LABPLAS

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Land-Based Solutions for Plastics in the Sea

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D7.5 Biogeochemical transport-reaction model: Report on MP leachates and degradation in the Elbe-Thames-North Sea system

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ABBREVIATIONS AND ACRONYMS

Abbreviation / Acronym	Description
a	year
B	Biot number
BDE	Brominated Diphenyl Ether
C	Concentration
cm	centimeter
LDPE	Low-Density Poly Ethylene
MP	Micro Plastic
PA	Poly Amide
PBDE	Poly Brominated Diphenyl Ether
PCB	Poly Chlorinated Biphenyl
PE	Poly Ethylene
PET	Poly Ethylene Theraphthalate
POC	Particulate Organic Carbon
x	depth

1 INTRODUCTION

Although the industrial production of plastic started only 70 years ago, plastic waste is accumulating heavily in the environment. The durability of polymers, a wanted and designed product characteristic, prevents this type of waste from complete degradation. Instead of vanishing from ecosystems, plastic tends to decompose into smaller parts, the microplastic (MP) particles. The environmental impact of MP particles is driven by their size, shape and composition (i.e., polymer properties, particle size, shape and chemical additives determine environmental fate and ecotoxicological effects). Among those parameters, the leaching of harmful polymer additives has been identified as the main hazard for organisms. The distribution of leachates is determined by different transport processes: The MP particles act as carriers for the chemicals before they are leached into the environment. Leached additives dissolve in surrounding fluid phases and are transported by advective and diffusive processes. In the benthic environment, desorbed molecules dissolve into the pore water and are distributed within the sediment. The aim of LABPLAS task 7.4 was the development of a numerical model that can describe the transport and accumulation of MPs and leachates in the benthos.

2 THE BIOGEOCHEMICAL TRANSPORT REACTION MODEL C.CANDI

C.candi is a one-dimensional numerical transport-reaction model for benthic biogeochemical processes (Luff et al., 2001). It was first used by Luff et al. (2000) for modelling of benthic processes in the deep Arabian Sea and by Haeckel et al. (2001) for quantifying early diagenetic processes in polymetallic nodule habitats of the Peru Basin in the Southeast Equatorial Pacific. Luff and Moll (2004) connected C.candi to the ECOHAM model to simulate seasonal carbon cycle processes in North Sea sediments. C.candi includes transport and reactions of 25 dissolved and 16 solid species in the sediment (O_2, NO_3^-, MnO_2, Mn^{2+}, $Fe(OH)_3$, Fe^{2+}, SO_4^{2-}, CH_4, PO_4^{3-}, HPO_4^{2-}, $H_2PO_4^-$, H_3PO_4, NH_3, NH_4^+, POC_0, POC_1, POC_2, $CaCO_3$ (calcite, aragonite), $MnCO_3$, $FeCO_3$, $BaSO_4$, $CaSO_4$, Ca^{2+}, Ba^{2+}, H_2S, HS^-, S^{2-}, CO_2, HCO_3^-, CO_3^{2-}, $B(OH)_3$, $B(OH)_4^-$, TAlk, FeS, clay-Fe(II), clay-Fe(III), ^{210}Pb, Br^-, Cl^-, methane hydrate). Six primary redox reactions for three fractions of organic matter, 11 secondary redox reactions, as well as several mineral precipitation/dissolution reactions, acid/base equilibria and adsorption/desorption processes, are considered. These reaction equations are coupled with the transport equations of the particles and the dissolved species in the sediment as well as the interchange of constituents across the sediment-water interface. The corresponding differential equations are coded as finite difference approximations for derivatives in depth dimension and solved by a numerical solver for the time dimension. Model outputs are the concentrations of the model species as a function of depth below the seafloor. The current version of C.candi is a MATLAB code (The Mathworks, Nattick, MA, USA) and is frequently used at GEOMAR for the investigation of a diverse range of transport-reaction processes in marine sediments.

3 THE C.CANDI MICROPLASTIC MODULE

3.1 Objective

The objective of this task is the adaptation of C.candi to microplastic (MP) applications. The model was extended to treat the kinetics and thermodynamics of MP transport, leaching and degradation in marine and freshwater sediments. Instead of integrating the MP processes within the main C.candi code, a separate module has been added to the package since there is so far no interaction between the original model species and the MP species. The reduction of the MP module to only the necessary species and equations saves computation time. A complex model that involves a multitude of coupled processes is always a compromise between the accurate description of the underlying physical and chemical processes and the required computation time. This model

emphasizes on the leaching process of additives from MP and uses more simplified approaches for the adsorption of chemicals on the MP surface and MP degradation.

3.2 Transport of MP in marine sediment

When MP particles are deposited on the sediment surface, they can be transported into the sediment body and distributed within the sediment. Two processes are responsible for this transport: sedimentation and bioturbation. Sedimentation means the deposition of additional sediment from the water column on top of the layer that includes the MPs. Its mathematical representation corresponds to a downward movement with a velocity that equals the sedimentation rate. For this model, it is assumed that particles are not resuspended into the water column. Bioturbation is a mixing process that is caused by the movement of the benthic fauna. It can be described as a diffusive flux with a diffusion constant that depends on the depth x within the sediment. Benthic fauna typically inhabits only the upper 5-20 cm of the sediment and the diffusive mixing ceases below the inhabited zone. Bioturbation is a very effective transport process for solid particles in sediment, but it is difficult to quantify since it depends on the type, abundance and activity of the local fauna.

3.3 Transport of dissolved molecules in marine sediment

Dissolved molecules are more mobile than solid particles and are subjected to two additional transport processes. Similar to the transport of solid particles, dissolved particles are buried within the sediment by sedimentation and they are also affected by the local fauna. The corresponding fauna-induced process is called bioirrigation. Bioirrigation is the redistribution of pore water from actions of living species, like flushing of burrows or ingestion and egestion. The two additional processes are the diffusion of the molecules in the pore space of the sediment and their transport with an advective flux. In summary, there are two advective processes, pressure-induced flow and sedimentation, and two diffusive processes, diffusion and bioirrigation.

3.4 Leaching of additives from MP

The leaching of additives from microplastic particles into the environment can be described by up to four processes:

- The diffusion of the chemical inside the polymer to the polymer surface
- The transfer of the chemical through the boundary layer at the polymer surface
- Readsorption of part of the leached chemical onto the polymer surface
- Transport of the chemical in the pore water by diffusion, advection and bioirrigation

Desorption of additives from polymers is often a slow process and the concentrations of the desorbed species in the surrounding porewater are small. Hence, we make the simplificating assumption that the pore water is not close to its saturation limit of the corresponding leachates and that the desorption is not affected or limited by the pore water concentration.

A molecule desorbs from a polymer particle after it has diffused to the surface of the particle and transferred through the boundary layer at the surface. For most systems, one of these latter processes is rate limiting, and hence the kinetics of the other step can be neglected. The Biot number B, which is defined as the ratio of the plastic boundary layer times the boundary layer mass transfer coefficient and the diffusion coefficient in the plastic matrix, determines if the desorption is limited by diffusion or by boundary layer transfer (Vitrac and Hayert, 2006). Consequently, the model considers only one process for the mass transfer from the polymer to the pore water phase. The model user needs to specify, which of the two processes is included.

