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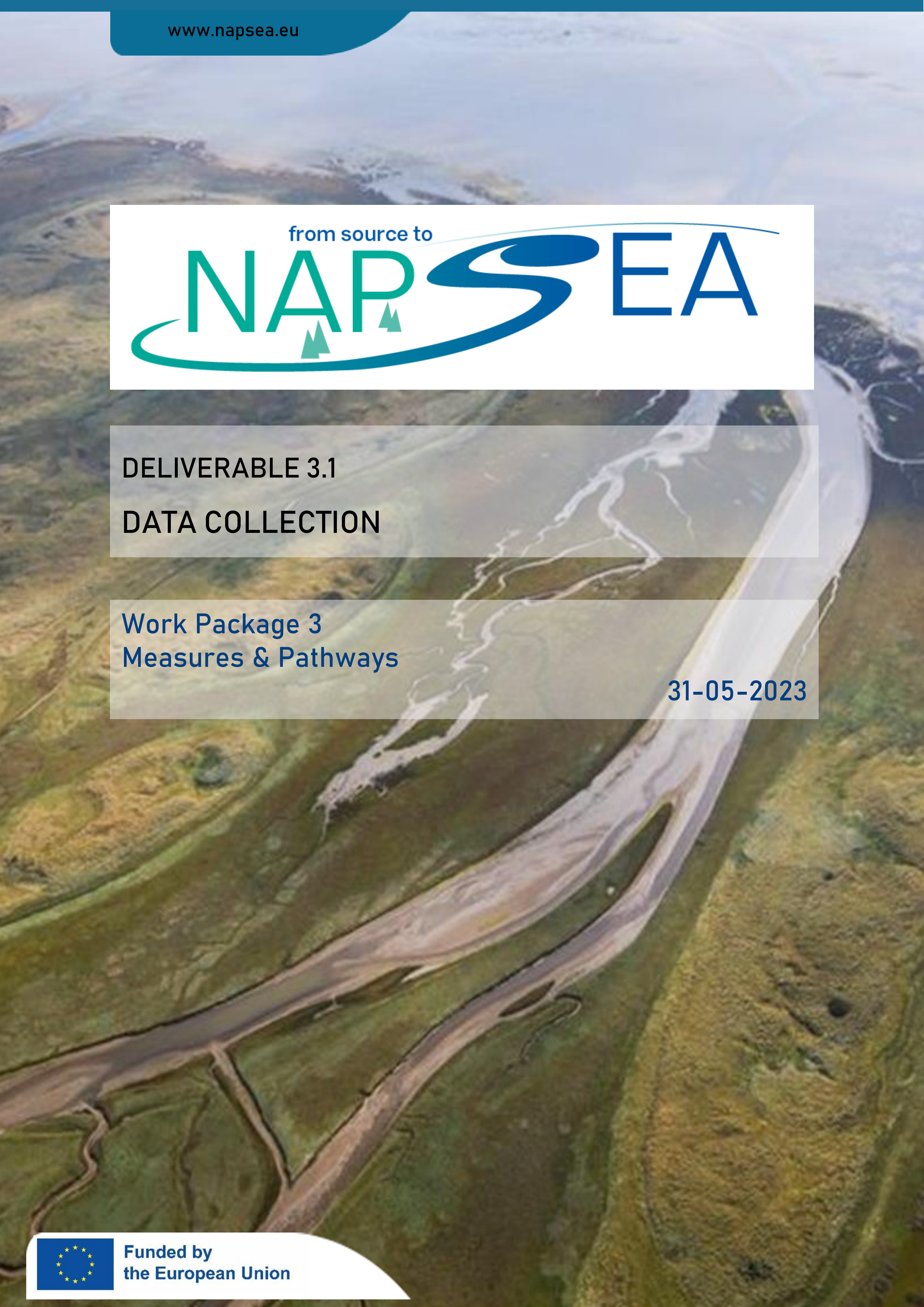

from source to NAPSEA

DELIVERABLE 3.1

DATA COLLECTION

Work Package 3
Measures & Pathways

31-05-2023

Funded by
the European Union

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Project Officer	Blanca Saez-Lacava/Christel Millet
Abstract	Data required for modelling including climate, land use, soil type, discharge, observed nutrient concentrations, agricultural practices, and point source.
Keywords	Elbe, Rhine, mQM, hydrological model, water quality, Nitrogen, Phosphorus, diffuse source, point source, mitigation measure.

Contents

1. ACRONYMES

AMSL	Above mean sea level
C^nANDY	Coupled Complex Algal-Nutrient Dynamics
FAIR	Findability, Accessibility, Interoperability, and Reusability
FGG	Flussgebietsgemeinschaft/ Riverine Commission
GRQA	Global River Water Quality Archive
MOSES	Modular Observation Solutions for Earth Systems
mQM	multiscale water Quality Model
mHM	mesoscale Hydrological Model
PE	Population equivalent
TERENO	Terrestrial Environmental Observatories
WP	Work package
WWTP	wastewater treatment plant

2. EXECUTIVE SUMMARY

Deliverable 3.1 summarizes the data availability, data sources and their spatiotemporal extent for the NAPSEA project basins draining into the Wadden Sea with a specific focus on the case sites Elbe, Rhine and Hunze. The data will be used to setup the water quantity and quality models in task 3.2 (mHM, mQM and C^{n}ANDY) to backcast concentrations and loads and capture spatial patterns of nutrients (Nitrogen and Phosphorus). These models will serve for testing the efficiency of different stakeholders-selected mitigations measures to ensure the safe ecological boundaries of both case studies. Data include climatic forcing, land use properties, soil type, point-sources (sewage stations and their discharge), agricultural practices (manure, mineral fertilizer) and measured stream discharge and nutrients (Nitrogen and Phosphorus) concentrations. Observed data covering the longest time series were prioritized in the analysis to ensure a good historical coverage of nutrient-pollution background conditions. Table 1 and table 2 summarize the spatiotemporal coverage of data availability and sources.

