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Projected changes of the emission and transport of organic pollutants and metals from shipping in European seas 2018–2050

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ABSTRACT

The ChemicalDrift model is applied to predict concentrations of metals and polycyclic aromatic hydrocarbons emitted from shipping in European seas in 2050, compared to 2018. Sources include antifouling paints (AFPs), discharge water from scrubbers and atmospheric deposition. The fate of pollutants in the marine environment is presented, highlighting the effect of degradation and volatilization, with seasonal and regional differences. A simplified impact assessment is outlined, where predicted environmental concentrations of individual chemicals and whole effluent concentrations of scrubber discharge water are compared to predicted no-effect concentrations (PNECs) or lowest observed effect concentration (LOEC). The 2018 assessment shows scrubber effluent concentrations exceeding LOEC in Baltic and North Sea coastal regions. By 2050, assuming high use of scrubbers, elevated concentrations may extend to all European seas. For AFPs, assuming continued use of primarily copper-based paints, the highest copper concentrations are projected in 2050 for North Sea ports and coasts, potentially exceeding PNECs.

1. Introduction

In the context of rapidly increasing exploitation of marine resources (DNV, 2021; IEA, 2021), it is urgent to develop tools enabling scientists, industry, and regulators to assess the risks and impacts of human activities to the marine environment, and enable sustainable planning and development (Oliveira et al., 2022b; Depellegrin et al., 2021; Olsson et al., 2023).

The ChemicalDrift open-source model for transport and fate of organic compounds and metals in the water column and sediment layer has been recently introduced by Aghito et al. (2023) where model functionality, parameters, and possible applications are described in details, and successively validated by Aghito et al. (2024). In the validation study, the model was applied to emissions of polycyclic aromatic

hydrocarbons (PAHs) discharged to the ocean as *produced water* from oil and gas production facilities in the North Sea, and model results were compared to field measurements acquired by deployment of passive samplers and caged mussels during the 2021 Water Column Monitoring environmental survey in the Ekofisk area (WCM2021, Brooks et al., 2023). The model is available at opendrift.github.io as a module in the Lagrangian framework OpenDrift (Dagestad et al., 2018).

The model was developed and applied within the scope of the Horizon 2020 project Evaluation, control and Mitigation of the Environmental impacts of shipping Emissions (EMERGE). The overall goal of the project is to achieve a comprehensive assessment of the impacts from shipping to the atmosphere and to the marine environment, with focus in the European region (Kukkonen et al., 2022). Some of the results from, e.g., chemical analyses, toxicological tests and modelling were

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summarised by Jalkanen et al. (2024). Shipping generates a range of contaminants that are emitted to the atmosphere and directly discharged to the ocean, e.g., through bilge water, grey water, sewage, antifouling paints and exhaust gas cleaning systems (EGCSs, also known as scrubbers).

The use of scrubbers has emerged in recent years as an alternative method to comply with regulations aiming to reduce sulphur oxides emissions to the atmosphere. Sulphur emissions control areas (SECAs) have been enforced gradually since 2006 in North American coasts, US Caribbean, North Sea, and Baltic Sea, by regulating the maximum allowed sulphur content in marine fuels to 0.1 % by mass since 2015. In addition, global restrictions have been applied (maximum 0.5 % sulphur) since January 2020, and the Mediterranean Sea will become a SECA in January 2025. When using scrubbers, the ship owner may continue to use cheaper heavy fuel oil (HFO) instead of switching to more expensive low sulphur fuel oils or liquefied natural gas (LNG). While reducing atmospheric sulphur oxide emissions, scrubber operation produces large volumes of waste water containing metals, PAHs, including alkylated derivatives, which are discharged directly to the sea (ICES, 2020; Hasselöv et al., 2020). Since the number of installed scrubbers has increased dramatically after the global sulphur cap was introduced, it is important to assess the risk and impact due to contaminants discharged by scrubbers to the marine environment.

The toxicity of scrubber effluents was reported in previous studies (Magnusson et al., 2018; Koski et al., 2017; Teuchies et al., 2020). In the EMERGE project, five research labs have conducted further ecotoxicological experiments and tests, considering field samples of endemic species from many different organism groups and life stages, exposed to scrubber effluents at multiple dilution rates (Chen et al., 2024; Monteiro et al., 2024; Picone et al., 2023; Genitsaris et al., 2024; Magnusson and Granberg, 2022). The most sensitive endpoint was the fertilisation of eggs from the green sea urchin (*Strongylocentrotus droebachiensis*), with a lowest observed effect concentration (LOEC) of 0.0001 % (dilution factor 1×10^6). The no-observed effect concentration (NOEC) was not determined for this endpoint since effects were observed at all tested concentrations.

Antifouling paints (AFPs) are applied to ships to prevent biofouling on the vessel's hull. These paints are generally categorized into two types: those that prevent biofouling by releasing biocides (biocidal AFPs) and those that use non-stick properties to inhibit fouling, known as fouling release (FR) coatings (Lagerström et al., 2022). FR coatings are either free of biocides or contain low concentrations of booster biocides, such as zinc pyrithione. Although interest in foul release coatings has grown among ship owners over the past few decades, the hull coating market is still predominantly dominated by biocidal AFPs, which account for about 90 % of all coatings used (Weber and Esmaili, 2023). Today, the majority of biocidal AFPs contain inorganic copper, with 76 % containing cuprous oxide (Cu_2O) and 8.8 % containing cuprous thiocyanate (CuSCN) (Paz-Villarraga et al., 2022). Ships coated with these copper-based AFPs have been identified as one of the largest anthropogenic sources of copper in marine environments with high shipping traffic. For instance, AFPs are estimated to contribute to about one-third of the total copper input into the Baltic Sea (Ytreberg et al., 2022).

The aim of this work is to model the distribution of pollutants from shipping, with special emphasis on antifouling paints and scrubbers in the European Seas, and to compare results for 2018 with projections for the year 2050.

2. Material and methods

2.1. ChemicalDrift simulations

The ChemicalDrift model is here applied to European regional scale emissions from shipping and from atmospheric depositions for the baseline year 2018 and for two emission scenarios for the target year

2050.

The model is based on a Lagrangian approach where the mass of emitted chemical is distributed (or seeded) to a number, N , of Lagrangian elements. The model calculates and stores the complete trajectory (latitude, longitude, z) and the history of each Lagrangian element, including the physico-chemical transformations occurring along the trajectory. Important properties considered here are the *mass*, i.e., the residual mass of a chemical substance in the environment after degradation and volatilization processes are calculated, and the removed fractions, stored in the *mass_degraded* and *mass_volatilized* properties; the partitioning of each Lagrangian element in the environment is updated dynamically at each time step, specifying whether the chemical mass is dissolved in sea water, adsorbed to suspended particles (SPM), adsorbed to dissolved organic matter (DOM) or deposited to the sediment layer. Sorption and desorption transfer rates for PAHs were derived by Aghito et al. (2023), based on mean octanol-water partition coefficient (K_{OW}) values and empirical relationships linking K_{OW} to the organic carbon-water partition coefficient (K_{OC}). For metals, transfer rates were determined as described by Simonsen et al. (2019), using average solid-water distribution coefficient (K_d) values reported by Tomczak et al. (2019) and IAEA (2004). Parameters governing partitioning, degradation, and volatilization are influenced by sea water temperature and salinity. Additional details can be found in Aghito et al. (2023). One snapshot from a ChemicalDrift simulation is shown in Fig. 1, with details explained in Sec. 2.1.2. The metocean physical and biogeochemical data utilised to force ChemicalDrift, including sea water velocity, temperature, salinity, mixed layer depth, surface wind, and SPM and DOC concentrations are listed in Table 1 and visualized in Fig. 2.

2.1.1. Preprocessing of emission data and seeding

Approximately 1 million Lagrangian elements were deployed in each simulation, based on spatio-temporal gridded data of emissions as described in Sec. 2.2. The very large emission datasets were pre-processed to reduce the computational complexity of the simulations. The Python `xarray.DataArray.coarsen` method was applied, reducing the spatial resolution to $0.2^\circ\text{N} \times 0.4^\circ\text{E}$ for shipping discharges, and $0.4^\circ\text{N} \times 0.4^\circ\text{E}$ for atmospheric deposition data. The time step was also reduced to 12 h for scrubber discharge data in 2018, 2 days for 2050 data, and weekly for all AFP and atmospheric deposition data. Further simplifications were applied (to all sources except 2018 scrubbers data) by filtering out the less significant grid cells, accounting for 5 % of the total mass of emitted chemicals, and distributing this to the other cells. The simplified emission data were divided in 16 or 32 slices defined by equal ranges of longitudes, fed to separate instances of ChemicalDrift, executed in parallel processes, significantly reducing the time needed for the simulations. Seeding of Lagrangian elements in each instance was done through the `seed_from_DataArray` method implemented in the model, which distributed the mass of each gridded emission data point to a number of Lagrangian elements in a radius of 10 km. The calculations main time step in the ChemicalDrift model was set to 6 h, with a higher time step applied internally for the vertical mixing sub process.

2.1.2. Raw and gridded output

Derived properties, such as the mass fractions in each environmental compartment described above, were extracted after a model run by the method `get_property`, and made available for manipulation and analysis. One snapshot of a ChemicalDrift simulation of dibenz(*a,h*)anthracene discharged from open-loop scrubbers showing the position and partitioning of $N = 1, 136, 133$ Lagrangian elements at the end of the simulated year 2050 is shown in Fig. 1.

Spatio-temporal maps of weekly mean concentrations for all the modelled emission sources, chemicals and scenarios, were provided for grid cells of $0.1^\circ \times 0.1^\circ$ at 10 vertical levels delimited by 0, -5, -10, -20, -30, -40, -50, -75, -125, -200 m, and sea floor depth (m), and

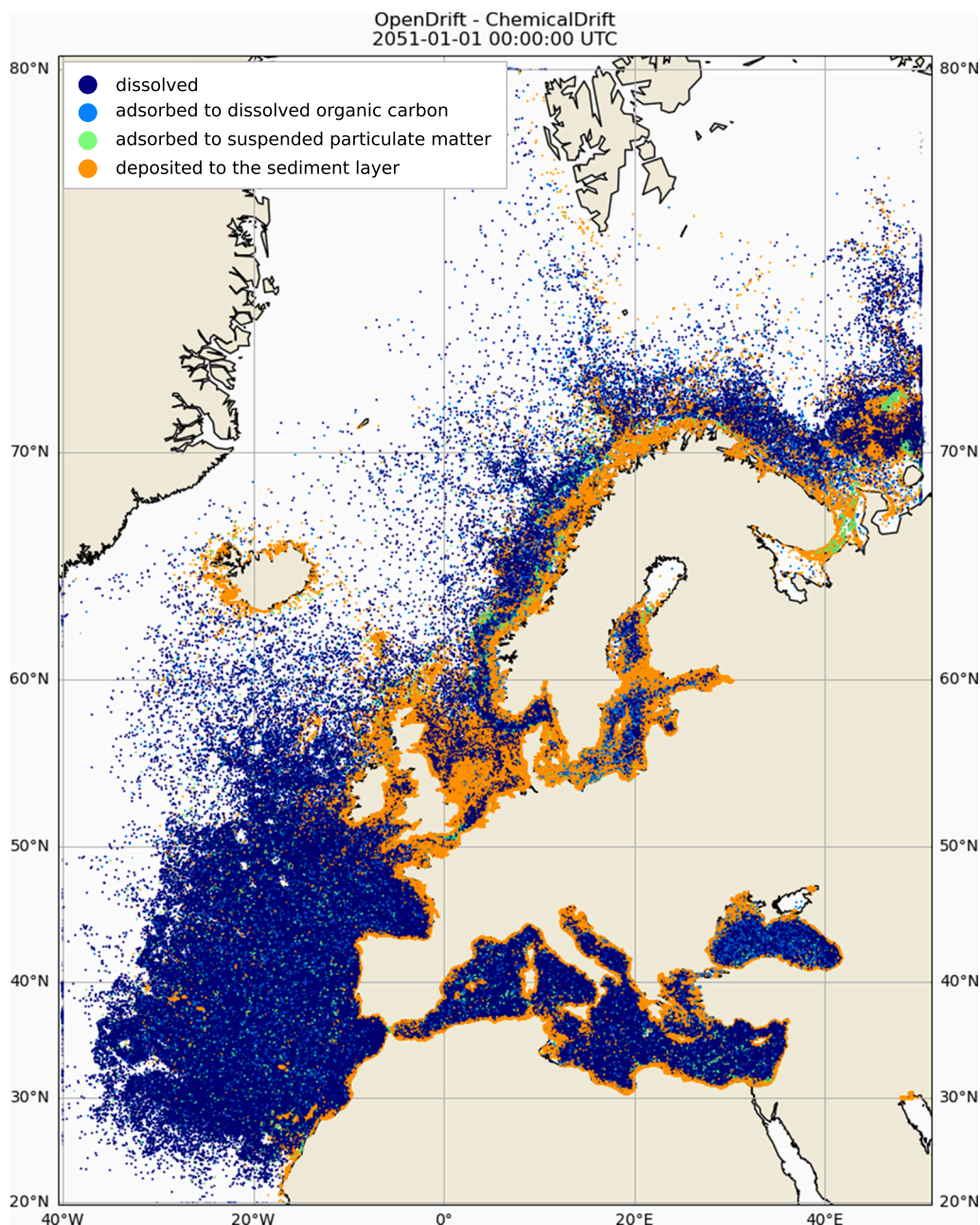


Fig. 1. The predicted spreading of dibenz(*a,h*)anthracene from open-loop scrubbers discharged in the year 2050, scenario 3, simulated by ChemicalDrift. The position of the Lagrangian elements and the partitioning between the modelled environmental compartments at the end of the year are shown. The different masses of each element are not represented in this plot.