Diffusion of additive molecules in a polymer matrix can be a highly complex process and depends on temperature, the state of the polymer (rubbery or glassy, crystalline and amorphous regions), the shape and size of the particle, the shape and size of the additive molecule, and the concentration in the surrounding medium. For small molecules in rubbery polymers, the diffusion process can be described by Fick's law. Small molecules from rubbery polymers are believed to be the main source of leached chemicals since the kinetics within glassy polymers are much slower or even neglectable. Therefore, the model calculates the diffusion-limited mass release of leachates from analytical solutions of Fick's law for three different geometries: Round particles, sheet-like particles and cylindrical shapes, which describe, for example, polymer fibres. Solutions for matrix diffusion limited release are taken from (Siepmann and Siepmann, 2012) with the full solution for spheres and sheets and the early time approximation for fibres, whereas the boundary layer limited process is implemented according to (Endo et al., 2013). Typical diffusion constants for small molecules are in the order of 10^{-14} m^2/s for PE and 10^{-16} m^2/s for PP (e.g. Lee et al., 2018). This is several orders of magnitude smaller than the self-diffusion coefficient of water, which has an order of magnitude of 10^{-9} m^2/s.

Especially for the matrix-diffusion-limited release, the desorption of molecules is strongly time-dependent at early times with high releases for molecules that reside close to the polymer surface and a very slow release kinetics at later times for molecules that need to diffuse towards the surface. For example, a particle, that has been drifting in the water body for a long time, enters the sediment with smaller release rates than a particle that is buried shortly after entering the water column. Simplified release models do not cover the transition from fast to slow release. Hence, we decided to incorporate the more complex solution of Fickian diffusion and implemented a water residence time, i.e. the time that a particle has already released additives into the water column while drifting, to account for the existence of pre-leached particles.

The time dependence of the additive release is a major challenge for the modelling of the transport reaction system: Particles of the same type, that are deposited at a later time point than the initial particle load, have a different chemical release rate and can be distinguished from the first set of particles by age. The transport reaction equations are only valid for indistinguishable particles. When a constant flux of particles from the water column into the sediment is assumed, the release of additives is underestimated since there is only a single release rate: The rate of the particles that were deposited at the starting time. The larger release rate of fresh particles is not applied. The exact solution for this problem would be the definition of every single distinguishable particle within the model, which would lead to incredibly large run times for a simulation. A proposed workaround is the definition of particle pulses: Particles are not deposited as a constant flux, but a set of particles is added at specific time points that ideally are close enough to each other that the particle distribution is not changed too much by transport processes during the time interval, but can also be more sparsely distributed if run time is critical. This concept is a compromise between a single deposition at the model starting time and a continuous particle influx.

3.5 Adsorption of additives and pollutants

Adsorption of particles can either be the readsorption of leached additives or the adsorption of pollutants from the surrounding pore water. Readsorption is increasingly important with increasing hydrophobicity of the leached chemicals. The description of the adsorption can be highly complex and depends on the properties of the molecule as well as the surface properties of the polymer, which change during weathering and degradation. To complicate the matter, cyclic adsorption/readsorption curves show a hysteresis. To keep the model simple, adsorption is described as the attachment of a fixed percentage of the surrounding pore water concentration to the polymer. The adsorption of a fixed percentage of the surrounding concentration follows the concept of

the adsorption isotherm as described by the Freundlich linear equation (Weber et al., 1991). This is a valid approximation as long as the pore water concentrations and the amount of adsorbed molecules are much smaller than the maximum solubility or adsorption capacity, respectively. A profound review of the adsorption behaviour of pollutants on microplastics can be found in (Fu et al., 2021). Due to their adsorption capacity, MPs can be either a source or a sink for pollutants. The adsorption of chemicals onto sediment grain surfaces is neglected within the model.

The C.candi MP module does not include a time-dependent term for the adsorption process. The general approach in the literature is the implementation of a (pseudo) first or second-order kinetic (see e.g. Wu et al, 2019), but adsorption processes can reach their equilibrium within hours or days, which is short compared to the release kinetics of the leachates and the diffusive transport of molecules in the pore water. Readsorption is therefore approximated as being instantaneous, although polymer/additive adsorption rates can be too small to justify this approach.

3.6 Polymer decomposition

When polymers are released into the environment, they are subjected to different degradation mechanisms that deteriorate the plastic particles. The most effective mechanisms are irradiation by UV light and mechanical abrasion. Once the plastic particle is buried in sediments, it is sheltered from these effects. UV light does not penetrate deeply into the sediment and is often absorbed in or reflected by the overlying water column, especially if the water is murky and opaque, and the mechanical drag of polymers among hard surfaces surface by waves or currents is stopped. For this reason, the degradation of plastic within seafloor sediments is extremely slow and practically non-existent on timescales that are associated with the appearance of man-made polymers (Krause et al. 2020). An exception could be the degradation of polymers by microorganisms. However, this is only effective when microbial strains are present that are able to crack the polymer matrix. In most cases, no degradation of polymers buried in seafloor sediments has been observed. This is also consistent with the observations from LABPLAS WP5, where buried PE sheets served as non-degradable reference for decomposition studies of biodegradable polymers. However, degradation kinetics for polymers subjected to specific microbial strains under laboratory conditions can be found in the literature. Hooda et al. (2023) have tested 14 different equations for their ability to describe their observed degradation process. They conclude that 5 out of those 14 equations can describe the degradation process sufficiently well, with the Michaelis-Menten equation as their best choice. Among those 5 suitable models is a simple exponential decay. We chose this exponential decay as a decay model for the C.candi MP module. One reason for our choice is the simplicity of the equation. Another reason is the fact, that this equation requires only the decay constant as a parameter. This parameter has a physical meaning and can be extracted from published decay curves. For regular MP model applications and time scales, no measurable decay is expected and the decay option is not used.

3.7 Summary of model parameters

The parameters within the C.candi MP module define different aspects of the modelled scenario:

The **model domain** is set by a **depth** vector. There is only one coordinate since the model is set for one-dimensional applications**. Boundary conditions** can be chosen to be either Dirichlet (constant flux) or Neumann (no flux). The modelled **time interval** is set by a **time** vector with start and end time.

C.candi takes the **pressure**, **temperature** and **salinity** as **environmental parameters**. For the MP module, pressure and salinity are not needed, while the temperature might be used to calculate temperature-dependent diffusion parameters.

The **sediment** is characterized by its **porosity**. The porosity defines the volume fraction that is occupied by the sediment grains (and solid species) and by fluids. After deposition, sediments undergo compaction due to further sediment accumulation. The equation used to calculate porosity changes over depth requires the input of three parameters. **Tortuosity**, a measure for the meandering path of diffusing molecules in pore space, is calculated from porosity based on established relationships.

Required **transport parameters** are **advection velocity**, **sedimentation rate**, and **parameters for the calculation of bioturbation and bioirrigation profiles.** Bioturbation and bioirrigation are caused by the benthic fauna and occur only within the inhabited sediment depths. Hence, a function of depth is required instead of a scalar value. The model includes functions for the calculation of these profiles from the provided parameters.

The plastic **degradation** needs only one parameter: The degradation **decay constant**. For almost all applications, decay can be neglected within the sediment.

Microplastic particles are characterized by the following parameters: their **size**, **shape** and **age**, the **type of leaching process** (matrix diffusion or boundary layer diffusion controlled), the **deposition time** when the particle is deposited on the seafloor and starts leaching into the sediment, and the **initial concentration** at the model start time for the initialisation of the solver.

Additives are defined for each MP and are described by **diffusion coefficients in polymer and water**, **polymer water partition coefficients**, **adsorption efficiencies** (fraction of adsorbed molecules), **initial concentration within the polymer**, **bottom water concentration** or **initial concentration profiles including bottom water**. The parameters with their corresponding parameter types and units are listed in Tables 1-3.