The deliverable was planned as a “data collection” in the project proposal. This document lists and describe the data, their data source and enables access to the data. The minimum data to run the model is available in FAIR repositories and open access publications such that everyone within the project consortium but also outside can access the data.

3. INTRODUCTION

3.1 Work package description

Measures and Pathways WP3 aims to evaluate the connection between nutrient concentration and load reduction measures, considering changed terrestrial inputs as well as enhanced retention processes (such as instream retention) and the safe ecological boundaries in the receiving waters of three case studies (Figure 1). An integral approach of testing stakeholders-approved pathways of nutrients reduction from the sources via streams and rivers to estuaries and coastal waters of the Wadden Sea will be adopted. To this end, scenarios for testing the efficiency of different nutrients reduction mitigations and enhanced retention measures will be conducted using process-based mHM (Samaniego et al., 2010, Kumar et al., 2013)[1,2], mQM (e.g., Nguyen et al, 2022)[3] and C^{n}ANDY (Yang et al. 2021)[4] models. This allows to prioritise nutrient reduction mitigation measures under short- and long-term perspectives and under different scenarios of climate change. Also, measures considering co-benefits aspects beyond the waterborne and airborne will be further explored. To this end, the integrated and time-variant modelling approach to nutrient transport and retention across nested scales from source to sea will be implemented (task 3.2). Modelling will be used for quantifying the effectiveness of proposed solutions under current and future climate change scenarios (task 3.3, 3.4 and 3.5). The modelling results will also be used as knowledge hubs for motivating stakeholders' solutions uptake of proposed actions. The model will be initially set up for the three case studies to capture the current observed state of nutrient concentrations in surface waters and exports to the Wadden Sea and to implement the measures and climate scenarios. Results from the case studies will be transferred to other basins draining into the Wadden Sea (task 3.6, e.g., Weser/ Ems basin, catchments north of the Elbe estuary) using data-driven methods, such as machine learning methods. To broaden the benefits of the modelling approach, other co-benefits aspects have also been considered, such as the capability of the developed modelling approach to offer further insights into the impacts of recently experienced climate-change-related problems (droughts after 2018 and connected long travel times of water in the main streams) on algae blooms and ecological state of the estuary. To this end, model usages' capabilities and its internal processes will be explored as additional sources of information to enhance our physical understanding. This requires further consideration of spatial and temporal resolution of model results and parameters to capture the instream processes at sufficient resolution (land-stream transfer).

3.2 Spatio-temporal data requirements for the envisioned modelling approach

A modelling approach is one of the most cost-effective tools for testing mitigation measures scenarios compared to any other approach before a real implementation. However, facilitating rigorous testing of mitigation measures requires adequate process detail in the modelling and adequate spatiotemporal resolution. Additionally, the model needs to acknowledge the spatial dimension of the modelled basins and the availability of data to run and calibrate the model. Consequently, not all small-scale measures

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[1] Samaniego L., R. Kumar, S. Attinger (2010): Multiscale parameter regionalization of a grid-based hydrologic model at the mesoscale. Water Resour. Res., 46, W05523, doi:10.1029/2008WR007327.

[2] Kumar, R., L. Samaniego, and S. Attinger (2013): Implications of distributed hydrologic model parameterization on water fluxes at multiple scales and locations, Water Resour. Res., 49, doi:10.1029/2012WR012195.

[3] Nguyen TV, Sarrazin FJ, Ebeling P, Musolff A, Fleckenstein JH, Kumar R. Toward Understanding of Long-Term Nitrogen Transport and Retention Dynamics Across German Catchments. Geophysical Research Letters 2022; 49: e2022GL100278.

[4] Yang S, Bertuzzo E, Büttner O, Borchardt D, Rao PSC. Emergent spatial patterns of competing benthic and pelagic algae in a river network: A parsimonious basin-scale modelling analysis. Water Research 2021; 193: 116887.

can be captured by a model running at the spatial scale of the entire multiscale case studies river basins (Elbe, Rhine and Hunze (Figure 2)). We argue that the mechanistic modelling approach applied in NAPSEA has advantages against established empirical and semi-empirical models in capturing the large-scale combined effect of measures to reduce nutrient inputs in the landscape and enhanced retention also under the changed boundary conditions of future climate developments.

Within NAPSEA we will combine the hydrological model mHM[1,2] (modelling discharge, evapotranspiration, soil moisture and river network water routing on a daily basis and in high spatial resolution) with the water quality model mQM[3] (modelling travel time-based nitrogen transport and retention in soil, groundwater and the stream network at annual time step at the spatial scale of sub-catchments) and C^{n}ANDY[4] (modelling dissolved phosphorous as well as benthic and pelagic-bound phosphorous transport in the river network at various time step) model.

Fundamentally different to other water quality modelling approaches is the *travel time concept* in mQM model - a unique mechanistic approach that can consider different time scales up to decades needed to capture different flow paths and connect retention processes to transport and turnover nutrients in soil and groundwater bodies before reaching streams. This will also allow us to quantify the time that a measure will take to impact stream water nutrient concentration and fluxes. Finally, the travel time concept will account for feedback on changed hydroclimatic drivers (e.g., prolonged drought periods) on the transport and retention of nutrients in the subsurface and the stream network.