Table 1

Datasets utilised to force ChemicalDrift.

GLOBAL_ANALYSISFORECAST_PHY_001_024 ^a
sea water velocity, sea water temperature, salinity, mixed layer depth
WIND_GLO_WIND_L4_REP_OBSERVATIONS_012_006 ^a
surface wind
OCEANCOLOUR_GLO_BGC_L4_MY_009_104-TDS ^a
SPM concentration
Compilation of DOM data (Hansell et al., 2021)
DOM concentration

^a Copernicus Marine Service products indicated with ID.

52 weeks. Gridded output was saved as NetCDF files with the `write_netcdf_chemical_density_map` method. One example of gridded output is visualized in Fig. 3.

In the following, concentrations in the water column refer to the sum of the dissolved, sorbed to DOC, and sorbed to SPM fractions, for each grid cell.

2.2. Emission data from STEAM and SILAM

Emissions of PAHs and metals were provided for the years 2018 and 2050 by the Ship Traffic Emission Assessment Model (STEAM) and the System for Integrated modelling of Atmospheric composition (SILAM). The overview of the scenarios, emission sources, and chemicals considered in this study is presented in Table 2.

Discharges from shipping were obtained from STEAM version 4.1. The STEAM model utilises Automatic Identification System (AIS) data to assess ship location and velocity and technical information of individual ships from the S&P Global and Global Information System for

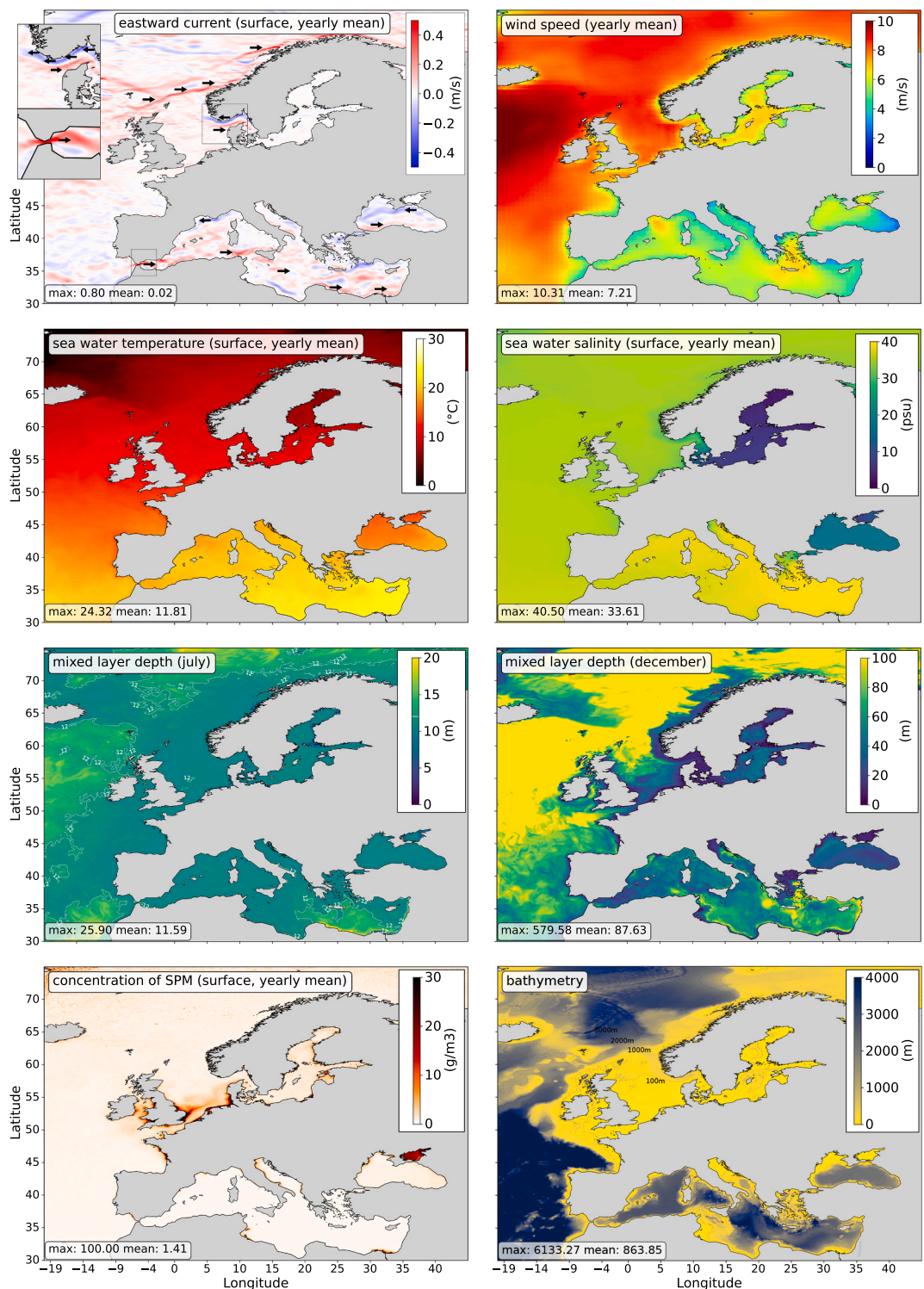


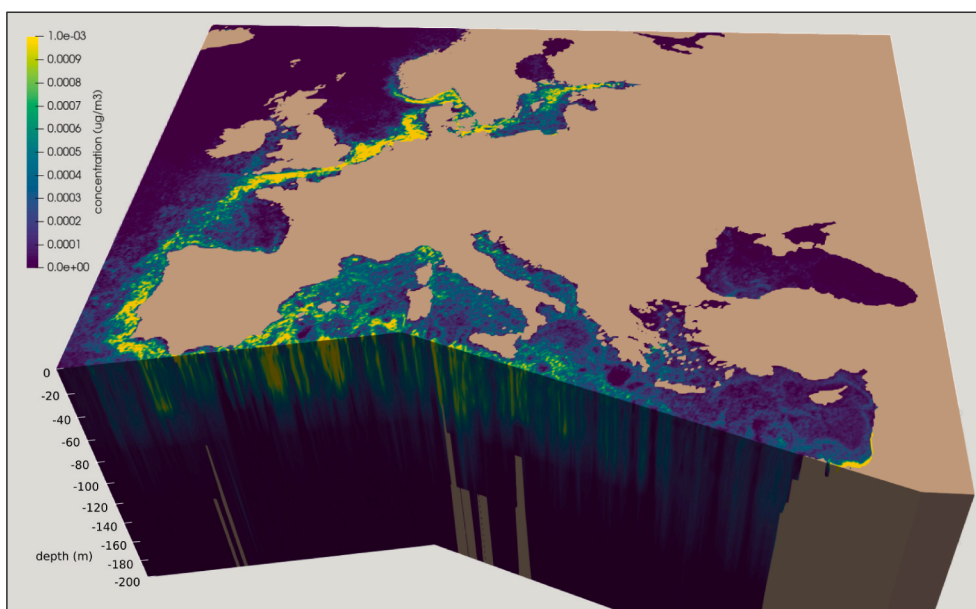
Fig. 2. Metocean and biogeochemical forcing data utilized by ChemicalDrift (Table 1).

International Shipping database. Ocean and weather conditions (winds, ocean currents, waves and sea ice) are combined with ship data to predict power output and emissions, including direct discharges to the sea and atmospheric emissions. More details are given by Johansson et al. (2017) and Jalkanen et al. (2021).

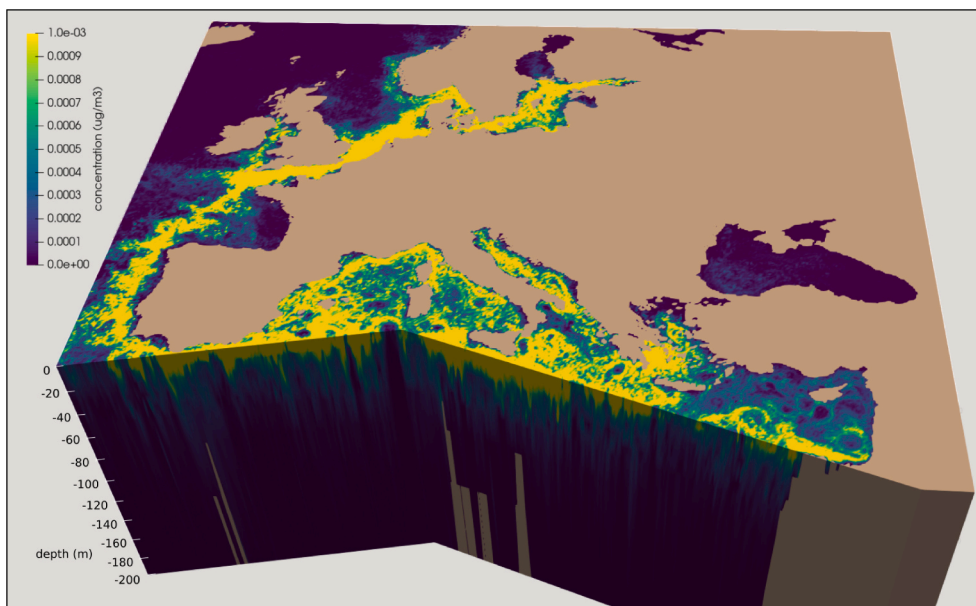
The STEAM provided estimates of leaching of copper (Cu) and zinc (Zn) from AFPs, and volumetric discharges of OL scrubber effluents. The mass of discharged chemicals from OL scrubbers were calculated for 6 PAHs, naphthalene (Nap), phenanthrene (Phe), fluoranthene (Flu),

benzo(a)pyrene (BaP), benz(a)anthracene (BaA), dibenz(a,h)anthracene (DahA) and 7 metals, Cu, cadmium (Cd), chromium (Cr), nickel (Ni), Zn, lead (Pb), vanadium (V), applying emission factors with the concentrations of pollutants in scrubber effluents described by Lunde Hermansson et al. (2021) and Ytreberg et al. (2021).

The depositions to sea surface of atmospheric emissions from ships and land sources (including aviation), were calculated using the SILAM chemistry transport model (see, e.g., Kouznetsov and Sofiev (2012); Wesely (1989), and <https://silam.fmi.fi>) that calculates atmospheric



(a) week 52



(b) week 25

Fig. 3. The predicted concentration of dibenz(*a,h*)anthracene from open-loop scrubbers in week 25 (b) and at the end of year, week 52 (a) modelled for 2050, in scenario 3. The mean weekly concentration in the water column at surface is shown (0 – 5 m) as well as the depth profile (0 – 200 m) along the main shipping route in the Mediterranean Sea between the Gibraltar Strait and the Suez channel.

composition and dry and wet depositions of gases and aerosols. Atmospheric deposition from shipping (AS) were calculated for the same set of 7 metals based on STEAM atmospheric emission data of ash particles and emission factors derived in EMERGE (Grigoriadis et al., 2022), integrated in ChemicalDrift. Atmospheric depositions from other sources (AO), i.e., land sources including aviation, were provided for Pb and Cd, based on EMEP emission inventory. Atmospheric depositions of PAHs were not available.

2.3. EMERGE scenarios

The year 2018 was selected as our baseline year to assess the reference state of European seas. Scrubbers were mainly used in the Baltic and the North Seas SECA, and in the other areas mostly used by cruise

ships which had to comply with the EU sulphur directive. Based on STEAM data, in the whole region less than 400 ships used scrubbers, with a total annual discharge of 718 million m³ from open-loop (OL) scrubbers, most of it, 80 %, in the SECA, and only 0.08 million m³ from closed-loop (CL) scrubbers. Based on average concentrations of a selection of metals and PAHs in OL and CL scrubber effluents, reported by Lunde Hermansson et al. (2021), these discharged volumes accounted for 540 tons of metals and 60 kg of PAHs from OL scrubbers, compared to 4.4 tons of metals and 0.5 kg of PAHs from CL scrubbers. Based on this, only OL scrubbers were considered in this study.