Model parameters	Unit	Type	Description
time	a	vector	first and last time point
depth	cm	vector	coordinates of the model domain
pressure	MPa	scalar	pressure at seafloor
temperature	°C	scalar	sediment temperature
salinity	g/kg	scalar	salinity of porewater
porosity_0		scalar	porosity at seafloor
porosity_end		scalar	porosity at full compaction
b		scalar	parameter to calculate the porosity profile
advection velocity	cm/a	scalar	porewater velocity within the sediment
sedimentation rate	cm/a	scalar	solids burial velocity due to sedimentation
bioturbation coefficient	cm^2/a	scalar	parameter to calculate bioturbation profile
bioturbation depth	cm	scalar	parameter to calculate the bioturbation profile
beta Db	cm	scalar	parameter to calculate bioturbation profile
number of MP		scalar	number of MP that differ in composition and/or deposition time
max number of additives		scalar	maximum number of additives per MP
MP parameters		Matrix	Matrix containing all MP related parameters, see Table 2
additive parameters		Matrix	Matrix containing all additive related parameters, see Table 3
decay constant	1/a	scalar	decay constant for MP degradation
MP initial concentration profile	$particles/cm^3$	vector	starting profile of each MP
additives' initial concentration profile	mol/l	vector	starting profile including bottom water concentration for each additive
boundary conditions		vector	choice of boundary conditions for solver

Table 1: Parameters to be set within the C.candi MP module

MP parameters	Unit	Description
size	cm	radius or thickness of the particle
shape		sphere / sheet / cylinder (fibre)
age	a	initial "age" of the particle, the time that the particle was under leaching conditions before settling
leaching type		diffusion controlled or boundary layer transfer controlled
initial concentration at the seafloor	particles/cm^3	initial concentration at the seafloor after settling and before the start of transport
deposition time	a	time within the modelled interval, when the particle is deposited.

Table 2: Detailed list of parameters that define the microplastic particle in the C.candi MP module

Additive parameters	Unit	Description
initial concentration in polymer	mol/particle	initial amount of additive in MP
diffusion constant polymer	cm^2/a	diffusion coefficient for solid-state diffusion in polymer
partition coefficient		polymer/water partition coefficient
diffusion coefficient water	cm^2/a	diffusion coefficient in water
adsorption factor		percentage of adsorbed additives
bottom water concentration	mol/l	concentration of additive in the water column at the seafloor

Table 3: Detailed list of parameters that define the additives in the C.candi MP module

4 APPLICATION OF THE C.CANDI MICROPLASTIC MODULE

4.1 Site selection

It was originally planned to use the model to simulate the microplastic deposition and leachate release for a field site and optimize model equations and parameters by comparing the model results to measured field data. At the current time, however, there is no site for which the essential model parameters have been determined. The parametrization of the model was therefore done with literature values and the model is used to demonstrate different effects and dynamics of the MP/leachate system. Microplastic concentrations in sediments were provided by LABPLAS WP2 for stations in the North Sea and the rivers Elbe and Thames. Since this is the only result from the North Sea – Elbe – Thames campaign that could be transferred to the model, no specific site was chosen, but three model sites were defined for the North Sea, Elbe and Thames, respectively, that were based on average MP concentration results to reduce the effect of the variability. Suitable available literature values were selected for the remaining parameters.

4.2 Parametrization

4.2.1 Model domain and location specific parameters

The industrial production of plastic started in the 1950s, about 70 years ago. Since then, the amount of produced plastic per year has been rising exponentially (Pilapitiya & Ratnayake, 2024). No MP depositions are expected for times prior to 70 years ago and not much MP accumulation is expected for the early years of the plastic era. Therefore, the time span of the model was set to **50 years**.

In typical coastal sediments, the most efficient transport mechanism for MPs and leachates are bioturbation and bioirrigation, respectively. These effects are limited to the inhabited layer of the sediment. Typically, North Sea sediments are well mixed within the uppermost centimetres (Dauwe et al., 1998) with little transport below the bioturbation/bioirrigation depth due to the comparably slow sedimentation and diffusion processes (de Haas et al., 1997). For this study, however, we chose to implement relatively large sedimentation rates because sites with substantial particle deposition are also expected to collect more MP particles. The model domain should be large enough for the modelled species to not reach the bottom of the domain within the time period. It is set to a length of **100 cm** with a depth increment of 0.1 cm.

The **temperature** is set to a mean sediment temperature to allow for the adjustment of diffusion constants, but most diffusion constants are not available for multiple temperatures. For this case study, a temperature was set, but not used within the model. **Pressure** and **salinity** are currently not needed for the MP module, but can be added in the future as relevant relationships for diffusion constants or other parameters become available.

Sediment porosities depend on the grain size of the sediment and are typically roughly about 0.5 for sand and 0.8 for silt/clay. The river beds with strong currents are composed of fine sediments while sand is deposited and accumulated in the river estuaries. Fine sediments are transported over long distances and accumulate in the North Sea sediment depot centre of the Skagerrak/Norwegian Channel.

The MP model assumes that MP particles are deposited on the seafloor and then buried over time. It does not consider the resuspension of already deposited particles. However, river currents of Elbe and Thames and tidal currents within the North Sea lead to resuspension of surface sediments, resulting in no net sedimentation or even riverbed erosion. To obtain meaningful results, only sites with net sedimentation were chosen for the model. These are the riverine estuaries of Elbe and Thames and a sediment depot centre of the North Sea.

Bioturbation and bioirrigation vary strongly with the type and activity of the local fauna and only limited data is available from literature. We either deliberately chose a site that is well characterized and where, as many parameters as possible are available from literature even if the site is not located within the main LABPLAS study area (North Sea) or compiled typical values from literature to design a “typical” and “meaningful” site within the LABPLAS area of interest (Elbe and Thames estuaries). Bioturbation parameters could not be found for both river estuaries and the North Sea parameters were taken for all three model sites.

4.2.1.1 North Sea

The main depot center for fine-grained sediments in the North Sea is located in the Skagerrak/Norwegian channel. The annual total sediment deposition in the Skagerrak is 46 · 106 tons per year (De Haas and Van Weering, 1997). Sediment composition varies between sand (<40% clay), mainly along the Danish coast, and fine-grained silt and clay sediments in the deeper parts (Stevens et al., 1996). Substantial animal burrows are present in the upper 10 - 20 cm in fine-grained areas (Canfield et al., 1993; Kristensen et al., 2018). Skagerrak

sediments are characterized by a large lateral input of mostly lithogenic material from the North Sea (Van Weering et al.,1993; De Haas and Van Weering, 1997).

A recent publication by Spiegel et al. (2023) provides a complete transport parameter dataset for sediment cores from the sediment depot centre in the Skagerrak. We use bioturbation and bioirrigation coefficients as well as porosities and the sedimentation rate of **0.12 cm/a** from core MC6, the core closest to the open North Sea, with coordinates 57° 38.086'N and 08° 23.998'E and a water depth of 185 m. Sedimentation rates for this site are much higher than in the central North Sea, where little to no net sedimentation is expected due to efficient sediment erosion. Table 4 summarizes the bioturbation and bioirrigation parameters as well as the porosity parameters. Advection does not occur at this location.

Mean bottom water temperatures in the central North Sea are about **7°C** (Schöne et al., 2005).

