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Tethys

Output 2.3

Fully operative transnational HS emissions model as a fit-for-purpose tool for risk assessment and evaluation of scenarios for policy support under new complex challenges and pressures

O2.3: Fully operative transnational HS emissions model as a fit-for-purpose tool for risk assessment and evaluation of scenarios for policy support under new complex challenges and pressures

PROJECT TITLE: Coordinated Danube Action for the titanic endeavor of tackling hazardous substances water pollution under changing pressures, challenges and targets

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Abstract

The developed MoRE model for the Danube River Basin (DRB) aims to manage and understand the relevance and impact of **metal, pharmaceuticals and PFAS emissions** in line with European legislative frameworks, like the Water Framework Directive (WFD). The emission model jointly further developed, upgraded with new data and algorithms and validated the HS emission model developed in the DTP Danube Hazard m^3c project, to enable a higher variety and complexity of scenarios, which is an essential step to make it a fit-for-purpose tool in view of the new complex challenges and required risk assessment approaches.

This Output 2.3. demonstrates the technical workflow and the results of the developed MoRE model, as a user guide extends the official MoRE manual.

The **background knowledge** to understand and use the upgraded transnational emission MoRE model described in **Chapter 1**, such as the general description, approach and main structure of the model, overview of the needed basic and the substance specific input data, the graphical user interface and application of the R mirrored version.

The **available and used data for final modelling** are listed in **Chapter 2**, such as applied analytical units, spatial and periodical input data (landuse, erosion, meteorological and hydrological data, population, sewerage data, the locations of WWTPs, industrial sites point sources), and data used for validation. The section 2.3. collects all emission factors were applied in the model for each pathway.

Chapter 3 serves an overview of the model results, by introducing the share of the pathways and the spatial distribution of specific emissions across the Danube River Basin (DRB). Pathway shares are presented for given sub-catchments of the DRB, this way highlighting differences between parts of the basin and highlighting pathways responsible for most emissions. Maps are introduced only to highlight major hotspots and to bring the attention to patterns, however, more detailed evaluation can be made based on pathway related maps, which can be found in Appendix 5.

Note: ***For the upgraded calculations and development results of the model*** *see the Output 2.1 "*Testing and demonstration of HS emissions model as an operative fit-for-purpose tool for transnational modelling-based risk and scenarios assessment under new challenges and pressures*".*

1 AIM AND SCOPE

1.1 GENERAL DESCRIPTION OF THE UPGRADED TRANSNATIONAL EMISSION MODEL

The MoRE emission model has been upgraded in order to provide estimates for all relevant pathways of three substance groups, six heavy metals and arsenic, two pharmaceutical compounds (diclophenac and carbamazepine), and two per- and polyfluorinated alkyl substances (PFOS and PFOA). The model

has been applied for such purpose previously on pilot scale[1], national scale[2] and regional scale[3] as well. Most pathways used in the current version have been involved in one of these applications, but new methods have been also introduced in the current version, especially for PFAS compounds. This substance group is challenging to quantify due to its ubiquitous presence in every matrix. An important improvement is the introduction of ways to regionalize concentrations with respect to groundwater, soil and atmospheric deposition, as these give a massive input for HM and PFAS substance groups.

New pathways have been introduced that focus on legacy pollution effects. These are the pollution under aerodromes and firefighting centres, municipal landfills, industry waste disposal sites (e.g. tailing facilities of mines and other landfills), and specific sites with high concerns (Gendorf legacy site for PFAS legacy pollution).

In the case of Pharmaceuticals, this is the first broad scale estimation that aims the pathway-oriented description of these substances. A challenging task that has been addressed, is the regionalisation of pharmaceutical use by inhabitants across the basin and also the evaluation of effluent concentrations of different size WWTPs and different treatment stages. This work has a value in terms of the scenario analysis of the emission patterns across the basin.

Industrial emissions are one of the most important inputs for some of the substances, therefore a proper estimation scheme for these has been developed, based on available information of industrial emissions for large plants (E-PRTR/IEPR facilities) and based on national scale information of smaller size plants, which required the cooperation of project partners. Valuable information has been gathered, which provided the base for the realistic estimation of industrial loads.

Retention of these substances in the river systems is not well known; to overcome this limitation, a river segment based analysis has been delivered that produced retention factors on segment scale, which was then also transferred to AU scale retention by observed empirical relationships. This upgraded retention scheme gives a chance for a more realistic description of riverine retention, specific to each substance groups.

An R based description of the calculation engine of the MoRE model has been prepared, which provides more flexibility for the better understanding of the model behaviour through sensitivity and uncertainty analysis of certain model parameters. Even though this is not a tool for the everyday use of the MoRE model, but it greatly supports the development of the model.

1.2 APPROACH AND MAIN STRUCTURE OF THE MODEL

In the current approach the set up of the MoRE model was delivered parallel with the development of a water balance model in the Danube Water Balance project and the development of a R version of the model engine, the retention algorithm and an uncertainty assessment tool. The interlinkage between these parallel processes can be seen in Figure 1.

[1] Gabriel, O., & Broer, M. B. (2023). Report on improved system understanding as basis for adapted transnational emission modelling at DRB scale - O T2.2 - Output Danube Hazard m3c project. https://dtp.interreg-danube.eu/uploads/media/approved_project_output/0001/56/52b44806c4c7637a97f77af4f9476a043bbcee60.pdf

[2] Kittlaus, S., Clara, M., van Gils, J., Gabriel, O., Broer, M. B., Hochedlinger, G., Trautvetter, H., Hepp, G., Krampe, J., Zessner, M., & Zoboli, O. (2022). Coupling a pathway-oriented approach with tailor-made monitoring as key to well-performing regionalized modelling of PFAS emissions and river concentrations. Science of The Total Environment, 849, 157764. https://doi.org/https://doi.org/10.1016/j.scitotenv.2022.157764

[3] Model application in the Promisces project, 2024. See also Liu et al, 2015.

The MoRE model structure is simple, there is one model instance for all three substance groups, so each group is calculated by running the relevant algorithm stacks in the MoRE model Graphical User Interface (GUI). The description of the algorithm stacks can be found in Annex I of this document (5.1).

The Tethys_Danube MoRE model instance contains several small modifications compared to earlier application, including the swapping of periodical data to simple analytical unit data or vice versa. Constant data was also swapped to regionalised analyitical unit data (e.g. groundwater concentration of heavy metals and PFAS substances).

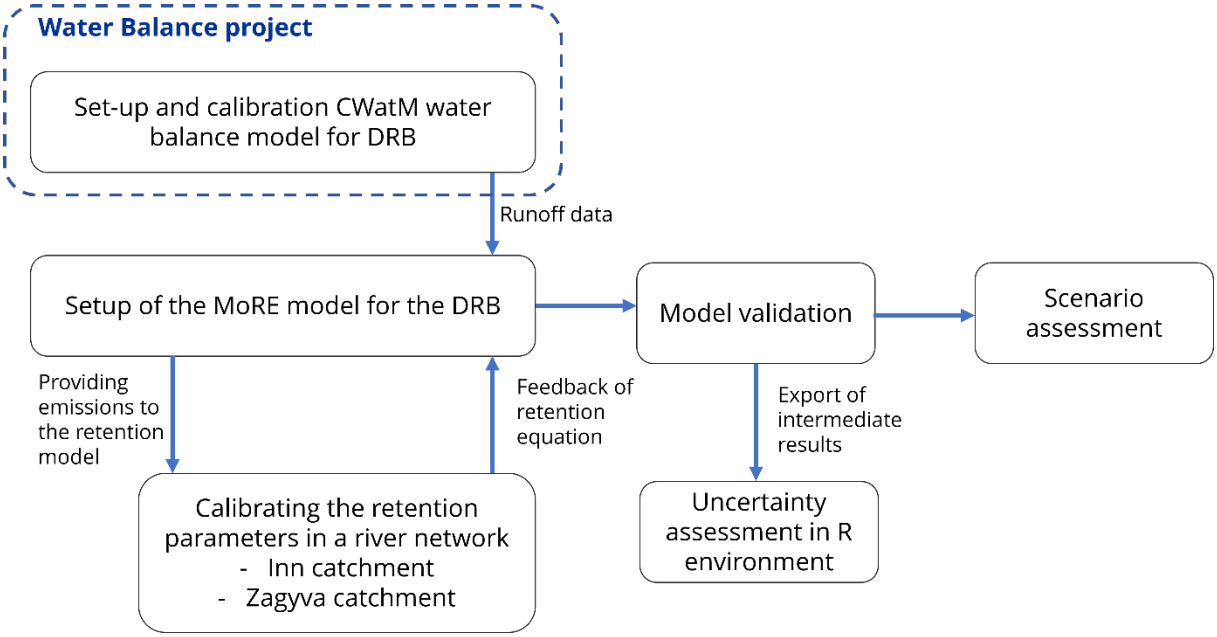


Figure 1 – workflow of the modelling approach used in the Tethys project

1.3 GENERAL DESCRIPTION OF THE MORE MODEL APPROACH

The MoRE model (Fuchs et al., 2017) is a semi-empirical emission model, which operates on the mesoscale (tenth to hundreds of square kilometres) and on annual time steps (in this model application period 2015-2020). It is a further development derived from the MONERIS emissions model (Behrendt et al., 2002) mainly developed for nutrients and differs in particular by a modified technical model realization.

The MoRE model, initially was available only in a German version for an extended number of organic and inorganic micro pollutants before this project. Additionally, a very basic application for nutrients was available in English. The latter was taken and built up into a fully functional English version for a wide range of substances and with a wide range of calculation approaches in the Danube Hazard m^3c project. In the current application the model is further translated and updated to fulfil some further requirements from the current work.

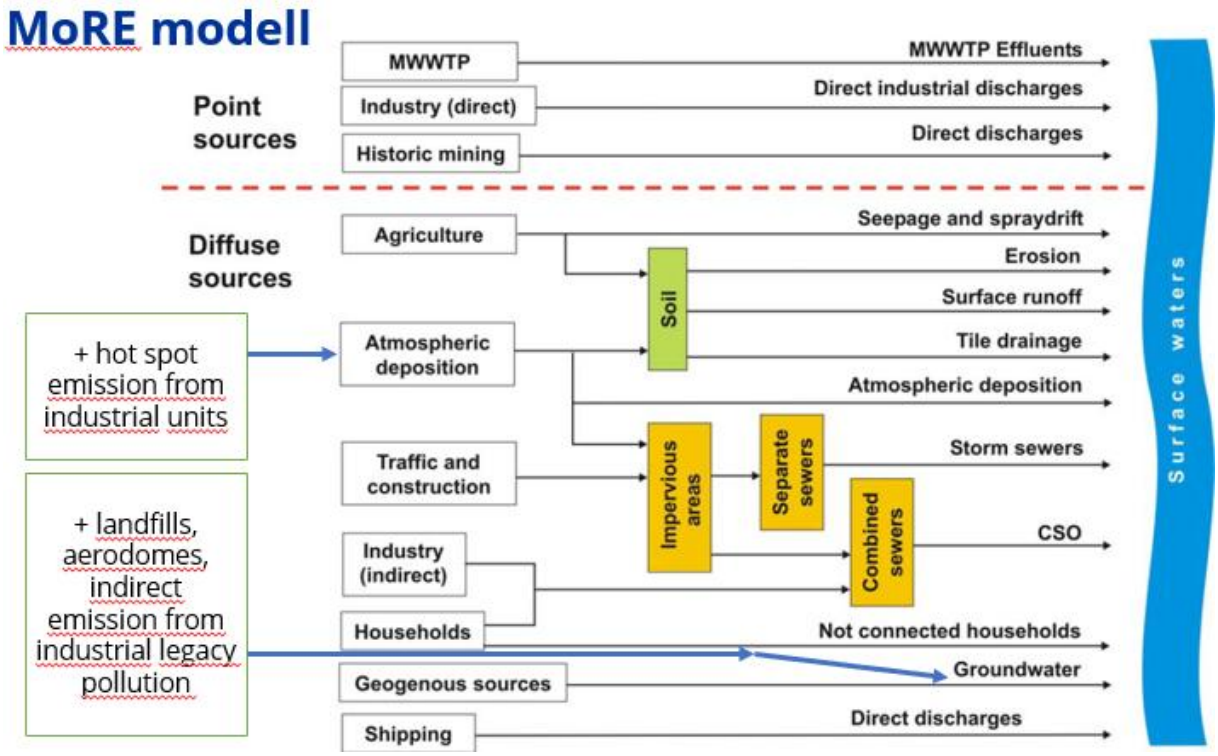


Figure 1 - Substance sources and emission pathways for water pollution (Fuchs et al., 2010)

In the current version, some modification of the pathways is undertaken, e.g. the historic mining is included as an industrial pathway, which is detailed to individual industry segments. Industrial indirect emission through the air is introduced, where the reported or estimated loads are distributed between the affected analytical units (see O2.1. 2.2.1 and 2.2.5). Legacy pollution from different activities have been introduced for three substance groups. These are landfills, aerodromes and fire-fighting centres and industrial legacy sites (LHSG – legacy hot spots via groundwater). The overview of the applied pathways per substance groups can be seen on Table 1.

Table 1 – pathways in the Tethys_Danube MoRE model

Process	Heavy metals	Pharmaceuticals	PFAS
Erosion	✓	×	✓
Surface Runoff	✓	×	✓
Tile drainage	✓	×	✓
Urban emission	✓	✓	✓
Groundwater	✓	×	✓
Atmospheric dep.	✓	×	✓
Atmospheric dep. - hot spot	✓	×	✓
Point source - communal	✓	✓	✓
Point source - industrial	✓	✓	✓
Industrial diffuse hot-spots	✓	×	✓
Landfills	✓	✓	✓
Aerodomes and other fire fighting centres	×	×	✓

Retention approach in the model

The MoRE model offers a simple retention calculation algorithm based on the Moneris nutrient retention scheme, which is an approach, where retention is a function of hydraulic load (which is related to retention time) and in the case of total phosphorus of area specific runoff. These built in algorithms

may be calibrated to other substances by the model parameters, however in case of organic pollutants the retention may be more specific, where other factors play an important role, such as photolytic transformation of diclophenac, where light conditions are related to river size, riverbank shading etc. In the upgraded model, a more complex retention approach is tested Figure 2, and used to fit new empiric approaches for AU level riverine retention.