Multiple ship emissions and discharge scenarios were constructed for the target year 2050, considering various degrees of traffic growth, energy efficiency improvements, fuel mixes and emission abatement technologies. Two extreme cases, scenario 3 (S3) and scenario 8 (S8)

Table 2

Overview of all the chemical compounds, emission sources, and scenarios simulated by ChemicalDrift. Mean concentrations over the whole domain are indicated, along with the corresponding change from 2018, and with the number of grid cells exceeding the predicted no-effect concentrations (PNECs), or fractions of PNEC.

Chem.	Source	Mean 2050 ($\mu\text{g L}^{-1}$)	Mean 2018 ($\mu\text{g L}^{-1}$)	Incr (%)	PNEC ($\mu\text{g L}^{-1}$)	cells > PNEC (#)	> 0.5 × PNEC 2050 (#)	> 0.1 × PNEC (#)	cells > PNEC (#)	> 0.5 × PNEC 2018 (#)	> 0.1 × PNEC (#)
Scenario 3											
Cu	AFP	4.7×10^{-3}	3.0×10^{-3}	56	1.45	721	1760	12,691	523	1267	7037
Zn	AFP	5.6×10^{-4}	3.7×10^{-4}	52	1.1	113	244	1768	86	187	1192
Cd	AO	6.8×10^{-6}	6.9×10^{-6}	0	0.2	0	0	8	0	0	13
Pb	AO	9.1×10^{-5}	9.1×10^{-5}	0	1.3	1	3	47	0	4	58
Cd	AS	1.9×10^{-9}	5.5×10^{-9}	-65	0.2	0	0	0	0	0	0
Cr	AS	6.6×10^{-8}	1.9×10^{-7}	-65	3.4	0	0	0	0	0	0
Cu	AS	1.2×10^{-7}	3.7×10^{-7}	-67	1.45	0	0	0	0	0	0
Ni	AS	2.8×10^{-5}	8.6×10^{-5}	-67	8.6	0	0	0	0	0	0
Pb	AS	2.1×10^{-8}	5.8×10^{-8}	-63	1.3	0	0	0	0	0	0
V	AS	4.8×10^{-5}	1.5×10^{-4}	-67	2.5	0	0	0	0	0	2
Zn	AS	6.3×10^{-7}	1.8×10^{-6}	-65	1.1	0	0	0	0	0	0
Nap	OL	6.8×10^{-6}	3.9×10^{-7}	1652	2.0	0	0	0	0	0	0
Phe	OL	1.0×10^{-5}	6.1×10^{-7}	1575	1.1	0	0	0	0	0	0
Flu	OL	1.3×10^{-6}	7.0×10^{-8}	1781	0.00076	0	0	31	0	0	0
BaP	OL	4.3×10^{-7}	2.1×10^{-8}	1922	0.00017	0	0	50	0	0	0
BaA	OL	1.0×10^{-6}	5.1×10^{-8}	1885	0.0012	0	0	1	0	0	0
DahA	OL	2.6×10^{-7}	1.3×10^{-8}	1935	5.66×10^{-5}	0	4	3576	0	0	0
Cd	OL	4.2×10^{-6}	2.5×10^{-7}	1588	0.2	0	2	12	0	0	0
Cr	OL	8.3×10^{-5}	4.9×10^{-6}	1608	3.4	0	2	16	0	0	0
Cu	OL	3.0×10^{-4}	1.7×10^{-5}	1710	1.45	4*	16	114	0	0	3
Ni	OL	5.4×10^{-4}	2.9×10^{-5}	1757	8.6	0	2	19	0	0	0
Pb	OL	2.8×10^{-5}	1.8×10^{-6}	1491	1.3	0	2	27	0	0	0
V	OL	1.7×10^{-3}	9.1×10^{-5}	1734	2.5	24*	72	457	0	2	15
Zn	OL	5.0×10^{-4}	3.0×10^{-5}	1560	1.1	47*	81	678	2	2	24
Scenario 8											
Cu	AFP	4.8×10^{-3}	3.0×10^{-3}	58	1.45	706	1748	12,825	523	1267	7037
Zn	AFP	5.6×10^{-4}	3.7×10^{-4}	52	1.1	126	256	1831	86	187	1192
Cd	AO	6.8×10^{-6}	6.9×10^{-6}	0	0.2	0	0	9	0	0	13
Pb	AO	9.2×10^{-5}	9.1×10^{-5}	0	1.3	1	5	60	0	4	58
Cd	AS	2.5×10^{-10}	5.5×10^{-9}	-95	0.2	0	0	0	0	0	0
Cr	AS	9.0×10^{-9}	1.9×10^{-7}	-95	3.4	0	0	0	0	0	0
Cu	AS	1.7×10^{-8}	3.7×10^{-7}	-95	1.45	0	0	0	0	0	0
Ni	AS	3.8×10^{-6}	8.6×10^{-5}	-95	8.6	0	0	0	0	0	0
Pb	AS	2.9×10^{-9}	5.8×10^{-8}	-95	1.3	0	0	0	0	0	0
V	AS	6.6×10^{-6}	1.5×10^{-4}	-95	2.5	0	0	0	0	0	2
Zn	AS	8.5×10^{-8}	1.8×10^{-6}	-95	1.1	0	0	0	0	0	0
	OL	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.

Nap: naphthalene, Phe: phenanthrene, Flu: fluoranthene, BaP: benzo(a)pyrene, BaA: benz(a)anthracene, DahA: dibenz(a,h)anthracene. Cd: cadmium, Cr: chromium, Cu: copper, Ni: nickel, Pb: lead, V: vanadium, Zn: zinc. AFP: antifouling paint, AO: atmospheric deposition from other sources, AS: atmospheric deposition from shipping, OL: open-loop scrubbers. *Modelling artefacts.

were selected. Both scenarios assume a high development of maritime transport (Longva et al., 2020), with number of modelled ships in the region increasing from approximately 100,000 in 2018 to 400,000 in 2050. Both scenarios also assume SECAs (0.1 % sulphur) applied in the Baltic Sea, in the North Sea, and in the Mediterranean sea, in addition to the 0.5 % global limit.

A wide adoption of open-loop scrubbers was assumed in S3, with 0.1 % sulphur limit additionally enforced in all European seas within 200 nautical miles from the coastline. Based on data from STEAM, the number of ships operating with a scrubber in 2050 is predicted to be 33,000 producing a total annual discharge from OL scrubbers of 17,000 million m^3 .

In S8 we assumed that measures to comply with the initial IMO strategy of reducing greenhouse gas emissions from shipping by 50 % by 2050 are taken. Extensive use of low sulphur alternatives was assumed, i.e., methanol, LNG, and conventional low sulphur marine fuels (accounting for 60 %, 20 %, and 20 %, respectively, of the produced ship energy) and scrubbers are not utilised.

For antifouling paints, the modelled scenarios assume that copper-based AFPs will remain the predominant choice in 2050, as they were in 2018, without considering advancements in AFP technology. As a

result, traffic growth is projected to significantly increase AFP emissions in both scenarios.

2.4. Risk and impact assessment

A simplified impact assessment of the emissions sources considered in this work is presented. Using the gridded output from ChemicalDrift, weekly mean concentrations in the top layer (0 – 5 m) of the water column are calculated adding the chemicals in the dissolved, sorbed to DOC, and sorbed to SPM fractions. Predicted concentrations of each modelled source and chemical were compared to the corresponding predicted no-effect concentrations (PNECs), based on values compiled by Lunde Hermansson et al. (2022). For the PAHs, the only source considered in this study was OL. For the metals, the total predicted concentrations were also calculated summing the contributions of each source, and compared to PNECs.

One limitation of the current approach is that other important sources were not available, e.g., riverine inputs and atmospheric depositions of PAHs. Furthermore, only the impact on the marine environment is studied, without considering, e.g., the health impact of atmospheric emissions. A holistic environmental impact assessment of

the emissions from shipping, which utilised also the gridded output from ChemicalDrift presented in this study, was described by Gueret et al. (2024).

2.5. Dilution approach

Scrubber effluents are a complex mixture of many chemicals. The ChemicalDrift model calculated the predicted environmental concentrations of single components, PEC_i , where $i \in \{1, 2, \dots, 13\}$ (6 PAHs and 7 metals), a fraction of the chemicals present in the mixture. The PEC_i were not directly comparable to LOEC derived from ecotoxicological experiments based on a whole effluent toxicity (WET) approach. To overcome this incompatibility, a method for estimating the degree of dilution of whole scrubber effluents (or other complex mixtures), when discharged in the environment and prior to its “deterioration” due to chemical processes, was recently developed by Zervakis et al. (2024), based on PECs of single components (Fragkou et al., 2023).

Dilution indices (DI_i , ratio of PEC_i over the concentration in scrubber wash water prior to discharge) were calculated for every component at each time step and grid cell. The method considers that the rate of dilution of a mixture discharged in the surface ocean is initially dominated by turbulent mixing, which acts to dilute all components at the same rate. Hence, the variance of these indices at the initial turbulent stage is low and relatively constant. On time scales of hours, chemical processes start affecting contaminant concentrations, e.g., through partitioning, degradation and volatilization, with rates depending on the different properties of each contaminant. At this stage, the variance of DI_i starts increasing. Associating this with the dilution index of the least reactive component (e.g. Cd), that acts as a proxy of scrubber water dilution, helps determine a “threshold” variance and allows us to set a criterion for the applicability of the method. The reader is referred to Zervakis et al. (2024) for a full description of the method, along with implementation examples.

In the most trafficked oceanic regions, the faster rate of removal of the less persistent components, e.g., Nap and Phe, may be compensated by the continuous replenishment from scrubber discharges. Nap and Phe are the two modelled components with the highest initial concentrations in scrubber effluents (Lunde Hermansson et al., 2021). More persistent chemicals, e.g., BaP and DahA, have higher affinity to particles and may exhibit faster removal from the water column by sedimentation. Hence, also depending on PECs spatial and temporal resolution and on the choice of threshold variance value, high concentrations of whole scrubber effluents may be estimated for longer time scales.

By applying the dilution method in 2018 and 2050 (S3) we computed maps with concentrations of scrubber whole effluent discharges considering only grid cells where the threshold was not exceeded at particular time instances. Estimated whole effluent concentrations were compared to LOEC values obtained from WET experiments (Chen et al., 2024; Magnusson and Granberg, 2022), and spatial distributions of the probability of exceeding LOEC were estimated.

2.6. European oceanic regions

Based on the ChemicalDrift scenario simulations, the mass budgets of chemicals discharged by OL scrubbers for the target year 2050 (S3) were calculated for different oceanic regions. The total discharged mass, the mass removed by degradation, volatilization, and the amount that drifted to other regions have all been estimated.

The following oceanic sub-regions defined by the Marine Strategy Framework Directive (MSFD) were utilised: Baltic Sea (Bal); Greater North Sea, including the Kattegat and the English Channel (Nrt); Celtic Seas (Cel); Bay of Biscay and the Iberian Coast (B–I); Western Mediterranean (W.Med); Ionian Sea and the Central Mediterranean Sea (C. Med); Adriatic Sea (Adr); Aegean-Levantine Sea (E.Med); Black Sea (Bla). The Norwegian Sea (Nwg) as defined by the International Hydrographic Organization (IHO) was also computed after removing a

small area overlapping the Celtic and North seas. The regions are shown in Fig. 4.

3. Results and discussion

The summary of the simulations results for each modelled scenario, source and chemical compound, is presented for the whole European domain in Table 2. Predicted mean concentrations in 2050 scenarios are reported and compared to baseline results, indicating the increments (% of 2018 levels). The increments reflect the changes in emissions described above; increments between 52 % and 58 % are modelled for Cu and Zn from AFP in S3 and S8 due to increase of ship traffic; the contributions of Cd and Pb from atmospheric depositions from land sources (AO) are the same as in 2018; predicted concentrations of metals and PAHs from scrubbers (OL) are increased in S3 by 1500 – 2000% compared to baseline levels, which is a direct consequence of the use of scrubbers assumed in this scenario; the contributions from depositions from shipping atmospheric emissions (AS) are significantly reduced in both scenarios (63 – 67% in S3, and 95% in S8) for different reasons; in S3, the reduction is due to the use of scrubbers, and in S8, the reduction is due the use of low sulphur alternatives, i.e., methanol and LNG. These reductions are considered insignificant with respect to the total concentrations in the water, since the contributions from OL and AO are much higher, by 2 – 3 orders of magnitude.

The total predicted concentrations were calculated for the metals, summing the contributions of the modelled sources (OL, AFP, AS and AO). These are summarised for each scenario in Table 3.