Parameter	Value	Unit
Bioturbation coefficient	26	cm^2/a
Bioturbation depth	4	cm
Bioirrigation coefficient	24	cm^2/a
Bioirrigation depth	1.5	cm
Sediment surface porosity	0.5	
Compacted porosity	0.49	
Porosity parameter	0.1	

Table 4: Bioturbation, bioirrigation and porosity parameters

4.2.1.2 Elbe

Sedimentation in riverine systems and estuaries depends on the local current velocity. While there are high sediment accumulations at stagnant zones, the river bed can also be subjected to erosion with negative sedimentation. Extensive sediment relocation takes place due to erosion and re-sedimentation enhanced by heavy storm surges. Sedimentation rates for the estuary are estimated in literature to be up to several cm per year. Due to the large relocations of sediments by natural causes as well as by dredging, it is difficult to get a sedimentation rate for this area. The chosen value for the model is therefore somewhat arbitrary. It was set to get the most meaningful results: High sedimentation rates in the order of several cm/a lead to a relatively fast transport of MPs out of the inhabited sediment zone, but MPs are most hazardous when they leach into the bioturbated layer. Hence, a value was chosen that is large enough to realistically describe a location with particle deposition from the sediment freight of a river, but also ensures a considerable residence time of the MPs in the bioturbated layer, where the leachates interact with the local fauna. With these prerequisites, we set **0.25 cm/a** as model parameter. Porosities for the Elbe estuary can be found in Deek et al. (2013). Close to Cuxhaven, a value around **0.6** can be expected. Advection does not occur. Bioturbation and bioirrigation coefficients could not be found in the literature and are set to the North Sea values.

Mean water temperatures in the Elbe River are about **10°C** (Markovic et al., 2013).

4.2.1.3 Thames

The sites within the Thames estuary suffer from the same lack of data as the Elbe estuary. The only parameter that is well characterized is the sedimentation rate since it is important for managing the river as a transport pathway for ship traffic. However, the sedimentation rates vary vastly across the river and the estuary. Tomes et al. (2006) estimate sedimentation rates for the lower Thames to be 1.2-2.5 cm/a, but we apply the same reasoning as we did for the Elbe estuary and use the smaller sedimentation rate of **0.15 cm/a** as model parameter to avoid a too fast transport of MP particles out of the inhabited sediment layer.

Exemplary sediment porosities for the inner Thames estuary are given by Trimmer et al. (2000) to be about **0.65** without a compaction curve. Advection does not occur. Bioturbation and bioirrigation coefficients could not be found in the literature and are set to the North Sea values.

Mean water temperatures in the Thames River are about **12°C** (Orr et al., 2010).

4.2.2 Microplastic particles and additives

LABPLAS WP2 (LABPLAS, 2024) extracted and analysed microplastic particles from sediment field samples from the North Sea, Elbe and Thames stations. Among the found polymer types, 3 polymers were selected for the model because of the availability of literature values for model parameters: PET, PA and PE. As explained in Section 3, MP particles start leaching additives as soon as they are in contact with the atmosphere or a liquid phase. At the time when they settle on the seafloor, they have already lost a certain amount of the chemicals. Weathering mechanisms like exposure to UV radiation or mechanical abrasion do even lead to higher leaching rates in surface waters compared to the more sheltered location in sediments (see e.g. Bridson et al., 2023, Bridson et al., 2024, Dhavami et al., 2022, Dimassi et al., 2023). MPs are even considered to be a vehicle for the long-range transport of chemicals in the ocean (Andrade et al., 2021) and low-density polymers can drift large distances before they are aggregated with organic matter and sink to the ocean floor (Galgani et al., 2022). The polymer selection for the model demonstration includes two polymers that are denser than water (PET and PA). Those particles are expected to settle more rapidly and spend less time leaching in the water column. Their water column residence time was set to 0.05 a, whereas PE has a lower density and a higher buoyancy and its residence time was set to 0.1 a to account for longer drifting times. Most detected particles in the field samples were in the size range of 10-50 µm (LABPLAS Project, 2024). Accordingly, the particle radius was set to 25 µm. PA MP originates mainly from clothing or ropes of fishnets and enters the environment predominantly as fibre. Hence, the shape for PA was set to cylindrical, while the shape for the other particles was set to spherical because they are most likely fragments from larger plastic products. Table 5 summarizes the MP particle parameters.

MP parameters	LDPE	PA	PET
size	25 µm	25 µm	25 µm
shape	spherical	cylindrical	spherical
age	0.1 a	0.05 a	0.05 a
additives	BDE7, BDE153, BDE209, PCB52	BDE153	BDE153

Table 5: Model parameters for microplastic particles

The number of potential additives in MP is huge and includes light stabilizers, heat stabilizers, nucleating agents, pigments, antistatics, flame retardants and fillers (Fauser et al., 2022, Chen et al., 2022, United Nations, 2023). It is impossible to determine and consider a complete set of additives for the selected polymers and for most additives, the needed kinetic parameters are not available. PE is a well-researched compound, but data are sparser for other polymers. Since data for partition coefficients are often lacking, octanol/water partition coefficients, which are more easily available, can be used instead. Diffusion coefficients for chemicals within polymer matrices are also hard to find in literature and they are highly dependent on the specifics of the polymer e.g. glass transition temperature, crystallinity and the state of weathering. Rusina et al. (2010) published a well-recognized compilation of diffusion coefficients for biphenyls and polycyclic aromatic hydrocarbons in Polydimethylsiloxane and LD-PE, while Valderrama et al. (2016) published diffusion coefficients of polybrominated diphenyl ethers in LD-PE and silicone rubber. The availability of these diffusion coefficients makes flame retardants a favourite subject of experimental studies (see Cheng et al. (2020) for a review). Most published diffusion coefficients were, however, determined with organic solvents and not water as the surrounding medium. A major problem in the compilation of literature data for the model is the use of different equations for the leaching process in publications (e.g. Dhavamani et al., 2022). Often, more simple equations are employed and the obtained parameters cannot be used with the C.CANDI MP model. We deliberately chose to implement Fickian diffusion since it is a fundamental law of transport with meaningful parameters and it can cover different stages of the transport process. Consequently, we can use only literature parameters from publications that use the same set of equations.

Another criterion for exclusion for the choice of the additives was an expected elevated concentration of the leachate in the surrounding pore water. When the pore water concentration is too high, some of the simplifications within the model no longer apply and it should not be used for this constellation. For bisphenol A, for example, it is discussed if MPs act as a source for the additive, or if they can rather be sinks and adsorb bisphenol A from the pore water (Liu et al., 2019).

Additives for the model demonstration were chosen based on their abundance in MP, which we take as a measure for the relevance of the additive, and on literature value availability as discussed in the preceding paragraph. These requirements limited the choice of additives to two sets of chemicals. The first set of considered additives are polybrominated diphenyl ethers (PBDE), which are added as flame retardants. According to Fauser et al. (2022), PBDEs are found in almost all recovered marine MPs and can therefore expected to be found in environmental matrices. The second set are polychlorinated biphenyls (PCB). PCBs have been widely used as stabilisers in polymer production and are known to have entered the environment in significant concentrations. While PCB concentrations in the water body are close to or below the actual detection limit (Lu et al. 2017) and enter the river systems only during events like flooding (Stachel et. al, 2004), they are still persistent in the sediments. Reported PCB52 concentrations in sediment pore water are 0.4-1.9 µg/kg in the North Sea (Klamer et al., 2005), 26-101 pg/l in the Elbe River (Schäfer et al., 2015) and 2-20 µg/kg (sum of 6 PCBs) for river Thames (Vane et al., 2020). PBDEs, on the other hand, are known to accumulate in fish and other marine fauna, but their concentration in the water column and the sediments is close to or below the detection limit (Sühring et al, 2015).

Parameters for the additives are listed in Table 6 and are taken from Endo et al. (2013) for PCB and from the compilation of Sun et al. (2019) for BDEs. Initial amounts of additives in the polymer have been calculated from typical values for PBDE in environmental MPs (Fauser et. al, 2022), and for PCB from the initial concentrations in acrylonitrile butadiene styrene, as determined by Sun et al. (2019). Each polymer is set with the same amount to enhance the comparability of the resulting distributions. The adsorption properties of the molecule in this

scenario are difficult to determine. Because of the hydrophobicity of the molecules, adsorption is expected to occur, but the amount varies for polymers and leachates. Adsorption efficiency has been set to 10%, which is probably an underestimation of the adsorbed fraction.