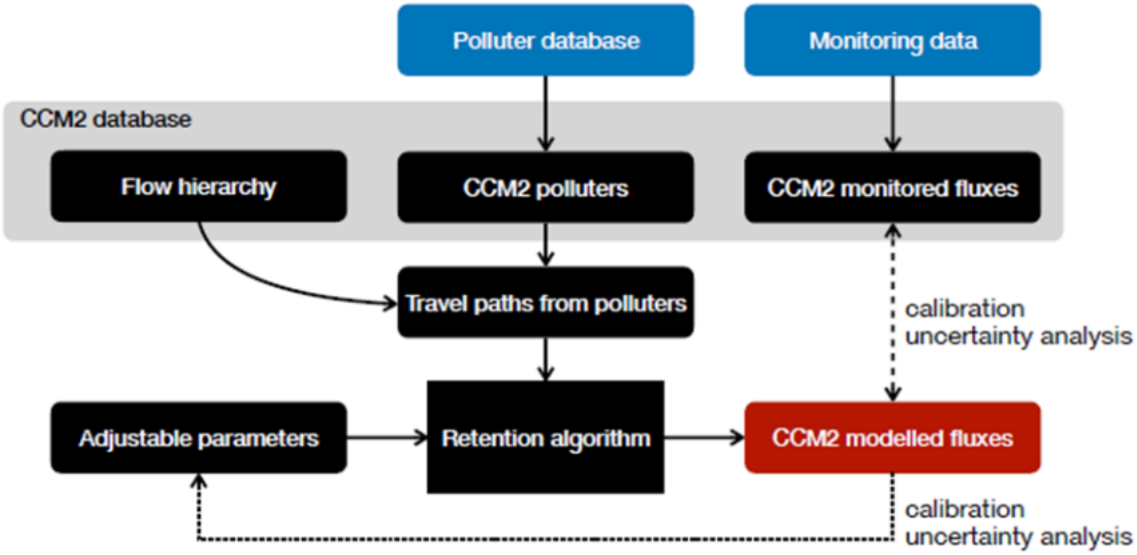


Figure 2 - Workflow of the river retention approach in river reach level. (outside of the MoRE model)

The approach is starting with a river segment level retention calculation of the substances based on the input data from the calculated emissions by the MoRE model and validation data available in test basin. The Inn catchment is the first test basin, where retention parameters were fitted. These were then transferred to model parameters by simple regression. Minor channel travel distance has been the strongest predictor or riverine retention of heavy metals (Figure 3).

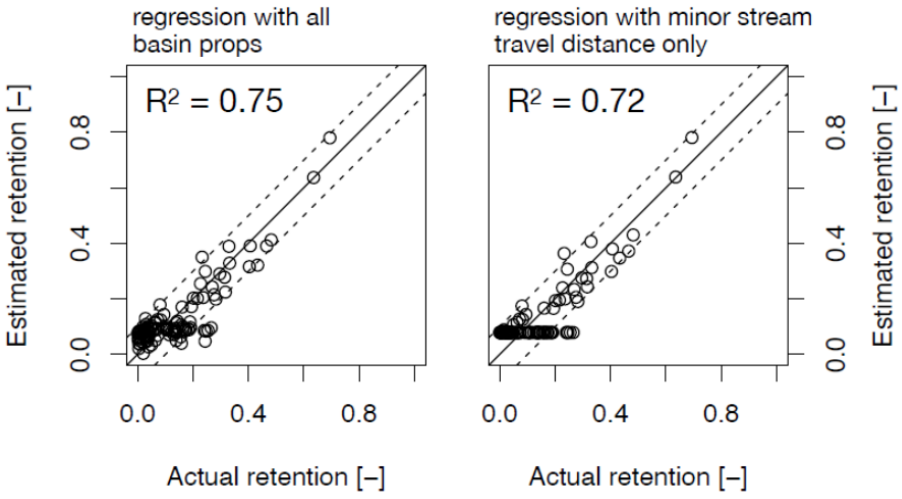


Figure 3 – fitting of prediction formulas to modelled retention in the Inn catchment for Cadmium.

1.4 INPUT DATA NEEDS

To see a full list of model variables, please see O.2.1 Annex III, which introduces all the model variables used in the current MoRE model. There is a very important notice about the naming convention of the model variables: The starting two letters always refer to the pathway or data type, these describe (e.g. BI stands for basic input, US stands for urban systems). The second part refers to further information (general terms) of the data (e.g. *A* stands for area, *PREC* for precipitation, *yr* for yearly, *lt* for long term, *E* for emission, *CONC* for concentration, *CONT* for content. The letters in the end with either the substance group name (*HM* for heavy metals, *PFAS* for per and polyfluorinated alkyl substances, and *PHAR* for pharmaceuticals) or the given substance (eg. ZN, PFOA, DI…).

1.4.1 Overview of the basic input data needed in the MoRE model

There are a high number if input data in the model, therefore, we do not introduce them here in full detail, but only introducing the most relevant basic input data (Table 2).

Table 2 – selected basic input data oft he MoRE model with regard to different pathways without a full listing of these.

Actual input data code	**Name**	**Description**	**Unit**	Spatial/Periodical
Analitical Unit (AU)				
BI_A	Area	Area of analytical units	km²	(x)
BI_ELEVA	Digital Elevation Model	Mean hights of subcatchments	m	(x)
Landuse				
BI_A_AL_slope_0-1	Arable land	5 slope classes: 0-1; 1-2; 2-4; 4-8; >8 % (if available)	km²	(x)/(x,t)
BI_A_PST	Pastures	Greenland, meadows	km²	(x)/(x,t)
BI_A_WS_mr	Water surface	Main river (also lakes; reservoirs)	km²	(x)/(x,t)
BI_A_WS_trib	Water surface	Tributaries (also lakes; reservoirs)	km²	(x)/(x,t)
BI_A_FOR	Naturally covered areas	Woods; scrubland	km²	(x)/(x,t)
BI_A_O	Open areas	Mountainous area without vegetation; beaches; dunes	km²	(x)/(x,t)
BI_A_OPM	Surface mining	Mining areas	km²	(x)/(x,t)
BI_A_URB	Settlements	Total urban areas	km²	(x)/(x,t)
BI_A_IMP	Impervious urban area	Paved areas inside urban areas: settlements; industrial estates; car parks….	km²	(x)/(x,t)
BI_A_WL	Wetlands	Area of Bog; swamp; floodplains	km²	(x)/(x,t)
BI_A_OR	Country roads	Paved road area; not included in settlements	km²	(x)/(x,t)
BI_A_REM	Other remaining areas	Other areas not listed above	km²	(x)/(x,t)
Drainages, Melioration cadastre				
TD_SHR_a_td_agrl	Tile drained areas	From arable land and pastures	km²	(x)
Meteorological Data				
AD_EVAPO_lt	Evapotranspiration	Longterm mean annual evapotranspiration	mm	(x)/(x,t)
BI_PREC_apr	Precipitation	Monthly values	mm	(x)
Hydrological data, river discharges				
BI_Q_net	Net runoff	Modelling period; annual data	m3/s	(x)
Erosion		**Soil loss**		
ER_agrl_SL_spec_lt_AL	Soil loss	Soil loss from arable land (optional from 5 slope classes)	t/(ha·a)	(x)/(x,t)
ER_agrl_SL_spect_lt_PST	Soil loss	Soil loss from pastures	t/(ha·a)	(x)/(x,t)
Sewer systems - Statistical data about inhabitants and waste water system				
BI_INH	Number of inhabitants	Populaltion	inh	(x,t)

Actual input data code	Name	Description	Unit	Spatial/Periodical
US_cso_VOL_spec_SOT	Stormwater overflow	Storage volume of stormwater overflow tanks in combined sewer systems, area-specific	m³/ha	(x)/(x/t)
US_L_CS	Combined sewers	Length of combined sewers	km	(x)/(x/t)
US_L_SS	Stormwater sewers	Length of stormwater sewers	km	(x)/(x/t)
US_SHR_inh_con_tot	Connection rate	Percentage of inhabitants that are connected to sewer systems	%	(x)/(x/t)
US_SHR_inh_conWWTP_tot	Connection rate	Percentage of inhabitants that are connected to sewer systems and waste water treatment plants	%	(x)/(x/t)
US_SHR_inh_nss_tot	Connection rate	Percentage of inhabitants that are not connected to sewer systems	%	(x)/(x/t)
US_INHC_H2O	Water consumption	Inhabitant specific water consumption	l/(inh·d)	
US_nss_SHR_inhl_towwtp_sept	Percentage of the inhabitant load that is transported from septic tanks to waste water treatment plants		%	(x)/(x/t)
US_Q_spec_COM	Runoff rate for commercial waste water		l/(ha·s)	
Point source data - urban wastewater				
WWTP_ps_INH_conWWTP	Connection rate	Number of inhabitants that are connected to sewer systems and waste water treatment plants (point sources)	Inh	(x)/(x/t)
WWTP_ps_CP	Capacity	Capacity of the waste water treatment plant (point sources)	PE	(x)
WWTP_ps_PE	Load	Nominal load of waste water treatment plant (point sources)	PE	(x,t)
WWTP_ps_TS	Treatment type	Current treatment type of waste water treatment plant (point sources)	-	(x)/(x/t)
WWTP_ps_Q	Discharge	Runoff via waste water treatment plant (point sources)	m³/a	(x/t)
Point source data - Industrial wastewater				
ID_ps_Q	Discharge	Runoff via industrial direct dischargers	m³/a	(x/t)

(x,t) = function of space and time; (x) = function of space;

1.4.2 Overview of the substance specific input data needed in the MoRE model

The modelling approach requires the definition of several pathway related substance specific data. These are either constants, analytical unit variables, periodical analytical units variables, point source variables or periodical point source variables.

Urban System emission

Table 3 - Substance specific variables and constants used for Urban System emission calculation in the Tethys MoRE model; SG abbreviates substance group, SS abbreviates specific substance

name	description	parameter	unit	Data source
US_CONC_ROAD_SG_SS	Concentration of roads	concentration	µg/L	Literature data
US_CONC_COM_SG_SS	Concentration in runoff from commercial areas	concentration	µg/L	Literature data
US_CONC_INH_FS	fine solids concentration from inhabitants	concentration	mg/L	MoRE old values
US_cso_CONC_FS	fine solids concentration in runoff via combined sewer overflows	concentration	mg/L	MoRE old values

US_ss_CONC_FS	Solids (AFS fine) concentration in stormwater runoff in the separation system.	concentration	mg/L	MoRE old values
US_INHL_SG_SS	inhabitant specific load	load from inhabitants	g/(inh·a)	Calculated from monitoring data
US_cso_CONC_SG_SS	Concentration in the discharge of the combined sewer during discharge	concentration	µg/L	Tethys HS database
US_KD_SG_SS	Solid-liquid partition coefficient in stormwater runoff (combined and storm water systems)	Distribution coefficient	L/kg	MoRE old values
US_nss_RET_SOIL_SG_SS	retention in soil	retention, soil	-	MoRE old values

Point source constants

Table 4 - Substance specific variables and constants used for WWTP emission calculation in the Tethys MoRE model; SG abbreviates substance group, SS abbreviates specific substance

name	description	parameter	unit	Data source
WWTP_CONC_SG_SS	Concentration in the effluent of the WWTP	Point source variable	µg/L	Tethys HS database
AM_CONC__SG_SS	Concentration from abadoned mining	Point source variable	µg/L	Tethys HS database
ID_CONC_SG_SS	Effluent concentration from industrial direct dischargers	Point source variable	µg/L	Tethys HS database
WWTP_ps_EF_inh_PFT_PFOA	Population-related PFOA emission factor for wastewater treatment plants	Point source variable	g/ing/a	Tethys HS database
WWTP_CONC_NOTREAT_SG_SS	Concentration in effluent	Constant	µg/L	Tethys HS database
WWTP_CONC_PRIM_SG_SS	Concentration in effluent	Constant	µg/L	Tethys HS database
WWTP_CONC_QUART_SG_SS	Concentration in effluent	Constant	µg/L	Tethys HS database
WWTP_CONC_SEC_SG_SS	Concentration in effluent	Constant	µg/L	Tethys HS database
WWTP_CONC_TERT_SG_SS	Concentration in effluent	Constant	µg/L	Tethys HS database
WWTP_CONC_WWTP_0to25kEW_PFAS	PFAS Concentration in the effluent of WWTP smaller than 25.000 p.e.	Constant	µg/L	Tethys HS database
WWTP_CONC_WWTP_25to250kEW_PFAS	PFAS Concentration in the effluent of WWTPs between 25.000 and 250.000 p.e.	Constant	µg/L	Tethys HS database
WWTP_CONC_WWTP_250kEWplus_PFAS	PFAS Concentration in the effluent of WWTPs larger than 250.000 p.e.	Constant	µg/L	Tethys HS database
WWTP_s_CONC_SG_SS	Concentration in the effluent of the WWTP	Constant	µg/L	Tethys HS database

Erosion emission

Table 5 - Substance specific variables and constants used for erosion emission calculation in the Tethys MoRE model; SG abbreviates substance group, SS abbreviates specific substance

name	description	parameter	unit	Data source
ER_agrl_CONT_SOIL_top_AL_SG_SS	Substance content in topsoil of arable land	analytical units variable	mg/kg	Tethys data from Gemmas and JRC
ER_agrl_CONT_SOIL_top_PST_SG_SS	Substance content in topsoil of grassland	analytical units variable	mg/kg	Tethys data from Gemmas and JRC
ER_CONT_ROCK_SG_SS	Substance content in crushed rock from glaciers	analytical units variable	mg/kg	MORE DH
ER_nat_CONT_SOIL_SG_SS	Substance content in topsoil of naturally covered areas	analytical units variable	mg/kg	MORE DH
ER_ENR_SG_SS	Enrichment ratio	Constant	-	MORE DH
ER_CONC_FS	Solids concentration during erosion events	Constant	mg/L	MORE DH
ER_EXP_ENR_HM_SS	Exponent, of heavy metal enrichment ratio	Constant	-	MORE DH
ER_EXP_SDR_nat	Exponent for calculating the SDR of naturally covered surfaces	Constant	-	MORE DH
ER_FCT_a_ENR	factor a, pollutant enrichment ratio	Constant	-	MORE DH

Surface runoff emission

Table 6 - Substance specific variables and constants used for surface runoff emission calculation in the Tethys MoRE model; SG abbreviates substance group, SS abbreviates specific substance

name	description	data type	unit	Data source
KD_SOIL_WATER_SG_SS	Distribution coefficient of substances between soil and water	Constant	L/kg	Tethys HS database
SR_CONC_SG_SS	Concentration in surface runoff	Constant	µg/L	Tethys HS database

Atmospheric deposition

Table 7 - Substance specific variables and constants used for atmospheric deposition, groundwater, tile drainage and open road emission calculation in the Tethys MoRE model; SG abbreviates substance group, SS abbreviates specific substance

name	description	Data type	unit	Data source
AD_RATE_SG_SS	Substance depositions rate	Analytical units variables	g/(ha·a)	Tethys HS database
AD_FACT_SOIL_RATE_dep_HM_AS	Conversion factor from soil to atmospheric deposition	Constant	-	Tethys HS database

GW_CONC_SG_SS	Concentration in ground water	Analytical units variables	µg/L	Tethys HS database
GW_FCT_CALIB_PFAS	Calibration factor to account for the retention of PFAS in groundwater	Constant	-	Tethys HS database
KD_OC_PFAS	Partition coefficient of PFAS between soil organic carbon and soil water	Constant	L/kg	Tethys HS database
GW_CONC_CALC_FOC_PFAS	Organic carbon content of soils	Constant	-	ESDAC SOIL DATABASE, ISRIC
TD_CONC_FS	fine solids concentration in runoff via tile drainage	Constant	mg/L	MORE DH
OR_CONC_FS	Solids concentration in runoff from non-urban roads.	Constant	mg/L	MORE DH
OR_SFL_SG_SS	Substance accumulation potential on non-urban roads	Constant	g/(ha·a)	MORE DH

1.5 MODEL APPLICATION

1.5.1 Graphical user interface (GUI) of the MoRE model

MoRE Developer is a database management tool that interfaces with PostgreSQL. It launches in reading mode by default, where only interface configuration can be adjusted. Switching to writing mode enables users to add, change, or delete variables, input data, and other items.