Also, the *spatially distributed model* implementation in sub-catchments is a unique feature for testing a spatially targeted mitigation measure locally and quantifying their effect on the overall nutrient export at the basin scale. In a scenario approach, we will be able to track back nutrients exported to the Wadden Sea to its source and test effectiveness of spatially targeted measures considering retention in the river network.

To achieve this level of enhanced understanding, intensive model calibration and validation is required. To this end, model setup and validation for nutrient retention and transport from source to sea become a data-demanding process. More specifically, the models need a large amount of data on the (1) meteorological forcing, (2) on nutrient inputs from point and non-point sources, on (3) landscape properties and (4) on water quantity and quality observations. Meteorological forcing comprises precipitation, potential evapotranspiration and air temperature data that drives the hydrological model mHM and allows estimations of the soil temperature needed for the soil nitrogen reactions in the water quality model mQM. Nutrient inputs are used for nitrogen fluxes in mQM and for phosphorous fluxes in C^{n}ANDY. Landscape properties comprise soil databases, land cover and topography shaping hydrological transport and retention of nutrients. Observational water quantity data are used to calibrate mHM while the water quality observations are used to calibrate and validate mQM and C^{n}ANDY. Since mQM will be calibrated against these observations for each sub-catchment, the availability of water quality observations dictates the spatial resolution of the model. At the moment, we envision a spatial resolution of approximately 100 km^2 matching 2nd to 3rd Strahler order streams (see chapter 3.4). This also matches the spatial resolution of the diffuse N inputs that will be used in the model (Batool et al. 2022).

Observational data on water quality and quantity for the German part have been collected before and published following the FAIR data principle (QUADICA database)[5]. These data have been updated and extended considering the case studies requirement and project needs. In addition, spatiotemporally monitored water quantity and quality data during the last ten years with the monitoring activities of

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[5] Ebeling P, Kumar R, Lutz SR, Nguyen T, Sarrazin F, Weber M, et al. QUADICA: water QUAlity, DIscharge and Catchment Attributes for large-sample studies in Germany. Earth Syst. Sci. Data 2022; 14: 3715-3741.

TERENO[6] and MOSES[7] activities are available for internal processes understanding and validating the modelling results. Collected data at the first phase of the project, their spatial and temporal resolution and their repositories are summarized in Table 1. Furthermore, more detailed data will be gathered continuously over the course of the project implementation within each of the local case studies specifically focusing on the local issues at hand and depending on the further requests and needs.

All required data to setup the models in all basins are available and freely accessible in different repositories (Table 1). These data are originally reviewed and published separately in international and highly ranked journals using the FAIR principal. These data are considered as the minimum data needed for our models' setup. However, modelling results can be further analysed and improved when additional in-situ observations about the model's internal processes are available. Additional data that can help constraining the models are soil organic and mineral N data, groundwater quality data (see Table 1) and water age measurements. Table 2 lists additional local data that is available to calibrate and validate the Hunze test basin.

3.3 Data availability and access

All data used to run and calibrate the models mHM, mQM and C^{n}ANDY are available in FAIR open data repositories or part of open access publications that can be assessed by everyone. We refrain from duplicating this data in another repository to avoid redundancy and to account for the fact that some of the data is updated (e.g., meteorological drivers) on the data website.

Additional data for local calibration and validation of the Hunze basin was provided from local authorities and is available on request for everyone in the consortium.

3.4 Data availability per case study

3.4.1. Rhine river basin

The Rhine river basin drains an area of 220,000 km^2 and is one of the most heavily used waterways in the world. Precipitation of the Rhine River ranges from less than 200 mm y^{-1} in the central part to 3500 mm y^{-1} in the mountains. The Rhine has an average discharge of about 2,900 m^3 s^{-1}. In the past, the Rhine experienced strong anthropogenic impacts with strong modification of the hydromorphology and heavy industrial pollution. While industrial pollution has been greatly reduced, the Rhine is still a major contributor of nutrients from diffuse agricultural sources and from wastewater discharges to the Wadden Sea. In recent years, the Rhine experienced a series of droughts (2018, 2022) with severe impacts on the instream ecosystem such as algal blooms in tributaries.

3.4.2. Elbe river basin

The Elbe River basin, located in central Europe covers an area of 148.268 km^2, where approximately one third is the Czech Republic. Less than 1% belong to Austria and Poland. About 50% of Elbe River basin are lowlands below 200 m AMSL, dominating the north landscape of the basin. Overall, the river basin is characterised by sandy plateaus with loam-covered riparian zones and wetlands in between. The average annual precipitation of the Elbe River basin is about 628 mm. However, the annual precipitation reached higher levels in the Giant and Jizera Mountains where precipitation can reach 1700 mm per year[8]. Precipitation shows a rather uniform intra-annual distribution due to the low slopes, sandy soils, and relatively low rainfall intensity, the hydrological behaviour is governed by groundwater dynamics. Major land uses are grassland, forestry, and agriculture, often on poor soils. The long-term

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[6] https://www.tereno.net/

[7] https://www.ufz.de/moses/

[8] https://www.ikse-mkol.org/fileadmin/media/user_upload/E/06_Publikationen/08_IKSE_Flyer/2016_ICPER-Flyer_The_Elbe_River_Basin.pdf

annual mean discharge at the river mouth is about 861 m^3 s^{-1}, which is equivalent to an average evapotranspiration of 519 mm y^{-1} (FGG Elbe, 2005). With the onset of industrial revolution, the Elbe has developed from an increased chemical pollution primarily from wastewater inputs originating from urban and industrial and mining activities (Figure 3). Later, point sources pollution has been controlled through intensive building of sewer systems across the country, leading to rapid improvement of water quality and autotrophic river systems.