Additive parameters	BDE7	BDE153	BDE209	PCB52	BDE153	BDE153
Polymer	LDPE	LDPE	LDPE	PE	PA	PET
initial concentration in polymer/mol per particle	$1.4x10^{-6}$	$8.8x10^{-7}$	$3.76x10^{-4}$	$1.8x10^{-5}$	$8.8x10^{-7}$	$8.8x10^{-7}$
diffusion constant in polymer / cm^2/a	40.1	$1.51x10^{-3}$	$5x10^{-8}$	$3.07x10^{-2}$	$1.1x10^{-8}$	$3.46x10^{-15}$
partition coefficient	-	-	-	$3.89x10^{5}$	-	-
diffusion coefficient in water / cm^2/a	158.1	158.1	158.1	150.7	158.1	158.1
bottom water concentration	0	0	0	0	0	0
leaching type	diffusion controlled	diffusion controlled	diffusion controlled	boundary controlled	diffusion controlled	diffusion controlled

Table 6: Model parameters for additives.

The three sampling sites are characterised by different microplastic loads and microplastic compositions. From the results of WP2, we approximate the overall MP concentration at the seafloor to be 2, 1, and 0.5 particles per cm^3 for Elbe, Thames and North Sea, respectively. The field data compilation provides the amount of PE, PA and PET as a percentage of the overall MP concentration for the winter and the summer campaign, respectively. We chose the higher of the two percentages as the seafloor MP concentration for the model. Table 7 lists the concentrations that were taken as initial particle loads at the surface.

Initial MP concentration particle / cm^3	Elbe	Thames	North Sea
PE	0.1	0.16	0.13
PA	0.09	0.3	0.17
PET	0.06	0.05	0

Table 7: Initial MP concentrations at seafloor as model input parameters for three sites.

4.3 Results

The transport of MP particles into the sediment is shown in ***Figure 1*** for the North Sea setting, in ***Figure 2*** for the Thames River and ***Figure 3*** for the Elbe River. The graphs show the normalized particle concentration as a function of depth. On the left-hand side of the figures, an initial concentration has been deposited on the seafloor and no further particles are added. On the right-hand side, a constant flux of particles into the sediment is assumed. Since bioturbation is set equal for all scenarios, the differences originate from the different assumed sedimentation rates. The high sedimentation rates transport the particles effectively into deeper layers and the bioturbation mixes the upper 15 cm. For comparison, ***Figure 4*** shows the transport with only bioturbation and no sedimentation. This would be the case in central river beds and most of the North Sea. However, when no sedimentation occurs, also MP deposition is expected to be minimal. This effect can be seen in the low MP concentrations found by WP2 in some North Sea stations. Without sedimentation, the MP concentration is restricted to the bioturbated layer.

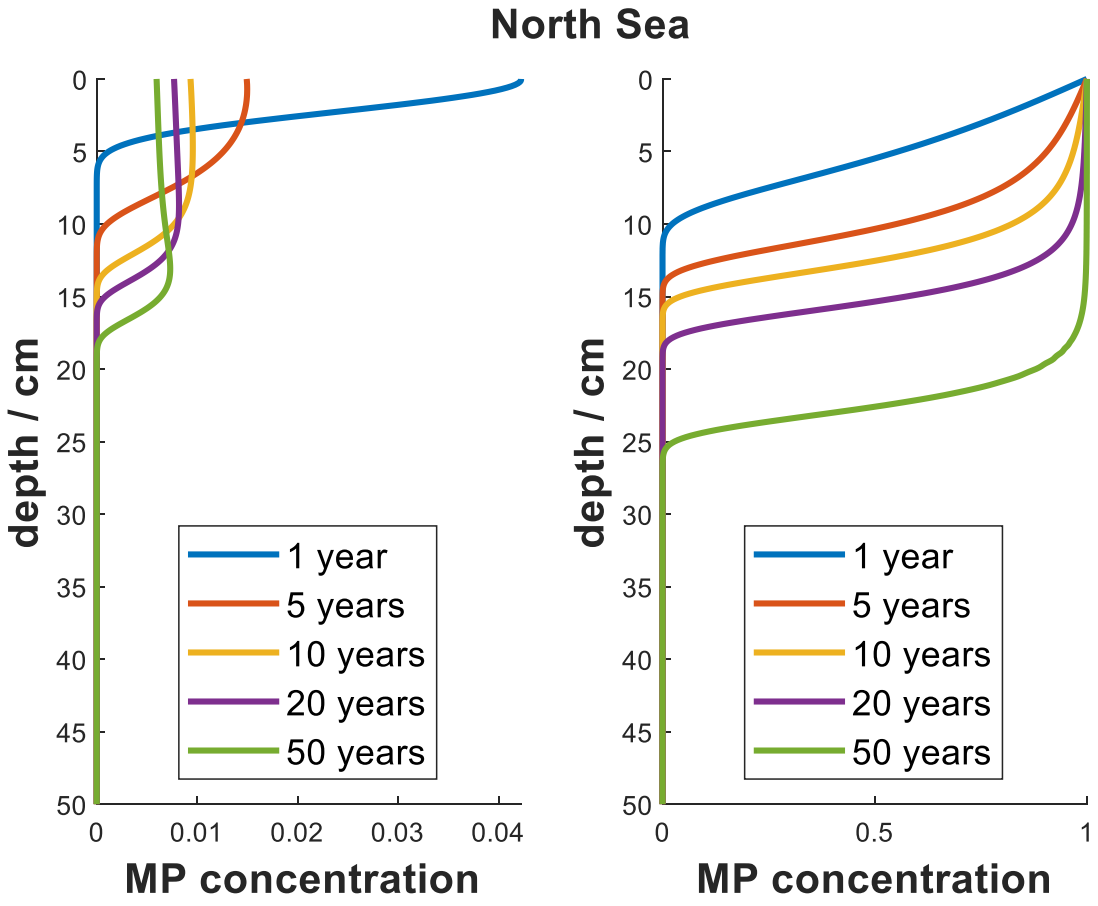

Figure 1: Normalized MP concentration in North Sea sediments as a function of time. Left-hand side: single deposition, Right-hand side: constant flux of particles on the seafloor.

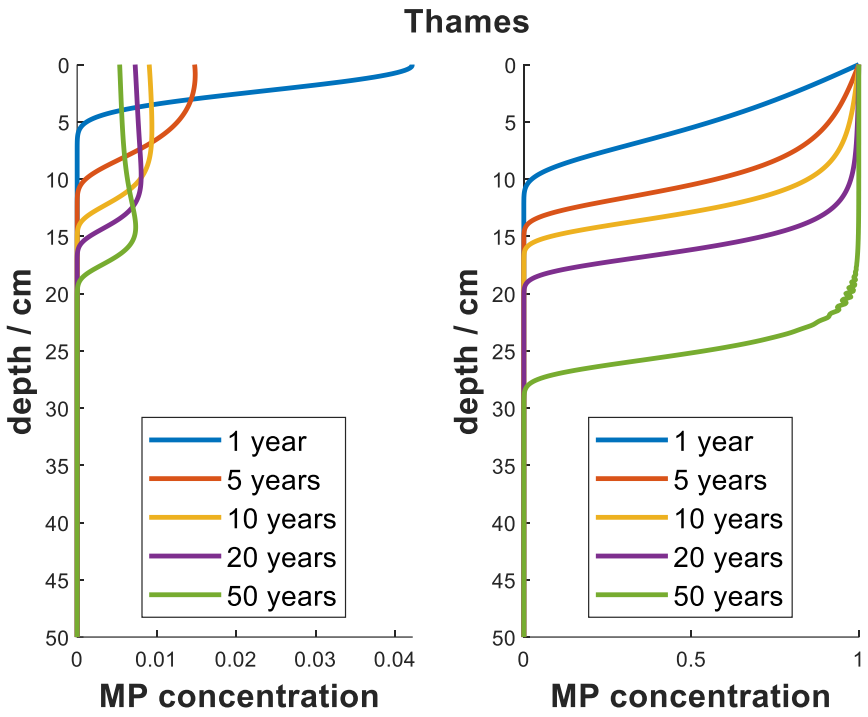

Figure 2: Normalized MP concentration in Thames sediments as a function of time. Left-hand side: single deposition, Right-hand side: constant flux of particles on the seafloor.