The MoRE Developer GUI consists of four main components arranged across the screen (Figure 4). On the left side, an overview of all object tables provides hierarchical access to the database content. The main categories include metadata, which contains variable information, types, and references; input data, comprising preprocessed analytical units, area properties, and aggregated spatial and temporal values; calculation, featuring algorithms for substance emission modelling organized into algorithm stacks with formulas and calculation steps; and results, storing calculation outputs, result sets, and runoff model data.

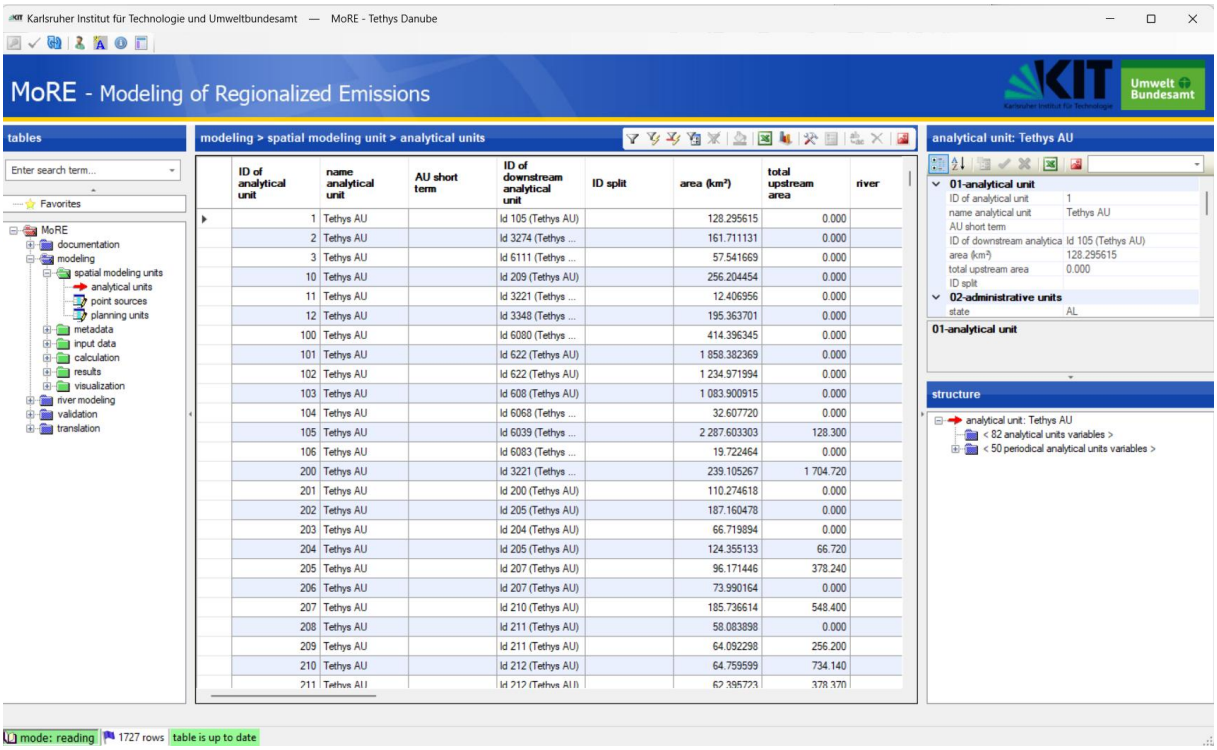


Figure 4 - The MoRE GUI – main window.

In the center of the interface, the data grid displays the contents of the selected object table in tabular format. Records can be selected by clicking on the left margin, which highlights them in blue. The window heading reflects the currently selected data record. Only one object table can be selected at a time, indicated by a red arrow and blue highlighting of the table name.

On the right side, two windows provide additional information. The attribute window at the top shows detailed information for selected data records and serves as the primary interface for creating and modifying records in writing mode. Below it, the structure window displays the hierarchical structure of selected records, which is particularly useful for examining calculation objects such as formulas, algorithms, and algorithm stacks. Clicking on elements within the structure window updates the data grid view to show further details.

MoRE features two toolbars that enable interaction with the PostgreSQL database. The data grid toolbar offers functions for filtering and searching records, exporting content to Excel, deleting records, performing search-and-replace operations to change multiple entries simultaneously, creating statistical diagrams, and executing calculation engine functions. The attribute window toolbar provides tools for ordering and sorting entries, creating new records, exporting content, and uploading PDF documents to data records. These toolbars adapt their available tools depending on which object table is currently selected.

1.5.2 Application of the R mirrored version

In order to provide flexibility to the model calculations and implement uncertainty analysis of certain model parameters, the calculation engine of the MoRE model has been mirrored in R language.

Due to the dynamic structure of the MoRE model—where calculation equations are stored in the same database as the data—the underlying algorithm may change over time. A static implementation in R would therefore require continuous and labor-intensive synchronization with updates to the original model. To avoid this, the R implementation is designed to be fully dynamic and is based on an exported formula heap from MoRE. This formula heap can be the algorithm stack of any pathways or the river retention module.

The formula heap contains the equations defining all relevant calculated variables in an undefined order, while ensuring completeness. At a minimum, it stores the name of each calculated variable and the corresponding equation. Prior to loading the heap into R, minor preprocessing steps are required, including translating conditional expressions into valid R syntax and renaming specific function calls to ensure compatibility.

Following preprocessing, the formula heap is analysed automatically. Variable identifiers are extracted from the equations, and dependency relationships between variables are derived by linking each left-hand-side variable to all variables appearing on the right-hand side. Based on these dependencies, a directed calculation graph (Figure 5) is constructed. This graph is used to identify input variables, terminal variables, and to determine a valid calculation sequence through dependency-aware ordering.

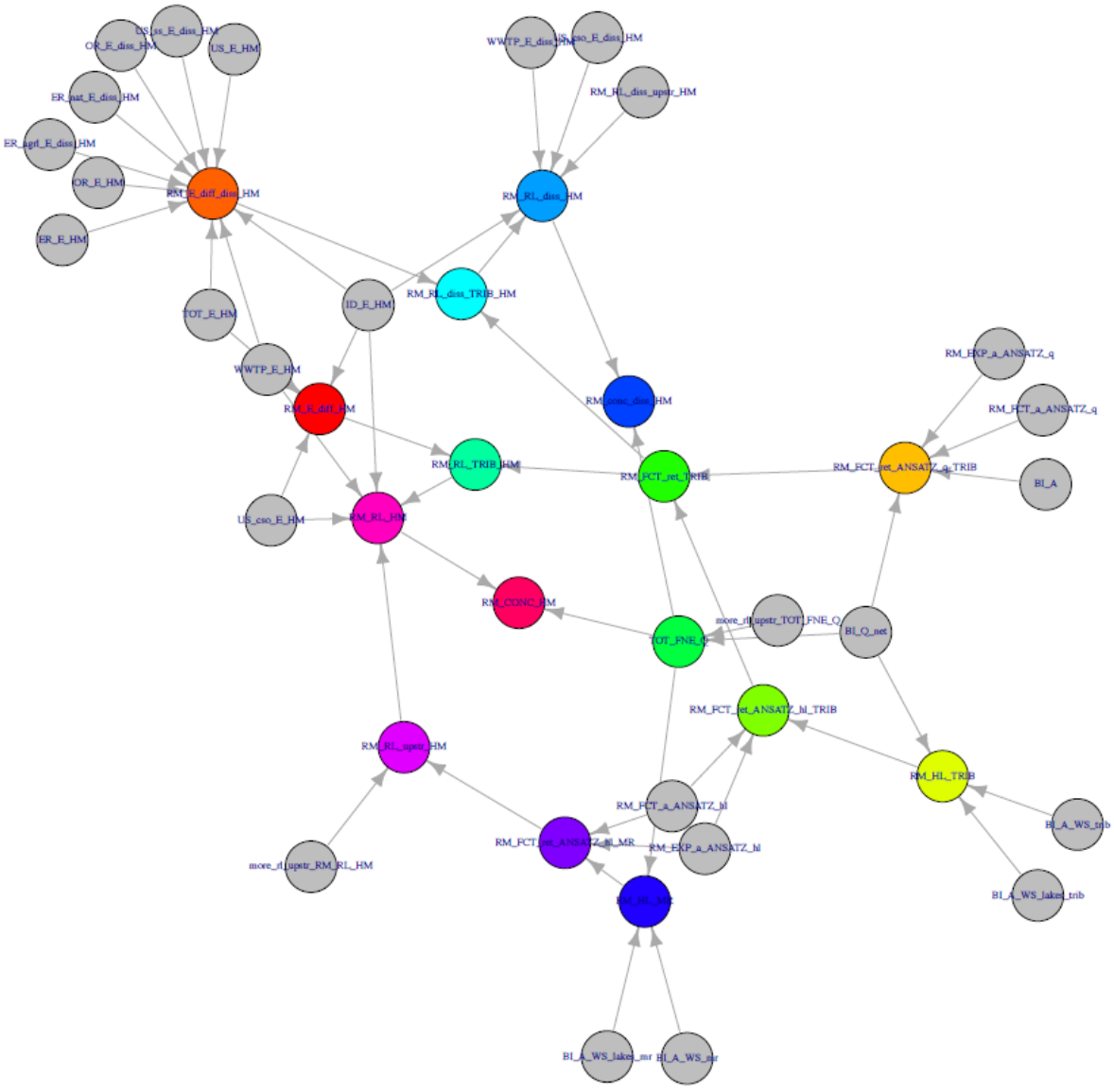


Figure 5 - dependency graph of the MoRE-R engine

The analysed formula heap and the resulting graph structure are stored in a compact data object that contains all algorithmic information required to evaluate the model for a single spatial unit (AU). At this stage, neither the input data nor the interconnections between AUs are specified. To fully mirror the MoRE model, the algorithm must therefore be executed for all AUs in a logical dependency order, with the required inputs provided externally. This task is handled by a separate routine capable of

iterating over AU collections and selecting AU-specific inputs from a pooled data source. For further details about the R package and its use, see Appendix II.

1.6 SUBSTANCES APPLIED IN THE MODEL

Seven heavy metals, two pharamaceutical compounds and two PFAS compounds have been implemented parametrized and validated in the model (Table 8).

Table 8 – substances applied in the Tethys_Danube MoRE model

Substance group	Substance	Implemented	Parametrized	Validated
Heavy metals	Cadmium (Cd)	x	x	x
Heavy metals	Copper (Cu)	x	x	x
Heavy metals	Chrome (Cr)	x	x	x
Heavy metals	Nickel (Ni)	x	x	x
Heavy metals	Lead (Pb)	x	x	x
Heavy metals	Zinc (Zn)	x	x	x
Heavy metals	Arsenic (As)	x	x	x
Pharmaceuticals	Diclofenac	x	x	x
Pharmaceuticals	Carbamazepine	x	x	x
PFAS	PFOS	x	x	x
PFAS	PFOA	x	x	x

2 TECHNICAL WORKFLOW OF THE MODEL SETUP

2.1 BASIC INPUT DATA PREPARATION

The very first step of the modelling exercise is the selection of the most appropriate data source and the pre-processing of this data to create model compatible input data. The term, basic input data, refer to data that describes geographical, geo-physical and hydrological data of the analytical units and that do not refer specifically to a given pathway. Land use information, elevation, slope, precipitation, population and runoff are the main data included in this category. For detailed description refer to O.2.1 section 3 and Annex III.

Data availability and contribution of the project partners

2.1.1 Analytical units (AUs)

The MoRE model calculates emissions for analytical units (AU), these are the units of aggregation in the model, variables within this unit is constant, therefore the resolution of the model outputs will be equal of the resolution of the AUs. Most data is defined for these units in the preprocessing steps, e.g. the soil concentration for an AU is determined from base soil concentration maps with finer resolution by statistical methods (mean, median or quantiles in most cases). The sizes of the analytical units of the Danube River Basin (DRB) varies country by country with smallest sizes in Austria and larges sizes in Hungary, Romania and the countries in the western Balkans (Figure 6). The Danube River Basin contains 1727 units in total. The average area of the units is 468.6 km^2, while the median value is 322 km^2.

It is hugely important to use a hydrologically coherent delineation of watersheds, when preparing AUs. In the case of AUs next to administrative boarders, this requirement is breached in most cases, however this limitation serves country reporting. In the current delineation several such forced delineation

exists as these units were created and/or approved by countries for the 2021 RBMP application of the Moneris nutrient emission model[4].