3.4.3. Hunze river basin

The Hunze river basin is an intensively farmed catchment of ~350 km^2 draining into a freshwater lake (Zuidlaardermeer) with important recreational functions. Stakeholders around the lake, like holiday park and marina owners, are directly affected by harmful algal blooms. At the same time, the upstream low-reactive, sandy agricultural soils are susceptible to nutrient losses. The close link between the nutrient sources and the nearby eutrophication issues in lake Zuidlaardermeer make this case interesting. Further downstream, the Hunze river basin influences the channels of the city of Groningen before draining into the Wadden Sea.

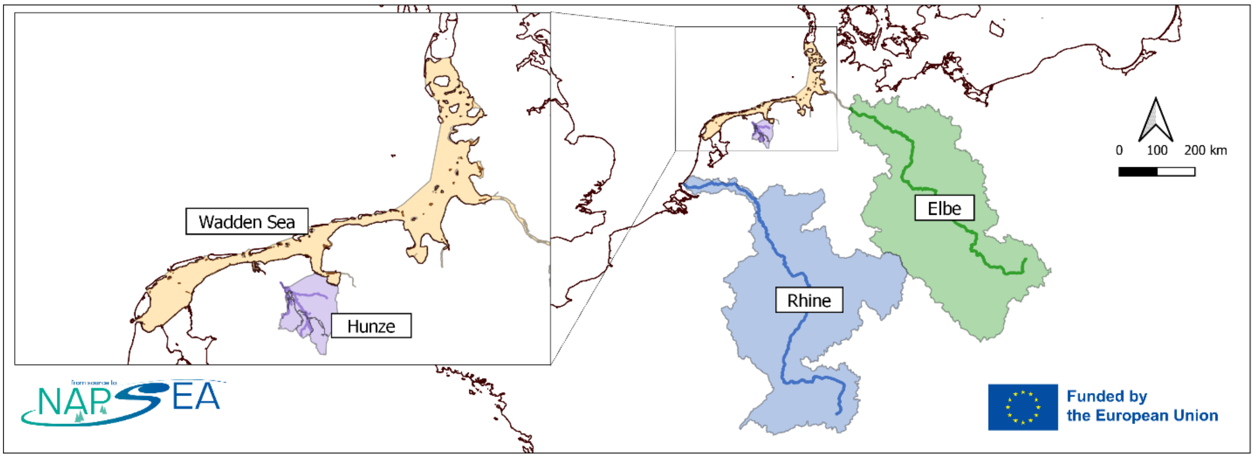

Figure 1. Case studies of NAPSEA project from sources to Wadden Sea: Hunze, Rhine and Elbe river basins, and Wadden Sea.

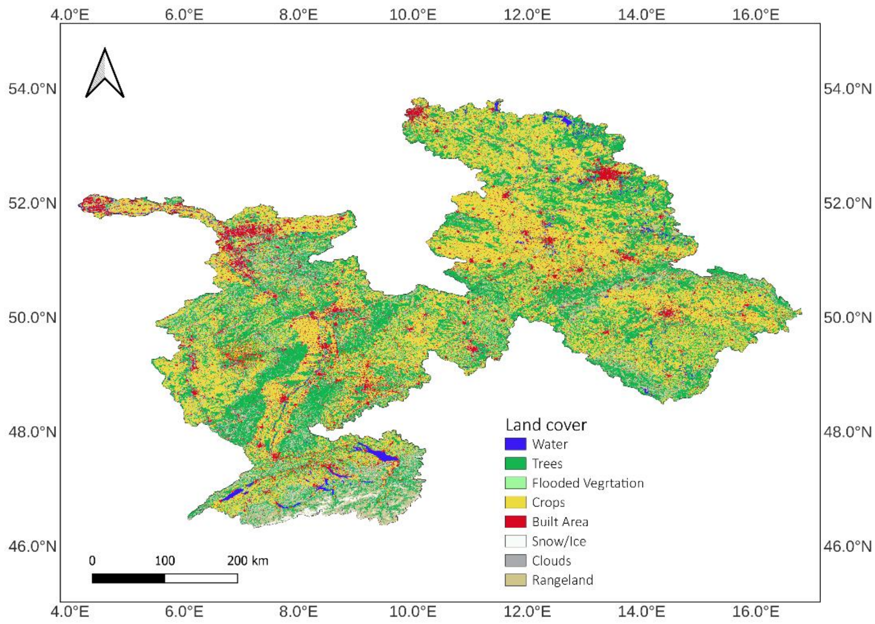

Figure 2. Land cover maps for the Elbe and Rhine River basins.