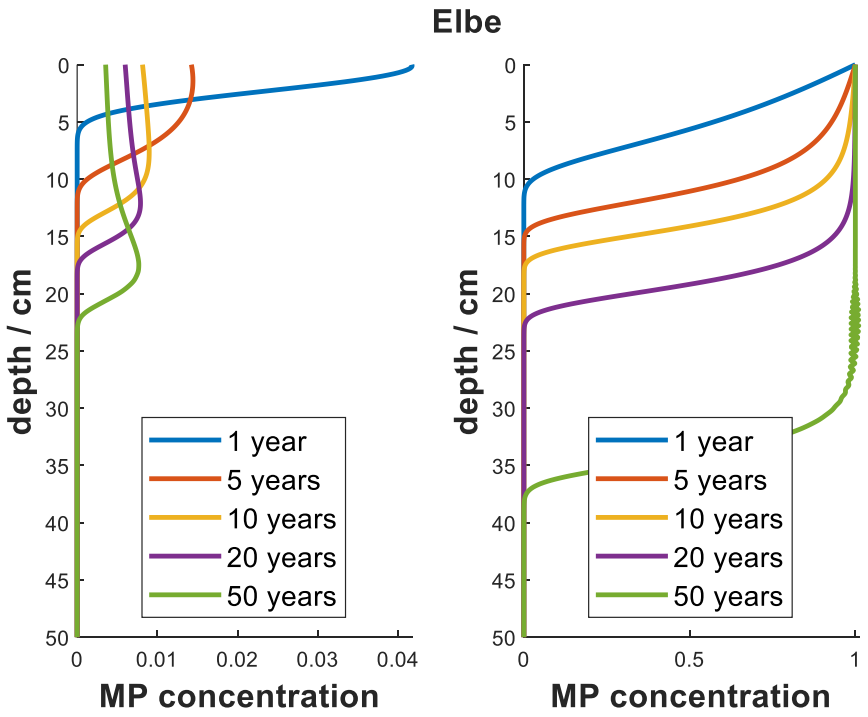

Figure 3: Normalized MP concentration in Elbe sediments as a function of time. Left-hand side: single deposition, Right-hand side: constant flux of particles on the seafloor.

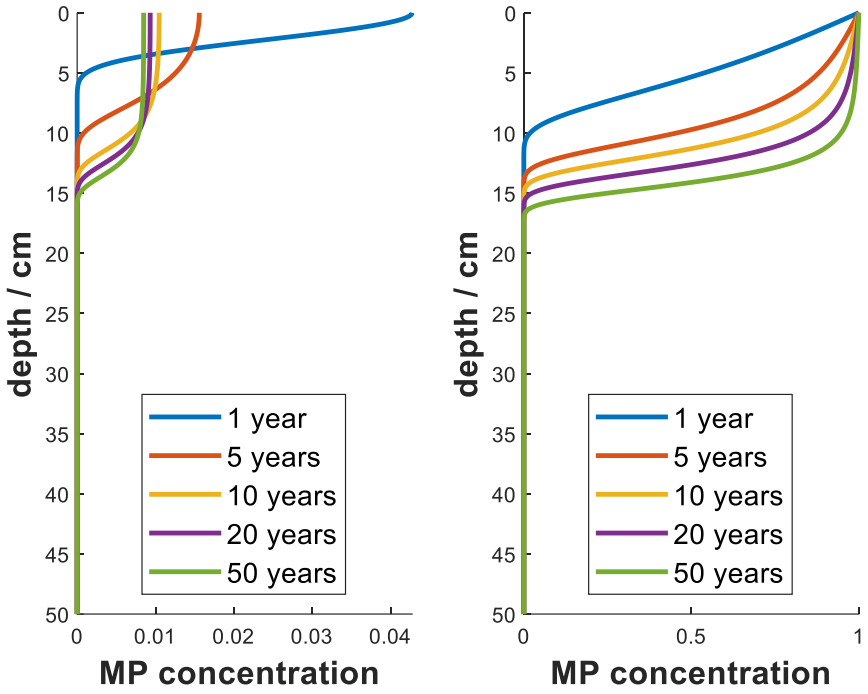

Figure 4: Normalized MP concentration without sedimentation as a function of time. Left-hand side: single deposition, Right-hand side: constant flux of particles on the seafloor.

Figure 5 shows the release rate of additives from MP particles with a radius of 50 µm, which corresponds to the radius of the majority of found MP. Three of the additives are released within days: BDE153 in LDPE (upper left), BDE7 in LDPE (lower left) and PCB52 in LDPE (lower right). These additives can be considered to be completely leached before they reach the seafloor or while they are still on the seafloor and in contact with bottom water. The release of BDE7 in LDPE is instantaneous on the presented time scale (not resolved on this time scale). BDE153 in PET, on the other hand, is shown in the upper right part and has extremely low release rates. This additive can be considered to be retained in the polymer. ***Figure 6*** and ***Figure 7*** show the release rates for larger particles with 100 and 200 µm radii, respectively. These particle sizes correspond to the larger particles that were recovered by WP2. Although additive release takes more time for larger particles, the time scales are about the same for fast release, and the slow release is even more inhibited. The depth distribution of leachates is therefore only modelled for BDE153 in PA and BDE209 in LDPE.

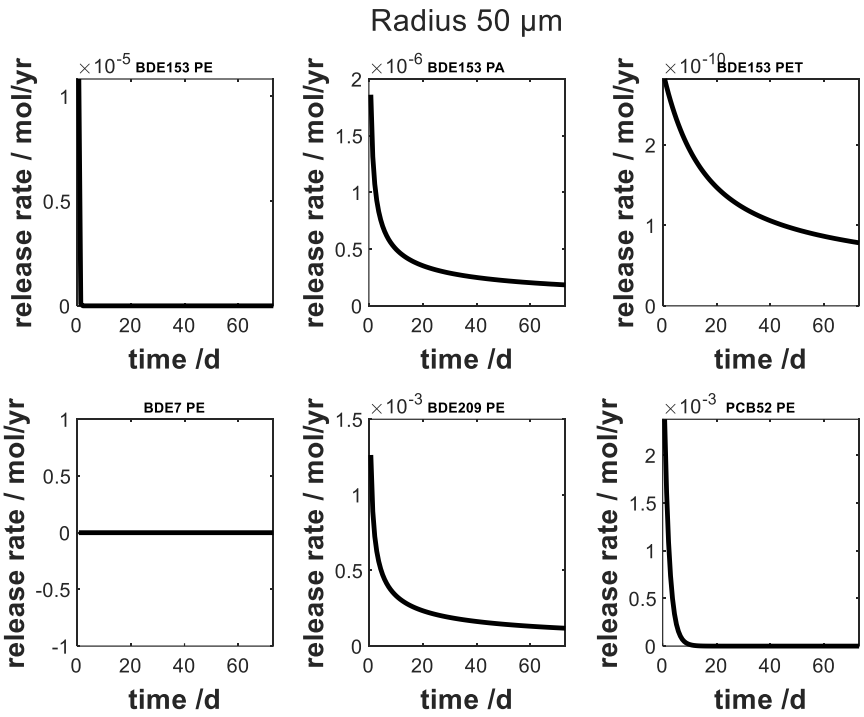

Figure 5: Release rate of additives from polymers with radius 50 µm: LDPE with BDE153 (upper left), BDE7 (lower left), BDE209 (lower middle) and PCB52 (lower right); PA with BDE153 (upper middle); and PET with BDE153 (upper right).

