ensure robust assessments of contaminant behavior under varying environmental conditions.
- Further research and method development.
  - Conduct experimental (preferably using mesocoms) and field studies across a broader range of compound properties to validate turbidity- and hydrophobicity-driven contaminant release under varying environmental conditions.
  - Further investigate the role of sediment grain size distribution and water DOC on contaminant release from sediment.
  - Explore possibilities for integrating turbidity – specifically from sediment resuspension – as a covariate in Environmental Quality Standards (EQS) for HOCs and metals to improve the ecological relevance and accuracy in risk assessments. This would allow EQS values to be dynamically adjusted based on local turbidity measurements, enhancing comparability of the bioavailable contaminant fraction across variable environments, and supporting the development of more adaptive regulatory frameworks, particularly in systems where resuspension and particle-associated transport are significant. Such dynamic approach would be analogous to how metal concentration thresholds in sediments are normalized to total organic carbon (TOC). Turbidity would thus serve as an operational proxy for the particle load influencing contaminant transport and partitioning, particularly for substances with high particle affinity. This could improve cross-site comparability of bioavailable fractions and support the development of more adaptive, context-sensitive regulatory frameworks. Without accounting for the differential response of low and high $K_{OW}$ compounds to resuspension, EQS may underestimate contaminant risks under conditions of elevated turbidity, such as during storms, dredging operations or high sediment resuspension events. This is particularly critical in environments where fine-grained sediments remain suspended for extended periods, increasing potential exposure.

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# Appendix A. Supplementary Material and Methods

**Preparation of brackish water.** Brackish water (salinity of ca 7 ‰) was prepared from MilliQ water, 4.84 g $L^{-1}$ NaCl, 0.17 g $L^{-1}$ KCl, 0.18 g $L^{-1}$ $CaCl_2$, 1.12 g $L^{-1}$ $MgCl_2{\cdot}6H_2O$ and 0.73 g $L^{-1}$ $MgSO_4{\cdot}7H_2O$. The water was pH adjusted (pH 7 to 8 using 3.5 g $L^{-1}$ NaOH) and autoclaved before use.

**Preparation of artificial sediment.** The artificial sediments were prepared from coarse sand, quartz sand, kaolin and peat following modified OECD n°218 guidelines (OECD, 2004). For experiments I, the sediments were prepared to mimic a typical Baltic Sea sediment with respect to grain size distribution and organic carbon content (coarse sand, quartz sand, kaolin and peat dry weight ratio of 13:61:3.8:1, final organic carbon content; TOC; of 2.2 %). These proportions were chosen after a field survey performed in Askö (Sweden) to determine the average particle size distribution in this area and use it as a reference for our experiments. The same artificial sediments were used in all our experiments (with varying grain size distribution in Experiment II) to control these parameters (particle size distribution and TOC). Having standardized artificial sediments allows comparison across experiments.

The peat was initially freeze-dried, grounded, and sieved to a fine consistency. A portion of the peat was combined with artificial brackish water in a beaker, along with a stir bar. The mixture was left to soak for two days, and the pH was adjusted to a range of mildly acidic conditions using calcium carbonate ($CaCO_3$). In experiment II, the ratio of quartz sand, kaolin, and coarse sand was altered in order to prepare sediments ranging in fine grain size (< 63 µm) from 43 to 72 %. The pH of prepared sediment slurries was adjusted to 5.5–6.0 using $CaCO_3$.

**Spiking of sediment with organic contaminants (following OECD guideline n°218)** Briefly, the model compounds were first dissolved in acetone and then mixed with Fontainebleau (coarse) sand. The acetone was then let to evaporate at room temperature before the spiked sand was mixed with quartz sand, kaolin, and of a peat slurry. MeHg was spiked through the peat slurry. A stock solution of MeHg (dissolved in MilliQ water) was added to the peat during its preparation. The sediments were then prepared as described above. Once prepared, the cores were left to equilibrate for only two days to avoid MeHg degradation.

For all the experiments, un-spiked sediments were prepared in the same way described above.

**Preparation of PE film.** To prepare the polyethylene passive samplers, a 35 µm polyethylene (PE) sheet was cut into pieces, each measuring 2 × 1.8 cm and weighing 11.9 mg. Before use, the pieces were cleaned by soaking them for 24 hours in methanol while being mixed on a roller, followed by sequential treatments with acetone and n-hexane. After cleaning, the PE sheets were stored in n-hexane until use.

**Extraction and analysis of PAHs from PE film.** After exposure, the passive samplers were rinsed with Milli-Q water and dried with a lint-free tissue. They were placed in a vial with n-hexane and internal standards. The vial was mixed on a roller overnight at room temperature in the dark. The extract was transferred to a new vial, and the passive samplers were rinsed again with more n-hexane on the roller for a few hours. The two extracts were combined and dried with sodium sulfate. After vortexing and centrifuging, a portion of the liquid was collected, avoiding any sodium sulfate, placed in a GC vial, and a recovery standard was added. The samples were then stored in the freezer until analysis.

**Preparation of DGTs**. Deploying DGT devices followed the supplier guidelines. Briefly, the DGTs were always handled in a clean environment and using gloves. Prior the deployment, the DGT was quickly removed from its clean bag, attached with a pre-cleaned fishing line threaded through the hole on the rim of the unit, rinsed with MQ water and attached to the lead of the core used for our experiment. Temperature and pH were kept stable before and after deployment.

Extraction and analysis of THg and MeHg from DGTs. After 7 days of exposure, the DGTs were retrieved, immediately rinsed with MQ water and stored in clean bag. In a fume hood, the DGTs were cleaned again with MQ water and opened with a screwdriver (inside a clean glove). The binding layer was peeled off and placed in a sterile tube. An isotopically enriched $Me^{200}Hg$ tracer (0.5 ml, standard concentration of 1 µg $L^{-1}$) was added as internal standard (IS). An additional 0.5 ml of MQ water was added to allow the binding layer to be fully immersed. The samples were kept at −20 °C before further analysis.

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# Mobility, Bioavailability and Toxicity of Sediment Contaminants (MOBILITY)

Sediment resuspension increases contaminant bioavailability and ecological risks. The MOBILITY project focused on the environmental risks of contaminants stored in sediments by studying the release, bioavailability, and toxicity of organic contaminants and methylmercury from contaminated sediment during resuspension. Lab studies were conducted in cores containing artificial sediments with added contaminants, where resuspension was simulated to evaluate the effect of turbidity, hydrophobicity, and grain size on contaminant release and uptake by algae. Passive samplers were used to measure the freely dissolved and bioavailable fraction of the contaminants. Results showed turbidity and grain size influenced contaminant desorption and diffusion. In experiments where algae were exposed to resuspended sediments, the algal uptake correlated with the uptake in passive samplers and, for organic model substances, also with photosynthesis inhibition (reflecting toxic effects linked to bioaccumulation). The study recommends the use of passive samplers in contaminated sediment risk assessments and to consider variations in turbidity as an indicator for use in monitoring protocols for contaminated sediments.

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