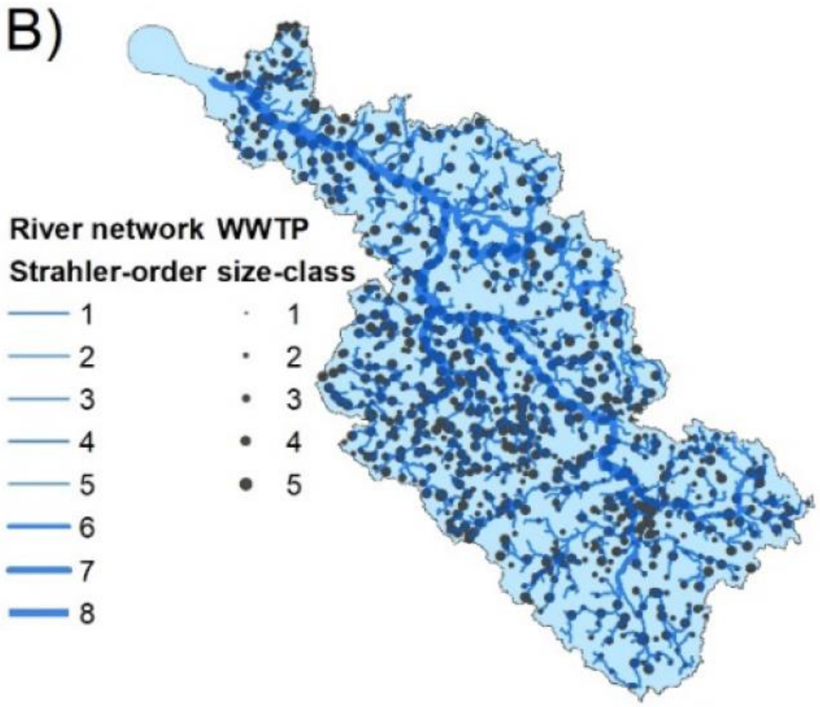

Figure 3. Wastewater treatment plants (WWTP) with population equivalents > 2000 in the Elbe River basins reported under the umbrella of the European wastewater treatment directive taken from Büttner et al. (2022)[9]. Map shows the Elbe catchment with its river network and the WWTP indicating the size-class related to the number of population equivalents (WWTPs size classes 1- 3 (population equivalent, PE < 10,000), while size class 4 or 5 (PE > 10,000)).

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[9] Büttner O, Jawitz JW, Birk S, Borchardt D. Why wastewater treatment fails to protect stream ecosystems in Europe. Water Research 2022; 217: 118382.

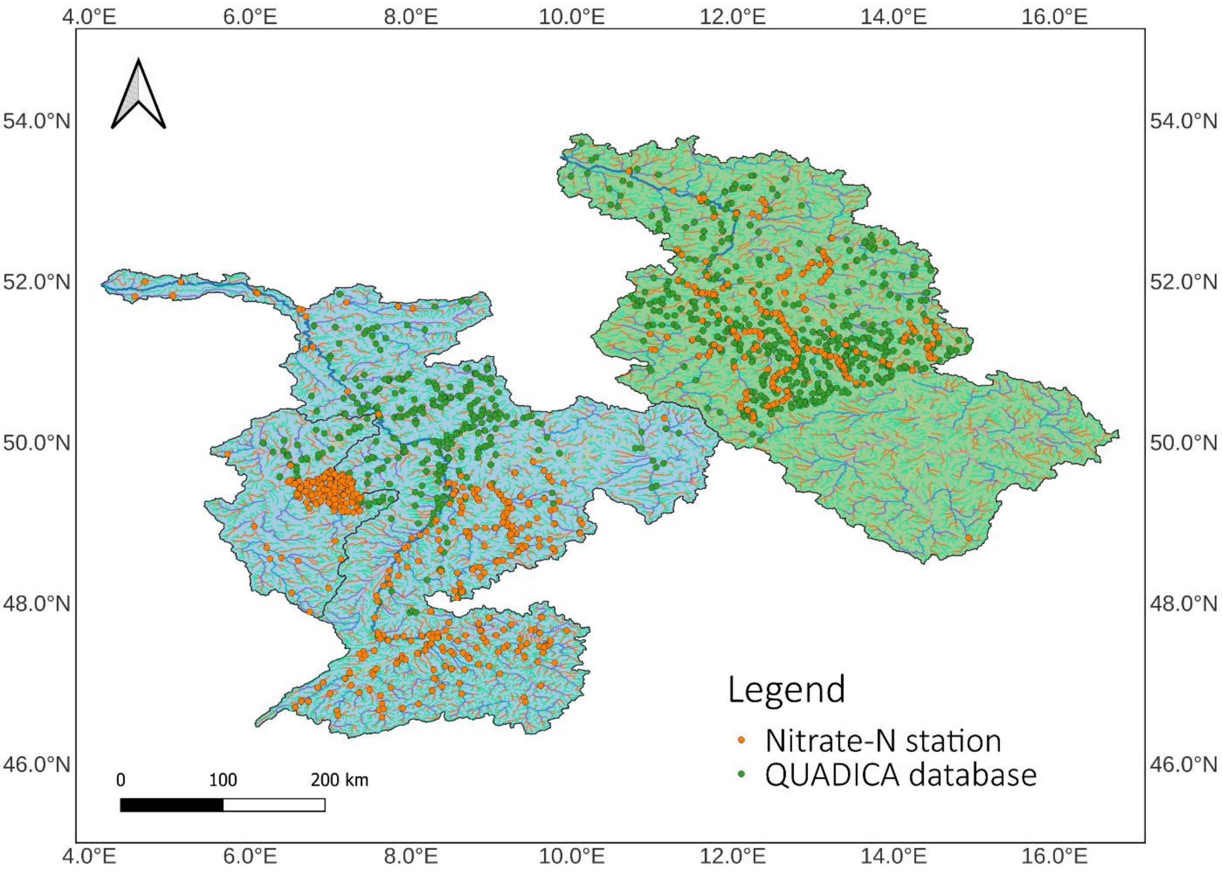

Figure 4. Spatial extent of nitrate-N gauging stations from QUADICA (Ebeling et al. 2022) and Global River Water Quality Archive GRQA (Virro et al. (2021)[10] *databases in the Rhine and Elbe River basins.*

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[10] Virro H, Amatulli G, Kmoch A, Shen L, Uuemaa E. GRQA: Global River Water Quality Archive. Earth Syst. Sci. Data 2021; 13: 5483-5507.