Modelling results are reported in detail in the following examples, presenting the spatial and temporal distribution, the chemical fate, and the transport between sea regions for selected representative chemicals. Nap and Phe are low molecular weight PAHs (2 – 3 benzene rings), while BaP and DahA are examples of high molecular weight PAHs (5 rings), which exhibit higher affinity to solids, slower degradation and volatilization, hence longer persistence in the environment. Flu and BaA are 4-ring PAHs, with chemical properties within the range of the presented extremes. Based on the overview in Table 2, DahA is the PAH with highest modelled impact (number of cells above $0.1 \times$ PNEC). For the metals, Cd was selected in the examples for its environmental relevance and since emission data was available for OL, AO and AS, while Cu was discussed for AFP, based on the high PNEC exceedance reported in Table 2. Metals are not affected by degradation and volatilization and exhibit more similar behaviors, with some differences due to variations in affinity to solids. For each source, similar concentration patterns were obtained for the other PAHs and metals.

3.1. Predicted concentrations of benzo(a)pyrene and cadmium

The mean concentrations of BaP in the water column (top 5 m, yearly mean) for 2050 (S3) and 2018 are shown in Fig. 5. It can be observed that in 2018 the highest concentrations, in the order of $10^{-6} \mu\text{g L}^{-1}$, were modelled in the Baltic Sea, in the North Sea and in the English channel, while the concentrations in the Bay of Biscay, Atlantic Ocean and Mediterranean Sea were significantly lower (by 1 – 3 orders of magnitude). This is as expected since in 2018 SECA was enforced only in Northern Europe, hence only a small number of ships with scrubbers were sailing in the Atlantic Ocean and in the Mediterranean Sea. In 2050, with global sulphur restrictions and SECA enforced also in the Mediterranean, higher concentrations are predicted over the whole region, particularly along the main shipping routes from the Baltic, through the English channel and Gibraltar, to Suez.

The concentrations of BaP accumulated in the sediment after one year of emissions for OL in S3 and baseline are shown in Fig. 6 (assuming an accumulation layer of 3 cm, porosity 0.6, sediment density 2600 kg m^{-3}). A similar trend is observed also in this case, with significantly higher concentrations modelled for the year 2050 compared to 2018. Accumulation in sediments is predominantly affecting the shallower

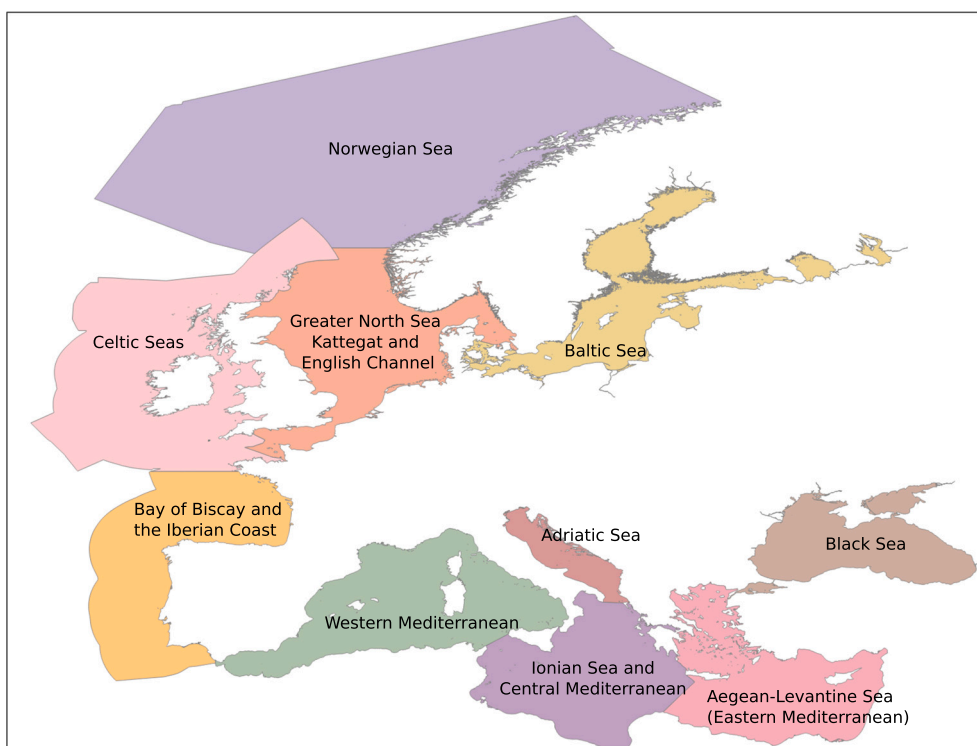


Fig. 4. Sea regions used in this study.

Table 3

Overview of the predicted total concentrations of metals, obtained summing the contributions from each source. Mean total concentrations over the whole domain are indicated, along with the corresponding change from 2018, and with the number of grid cells exceeding predicted no-effect concentrations (PNECs), or fractions of PNEC. PAHs were only modelled for open-loop scrubbers, and Cr, Ni, and V were only modelled for atmospheric depositions of shipping emissions, and are not included here as already reported in Table 2.

Chem	Sources	Mean 2050 ($\mu\text{g L}^{-1}$)	Mean 2018 ($\mu\text{g L}^{-1}$)	Incr (%)	PNEC ($\mu\text{g L}^{-1}$)	cells > PNEC 2050 (#)	> 0.5 \times PNEC 2050 (#)	> 0.1 \times PNEC 2050 (#)
Scenario 3								
Cu	OL, AS, AFP	5.1×10^{-3}	3.1×10^{-3}	64	1.45	780	1872	14,098
Zn	OL, AS, AFP	1.1×10^{-3}	4.1×10^{-4}	161	1.1	159	390	2878
Cd	OL, AS, AO	1.1×10^{-5}	7.3×10^{-6}	54	0.2	0	2	32
Pb	OL, AS, AO	1.2×10^{-4}	9.4×10^{-5}	27	1.3	2	8	85
Cr	OL, AS	8.3×10^{-5}	5.1×10^{-6}	1543	3.4	0	2	16
Ni	OL, AS	5.7×10^{-4}	1.2×10^{-4}	393	8.6	0	2	21
V	OL, AS	1.7×10^{-3}	2.4×10^{-4}	616	2.5	26	73	462
Scenario 8								
Cu	AS, AFP	4.8×10^{-3}	3.0×10^{-3}	58	1.45	706	1748	12,825
Zn	AS, AFP	5.6×10^{-4}	3.7×10^{-4}	51	1.1	126	256	1831
Cd	AS, AO	6.8×10^{-6}	6.9×10^{-6}	0	0.2	0	0	9
Pb	AS, AO	9.2×10^{-5}	9.1×10^{-5}	0	1.3	1	5	60

Cd: cadmium, Cr: chromium, Cu: copper, Ni: nickel, Pb: lead, V: vanadium, Zn: zinc. AFP: antifouling paint, AO: atmospheric deposition from other sources, AS: atmospheric deposition from shipping, OL: open-loop scrubbers.

coastal regions and the continental shelf. This is because concentrations of suspended solids are typically high close to the coasts (Fig. 2), and also decrease with depth, as considered in the model (Aghito et al., 2023).

The contributions of the modelled sources to concentration levels of Cd in the water column in S3 are presented in Fig. 7, illustrating that the main sources are OL and AO, with a minor contribution from AS, as already indicated in Table 2. It is important to note that other water-borne sources like loads from rivers were not included in this study since data was not available for the whole European domain, though expected to be significant. For the Baltic Sea, a total water-borne input of

Cd of 17 tons and total deposition of 4 tons were reported (Sonesten et al., 2024).

3.2. Seasonal differences

The predicted gridded concentrations of DahA from open-loop scrubbers in S3 are found in Fig. 3, showing mean weekly concentrations in the surface layer (0 – 5 m) and vertical transects along the main shipping route in the Mediterranean Sea from Gibraltar Strait to Suez. Results are presented for a typical summer (week 25) and winter (week 52) situation. Higher concentrations at the surface in summer are

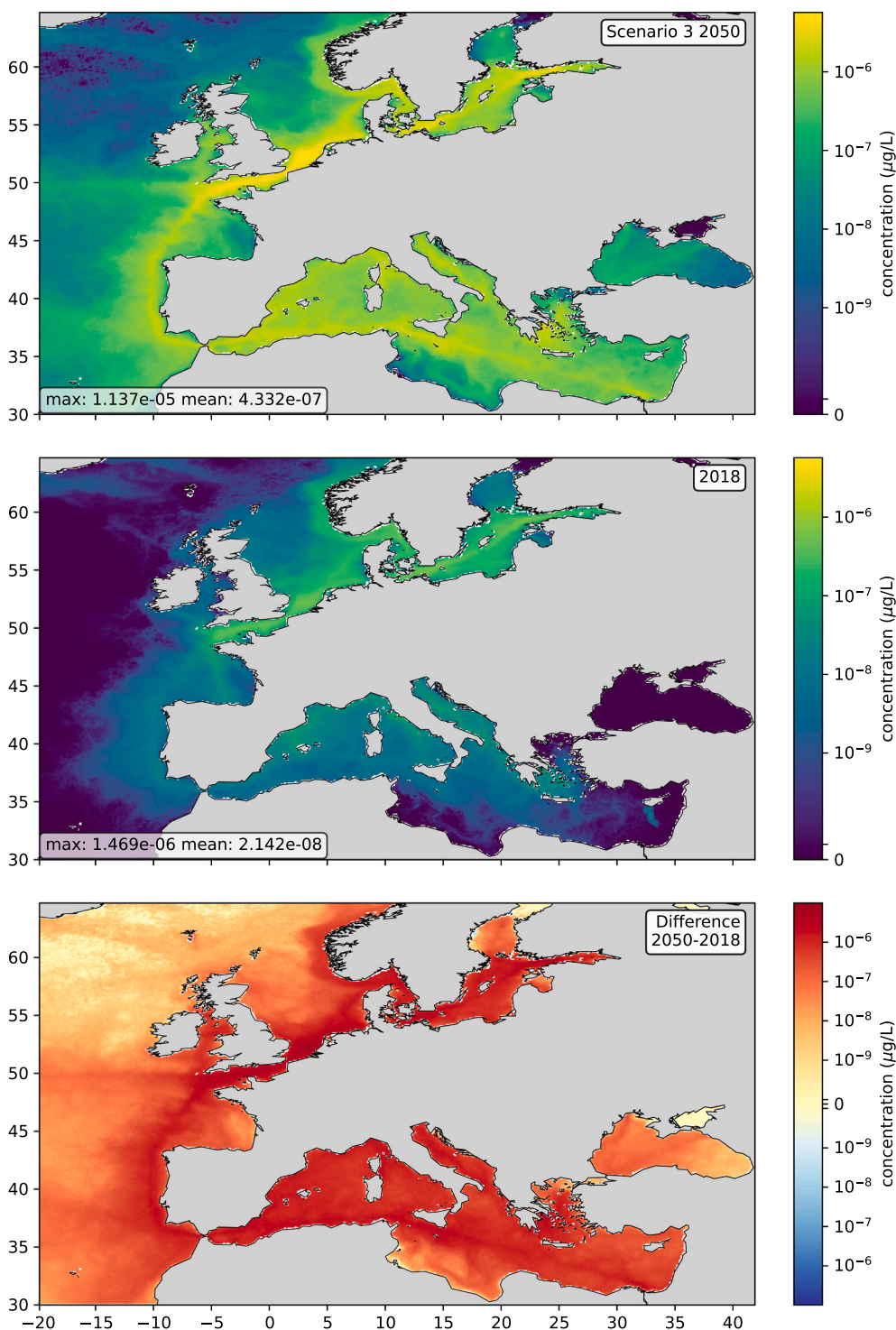


Fig. 5. Modelled yearly mean concentrations of benzo(a)pyrene in the water column (top 5 m), discharged from open-loop scrubbers in 2050 scenario 3 (top), compared to 2018 (middle). The change from 2018 to 2050 in shown in the bottom panel.

observed, which is expected since scrubber effluents are discharged near the surface and the formation of a narrow mixed layer limits mixing with the deeper colder and heavier waters.

3.3. Simplified impact assessment for single chemicals

The number of grid cells exceeding PNEC (or fractions, 50 %, 10 % of PNEC) in each simulation are also presented in Table 2 in order to identify the emissions sources with largest impact. In both scenarios, the

emissions of Cu and Zn from AFP are the contributions that produce the highest number of grid cells exceeding PNEC (113 – 721 grid cells). The predicted impacts in 2050 also reflect the projected increased concentrations with respect to the baseline year 2018, as seen for example for Cu from AFP in S3 (from 523 to 721 cells exceeding PNEC).