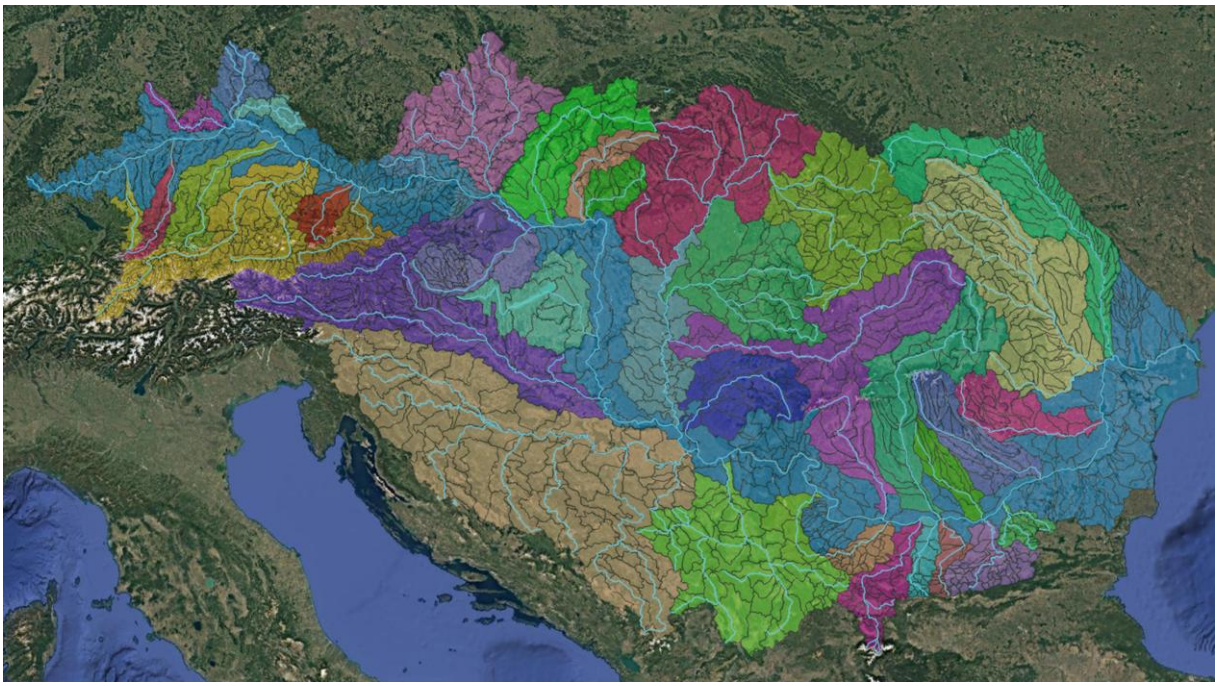


Figure 6 - Analytical units in the DRB for the MoRE model in the Tethys project. Colouring refers to subbasins.

2.1.2 Spatial and periodical input data

2.1.2.1 Landuse

As it is described in O.2.1. S.3.2.1, land use information was taken from the Moneris model dataset[4], which was derived from Corine Land Cover 2018 land use map. Land use categories also follow Moneris methodology, according to which the following distinctions are made: agricultural land use is divided into arable land by slope categories and pastures. Natural vegetation equals to forests. Urban land cover is comprising of two categories: impervious areas (determined by High Resolution Layer Imperviousness[5]) and other urban areas (Corine urban areas minus the impervious lands). Other important land use for the pathway calculations is the water surface, the open roads, while wetlands, open spaces, glaciers and open mines are also part of the model. From these latter categories, not all are used directly in the model, but they are used when summing up the land uses to calculate land use balance (See Annex I). This step provides the quality check for the input data.

2.1.2.2 Erosion, soil loss

Soil loss data is also a critically important information for the MoRE hazardous substance application, as erosion is a dominant pathway for many substances.

[4] Gericke, A. (IGB-B., & Venohr, M. (IGB-B. (2021). *Nutrient Emissions and Loads in the Danube River Basin - Current situation and scenarios for the 3rd Danube River Basin Management Plan – Final report*. https://www.icpdr.org/sites/default/files/2023-09/2021 Report on nutrient emission modelling in the DRB_1.pdf

[5] https://land.copernicus.eu/en/products/high-resolution-layer-imperviousness/imperviousness-density-2018

Erosion data for agricultural soils is based on RUSLE 2015[6] data of the JRS ESDAC product, which was processed for the Moneris application in the RBPMP 2021. This data has been received and applied for the model, however, erosion data for the pastures and natural land has been revised as the originally received values were unrealistically high. The new values were gathered from two data sources: for EU countries, the RUSLE 2015 data has been used, while for Non-EU countries the GLOSEM high resolution erosion database[7] was used.

The model calculates erosion on annual basis, however, currently land use data in permanent in the model, which means that annual erosion estimation is constant. Sediment input to the rivers is calculated by the aggregated soil loss from different slope classes (5 classes with division values of 1, 2, 4, 8%) multiplied by the sediment delivery ratio. For the detailed description, please see O.2.1-section 2.2.6. Resulting sediment input that gives the base for pollutant transport is presented in Figure 7 and Figure 8 for agricultural and natural land use respectively.

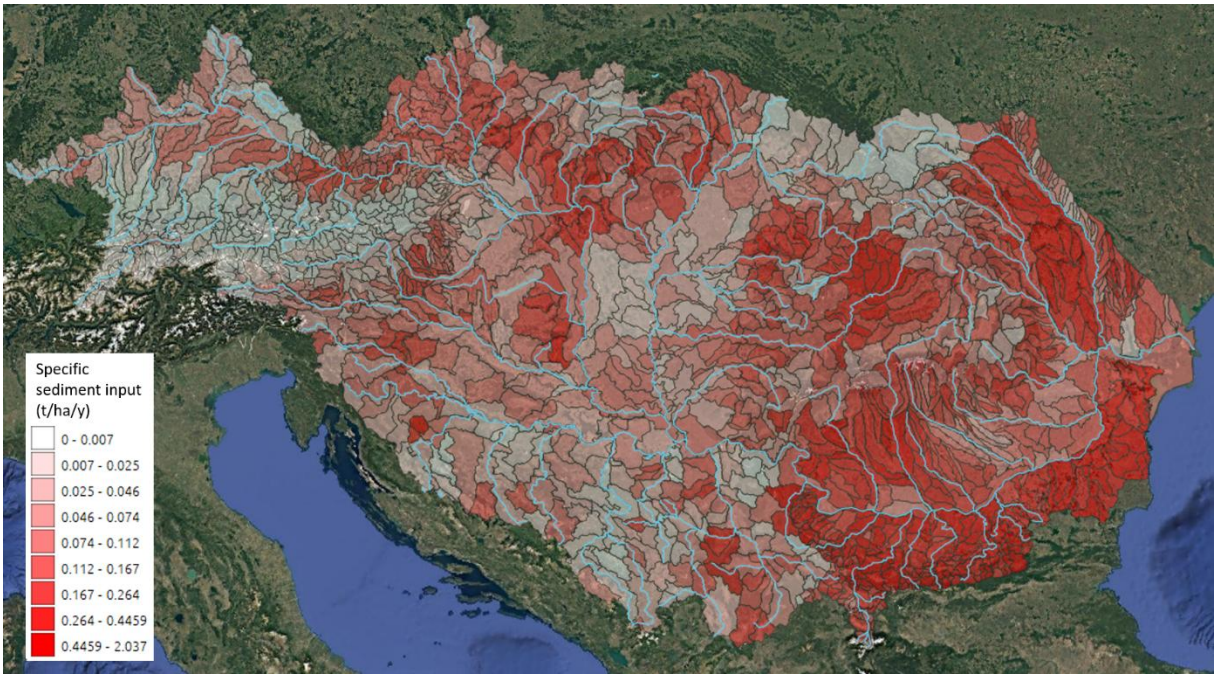


Figure 7 – Specific sediment input from agricultural land from the AUs in the DRB as calculated by the MoRE model.

[6] Panagos, P., Borrelli, P., Poesen, J., Ballabio, C., Lugato, E., Meusburger, K., Montanarella, L., Alewell, .C. 2015. The new assessment of soil loss by water erosion in Europe. Environmental Science & Policy. 54: 438-447. DOI: 10.1016/j.envsci.2015.08.012

[7] Borrelli, P., Ballabio, C., Yang, J.E. et al. GloSEM: High-resolution global estimates of present and future soil displacement in croplands by water erosion. Sci Data 9, 406 (2022). https://doi.org/10.1038/s41597-022-01489-x

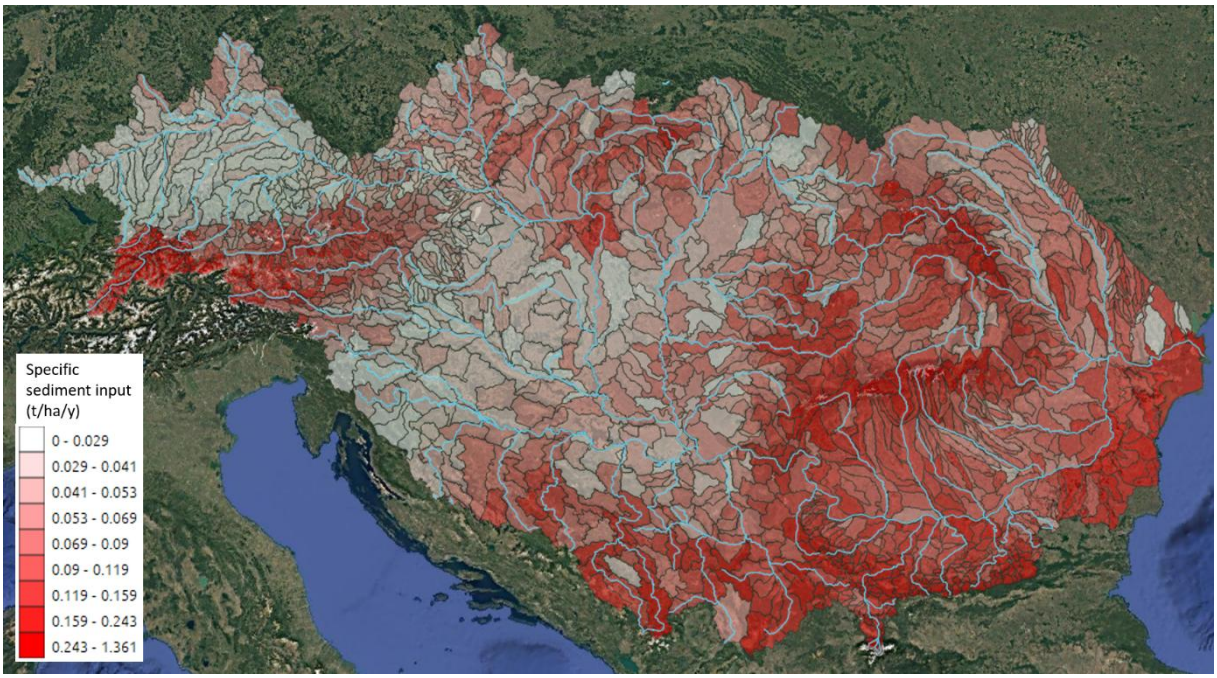


Figure 8– Specific sediment input from natural land cover from the AUs in the DRB as calculated by the MoRE model.

2.1.2.3 Meteorological data

The MoRE model uses precipitation and evapotranspiration data for multiple calculations. Precipitation is used for the annual diversion of the R factor (USLE model for erosion estimation) from long term averages precipitation data. For this, summer and winter precipitation is needed, which is calculated from monthly precipitation values. This is therefore a basic input data to the model. Runoff from impervious areas is also estimated based on annual precipitation. For total recharge estimation of legacy pollution sites, annual precipitation and annual evapotranspiration is used as a point source data.

In our model application, this has been received from the CWATM model application[8], where the EMO[9] datasets were used as source of precipitation (Figure 9) and evapotranspiration (Figure 10) is calculated by the model. These data have been provided as netcdf files. These has been processed either to calculate zonal statistics for analytical units or sampled to get values for sites of interest.

[8] Received from data exchange from Danube Water Balance project, where IIASA has been developing the CWatM hydrological model for the entire Danube River Basin.

[9] Thiemig, V., Gomes, G. N., Skøien, J. O., Ziese, M., Rauthe-Schöch, A., Rustemeier, E., Rehfeldt, K., Walawender, J. P., Kolbe, C., Pichon, D., Schweim, C., & Salamon, P. (2022). EMO-5: a high-resolution multi-variable gridded meteorological dataset for Europe. *Earth System Science Data*, *14*(7), 3249–3272. https://doi.org/10.5194/essd-14-3249-2022

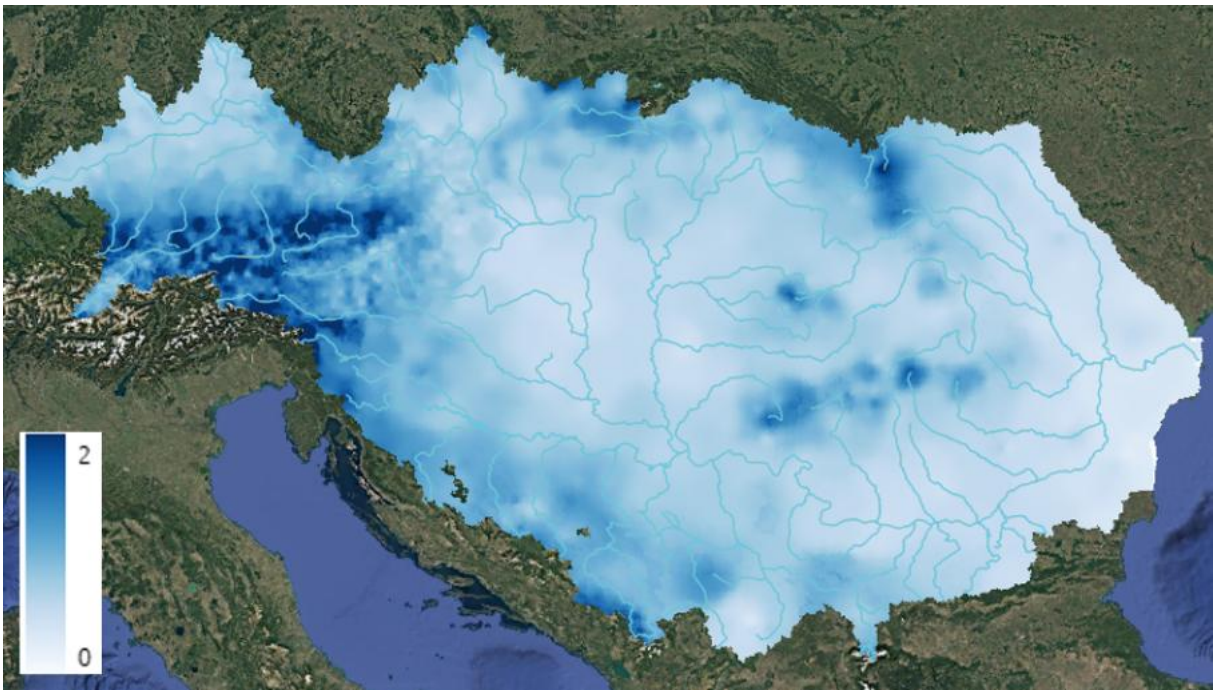


Figure 9 – Annual total precipitation as used in the CWatM model of the Danube Water Balance application