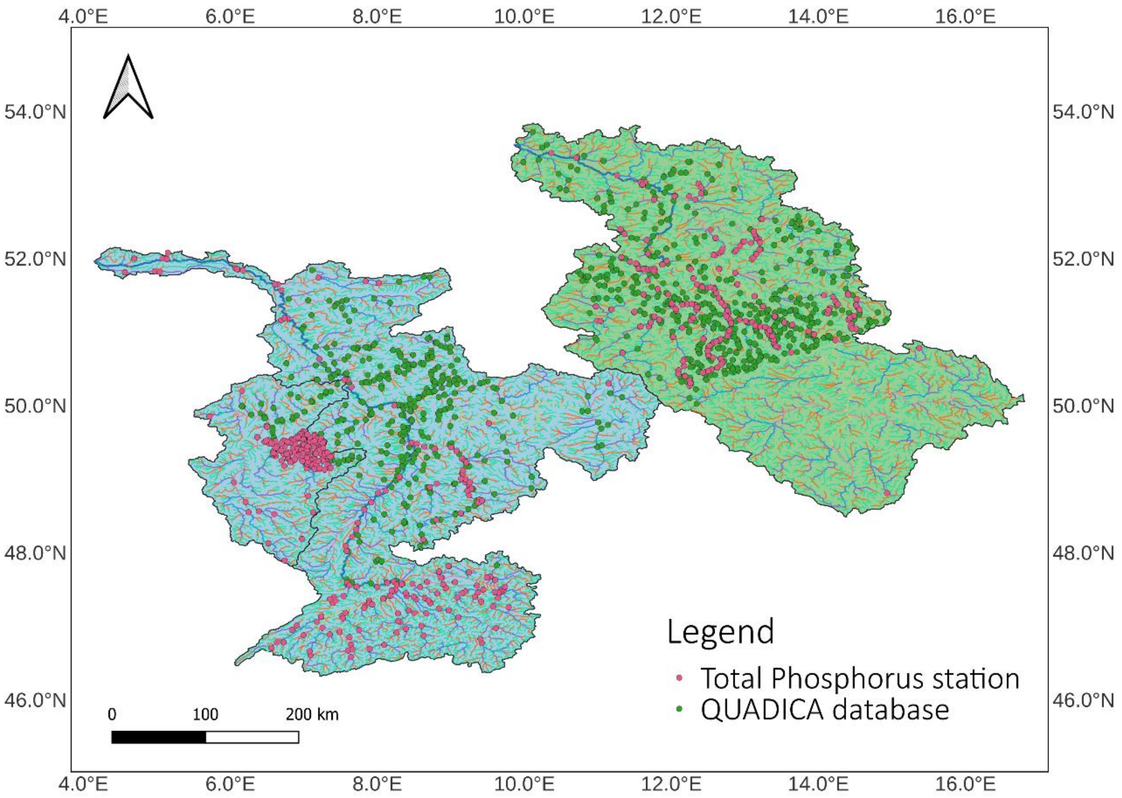

Figure 5. Spatial extent of Total Phosphorus gauging stations from QUADICA (Ebeling et al. 2022) and Global River Water Quality Archive GRQA (Virro et al. 2021) databases in the Rhine and Elbe River basins.

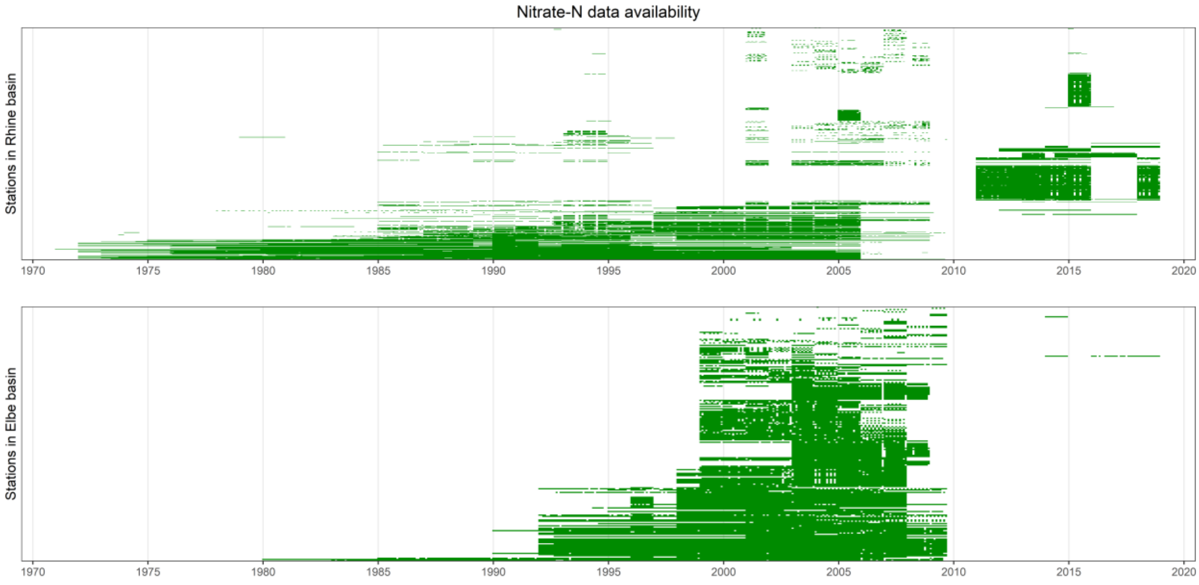

Figure 6. Heatmap of the spatiotemporal extent of measured Nitrate-N time series concentrations for the Elbe and Rhine River basins using GRQA database.