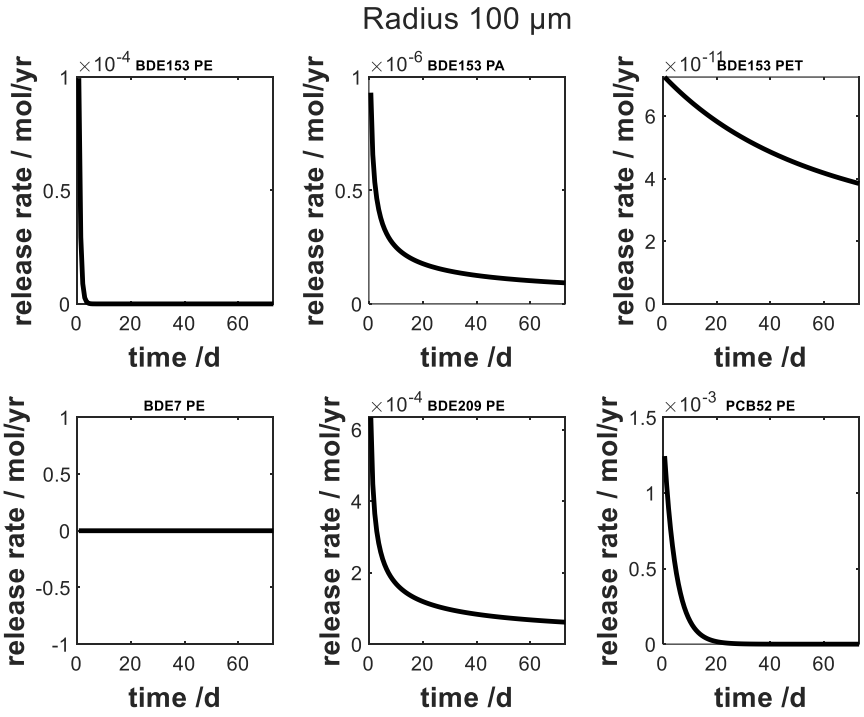

Figure 6: Release rate of additives from polymers with radius 100 µm: LDPE with BDE153 (upper left), BDE7 (lower left), BDE209 (lower middle) and PCB52 (lower right); PA with BDE153 (upper middle); and PET with BDE153 (upper right).

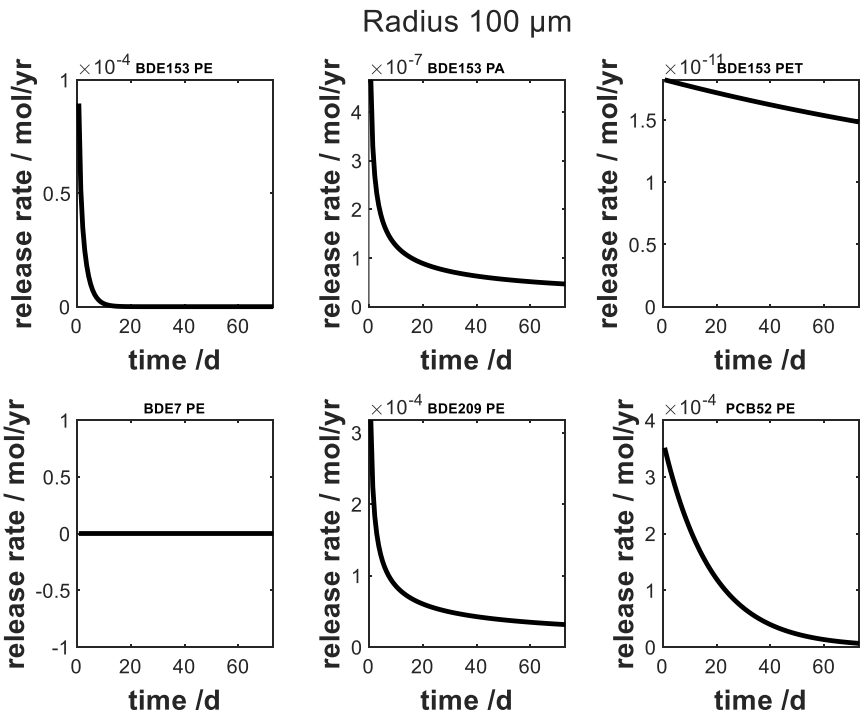

Figure 7: Release rate of additives from polymers with radius200 µm: LDPE with BDE153 (upper left), BDE7 (lower left), BDE209 (lower middle) and PCB52 (lower right); PA with BDE153 (upper middle); and PET with BDE153 (upper right).

Figure 8 and ***Figure 9*** show the distribution of leached BDE153 after one and 50 years after deposition, respectively. After one year, the distribution is still defined almost exclusively by bioturbation, whereas sedimentation strongly influences the 50-year distribution. The location of the concentration profiles follows the profiles of the solid source particles. A fraction of the leached molecules is transferred from the surface sediments into the water column. Peak concentrations are 3.6×10^{-10} mol/l after 1 year and 1×10^{-8} mol/l after 50 years for the more heavily polluted Thames.

The distribution of BDE209 is shown in ***Figure 10*** after a time span of one year and in ***Figure 11*** for a time span of 50 years. The profiles are similar, but the concentration is higher because of the higher additive load in the polymer, The maximum concentration is 6.9×10^{-8} mol/l after one year and 2×10^{-6} mol/l after 50 years. As shown by these profiles, the transport of additives into deeper sediment layers is effectively caused by the bioturbative mixing of MPs into depth. Therefore, a significant fraction of potentially toxic additives are released in the sediment and should not be neglected when assessing the environmental impacts of MP pollution.

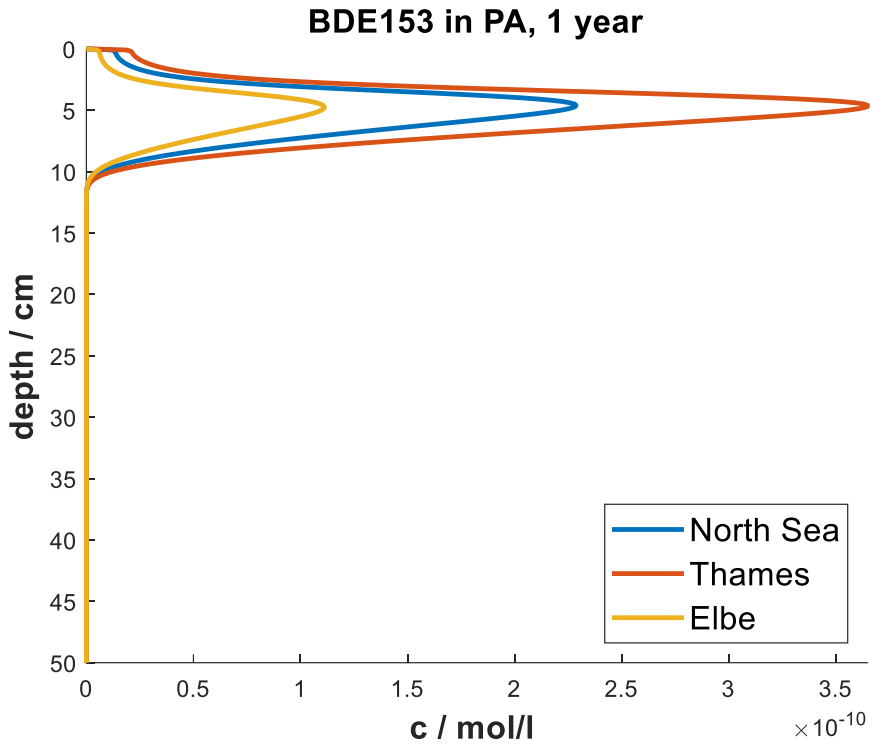

Figure 8: Distribution of BDE153 in sediment pore water after 1 year.