The concentrations obtained summing the contributions from each source are also evaluated and reported in Table 3. For Cu and Zn, PNEC exceedance is slightly increased (126 – 780 grid cells) in S3 due to the additional input from AO. In S8, the total concentration and PNEC

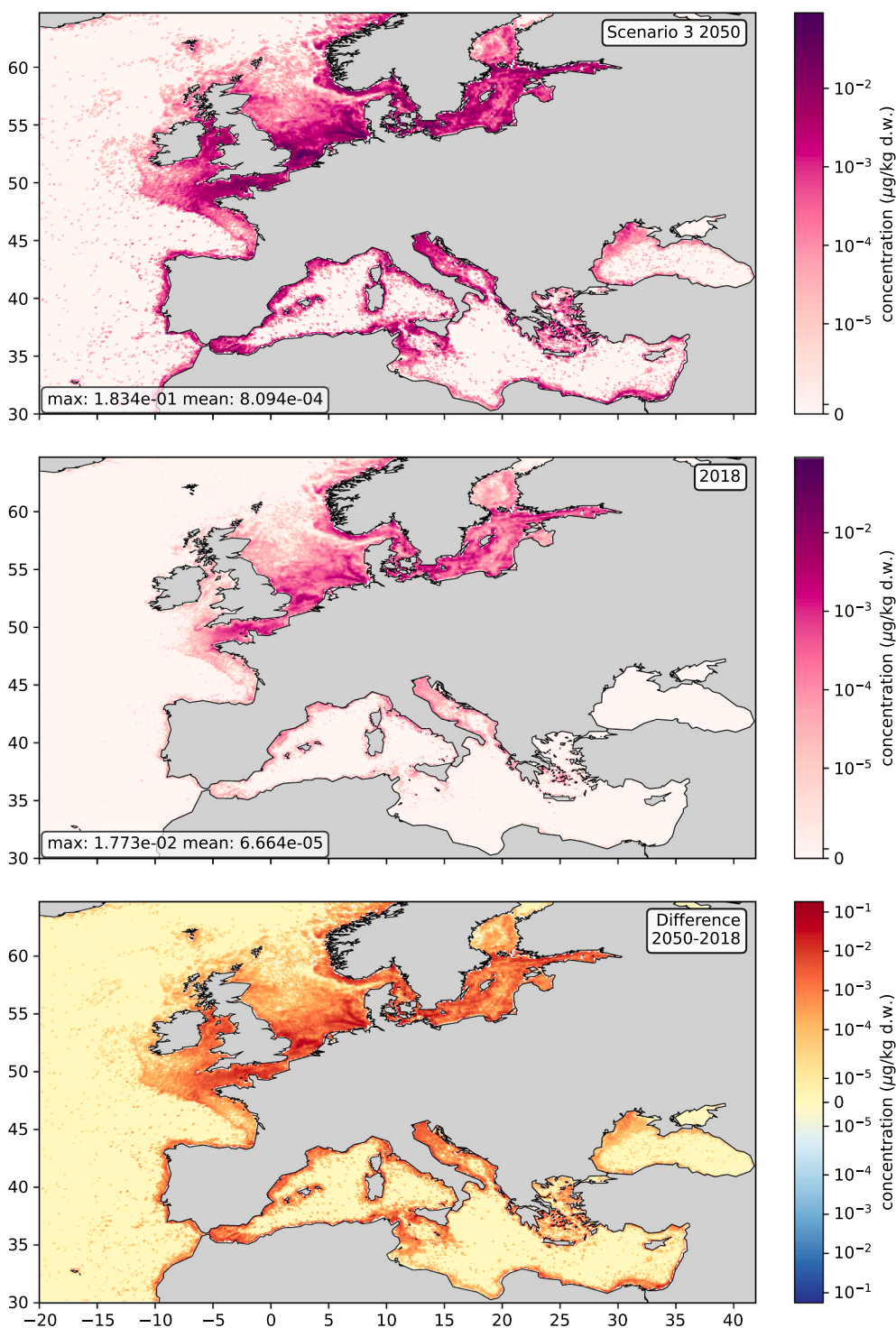


Fig. 6. Modelled dispersion of benzo(a)pyrene discharged from open-loop scrubbers and deposited to the sediment layer at the end of a year long simulation, in 2050 scenario 3 (top) compared to 2018 (middle). The change from 2018 to 2050 is shown in the bottom panel.

exceedance obtained adding the contributions from AFP and AS are identical to the results reported for AFP in Table 2, confirming that the impact of AS is not significant.

An exceedance map of Cu from AFP in S3 is found in Fig. 8 (top panel), indicating the northern coast of Netherlands and Germany as the most severely affected region. This is explained by the number of large commercial ports along this coastline (Antwerpen, Rotterdam, Amsterdam, Emden, Bremehaven, Hamburg) and the associated ship activity. Only the spatial distribution of the exceedance is shown, but not the

frequency, i.e., pixels where PNEC is exceeded in one week, or in all 52 modelled weeks, are equally indicated as red pixels. It should be noted that the target of the simulation was a regional modelling of all European seas. The high levels predicted in the Wadden Sea and in the IJsselmeer are likely to be modelling artefacts, due to the insufficient resolution of the ocean model utilised, and missing geographical features that are not included in the GSHHS land mask utilised by default in ChemicalDrift, i.e. the Afsluitdijk dam and the navigation channel between Amsterdam and the North Sea. High resolutions simulations

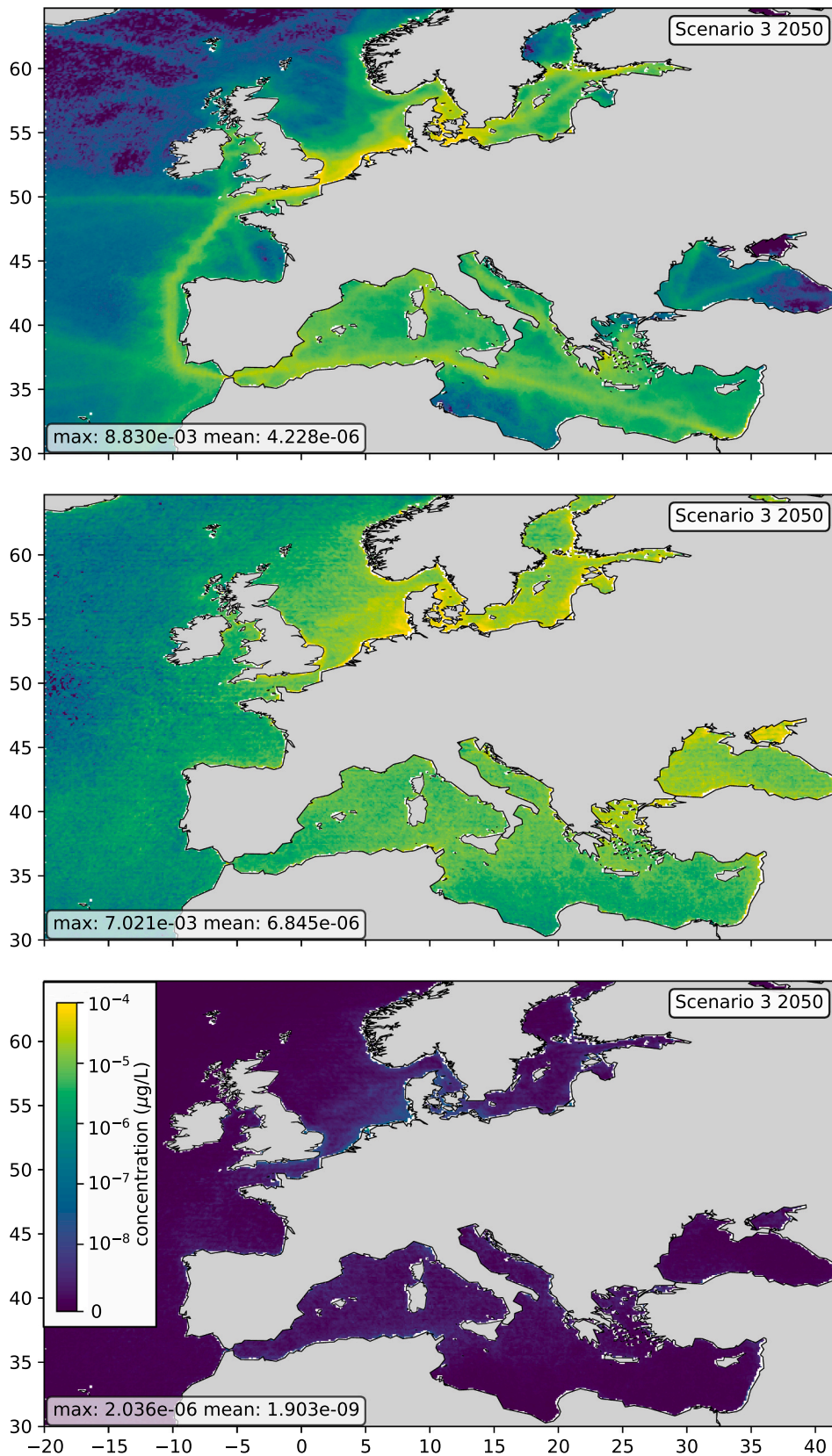


Fig. 7. Simulated dispersion of cadmium in the water column (top 5 m) in 2050 scenario 3, from open-loop scrubbers (top), atmospheric depositions from land and aviation (middle), and atmospheric depositions from shipping (bottom). The same color scale is utilised in all plots.

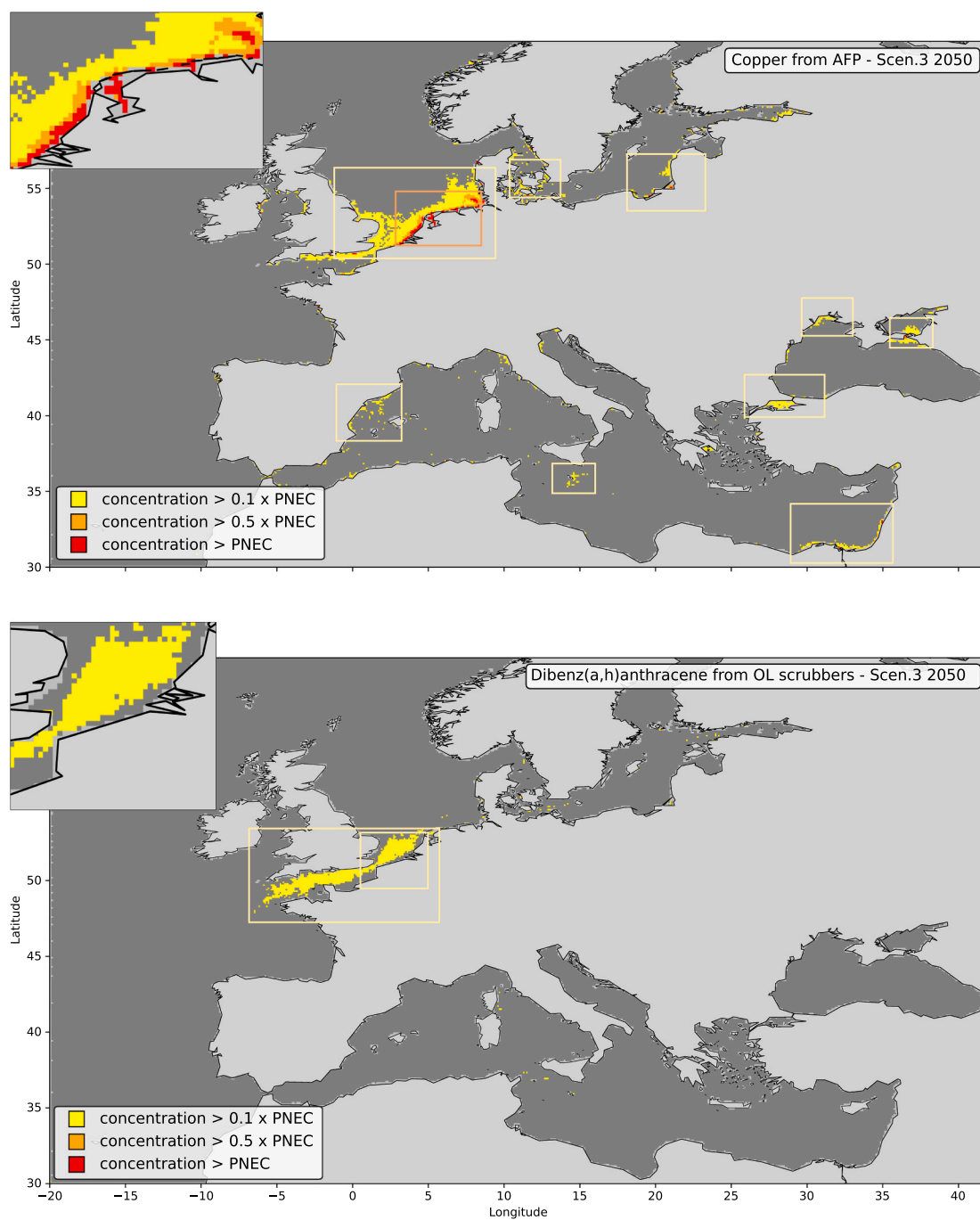


Fig. 8. Exceedance maps of areas where predicted weekly mean of surface concentration of compounds from specific sources may be above predicted no-effect concentration (PNEC) values, or fractions of PNEC, for the year 2050, scenario 3. Copper from antifouling paint (top), and dibenz(*a,h*)anthracene from open-loop scrubbers (bottom).

should be performed for detailed modelling of complex coastal areas. For the same reason, the few grid cells exceeding PNEC for Cu, V, Zn from OL in S3 are assumed to be modelling artefacts as indicated in Table 2.