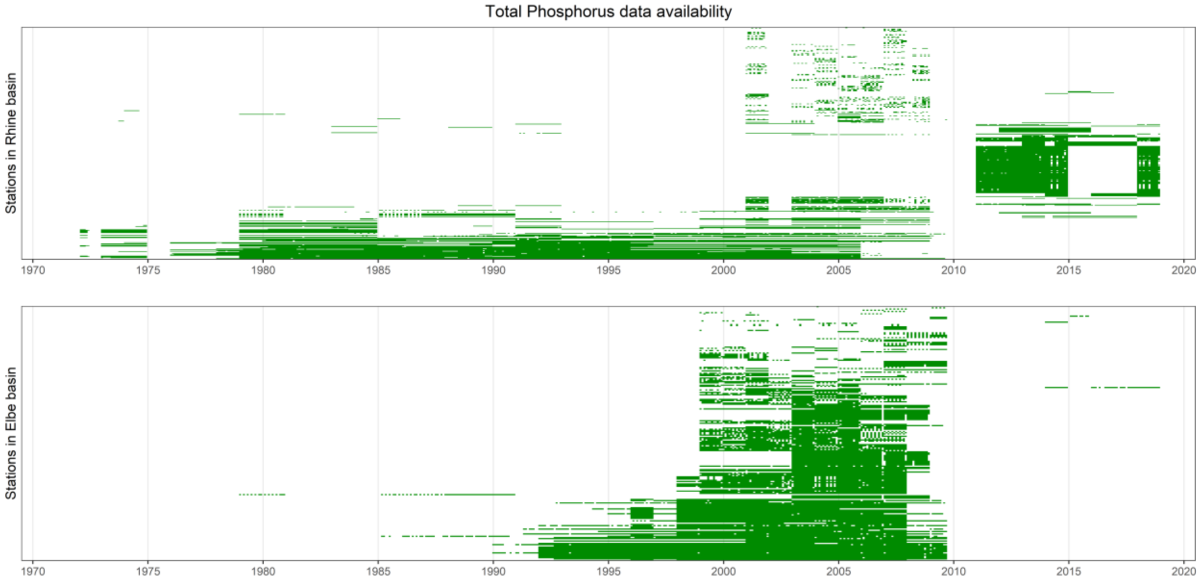

Figure 7. Heatmap of the spatiotemporal extent of measured total phosphorus time series concentrations for the Elbe and Rhine River basins using GRQA database.

Table 1. Data needed for mQM and C^{n}ANDY model setup considering the Elbe and Rhine River basins.

Data type	Variable	Resolution/ Extent	Period	Source and Data format
		Model input data		
Meteorological data	Precipitation	Daily at 1x1 km/ entire Europe	1950-2020	Interpolated daily data based on observations: E-OBS (Cornes et al. 2018)[11] NetCDF format https://surfobs.climate.copernicus.eu/dataaccess/access_eobs.php
	Temperature (mean, min, max)			
Hydrological data	Predicted discharge and soil moisture	Daily at 4x4 km/ entire Germany Daily at 5x5 km/ entire Europe	1950-2020 scenarios until 2100	Predicted discharge at the UFZ using the mHM hydrological model results[12,13] NetCDF format Germany: https://www.ufz.de/index.php?en=41160 Europe scenarios, temporally aggregated values: https://doi.org/10.24381/cds.ccf781a2 Europe scenarios, daily data under representative concentration pathway rcp2p6: http://www.ufz.de/record/dmp/archive/7074 http://www.ufz.de/record/dmp/archive/7093 Europe scenarios, daily data under representative concentration pathway rcp6p0: http://www.ufz.de/record/dmp/archive/7079 http://www.ufz.de/record/dmp/archive/7096
	Measured discharge	Daily observations at gauging stations/ Germany, Europe, global	1950-2020	Global data ASCII table format https://portal.grdc.bafg.de/ For additional stations: QUADICA database for German water quantity observations described in Ebeling et al. (2022), ASCII table format

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[11] Schrier, E.J.M. van den Besselaar, and P.D. Jones. 2018: An Ensemble Version of the E-OBS Temperature and Precipitation Datasets, J. Geophys. Res. Atmos., 123.

[12] Samaniego L., R. Kumar, S. Attinger (2010): Multiscale parameter regionalization of a grid-based hydrologic model at the mesoscale. Water Resour. Res., 46, W05523.

[13] Kumar, R., L. Samaniego, and S. Attinger (2013): Implications of distributed hydrologic model parameterization on water fluxes at multiple scales and locations, Water Resour. Res., 49.