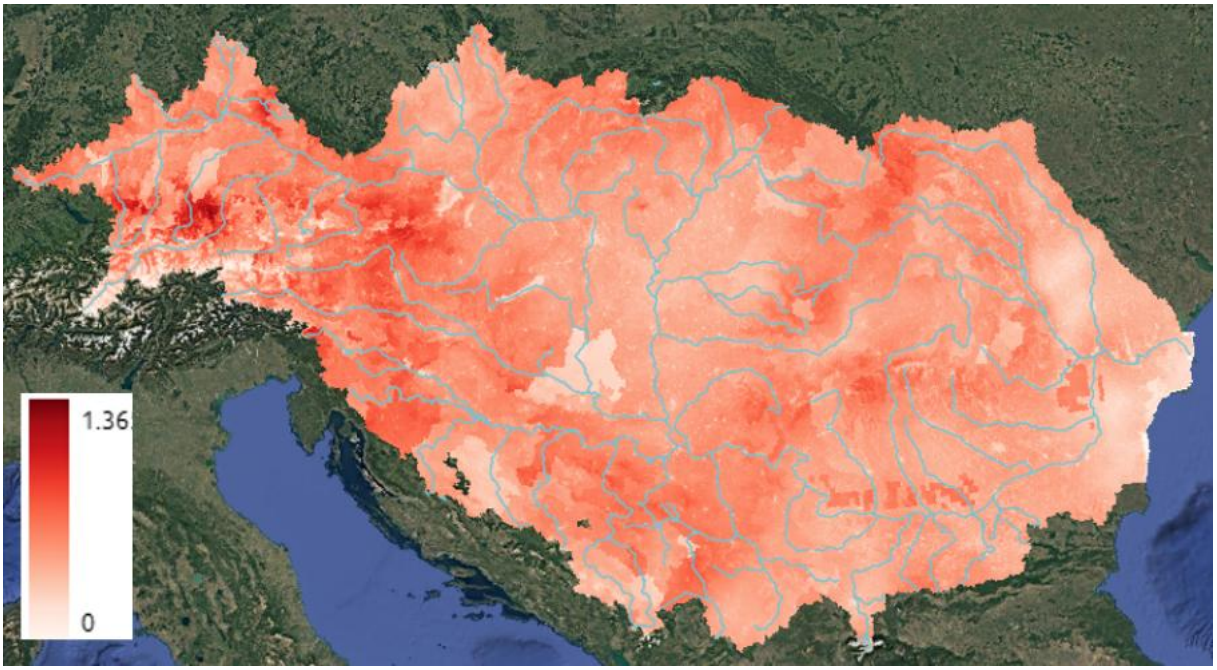


Figure 10 - Annual total evapotranspiration as calculated by the CWatM model of the Danube Water Balance application

2.1.2.4 Urban data (population, sewerage)

Urban emissions are very relevant for many substances, including some heavy metals, pharmaceutical compounds and PFAS compounds. Urban systems in the MoRE model is also quite complex (see O2.1, section 2.2.1.2 for details) as there are multiple pathways that contribute to the so called urban systems („US_“ notation in the model). Diffuse loads from the sewer systems, overflow from the combined systems, or discharge from the sewer systems without treatments produce relevant loads in some large or smaller cities. These estimation requires data about connection rates, connected population numbers, sewer lengths etc, parameters, which are related these are introduced in Table 9. Some of the pathway data is further discussed below:

Runoff from commercial areas: As no data is available about this, a constant value of 0.8% is used in the model for all commercial areas. CSO storage volumes and its development stage is given by estimates originate from Moneris application 2021.

Inhabitant water consumption data (US_INHV_H2O) is taken from ICPDR River Basin Management Plan 2021[10]. This is used to calculate discharge from inhabitants not connected or only connected to sewer systems.

Connection rates of inhabitants are primarily based on ICPDR datasets, that were also used in the Moneris application in 2021.

Table 9 – input variables related to urban systems

name	**description**	**unit**	
US_cso_DUR	duration of overflow from stormwater overflow tanks caused by heavy stormwater events (duration of overflow)	d/a	Constant of 17 is used for each AU. Need to be updated
US_cso_Q_inp	CSO direct storm runoff from input data	m^3/a	Not provided in the current application
US_cso_SHR_vol_real_tot_STO	Percentage of storage volume of stormwater overflow basins compared to full-scale development (degree of development).	%	Moneris data is used
US_cso_VOL_SOT	storage volume of stormwater overflow tanks in combined sewer systems	m^3	Moneris data is used
US_cso_VOL_spec_SOT	storage volume of stormwater overflow tanks in combined sewer systems, area-specific	m^3/ha	Moneris data is used
US_SHR_a_cs_tss	Proportion of the area drained by the combined system to the total area drained by the sewage system.	%	Moneris data is used
US_ss_Q_inp	Storm sewer runoff from input data	m^3/a	Not provided in the current application
US_ss_VOL_SST	storage volume of stormwater sedimentation tanks in separate sewer systems	m^3	Calculated form Moneris data
US_ss_SHR_vol_tft_sst	percentage of storage volumes of throughflow tanks in the total storage volume of stormwater sedimentation tanks	%	Estimated in Tethys project

[10] ICPDR. (2021). *Danube River Basin Management Plan - Update 2021*. ICPDR.

US_A_IMP_com_dlm	commercial area connected to sewer systems	km²	Not data available.
US_SHR_inh_con_tot	percentage of inhabitants that are connected to sewer systems	%	Calculated based on Moneris data
US_SHR_inh_conWWTP_tot	percentage of inhabitants that are connected to sewer systems and waste water treatment plants	%	Calculated based on Moneris data
US_SHR_inh_oss_tot	percentage of inhabitants only connected to the sewer system	%	Calculated based on Moneris data
US_SHR_inh_nss_tot	percentage of inhabitants that are not connected to sewer systems	%	Calculated based on Moneris data
US_imp_Q_mod	Urban runoff from impervious areas from model	m³/s	Runoff from hydrological model.
US_INHC_H2O	Inhabitant specific water consumption	l/cap/day	European statistical data and country data

Total inhabitant number has been received from the Moneris dataset, which was based on country scale statistical data from Eurostat and distributed by GHS-POP gridded dataset[11]. This data was available until 2018, for the current application this has been extended with further data from Eurostat and was distributed by the same GHS-POP dataset, which provides high-resolution, regularly updated population and settlement data based on satellite imagery and census information.

2.1.2.5 Point source data (WWTPs, industrial sites)

WWTPS

Two main data sources were used to create a DRB-wide point source discharges database. For EU countries, the UWWTD database was used. In particular, the version created based on reports covering 2019-2020 was used (because this data refers to the modelled period). For non-EU countries, a database compiled by ICPDR, referring to years 2016-2018 was used. The merged database contains following data: Identifier of treatment plant / discharge point, location (coordinates) of treatment plant / discharge point, constructed capacity of the treatment plant (if any), amount of discharged wastewater, [number of connected inhabitants], [incoming load (p.e.)], treatment technology of the

[11] Schiavina, Marcello; Freire, Sergio; MacManus, Kytt (2019): GHS population grid multitemporal (1975, 1990, 2000, 2015) R2019A. European Commission, Joint Research Centre (JRC) DOI: 10.2905/42E8BE89-54FF-464E-BE7B-BF9E64DA5218 PID: http://data.europa.eu/89h/0c6b9751-a71f-4062-830b-43c9f432370fConcept & Methodology:
Freire, Sergio; MacManus, Kytt; Pesaresi, Martino; Doxsey-Whitfield, Erin; Mills, Jane (2016): Development of new open and free multi-temporal global population grids at 250 m resolution. Geospatial Data in a Changing World; Association of Geographic Information Laboratories in Europe (AGILE). AGILE 2016.

discharge point. The treatment technology can take five values from “no treatment” to “quaternary treatment”.

Table 10 - Number of plants by treatment stage and country

			treatment stage				
country	**unknown**	**notreat**	**prim**	**sec**	**tert**	**quat**	**total**
AT	0	0	0	1	597	6	604
BA	0	73	1	11	0	0	85
BG	94	0	2	5	46	0	147
CZ	0	0	0	163	40	1	204
DE	1	0	0	36	596	35	668
HR	0	54	9	26	11	0	100
HU	0	32	3	207	581	0	823
MD	0	20	6	7	0	0	33
ME	0	3	0	2	2	0	7
RO	5	192	37	620	256	0	1110
RS	0	283	9	34	3	0	329
SI	0	54	0	44	86	0	184
SK	22	0	2	66	279	0	359
UA	0	21	2	12	0	0	35

Industrial sites

The MoRE model incorporated mainly industrial **facilities covered by E-PRTR**, supplemented with some of the **more significant emitters obtained from national databases**. All E-PRTR activities were considered in the modelling, except for Intensive Rearing of Poultry or Pigs (farms), as metal emissions from these farms are irrelevant and usually discharge their wastewater to the public sewer system. These emissions are included in the emissions from municipal wastewater treatment plants. Many production facilities have more than one installation, with different production types or technologies. For modeling, **we selected the main activity** to which we could later assign an emission factor. We consider facilities that were **in operation for at least one year between 2015 and 2023** based on E-PRTR or national databases. **Totally of 4205 production facilities** were considered for MoRE modeling in the Danube Basin (Figure 11 and Figure 12). Industrial data not available from Bosnia, Montenegro and Moldova.

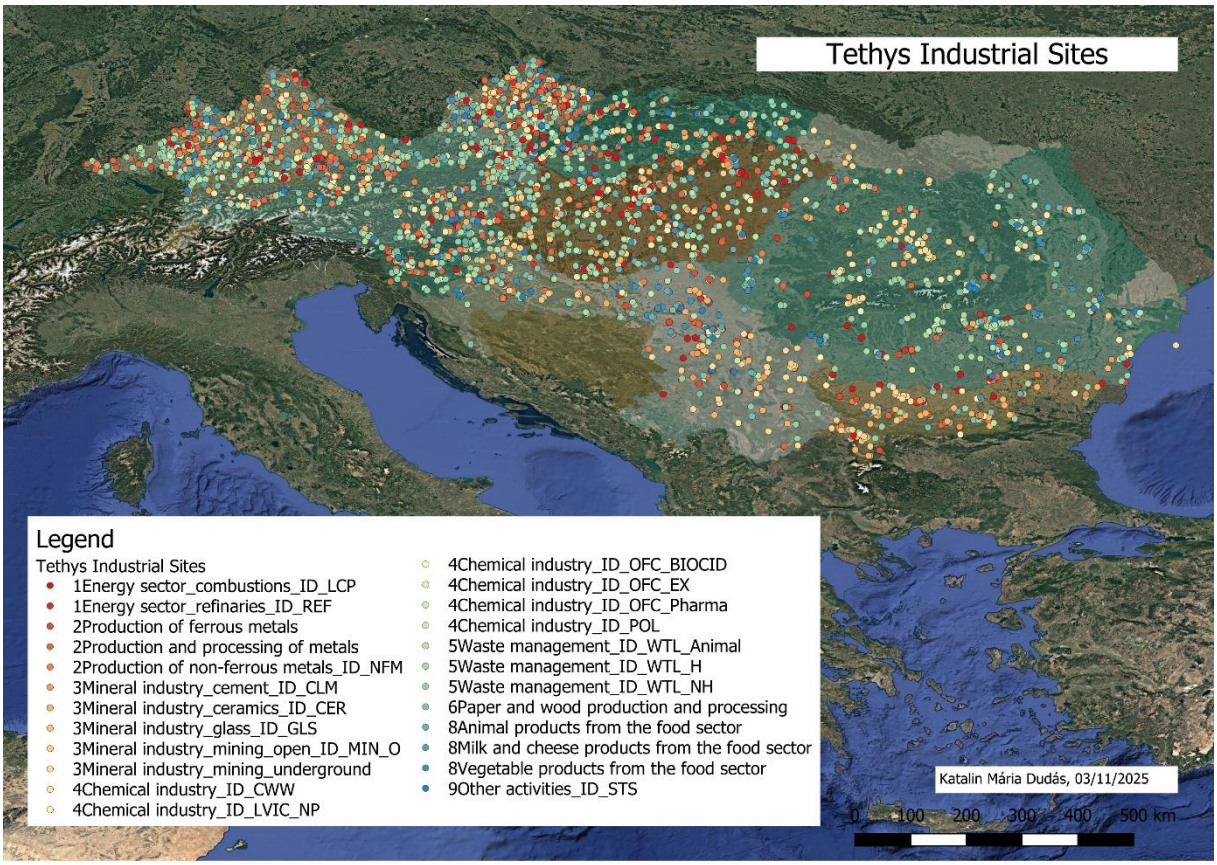


Figure 11 – Industrial facilities across the Danube River Basin based on IEPR database

The facilities belonging to each industrial activity category belong to the same statistical group. The emission factor is applied to each such group. Based on the available information, the E-PRTR categories are the most suitable for categorization. In some cases, some restructuring was necessary, including separation and addition of new types, due to the nature of the activity. It was also important to establish a connection with the BREFs, as this is the main literature source regarding the expected emission levels. A category conversion was necessary, for example, in the case of waste incinerators, which we merged with LCPs (large combustion plans), since these incinerators also partially burn waste for energy production. The final activity list is shown in the Figure 11.