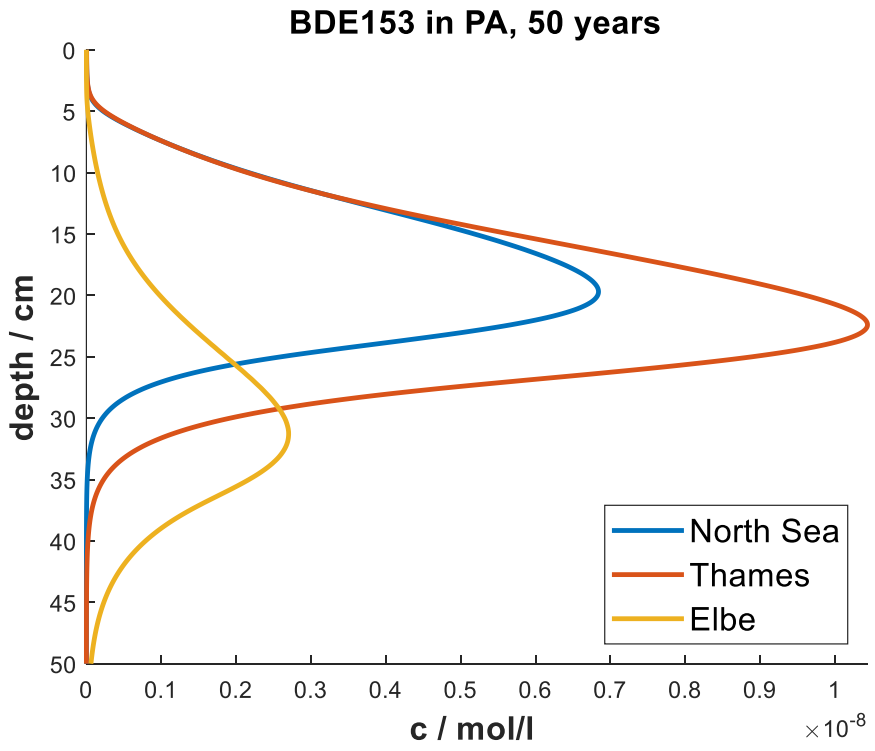

Figure 9: Distribution of BDE153 in sediment pore water after 50 years.

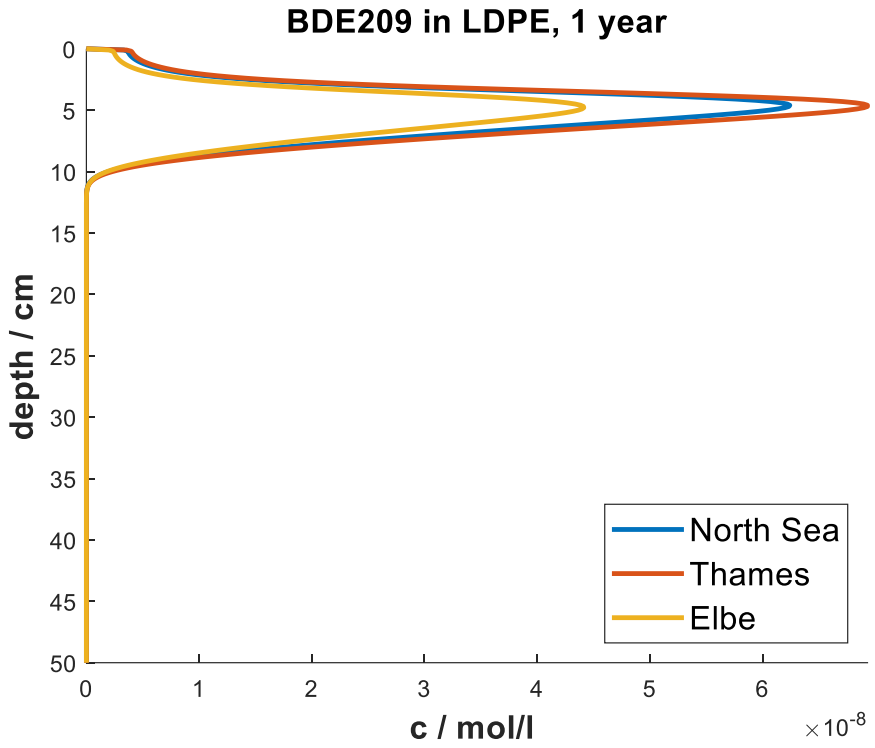

Figure 10: Distribution of BDE209 in sediment pore water after 1 year.

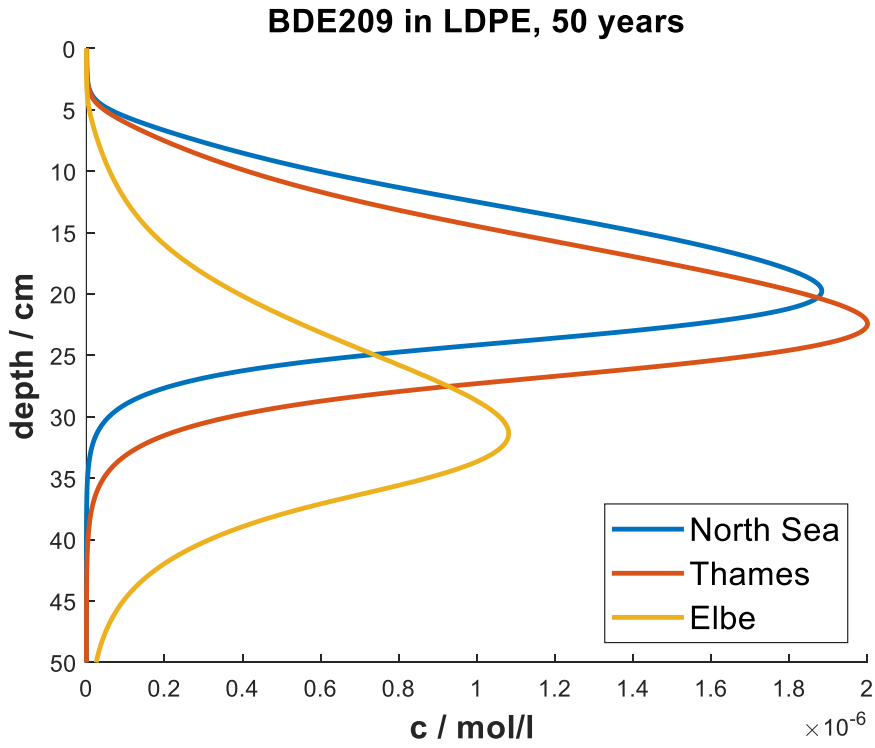

Figure 11: Distribution of BDE209 in sediment pore water after 50 years.

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