			2009-2023	https://doi.org/10.4211/hs.88254bd930d1466c85992a7dea6947a4
Soil data	Soil type	1 x 1 km, entire Europe	-	European Soil Database, GIS raster format https://esdac.jrc.ec.europa.eu/content/european-soil-database-v2-raster-library-1kmx1km
Agricultural data, Nitrogen inputs	- Nitrogen surplus including diffuse sources from non-agricultural land, - Application of mineral fertilizer and manure	Annual at 10 x 10 km/ entire Europe	1850-2019	Nitrogen surplus based on spatially disaggregated national statistical data on fertilizers, crop yield, lifestock density and atm. deposition; data described in Batool et al. (2022)[14] NetCDF format https://doi.org/10.5281/zenodo.6581441
Land use depended diffuse phosphorous land to stream transfers	Dissolved phosphorus inputs	Average loads and concentrations, derived for Germany	-	Yang et al. (2021)[4] and UBA (2010)[16] Average loads and concentration delivered from land to stream depending on the land use class. This is information in a table format and not a downloadable data set.
Nutrient point sources	Total annual N and total P loads from wastewater point sources (wastewater treatment plants - WWTP)	Germany: all WWTP EU: WWTP with population equivalents (PE) > 2000 are considered	average	In Germany following Buettner et al. (2020)[17], Büttner et al. (2022)[9] Metadata, text format: https://doi.org/10.4211/hs.2f2c2fa04e6e417ba0eb7b0fb14b1090 Data in XLSX and shape format: https://www.ufz.de/record/dmp/archive/7800/en/ Entire EU: EEA (2022) UWWTD database[15] ASCII table format https://www.eea.europa.eu/data-and-maps/data/waterbase-uwwtd-urban-waste-water-treatment-directive-9
Morphological data	Digital Elevation Model	90 m/ entire Europe	-	SRTM – Shuttle Radar Topography Mission https://doi.org/10.5066/F7F76B1X Data retreaved via EarthExplorer, GIS raster format https://earthexplorer.usgs.gov/
	Land cover	25 ha minimum unit/ entire Europe	1990-2018	CORINE land Cover Data, shape format https://land.copernicus.eu/pan-european/corine-land-cover

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[14] Batool, M., Sarrazin, F.J., Attinger, S. *et al.* Long-term annual soil nitrogen surplus across Europe (1850–2019). *Sci Data* **9**, 612 (2022). https://doi.org/10.1038/s41597-022-01693-9

[15] EEA (2019). https://www.eea.europa.eu/data-and-maps/data/waterbase-uwwtd-urban-waste-water-treatment-directive-7

Model evaluation data				
Measured nitrogen and phosphorus concentrations, surface water	Nitrogen and Phosphorous species concentration	Weekly to monthly observations/ Germany, Europe and global	1968-2020	**Elbe and Rhine** Entire Germany: Ebeling et al. (2022)[5] ASCII table format, data from: https://doi.org/10.4211/hs.88254bd930d1466c85992a7dea6947a4 Europe and global: Virro et al. (2021)[10] ASCII table format, data from: https://doi.org/10.5281/zenodo.5097436
Measured nitrogen concentration, groundwater	Nitrogen species concentration	bi-annual to annual observations/ entire Europe	1990-2017	EEA database containing observational raw data (Part 1: DisaggregatedData, ASCII table format) https://www.eea.europa.eu/data-and-maps/data/waterbase-water-quality-icm-2

Table 2: Additional data sources allowing for mQM and C^nANDY model setup in the Hunze test catchment.

Data type	**Variable**	**Resolution/ Extent**	**Period**	**Source**
Measured nutrient concentrations, surface water	TN, TN and other water quality parameters (such as Chloride, dissolved oxygen, pH, NO_3, PO_4 etc)	Weekly to monthly observations/ nine stations	2000-2023	Biweekly measured concentrations data at nine gauging stations from upstream to downstream area of the Hunze catchment was collected from the responsible authorities.
Hydrological data	Measured discharge	Daily observations at six gauging stations/ Hunze	2010-2022	Daily measured discharge data was collected from the responsible authorities.

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2. Kumar, R., L. Samaniego, and S. Attinger (2013): Implications of distributed hydrologic model parameterization on water fluxes at multiple scales and locations, Water Resour. Res., 49, doi:10.1029/2012WR012195.
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4. Yang S, Bertuzzo E, Büttner O, Borchardt D, Rao PSC. Emergent spatial patterns of competing benthic and pelagic algae in a river network: A parsimonious basin-scale modelling analysis. Water Research 2021; 193: 116887.
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6. https://www.tereno.net/
7. https://www.ufz.de/moses/
8. https://www.ikse-mkol.org/fileadmin/media/user_upload/E/06_Publikationen/08_IKSE_Flyer/2016_ICPER-Flyer_The_Elbe_River_Basin.pdf
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10. Virro H, Amatulli G, Kmoch A, Shen L, Uuemaa E. GRQA: Global River Water Quality Archive. Earth Syst. Sci. Data 2021; 13: 5483-5507.
11. Schrier, E.J.M. van den Besselaar, and P.D. Jones. 2018: An Ensemble Version of the E-OBS Temperature and Precipitation Datasets, J. Geophys. Res. Atmos., 123.
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13. Kumar, R., L. Samaniego, and S. Attinger (2013): Implications of distributed hydrologic model parameterization on water fluxes at multiple scales and locations, Water Resour. Res., 49.
14. Batool, M., Sarrazin, F.J., Attinger, S. *et al.* Long-term annual soil nitrogen surplus across Europe (1850–2019). *Sci Data* **9**, 612 (2022). https://doi.org/10.1038/s41597-022-01693-9
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