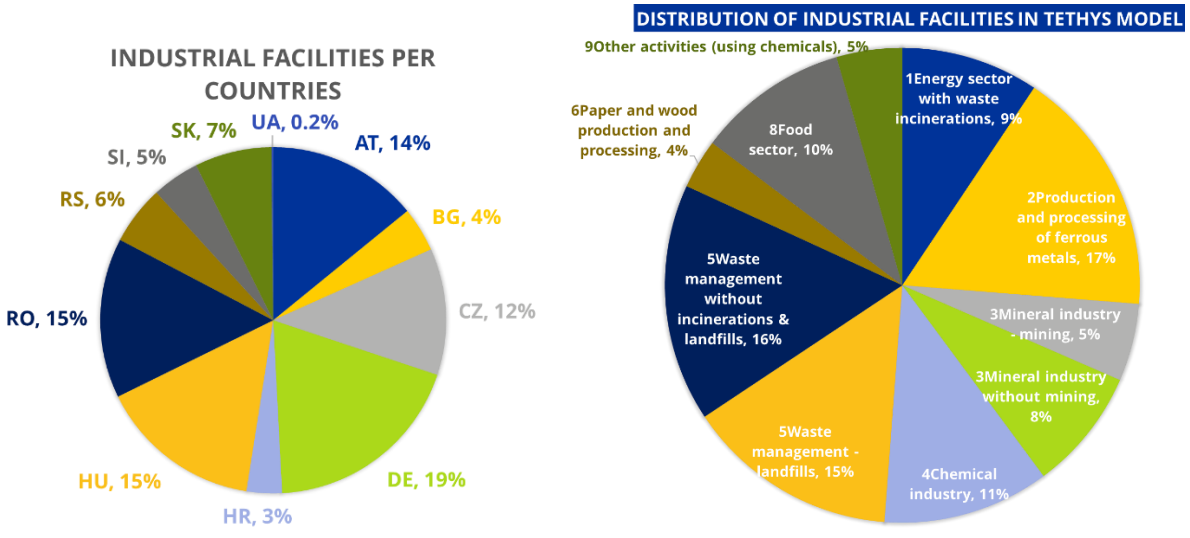


Figure 12 - Portion of Industrial facilities in the Danube Basin per country (a) and per activity (b) after dataprocess

2.2 RUNOFF AND WATER BALANCE

2.3 SUBSTANCE SPECIFIC INPUT DATA

2.3.1 Municipal wastewater concentrations (Máté)

Currently, the following emission factors are applied in the model (Table 11). See document Output 2.1 "Testing and demonstration of HS emissions model as an operative fit-for-purpose tool for transnational modelling-based risk and scenarios assessment under new challenges and pressures" for details.

Table 11 - Emission factors used in the current version of the model. All values are in µg L^{-1}. Basis for the values for the various treatment type is data-based expert estimation; for small plants, emission factors are calculated based on the DHm³c inventory data.

	NOTREAT	PRIM	SEC	TERT	QUART	small
AS	6	4	3	2.5	0.1	1.55
CD	1	0.5	0.1	0.02	0.001	0.00221
CR	50	20	5	4	0.4	2.81
CU	36	21	15	9	0.9	4.51
NI	180	90	9	8	0.8	6.81
PB	15	7.5	3	1	0.1	1.43
ZN	420	210	150	60	6	36.8
PFOA	0.01	0.01	0.01	0.01	0.001	0.03
PFOS	0.01	0.01	0.01	0.01	0.001	0.05
CAR	0.5	0.5	0.5	0.5	0.05	0.59
DI	1	1	1	1	0.1	1.98

2.3.2 Industrial wastewater concentrations

The measured values are indeed included in the MoRE model in an unchanged form (except for the measured value 0, see later). At those discharge points where there was no measurement in the given year, but there was in other years, the average of the measurement results is considered. Where no emission load could be determined based on the above, the 'Sectoral Emission Factor' was applied, which was estimated using the following method.

The Sectorial Emission Factor is based on the median emission values (loads) of the given activity type. For the variant 1 (normal case) to use median value instead of mean allows the exclusion of plants with high emissions, whose measured values added to the model anyway. The method uses the 20% percentile to estimate the 'best case' for calculating minimal industrial loads (variant 2). The national databases contains many 0 values, without indicating LOQ-s or other information related to 0 value. The huge number of zero have a significant statistical distorting effect, therefore variant 4 'modified normal case' omitted zero values from delivering EF (statistics) and the variant 4 uses 20% percentile to estimate emission load instead of 0; and uses sectorial median of the modified statistics. The variant 3 describe the 'worst case', uses 20% percentile to estimate emission load instead of 0; and uses sectorial 80% percentile of the modified statistics. (Table 12)

The used emission factors are presented with statistical data in O2.1. Section X. The used industrial emission data are listed in Annex 3, table X.

Table 12 – Explanation of the variants used for industrial load estimations

Used variants for modelling	Measured 0	Not measured facilities
VAR1 = Normal case	Considering for delivering EF	EF = Sectorial median
VAR2 = Best case (minimum)		EF = Sectorial 20% percentile

VAR3 = Worst case (maximum)	Omitted from delivering EF, & using Sectorial 20% percentile instead of measurements	EF = Sectorial 80% percentile
VAR4 = Modified normal case		EF = Sectorial median

2.3.3 Concentration in CSOs

CSO concentration data for micropollutants is very scarce, therefore no upgrade was made I the current model application (Table 13). CSO concentration for heavy metals was used from previous model application, which was based on a database of Austrian measurements. In the Tethys project further measurements have been conducted in Hungarian CSO outlets, which has not been implemented yet in the model. Pharmaceutical concentrations of waste water systems have been collected in the Danube Hazard project in Romania, Hungary and Austria. The results of these measurements have been used in the model to estimate CSO outflow concentrations. Concentrations has been distributed between countries based on vicinities.

Table 13 – Applied concentration values for CSOs in the DRB wide MNoRE model application

Name of variable	Number of variants	Conentration value	Unit of measure	Data source
US_cso_CONC_HM_AR	1	2	µg/L	median_value all data AT
US_cso_CONC_HM_CD	1	0.0245	µg/L	median_value all data AT
US_cso_CONC_HM_CR	1	50	µg/L	median_value all data AT
US_cso_CONC_HM_CU	1	3	µg/L	median_value all data AT
US_cso_CONC_HM_NI	1	1.35	µg/L	median_value all data AT
US_cso_CONC_HM_PB	1	0.604	µg/L	median_value all data AT
US_cso_CONC_HM_ZN	1	25	µg/L	median_value all data AT
US_cso_CONC_PHAR_CBZ_AT	1	0.4	µg/L	Danube Hazard pilot measurements
US_cso_CONC_PHAR_DCF_AT	1	0.85	µg/L	Danube Hazard pilot measurements
US_cso_CONC_PHAR_CBZ_HU	1	0.915	µg/L	Danube Hazard pilot measurements
US_cso_CONC_PHAR_DCF_HU	1	1.7	µg/L	Danube Hazard pilot measurements
US_cso_CONC_PHAR_CBZ_RO	1	0.54	µg/L	Danube Hazard pilot measurements
US_cso_CONC_PHAR_DCF_RO	1	0.99	µg/L	Danube Hazard pilot measurements

2.3.4 Concentration in the urban runoff

Similarly to CSO concentration, data form storm runoff is also very scarce, therefore real regionalisation cannot be done (Table 14). Previous monitoring has been conducted in Austria and Hungary, results from these campaigns has been used for all other countries.

Table 14 – concentration values for variables related to storm sewers

Name of variable	Concentration value Austria	Concentration value Hungary	Unit of measure	Data source
US_ss_CONC_HM_AS	1.350	1.350	µg/L	median value all data HU and AT

US_ss_CONC_HM_CD	0.024	0.070	µg/L	median value all data HU and AT
US_ss_CONC_HM_CR	3.630	2.280	µg/L	median value all data HU and AT
US_ss_CONC_HM_CU	21.000	17.600	µg/L	median value all data HU and AT
US_ss_CONC_HM_NI	2.000	3.970	µg/L	median value all data HU and AT
US_ss_CONC_HM_PB	2.210	5.100	µg/L	median value all data HU and AT
US_ss_CONC_HM_ZN	96.000	94.100	µg/L	median value all data HU and AT
US_ss_CONC_PFAS_PFOA	0.004	0.004	µg/L	median value all data AT
US_ss_CONC_PFAS_PFOA	0.003	0.003	µg/L	q25 all data AT
US_ss_CONC_PFAS_PFOA	0.009	0.009	µg/L	q75 all data AT
US_ss_CONC_PFAS_PFOS	0.003	0.003	µg/L	median value all data AT
US_ss_CONC_PFAS_PFOS	0.001	0.001	µg/L	q25 all data AT
US_ss_CONC_PFAS_PFOS	0.008	0.008	µg/L	q75 all data AT
US_ss_CONC_PHAR_CAR	0.490	0.490	µg/L	median value all data AT
US_ss_CONC_PHAR_DI	0.006	0.006	µg/L	median value all data AT

2.3.5 Groundwater concentrations

Groundwater concentration measurements are quite frequent for heavy metals in most countries, except some of the non-EU countries. PFAS measurements however are very sparse, only Austria and Germany can provide relevant number of monitoring sites with a few measurements. For this reason, different approach has been used for the two substance groups. Heavy metals concentrations were derived from groundwater well data, that has been collected from the Danube Hazard database and further country data from the wise reporting system. An example summary table for Zn is shown in Table 15.

Table 15 – statistics about groundwater wells used for calculating groundwater concentrations

Country	Well number	Average number of measure-ments	Zn med	Loq levels
AT	2110	16	48 ->loq n2101 <loq - n	3,5,20
SI	165	5	29 >loq n67 <loq n98	1.2
DE	2240	6	30 >loq n1393 <loq n847	1,6.5, 10

BG	99	4	27.5->loq n70 <loq n29	1,10,15,48.5
HR	64	16	221->loq n44 <loq - n20	2,5,10
HU	2619	3	17 >loq <loq 657	1,2,3,4,5,6,7,10,20,25,30,50,70,100
RO	441	7	107->loq n33 <loq - n407	10,25,30,37.5,50
SK	517	18	12.4 >loq n373 <loq n142	2,2.5,3
RS	53	9	282 >loq n53	-

Groundwater well concentration time series has been first analysed with regression on order statistics by the NADA2 R package[12]. Wells with at least 20% above limit of quantification (LOQ) levels are quantified only. Median and mean values from this analysis then were used for further statistical analysis. Groundwater levels were determined for subbasins of the Danube river (Figure 6). Median concentration of Arsenic is shown on Figure 13. For several heavy metals lots of wells show mean or median concentrations below loq. In these cases, the actual concentrations levels are unknown. To account for this uncertainty, three variants have been introduced, var1 referring to LOQ/2 levels, var2 to LOQ levels and var3 to 0 concentrations.

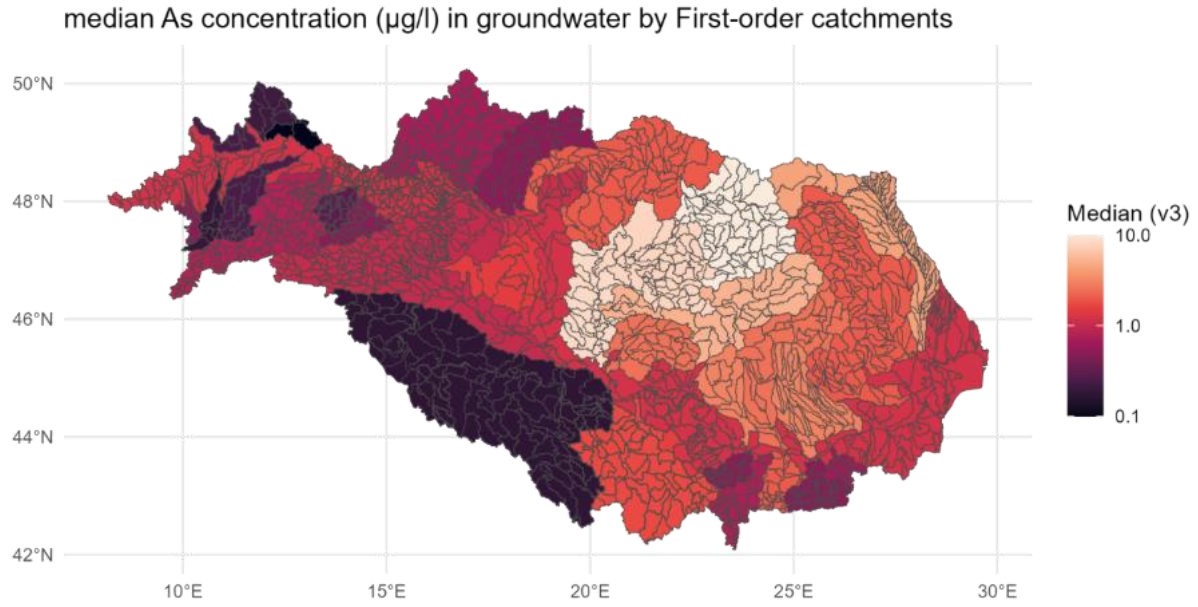


Figure 13 - median As concentrations for the Danube sub-catchments

PFAS concentration values are estimated in the model based on soil concentrations, which are also estimated values for each AU (See below).

[12] Julian P, Helsel D, Lee L (2025).
NADA2: Data Analysis for Censored Environmental Data.
R package version 2.0.0, https://github.com/SwampThingPaul/NADA2.

Groundwater concentrations are derived directly from soil concentrations with a distribution coefficient (KD_OC_PFAS in the model) that links soil-water concentration to concentrations on organic matter in the soil matrix (and subsequently on soil). To be able to calculate this pathway, soil organic carbon must be included, which is an available information from regional (JRC ESDAC SOM[13], which describes soil organic matter content, where carbon fraction needs to be estimated) or global datasets (ISRIC SOC[14] can be directly used). In the model this input data is defined by the input data parameter: GW_CONC_CALC_FOC_PFAS.

This calculated concentration is not equal to the groundwater concentration as the mixing of shallow and deep groundwater and the mixing of groundwaters of different ages cause dilution of these, while retention in the upper and deeper soil matrix also occurs. To account for this reduction effect, a calibration factor is introduced, which can be set by measured groundwater data. As an initial estimate these factors for PFOS and PFOA has been set to:

GW_FCT_CALIB_PFAS_PFOA = 0.25 (-)

GW_FCT_CALIB_PFAS_PFOS = 0.1 (-)

For further details about the calculation please refer to O2.1 section 4.6.2.