The exceedance map of DahA from OL scrubbers in 2050 (S3) is shown in Fig. 8 (bottom panel). In this case no values above PNEC are modelled, but concentrations above 10 % of PNEC are calculated in 3576 grid cells, the highest number for the chemicals discharged by OL scrubbers in 2050 (S3), as reported in Table 2. DahA is also the chemical with the lowest PNEC, $5.66 \times 10^{-5} \mu\text{g L}^{-1}$. As shown in the map the grid cells where exceedance is modelled are located in the southern North

Sea and in the English channel.

It can be observed that while emissions from AFP are concentrated in ports and coastlines, emissions from scrubbers are mostly offshore. This is expected since AFP is leaching from ship hulls at all times also when ships are in the ports whereas scrubber effluents are produced when ships are moving, and discharges are highest when high engine power is produced.

3.4. The chemical fate of different compounds

The mass balances of emissions of Cd, BaP and Nap from OL in 2050

(S3) modelled by ChemicalDift are plotted in Fig. 9, highlighting the different chemical behaviour of each compound and the importance of considering this in the model. Cd is not affected by degradation and volatilization hence the discharged mass is continuously accumulated in

the environment. The largest fractions (7458 kg, 55 %) are dissolved in sea water, and accumulated in the sediment layer (5198 kg, 39 %) and a smaller fraction is adsorbed to SPM (791 kg, 6 %). BaP is a highly persistent PAH with relatively low degradation and volatilization rates

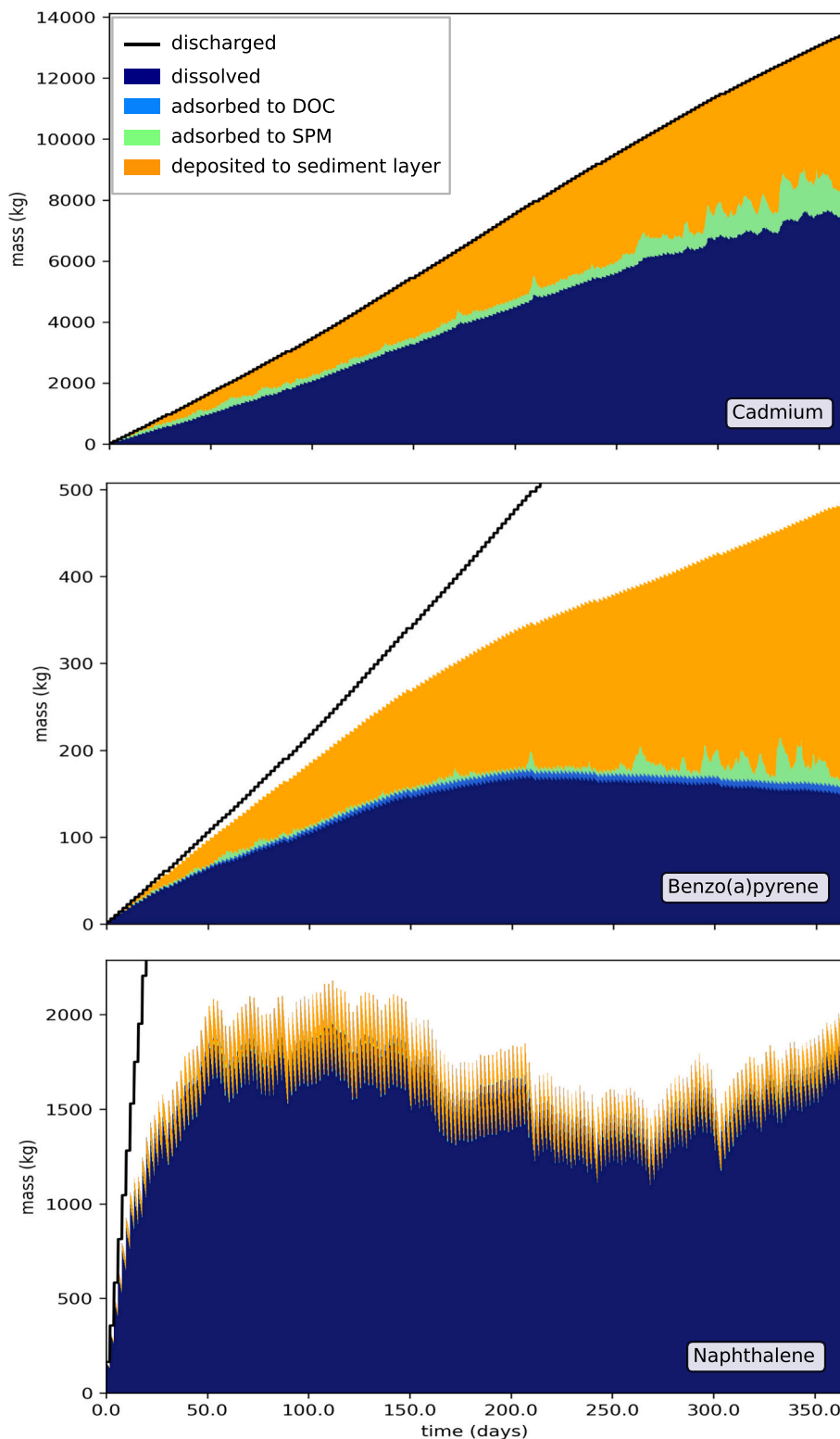


Fig. 9. Mass budget of cadmium (top), benzo(a)pyrene (middle), naphthalene (bottom) discharged from open-loop scrubbers in European waters in 2050, scenario 3. The discharged and residual mass are shown, separating the fractions of residual mass in the modelled environmental compartments: dissolved in sea water, sorbed to dissolved organic matter and suspended solids, and deposited to the sediment layer. For the organic compounds, the gap between discharged and residual mass represents the mass removed by degradation and volatilization.

hence most of the total discharged mass (840 kg) is still in the environment at the end of the simulation (482 kg, 57 % of the discharged mass). This residual mass is mostly in the sediment layer (317 kg, 66 %) and dissolved in sea water (148 kg, 31 %), with small fractions in the

DOC (8 kg, <2%) and SPM (9 kg, <2%). Nap is a highly volatile and degradable compound with low affinity to solids, hence only a small fraction (1843 kg, 4 %) of the discharged mass (47 tons) is still present in the environment at the end of the simulation. The residual mass in

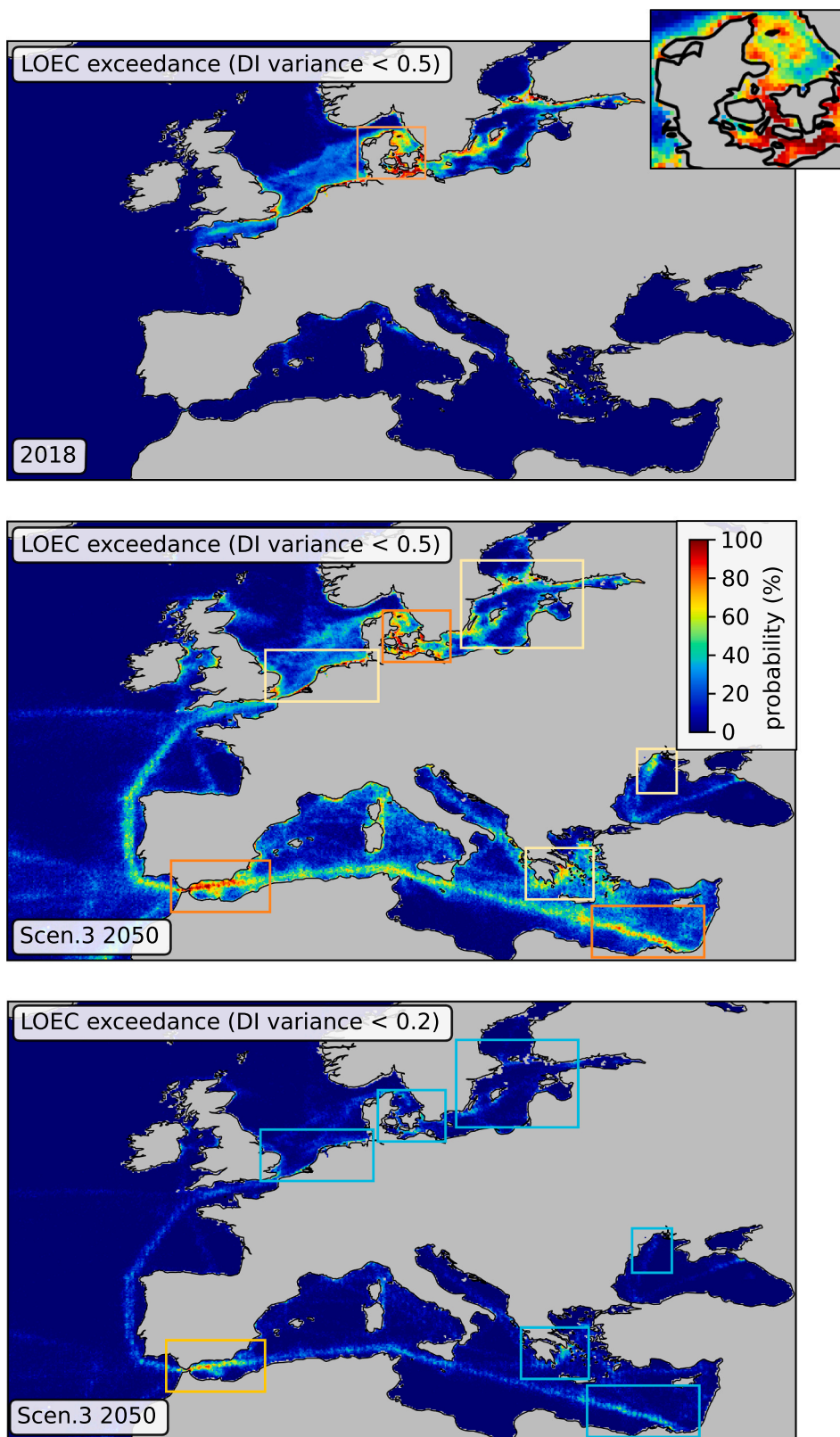


Fig. 10. Predicted occurrence of scrubber water with weekly mean whole effluent concentration exceeding LOEC (dilution 1:1000000) in 2018 (top), and in 2050 scenario 3 (lower panels). The normalised variance of dilution indices is below 0.5 and 0.2. The frequency of occurrence is expressed as a probability.

almost entirely dissolved in sea water (90 %) with a small fraction in the sediments (9 %). The jittery appearance of the curve is an artefact due to the coarsened time step of emission data (2 days) compared to the shorter time step of the simulations (6 h). While the mass of Cd and BaP are increasing in the whole simulated period, Nap emissions seem to reach an equilibrium with removal by degradation and volatilization after approximately 50–100 days, with levels in the environment remaining roughly constant after that. This indicates that with respect to the most persistent compounds, one year of emissions, as simulated in this work, seems to be insufficient in order to estimate steady-state concentrations. Concentrations are likely underestimated and longer simulations, with a buffer time prior to the period of interest, should be carried out to resolve this issue.

3.5. Dilution of scrubber effluents

Concentrations of OL scrubber effluents were calculated applying the dilution method. Maps showing the frequency of exceedance of LOEC determined from ecotoxicological experiments (Chen et al., 2024; Magnusson and Granberg, 2022) are presented in Fig. 10. In the maps a probability of, e.g., 50 % indicates that the LOEC was exceeded in 26 of 52 modelled weeks, and 100 % would indicate exceedance in all modelled weeks.

Setting the variance threshold to 0.5 showed that in 2018, high concentrations with a probability of exceeding the LOEC above 50 % were limited to the Baltic Sea and the North Sea. In several coastal areas, particularly in the narrow and highly trafficked shipping route between Denmark and Germany, probabilities of exceedance between 80–100% were modelled. Predictions for 2050 (S3) indicated a striking extension of exposed areas to almost all European sea regions along the main shipping routes (probabilities above 50 %). New areas with probabilities of exceedance above 80 % will include the Gibraltar Strait, mostly on the Mediterranean side, the shipping route in the proximity of the Suez Canal and the Aegean Sea.

Different values for the variance threshold were tested. With a threshold set to 0.2, probabilities of exceeding LOEC in the range 30–50% were obtained along the main shipping routes in 2050 (S3), as is also shown in Fig. 10. Further, an unrealistic case was calculated, without imposing a limit to the variance, resulting in exceedance probabilities up to 100 % in wide areas in all European sea regions. This confirmed that limiting the variance had the intended effect of eliminating grid cells where the scrubber mixture was not considered intact, but also indicated that results are strongly dependent on the value selected for threshold.