2.3.6 Concentration in tile drainage

Estimation of concentration in tile drainage runoff is similar to how groundwater concentrations are estimated for PFAS substances. The same process applies: estimation of soil PFAS concentration, the definition of TD_CONC_CALC_FOC_PFAS variable to the model, that describes soil organic carbon fraction. For data sources, please refer to the above section (groundwater concentration). Research on PFAS and heavy metals in this matrix suggests that tile drainage have higher concentration values than groundwater. The approach is similar, a reduction factor is introduced, which in principle needs to be calibrated, but in this case calibration data is not available. To temporarily overcome this burden, a very rough expert judgment is used and these constant factors are set as follows:

TD_FCT_CALIB_PFAS_PFOA = 0.5 (-)

TD_FCT_CALIB_PFAS_PFOS = 0.25 (-)

In case of metals (HMs and As), the estimation is based on groundwater concentration values and a simple conversion factor is used to get concentration values for tile drain flows (Figure 14).

TD_E_HM = (TD_Q * 86400 * 365 * GW_CONC_HM) / (1000 * 1000)*TD_FCT_GW_CONC_RATE_HM

where
TD_E_HM is the Metal emission through tile drainage (t/y)
TD_Q is the discharge in the AU vie tile drainage (m^3/s)
GW_CONC_HM is heavy metal concentration in groundwater (ug/l)
TD_FCT_GW_CONC_RATE_HM (-) is the conversion factor between groundwater concentration and tile drain flow (please refer to O.2.1 section 4.7 for the derivation of these values).

[13] Lugato, E., Lavallee, J. M., Haddix, M. L., Panagos, P., & Cotrufo, M. F. (2021). Different climate sensitivity of particulate and mineral-associated soil organic matter. Nature Geoscience, 14(5), 295–300. https://doi.org/10.1038/s41561-021-00744-x

[14] Poggio, L., de Sousa, L. M., Batjes, N. H., Heuvelink, G. B. M., Kempen, B., Ribeiro, E., and Rossiter, D.: SoilGrids 2.0: producing soil information for the globe with quantified spatial uncertainty, SOIL, 7, 217–240, 2021. DOI

variable	variant number	variant description	value
TD_FCT_GW_CONC_RATIO_HM_AS	1	Tethys	2
TD_FCT_GW_CONC_RATIO_HM_CD	1	Tethys	30
TD_FCT_GW_CONC_RATIO_HM_CR	1	Tethys	2
TD_FCT_GW_CONC_RATIO_HM_CU	1	Tethys	3.3
TD_FCT_GW_CONC_RATIO_HM_NI	1	Tethys	2
TD_FCT_GW_CONC_RATIO_HM_PB	1	Tethys	2
TD_FCT_GW_CONC_RATIO_HM_ZN	1	Tethys	2

Figure 14 – Conversion values between groundwater and tile drain flows in case of heavy metals and arsenic.

2.3.7 Soil concentrations

Metals have been mapped across Europe through several large-scale monitoring surveys. Within the framework of the GEMAS monitoring campaign[12], soil samples were collected in 2008 from agricultural and pasture soils in several Danubian countries, including the Western Balkan countries.

The second major monitoring initiative is the LUCAS soil survey, coordinated by the JRC, which covered most European countries in 2009 and was later extended to Romania and Bulgaria in 2012. However, the Western Balkan countries were excluded from this campaign (although they were covered in 2015, corresponding soil concentration maps are not available).

As the JRC/LUCAS campaign has more extensive spatial coverage and greater methodological consistency, JRC-derived soil concentration maps[13] were used to generate mean soil metal concentrations for analytical units (AUs) within those parts of the Danube River Basin (DRB) covered by the maps. For areas not included in the JRC dataset—namely the Western Balkan countries, Ukraine, and Moldova—GEMAS datasets were used where available, or values were extrapolated from nearby regions.

Due to methodological differences in soil sampling and laboratory analysis between the two monitoring campaigns, transfer functions were developed and applied to harmonize and adjust the concentration values. A detailed description of this procedure is provided in Section 4.3 of Deliverable O2.1. **As a result, a combined map was produced that covers the entire basin and is suitable for deriving mean concentrations for the MoRE model input** (Figure 15). **The derived concentrations are provided in the MoRE data tables in Annex 3.**

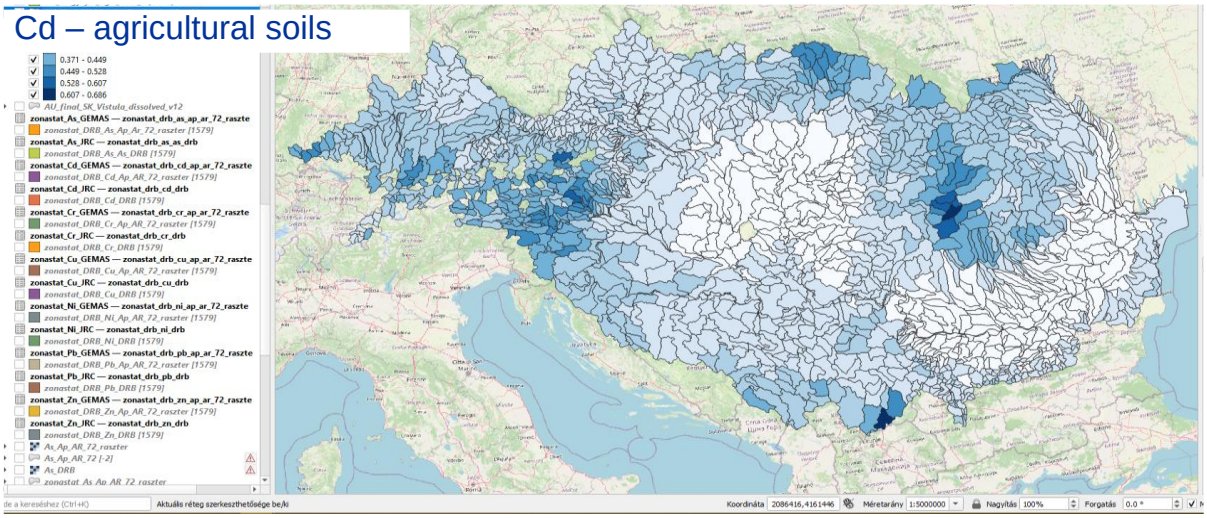


Figure 15 - Cadmium concentration in agricultural soils in the Danube River Basin

The interpolation of soil metal concentrations from point observations is inherently uncertain and depends on the interpolation technique applied. In the JRC mapping process, co-kriging was used, which also resulted in uncertainty maps. However, these uncertainty estimates are expressed in relative terms and are therefore not suitable for deriving quantitative uncertainty ranges or concentration quantiles. Consequently, alternative soil concentration variants are currently not available. Such information may become accessible from the JRC in the future.

2.3.8 Atmospheric deposition (Kata+Zsolt)

Generally, the source of metals in the atmosphere is related to industrial activities, traffic, agriculture, and some other sources. The emitted particles and dissolved phase elements are then transported by atmospheric processes to various parts of the basin or outside of it.

Atmospheric deposition (AD) is given by the sum of two sources:

1. There is a background value, which is determined from the extrapolation of monitoring results carried out for seven pilot sites within the Danube Hazard m^3c project. (Table 16)
2. Hot spot emissions in the vicinity of known aerial sources, such as oil refinery emissions, or chemical industry sites, where these substances are used. The value of the emitted load comes from industrial site emissions (Figure 16).

Table 16– Mean deposition rate values of 7 pilot catchment in the Danube Hazard model

AD_RATE_HM (g/ha/a)	Wulka	Ybbs	Vit	Koppany	Zagyva	Somes	Viseu
As	1.0	1.5	3.2	1.0	0.8	0.8	1.6
Cd	0.3	0.2	0.4	0.1	0.2	0.2	0.3
Cr	1.0	2.9	2.2	4.5	4.8	2.2	0.4
Cu	14.5	30.2	36.6	13.7	25.1	13.2	36.3
Ni	1.4	9.4	3.8	2.4	4.1	5.5	1.4
Pb	3.4	5.3	1.7	0.9	5.6	7.8	3.4
Zn	59.2	156.8	107.4	66.0	59.7	113.7	216.8

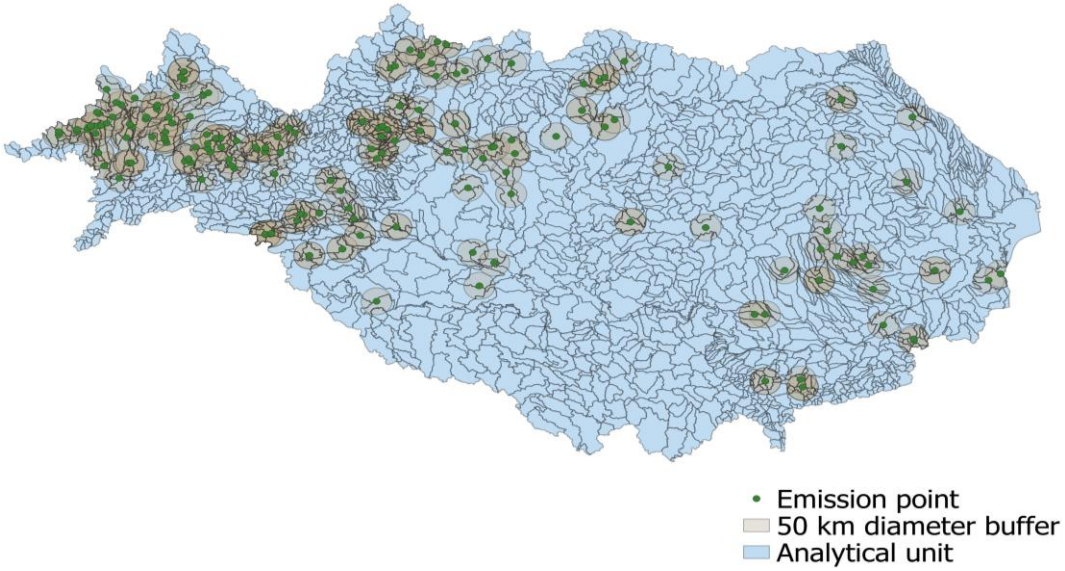


Figure 16 - Industrial site emissions with their 50 km diameter impact area

Atmospheric deposition from the chimneys of the industrial facilities estimated based on their discharged metal load to the air, considered only the 'large combustion plans' and 'waste incinerations'. In the case of measured atmospheric emissions (reported in the E-PRTR), we naturally use the measured results. At those facilities where there was no measurement in the given year, but there was in other years, the average of the measurement results is considered. Where no emission load could be determined based on the above ways, the 'AD Emission Factor' was applied. 'AD Emission Factor' estimate metal emissions to air based on NOx emissions into the air of the given facility with some corrections in low and high NOx emission ranges. (See the details in O2.1. Section 4.2.2.)

The metal emissions into the air of aerial emitters are aggregated for the analytical units. After that, **the deposition load on water surfaces is calculated by the proportion of the water surface area to the whole catchment area** in the model.

2.3.9 Concentrations for hot-spot type point source emissions via groundwater

Currently there are four different types of point sources emissions, where loads are estimated as 'direct groundwater' loads, which is a virtual pathway, as in reality these loads end up in the groundwater and mixing up with the groundwater from different ages and different concentrations, which would result in a different load. In this case the assumption is that the load from these sites directly reach the nearby surface water bodies. This, of course would result in an overestimation of real loads. To compensate for these a retention (or calibration) factor is applied, which with a rough estimation can be set initially to 0.5. Concentrations for these pollution sites come from research literature, which are not entirely from the Danube River Basin, but from the same economic area, including Poland, Serbia, Bosnia&Herzegovina. PFAS values rely on the Promisces database[15]. Concentration values applied, are found in Table 17.

Table 17 - Concentrations used for legacy hot-spots in the MoRE model

Substance	Stat.	Aerodromes	Landfills

[15] Liu, M., Saracevic, E., Oudega, T. J., Obeid, A. A. A., Nagy-Kovács, Z., László, B., Kittlaus, S., Zoboli, O., Krampe, J., Derx, J., & Zessner, M. (2025). Investigating the extent of PFAS contamination in the Upper Danube Basin across environmental compartments. Environmental Sciences Europe, 37(1), 99. https://doi.org/10.1186/s12302-025-01141-6

PFOS (ng/l)	Median	261.6	223.8
	Q25	19.5	110.1
	Q75	1307.9	480
PFOA (ng/l)	Median	25.4	379.7
	Q25	6.5	151
	Q75	67.7	1124.5
As (µg/l)	Median	-	2.8
Cd (µg/l)	Median	-	2.4
Cr (µg/l)	Median	-	8.4
Cu (µg/l)	Median	-	17.8
Ni (µg/l)	Median	-	18
Pb (µg/l)	Median	-	14.7
Zn (µg/l)	Median	-	143

2.4 MODEL VALIDATION

2.4.1 Monitoring data used

Model validation was based on a combination of large-scale monitoring programmes and project-specific datasets covering both water quality and discharge information across the Danube River Basin.

Concentration data were derived from multiple sources, including the Danube Hazard m^3c inventory, the Transnational Monitoring Network (TNMN), the Joint Danube Surveys (JDS3 and JDS4), and the Tethys project. Together, these datasets provided complementary spatial and temporal coverage for metals, pharmaceuticals, and PFAS in surface waters.

Two main validation configurations were applied. JDS-based validation relied on datasets representing low-flow summer conditions, while validation under mean discharge conditions combined monitoring data from TNMN, Danube Hazard m^3c, and Tethys.

Discharge data used for load calculations were primarily obtained from the Danube Water Balance (DWB) project, providing measured daily flow data for a large number of stations. These data were complemented by model-based discharge estimates from CWatM and long-term reference discharges from the ICPDR–MONERIS framework. The combined use of measured and modeled discharge datasets ensured consistent hydrological support for load estimation and validation across different spatial scales.

A more detailed description of the datasets used is provided **in Sections 6.1 and 6.2 of O2.1.**

2.4.2 River load calculation - Timi

The preparation of validation data was carried out through a structured, multi-step workflow implemented in R, combining water quality monitoring data with discharge information at the scale of the MoRE model analytical units (AUs).

The process included the pre-selection and filtering of concentration data, the separate handling of total and dissolved fractions, and the generation of distinct validation outputs for JDS-based datasets and for datasets representing mean discharge conditions. Monitoring stations and discharge stations

were spatially linked to analytical units using a manual review process, with particular attention paid to station location relative to AU outlets and to the hierarchical structure of the AU system.

Concentration data were statistically processed to derive annual and long-term summary values, including the explicit treatment of censored data using the Regression on Order Statistics (ROS) method under defined conditions. Discharge data were prepared from daily time series, applying quality-controlled aggregation and campaign-specific averaging for the JDS3 and JDS4 survey periods.

Finally, concentration and discharge data were combined to calculate annual and long-term loads using multiple discharge scenarios.