It is important to consider that although the overall risk of exposure could be estimated by adding the contributions (e.g., $PEC_i/PNEC_i$) of the modelled components, this type of approach would inherently underestimate the risk, since: 1) it would be highly unpractical and likely not possible to model accurately all the known components, and to achieve a full characterization of the mixture, which would likely contain other unidentified chemicals; 2) the potential “cocktail” effect due to the simultaneous presence of different known or unknown chemicals in the environment would not be considered.

3.6. Regional differences and drift of chemicals across regions

The transport and fate of chemicals from OL scrubbers in 2050 (S3) are presented separately for each considered sea region for Cd, Phe and BaP in Tables 4–6, as examples for metals and PAHs of high and low volatility. In each region, the discharged mass (kg), the residual mass (kg) in the environment at the end of the simulated year, and the net mass balance (kg) are reported. The residual mass is also indicated as a percentage of the discharged mass (res %). The mass removed by degradation, volatilization, or advected outside the region are also indicated as percentages of the discharged mass (deg %, vol%, adv %). The advection component (adv %) is positive for mass exported (positive

removal) and negative for mass imported. The fractions of the residual mass that at the end of the simulation are in the water column or in the sediment layers are also indicated (w %, s %). The median depth of the chemicals deposited to the sediment layer is reported in the last column (s dep). Finally, the net mass exchange of chemical between regions is reported.

3.6.1. Cadmium from open-loop scrubbers

The two regions which export most Cd are the North Sea (111 kg, 5 % of the discharged mass) and the Biscaya-Iberian (419 kg, 25 % of the discharged mass). The regions that import most Cd are the Norwegian Sea (164 kg) and the Mediterranean regions (33, 112, 143 kg). The net export of Cd from the North Sea to the Norwegian Sea is 178 kg. This is expected due to the effect of the Norwegian Atlantic current and including the Norwegian Coastal Current component which flows from the Kattegat. The distribution of chemicals discharged in the North Sea and advected to the other regions is illustrated in Fig. 11, where the emissions are marked in black, and the exported chemicals to the Norwegian Sea are shown in green. In Table 4 it is also indicated that the Biscaya-Iberian region exports 254 kg of Cd over the Gibraltar Strait into the West Mediterranean, as also illustrated in Fig. 12. From the W.Med, 283 kg of Cd are advected to the C.Med region. From the C.Med region, 32 kg and 141 kg of Cd are advected to the Adr and E.Med, respectively. The Eastward flow from the Atlantic to the E.Med is also explained by the current systems in the region, as shown by the mean eastward sea water velocity field in Fig. 2. Scrubber discharges occur at surface, and in the Gibraltar Strait surface currents flow mainly toward the Mediterranean. Further, coastal currents in the Mediterranean basin are characterized by a counterclockwise boundary flow, with eastward currents along the North African coast, which to large degree overlap with the main shipping path from Gibraltar to Suez, as seen, e.g., in Fig. 7.

3.6.2. Phenanthrene and benzo(a)pyrene from open-loop scrubbers

The results for Phe and BaP are presented in Tables 5 and 6, describing the different chemical behaviour of the two PAHs. It is reported that the 24 % of the totally discharged mass of Phe is accumulated in the environment at the end of the year. Large fractions are removed by degradation (38 %) and volatilization (37 %). In comparison, 57 % of the emitted mass of BaP remains in the environment, 41 % is degraded, and a minor fraction, 2 %, volatilized. This is expected, since BaP is more easily bound to particles, and exhibits lower degradation and volatilization rates. Hence a larger fraction of BaP is preserved compared to Phe. It should be noted that although Phe has a significantly faster degradation rate than BaP (Aghito et al., 2023), the degraded fractions are similar (38 % and 41 %). This is explained by the fact that degradation and volatilization are competing processes, and since volatilization of BaP is weak, a larger fraction is exposed to degradation. The higher affinity of BaP to particles is also reflected by the largest fraction of residual chemical accumulated in the sediment layer (66 % in sediment, 34 % in water column), compared to Phe (43 %, 57 %).

It is important to observe that the total load of BaP from OL scrubbers might be low compared to other sources that were not included in this study; loads of approximately 3 tons per year were reported by Sonesten et al. (2024) for the Baltic Sea in the period 2015–2020, much larger than 78 kg of BaP discharged in the Baltic Sea from OL scrubbers (not including the Kattegat region) modelled here for the year 2050; higher contributions from atmospheric depositions in the Baltic Sea might be expected also for the other PAHs. The Baltic Sea is particularly exposed, since it is surrounded by land areas with high atmospheric concentrations of BaP (Horálek et al., 2021) and such high deposition rates may not occur in other European seas.

Comparing regional differences, the fractions of Phe removed by degradation are in the range 22–29% in the Baltic, North Sea, Celtic Seas (not considering the data for the Norwegian Sea which are strongly

Table 4

Yearly mass balance and netto transport of cadmium (kg) from open-loop scrubbers across modelled sea regions, for the year 2050, scenario 3.

Reg	Discharged (kg)	Residual (kg)	Balance (kg)	Res (%)	Deg (%)	Vol (%)	Adv (%)	W (%)	S (%)	S dep (m)
Bal	1256	1268	12	101	0	0	-1	26	74	-44
Nrt	2399	2288	-111	95	0	0	5	30	70	-36
Nwg	77	240	164	314	0	0	-214	81	19	-65
Cel	735	680	-55	93	0	0	7	37	63	-90
BI	1655	1236	-419	75	0	0	25	84	16	-86
out	845	931	86	110	0	0	-10	93	7	-80
wMed	3197	3230	33	101	0	0	-1	74	26	-48
cMed	1374	1486	112	108	0	0	-8	81	19	-60
Adr	428	463	35	108	0	0	-8	42	58	-44
eMed	1410	1554	144	110	0	0	-10	68	32	-30
Bla	71	71	0	100	0	0	0	66	34	-39
all	12,602	12,516	-86	99	0	0	1	59	41	-44
total	13,447	13,447	0	100	0	0	0	61	39	-46

to from	Bal	Nrt	Nwg	Cel	BI	out	wMed	cMed	Adr	eMed	Bla
Bal			1.05								
Nrt	13.5		178			2.3					
Nwg						17.7					
Cel		82.5	2.10								
BI		0.02		16.8		146	254	2.52			
out				12.8			67.5	0.44			
wMed								283	2.13	3.57	
cMed									32.3	141	
Adr											
eMed						0.01			0.54		0.16
Bla											

Bal: Baltic Sea, Nrt: Greater North Sea, Cel: Celtic Seas, BI: Biscay and Iberian, wMed: Western Mediterranean, out: outer ocean, cMed: Ionian and Central Mediterranean Sea, Adr: Adriatic Sea, eMed: Aegean-Levantine Sea, Bla: Black Sea, Nwg: Norwegian Sea; res: residual, deg.: degraded, vol: volatilized, adv: advected; w: residual in water column, s: residual in sediments, s dep: sediments median depth. The most significant transport pathways are written in bold.

Table 5

Yearly mass balance and netto transport of phenanthrene (kg) from open-loop scrubbers across modelled sea regions, for the year 2050, scenario 3.

Reg	Discharged (kg)	Residual (kg)	Balance (kg)	Res (%)	Deg (%)	Vol (%)	Adv (%)	W (%)	S (%)	S dep (m)
Bal	2370	871	-1499	37	24	37	2	37	63	-19
Nrt	4529	1268	-3260	28	22	44	6	38	62	-26
Nwg	144	120	-24	83	98	157	-238	61	39	-17
Cel	1388	379	-1009	27	29	33	11	51	49	-45
BI	3124	522	-2602	17	29	27	28	89	11	-28
out	1596	336	-1260	21	57	48	-25	93	7	-44
wMed	6034	1369	-4665	23	41	30	6	64	36	-21
cMed	2593	515	-2079	20	55	41	-17	76	24	-32
Adr	808	231	-578	29	48	33	-10	45	55	-21
eMed	2662	546	-2116	21	55	42	-17	58	42	-18
Bla	134	37	-97	28	37	35	0	64	36	-17
all	23,786	5857	-17,928	25	37	37	2	55	45	-22
total	25,382	6193	-19,189	24	38	37	0	57	43	-23

to from	Bal	Nrt	Nwg	Cel	BI	out	wMed	cMed	Adr	eMed	Bla
Bal		7.90	0.70			0.04					
Nrt			70.1		0.19	4.02					
Nwg						14.9					
Cel		38.7	0.60								
BI				2.88		28.3	69.7	0.65		0.00	
out				2.88			22.1	0.08		0.00	
wMed								96.6	0.59	0.91	
cMed									11.8	27.5	
Adr											
eMed									0.09		0.01
Bla											

Bal: Baltic Sea, Nrt: Greater North Sea, Cel: Celtic Seas, BI: Biscay and Iberian, wMed: Western Mediterranean, out: outer ocean, cMed: Ionian and Central Mediterranean Sea, Adr: Adriatic Sea, eMed: Aegean-Levantine Sea, Bla: Black Sea, Nwg: Norwegian Sea; res: residual, deg.: degraded, vol: volatilized, adv: advected; w: residual in water column, s: residual in sediments, s dep: sediments median depth. The most significant transport pathways are written in bold.

Table 6

Yearly mass balance and netto transport of benzo(a)pyrene (kg) from open-loop scrubbers across modelled sea regions, for the year 2050, scenario 3.

Reg	Discharged (kg)	Residual (kg)	Balance (kg)	Res (%)	Deg (%)	Vol (%)	Adv (%)	W (%)	S (%)	S dep (m)
Bal	78	66	-13	84	17	1	-1	13	87	-28
Nrt	150	118	-32	79	16	1	4	11	89	-34
Nwg	5	7	2	144	66	3	-113	38	62	-31
Cel	46	28	-18	61	29	1	8	26	74	-66
BI	103	36	-68	35	37	1	27	79	21	-63
out	53	24	-29	45	74	3	-22	87	13	-70
wMed	200	102	-97	51	43	2	4	40	60	-27
cMed	86	37	-49	43	63	3	-8	58	42	-37
Adr	27	16	-10	61	49	2	-13	26	74	-24
eMed	88	45	-43	51	65	3	-19	37	63	-21
Bla	4	3	-2	59	40	2	0	43	57	-21
all	788	458	-329	58	39	2	1	32	68	-30
total	840	482	-359	57	41	2	0	34	66	-31

to from	Bal	Nrt	Nwg	Cel	BI	out	wMed	cMed	Adr	eMed	Bla
Bal			0.01								
Nrt	0.99		4.14		0.03	0.24					
Nwg						0.87					
Cel		2.05	0.04		0.46						
BI						3.53	7.34	0.04		0.00	
out				0.29			1.88	0.00			
wMed								8.19	0.07	0.19	
cMed									0.89	3.81	
Adr											
eMed						0.00			0.02		0.00
Bla											

Bal: Baltic Sea, Nrt: Greater North Sea, Cel: Celtic Seas, BI: Biscay and Iberian, wMed: Western Mediterranean, out: outer ocean, cMed: Ionian and Central Mediterranean Sea, Adr: Adriatic Sea, eMed: Aegean-Levantine Sea, Bla: Black Sea, Nwg: Norwegian Sea; res: residual, deg.: degraded, vol: volatilized, adv: advected; w: residual in water column, s: residual in sediments, s dep: sediments median depth. The most significant transport pathways are written in bold.

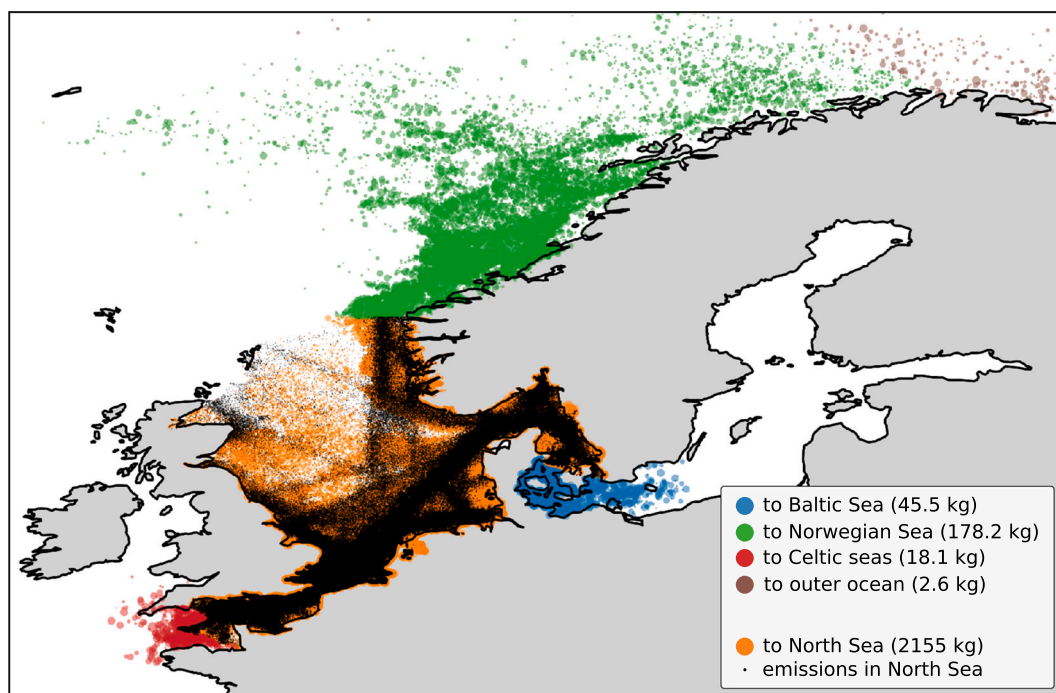


Fig. 11. Transport of cadmium discharged from open-loop scrubbers to the North Sea and exported to other regions for the year 2050, scenario 3. The black dots indicate the positions where the chemicals were discharged to the sea, the coloured dots indicate the final position of the chemicals in each region, at the end of the year. Total transported masses are indicated in the legend.

affected by import) and in the range 41 – 55% in the Mediterranean regions. The difference is explained by the strong dependency of degradation rates on the temperature, which is significantly higher in

the southern regions, as shown in Fig. 2. The corresponding fractions removed by volatilization are similar in northern and southern regions, 33 – 44% and 30 – 42%. The combined effect of temperature and

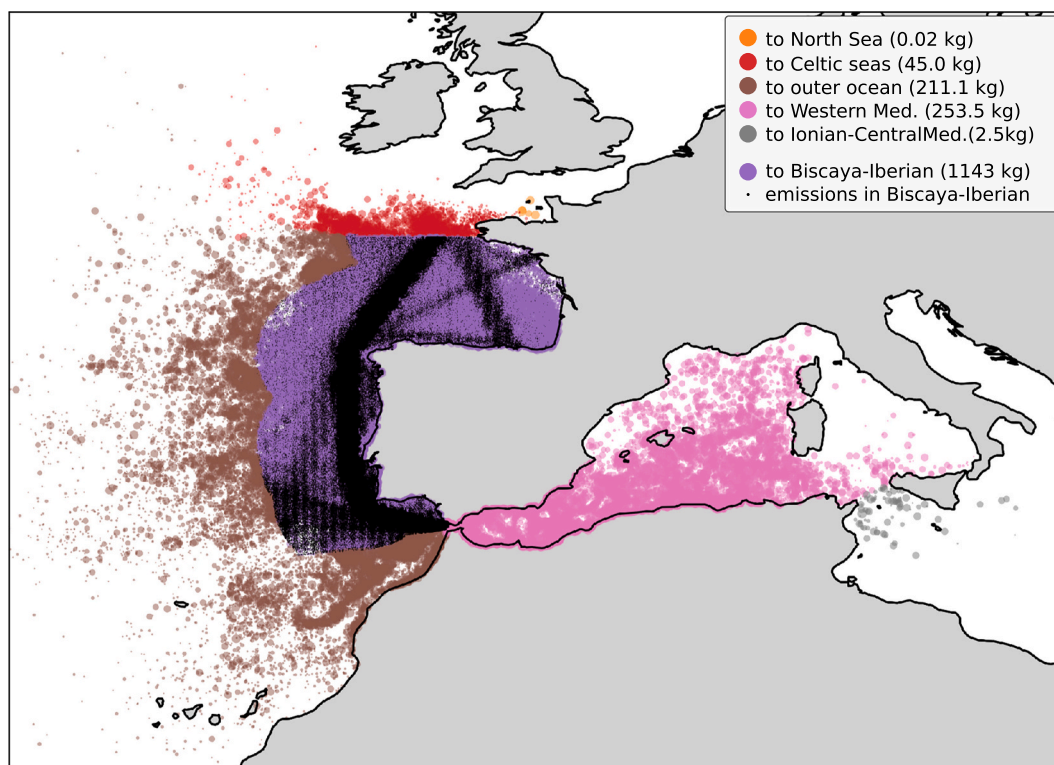


Fig. 12. Transport of cadmium discharged from open-loop scrubbers to the Biscaya Bay and Iberian coast region and exported to other regions for the year 2050, scenario 3. The black dots indicate the positions where the chemicals were discharged to the sea, the coloured dots indicate the final position of the chemicals in each region, at the end of the year. Total transported masses are indicated in the legend.

surface winds (stronger in the northern regions, also shown in Fig. 2) on volatilization rates are more complex and compound-dependent and thus the results are more difficult to interpret.

3.7. Summary and implications

The presented results indicate a significant increment of concentration levels of PAHs and metals from open-loop scrubbers in all European ocean regions, in 2050 (S3), compared to 2018, both in the water column and in the sediments. The most dramatic changes were predicted in the Atlantic and Mediterranean regions, as expected, since these areas were not affected by sulphur control regulations in 2018. The concentration levels of Cd and Pb from OL scrubbers in 2050 (S3) were predicted to be of the same order of magnitude of the levels due to atmospheric depositions from land sources, shown to be a dominant sources in a recent studies for the Baltic Sea (Ytreberg et al., 2022; Sonesten et al., 2024). To the authors' view, the most concerning result is the high predicted concentrations of OL scrubber effluents, considered as a mixture, obtained in the North Sea and Baltic for the year 2018, and across all European seas for the year 2050 (S3). The most affected areas are the highly trafficked routes in the waters around Denmark and across the Gibraltar Strait. Scrubber effluents concentrations exceeding observed toxic levels are likely to occur. The uncertainties were however not fully assessed and the method utilised for estimating concentration of complex mixtures was recently introduced by Zervakis et al. (2024) with higher resolution data. More work is needed to optimize the parameters and validate its robustness across different spatio-temporal scales.

A simplified impact assessment considering single compounds and emission sources was presented, comparing predicted levels to PNECs. Leaching of Cu and Zn from AFPs was predicted to be the source with most frequent PNEC exceedance, and the coast of Belgium, Netherlands, and Germany, in the North Sea, was predicted to be the most affected

area. Overall, the predicted frequency of PNEC exceedance for the other modelled sources was low, though substantial occurrences of concentrations exceeding 10 % of the PNEC were obtained for the chemicals discharged from scrubbers. The notably high predicted concentrations were obtained despite the fact that this study mostly focused on contaminants associated with shipping, with atmospheric emissions from other sources only considered for Cd and Pb.

This work should be extended by: 1) adding the contributions of important sources as riverine inputs, land based discharges as water treatment plants, offshore oil and gas production facilities, and atmospheric depositions of PAHs and other metals; 2) background levels should also be utilised, where data is available; 3) multi-year simulations should be calculated, and are expected to give higher predicted concentrations for metals and for the more persisting PAHs with slow degradation and volatilization rates; 4) the ChemicalDrift model supports also alkylated PAHs, which could be modelled deriving emissions factors with concentration of these compounds in scrubber effluents from the chemical analyses reported by Petrović et al. (2022); 5) a scenario assessing the impact of projected emissions of closed-loop scrubbers, not included in this study, should be modelled.

Furthermore, modelled concentration fields were calculated at relatively coarse scale, as a practical compromise, adequate to identify the most pressured areas. Higher resolution simulations are recommended for assessing local concentration maxima in the most exposed areas, as done in the complementary work carried out for the Aveiro, Øresund, North Adriatic, and Saronikos gulf case studies in the EMERGE project (Monteiro et al., 2024; Zervakis et al., 2024; Calgaro et al., 2024), which also included other sources such as riverine inputs not described here.

The calculated drift of pollutants from scrubbers across oceanic regions indicates two main export paths, from the North Sea to the Norwegian Sea, and from the Atlantic across the Strait of Gibraltar to the Mediterranean and further eastward along the shipping routes from

Gibraltar to Suez. These results highlight that also regions with relatively low traffic from ships may be affected. This underscores the importance of utilising an integrated chemical-fate and transport model.

Based on the additional evidence presented in this work, the authors share the growing concern (ICES, 2020) regarding the use of scrubbers and support a ban on open-loop scrubbers, as already proposed by countries such as Sweden and Denmark, and planned to be implemented from the 1st July 2025. It is important to note that CL scrubbers were not considered in this study, but the proposed model could be used to assess their impact.

Furthermore, given the predicted high concentrations of Cu and Zn from AFP in wide coastal regions of the North Sea, this study suggests that using alternative biocide-free products is preferable. Alternative exists, including FR coatings which have been shown to be as effective as biocidal copper-based AFP in preventing biofouling (Lagerström et al., 2022). In addition, Oliveira et al. (2022a) has shown both large socio-environmental cost savings as well as reduced operator costs when a ship is coated with a FR coating compared to copper-based AFP. Nonetheless, the market share of FR coatings is low, accounting for approximately 10 % (Lagerström et al., 2022). A major barrier to their adoption could be that ship owners prefer to “play it safe” by sticking with biocidal AFPs rather than trying a new FR coating. In addition, FR coatings are not suitable in ice conditions as they easily get damaged and destroyed (Oliveira et al., 2022a). Ionic liquid coatings (Baiju et al., 2023; Taylor et al., 2024) represent another promising technology, that could mitigate the risks associated with metal-based AFPs.

This study is the first attempt of model-based impact assessment of the pollution of PAHs and metals from shipping in the marine environment for future emission scenarios in all European seas. Recent related studies focused on smaller regions, e.g., Maljutenko et al. (2021) estimated the environmental concentrations of several contaminants from shipping in the Baltic Sea using a passive dispersion model, Liubartseva et al. (2023) presented a framework for analysing the pollution due to operational oil spills from shipping, which was applied to the Adriatic Sea; the impact of scrubbers with respect to ocean acidification in the North Sea was studied by Dulière and Baetens (2020). The coupling of STEAM and SILAM with the ChemicalDrift model allowed for a comprehensive account of the direct loads from shipping to the sea and the deposition to the sea surface of atmospheric emissions, with integrated support for both the hydrodynamical and the chemical processes affecting the emitted pollutants. This work further highlights the versatility and potential of the open-source ChemicalDrift package, which was recently validated using field data from a study on PAH discharges from oil platforms in the North Sea (Aghito et al., 2024). The model is readily adaptable for designing case studies in other regions and for various emission sources.

4. Conclusions

The chemical-fate and transport model ChemicalDrift model was applied to emissions of PAHs and metals from shipping and from atmospheric depositions in European seas, for the baseline year 2018, and for two scenarios for the year 2050. The highest levels of pollutants in the water column and in the sediments were, in the 2018, limited to the North Sea and the Baltic sea, where sulphur emission regulations were enforced and a significant number of vessels utilised scrubbers. With a wide adoption of scrubbers, a dramatic increase of concentration of pollutants directly discharged to the sea was predicted, for all European sea regions. Considering environmental concentrations of specific compounds emitted from shipping, the levels of Cu and Zn from AFPs were predicted to exceed safe thresholds in some coastal areas in the North Sea. The proposed method may be extended to include more compounds, e.g., alkylated PAHs, and other important sources like riverine inputs, water treatment plants, or offshore oil production facilities. Supported by ecotoxicological tests, preliminary modelling results which need to be confirmed by refinement and validation of the

methods utilised, indicate that toxic concentrations of the scrubbers mixture are likely to occur. High concentrations of scrubber effluents exceeding levels with observed negative effects on biota, may in the year 2050 extend to all coastal European oceanic regions.

CRedit authorship contribution statement

Manuel Aghito: Writing – original draft, Visualization, Validation, Software, Resources, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Elisa Majamäki:** Writing – review & editing, Software, Conceptualization. **Risto Hänninen:** Writing – review & editing, Software, Conceptualization. **Anna Lunde Hermansson:** Writing – review & editing, Conceptualization. **Ida-Maja Hassellöv:** Writing – review & editing, Project administration, Conceptualization. **Erik Ytreberg:** Writing – review & editing, Investigation, Conceptualization. **Vassilis Kolovoyiannis:** Writing – review & editing, Investigation, Conceptualization. **Vassilis Zervakis:** Investigation, Conceptualization. **Maria Granberg:** Writing – review & editing, Investigation, Conceptualization. **Jana Moldanová:** Writing – review & editing, Investigation, Conceptualization. **Knut-Frode Dagestad:** Writing – review & editing, Supervision, Software, Conceptualization. **Øyvind Breivik:** Writing – review & editing, Supervision, Investigation, Conceptualization. **Lars Robert Hole:** Writing – review & editing, Supervision, Project administration, Investigation, Conceptualization. **Jukka-Pekka Jalkanen:** Writing – review & editing, Project administration, Investigation, Conceptualization.

Disclaimer

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Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

Data will be made available on request.

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