A detailed description of the individual processing steps, selection criteria, and calculation methods is provided in **Section 6.3 of O2.1**.

An overview of the number of selected monitoring points for validation and the share of stations with long-term average concentrations below the limit of quantification (LOQ) can be seen in Table 18.

Table 18 : The total number of available monitoring stations and the subset selected for validation were quantified for each substance

Substance	Number of monitoring points (total form)	Share of monitoring points with avarage concentrations <LOQ (total form)	Number of monitoing points (dissolved form)	Share of monitoring points with avarage concentrations <LOQ (dissolved form)
Cr	239	25%	324	60%
Ni	240	13%	326	20%
Cu	236	5%	326	9%
Zn	240	8%	324	14%
As	237	14%	326	14%
Cd	239	68%	318	69%
Pb	240	24%	326	59%
PFOA	165	41%		
PFOS	197	21%		
CBZ	123	6%		
DCF	138	9%		

2.4.3 Results of the validation

Model validation has been done on annual bases. For heavy metals, the 6 years modelling period provided enough data for validation, for pharmaceuticals and PFAS the period had to be extended to the latest monitoring results from the Tethys project. In the latter case, average annual concentrations had been paired with annual discharge.

The annual data results pointclouds with relatively small variations around the mean values. To show regionality, country codes has been also shown as labels to each points.

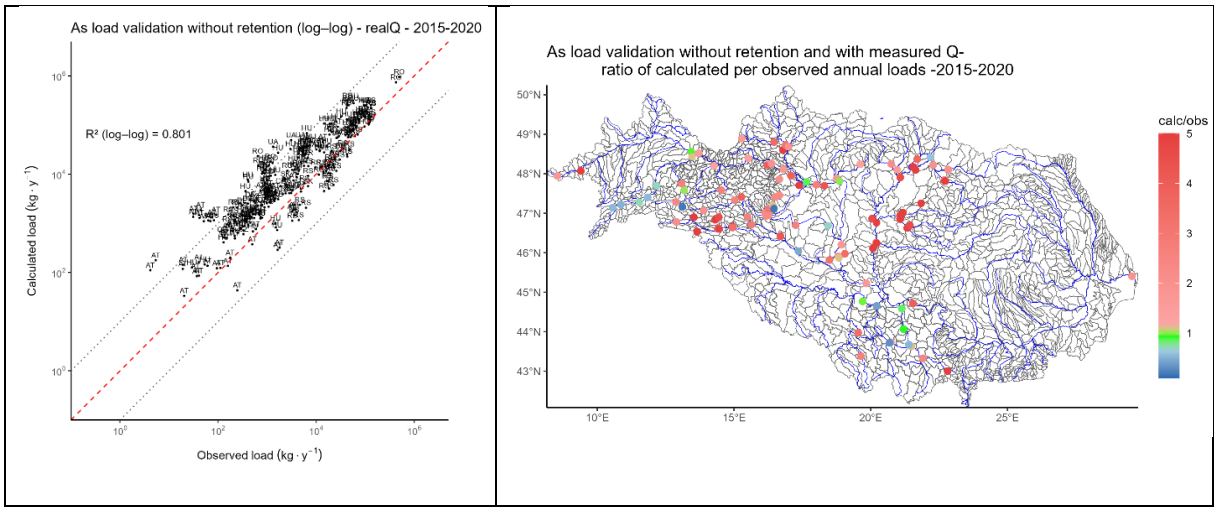
For the first validation run of the model, riverine retention has been turned off. The reason for this is that retention for each substance may vary significantly compared to nutrient retention, for which the original retention calculation of the Moneris model has been designed for. This is practical in the sense that one factor of uncertainty is removed from the model. This way we may also see clearly, if there is underestimation of emissions from analytical units at certain regions. As it is quite certain that some

of the emitted materials is retained in the river systems (by settling of particular phase pollutants), a good model should show slight overestimation of the river loads compared to actual measured loads.

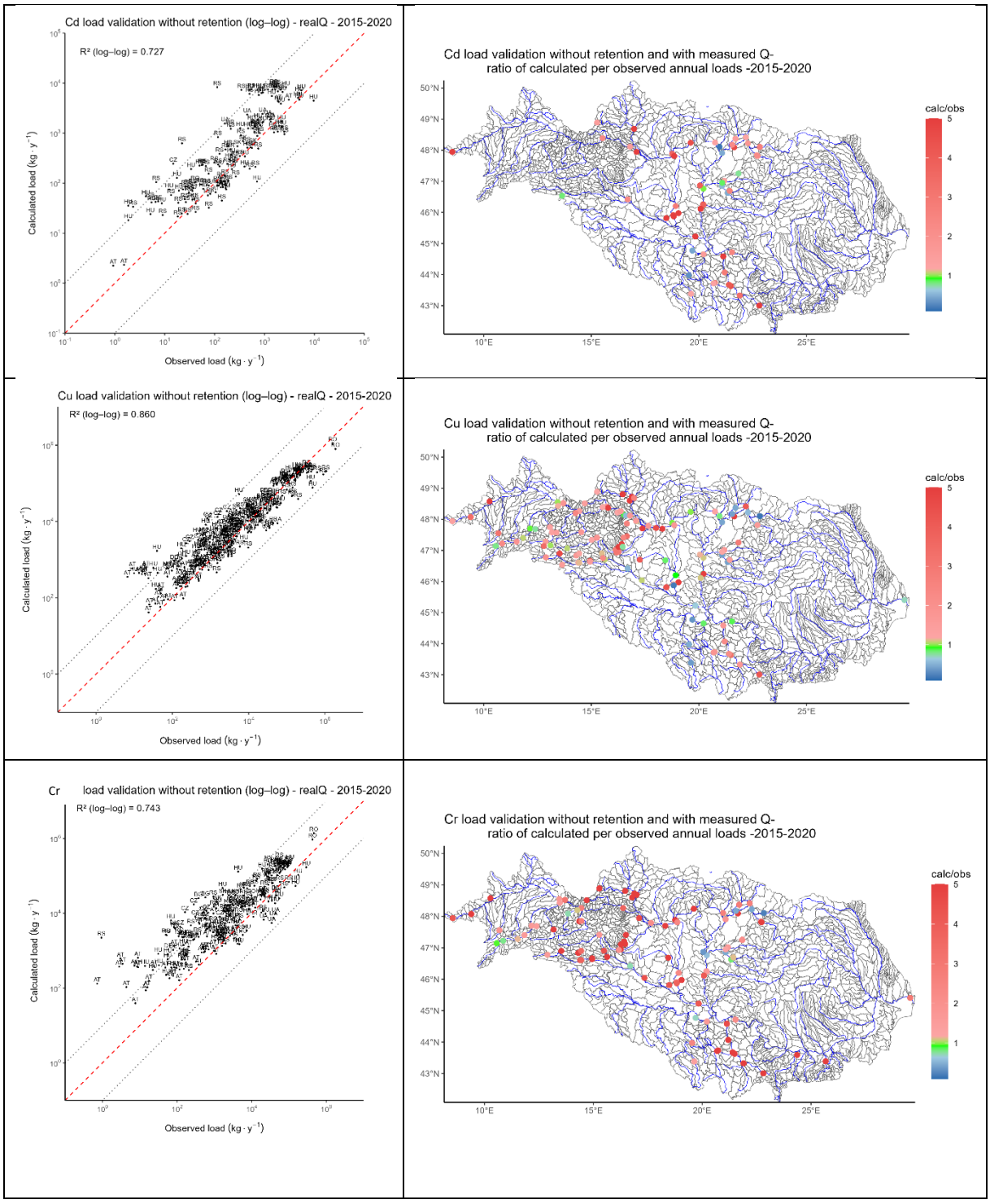
In the case of metalloids (Table 19), we see this slight overestimation for most substances. The only substance that seems to be underestimated (in average terms) is copper, as in the highest load range the loads are just met by the measured loads, or rather underestimate loads. The underestimation, in the case of copper shows underestimation at certain regions of the basin (Drava, Sava, Drina, upper Tisza), while show a fair overestimation at the upper Danube and Criș Rivers (Körösök). There are other signs of underestimation: arsenic is underestimated in the Inn catchment, and also in the Velika Morava catchment (Republic of Serbia, RS). This pattern of underestimation appears for other metals, which clearly highlights area, where higher concentrations in soils are present. These are areas, where minerals rich in some of these metals appear in the geological formations. This also means that mining activities are present, which are included in the model as point source loads, but actual emission levels might be also underestimated. In case of the Somes and Vit catchments this kind of underestimation became clear in the Danube Hazard m3c project[16]. The revision of industrial loads from operating and abandoned mines seems to be necessary.

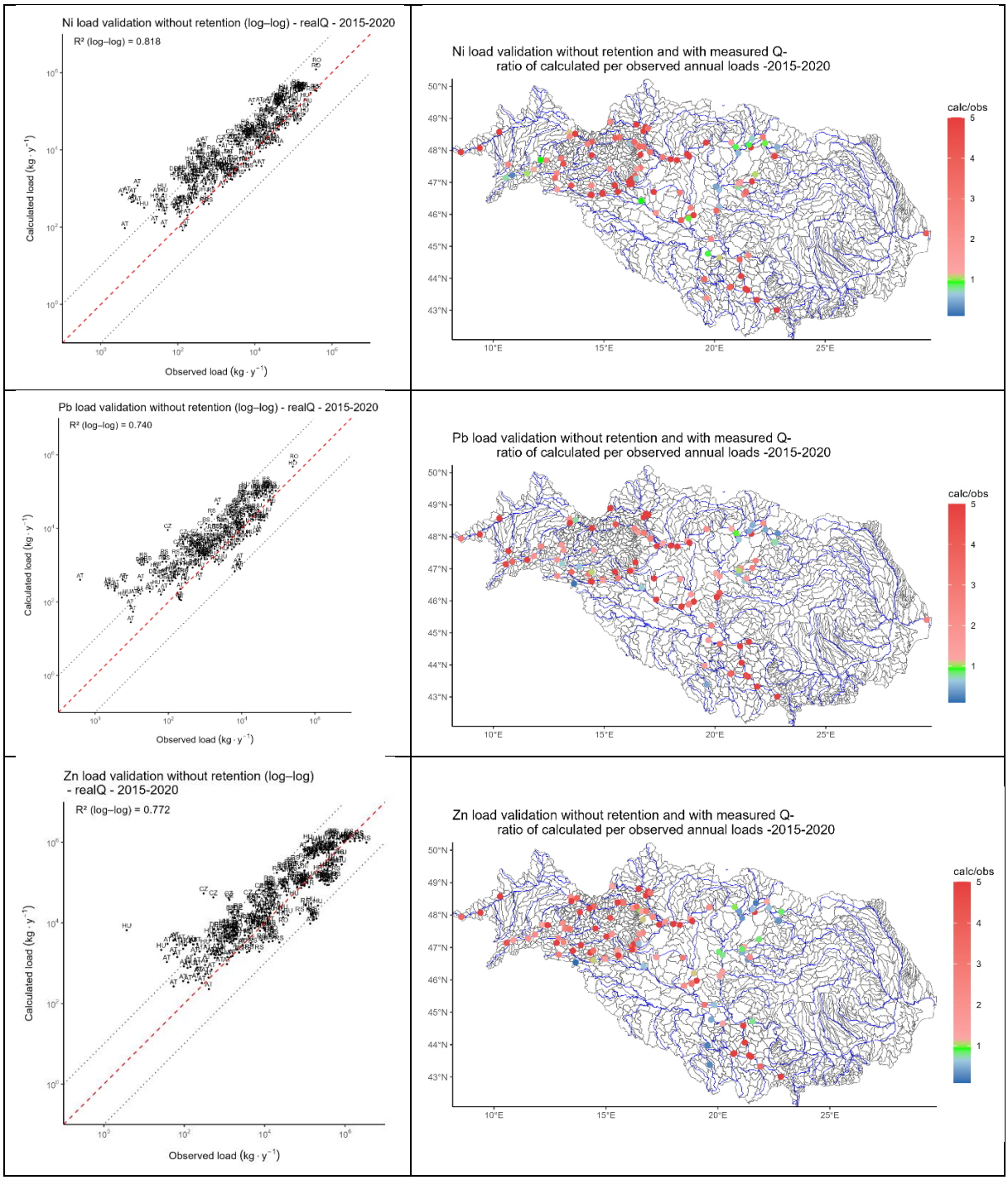
Overestimation also seems to be present for most metals. *Arsenic* shows overestimation in the Criș River system and at the lower Tisza section and at the upper Drava. *Cadmium* may be overestimated in the upper Danube, including the Morava (CZ) and the Drava. Clear signs of overestimation is not present for *copper*, apart from the areas, where it is underestimated, it seems to be balanced across the basin. In the case of chromium, overestimation seems to be more pronounced at the Velika Morava catchment (RS), the upper Drava, Raba, the upper Danube (DE section) and the Morava catchments. As the contribution of the sources in the total loads are different for these catchments, no common reason can be identified behind these, it might be unique at each catchment. The pattern for *nickel* is very similar to *chromium*, the difference is that the share of municipal point source load is higher in this case. *Lead* and *zinc* also show overestimation at the same catchments, while the share of loads between the pathways are different.

Table 19 – Validation results for 6 heavy metals and arsenic, without taking into account retention in river systems



[16] Gabriel, O., & Broer, M. B. (2023). Report on improved system understanding as basis for adapted transnational emission modelling at DRB scale - O T2.2 - Output Danube Hazard m3c project. https://dtp.interreg-danube.eu/uploads/media/approved_project_output/0001/56/52b44806c4c7637a97f77af4f9476a043bbcee60.pdf


Cd load validation without retention (log–log) - realQ - 2015-2020
R² (log–log) = 0.727
Calculated load (kg · y⁻¹)
Observed load (kg · y⁻¹)
Cd load validation without retention and with measured Q-
ratio of calculated per observed annual loads -2015-2020
calc/obs
Cu load validation without retention (log–log) - realQ - 2015-2020
R² (log–log) = 0.860
Calculated load (kg · y⁻¹)
Observed load (kg · y⁻¹)
Cu load validation without retention and with measured Q-
ratio of calculated per observed annual loads -2015-2020
calc/obs
Cr load validation without retention (log–log) - realQ - 2015-2020
R² (log–log) = 0.743
Calculated load (kg · y⁻¹)
Observed load (kg · y⁻¹)
Cr load validation without retention and with measured Q-
ratio of calculated per observed annual loads -2015-2020
calc/obs

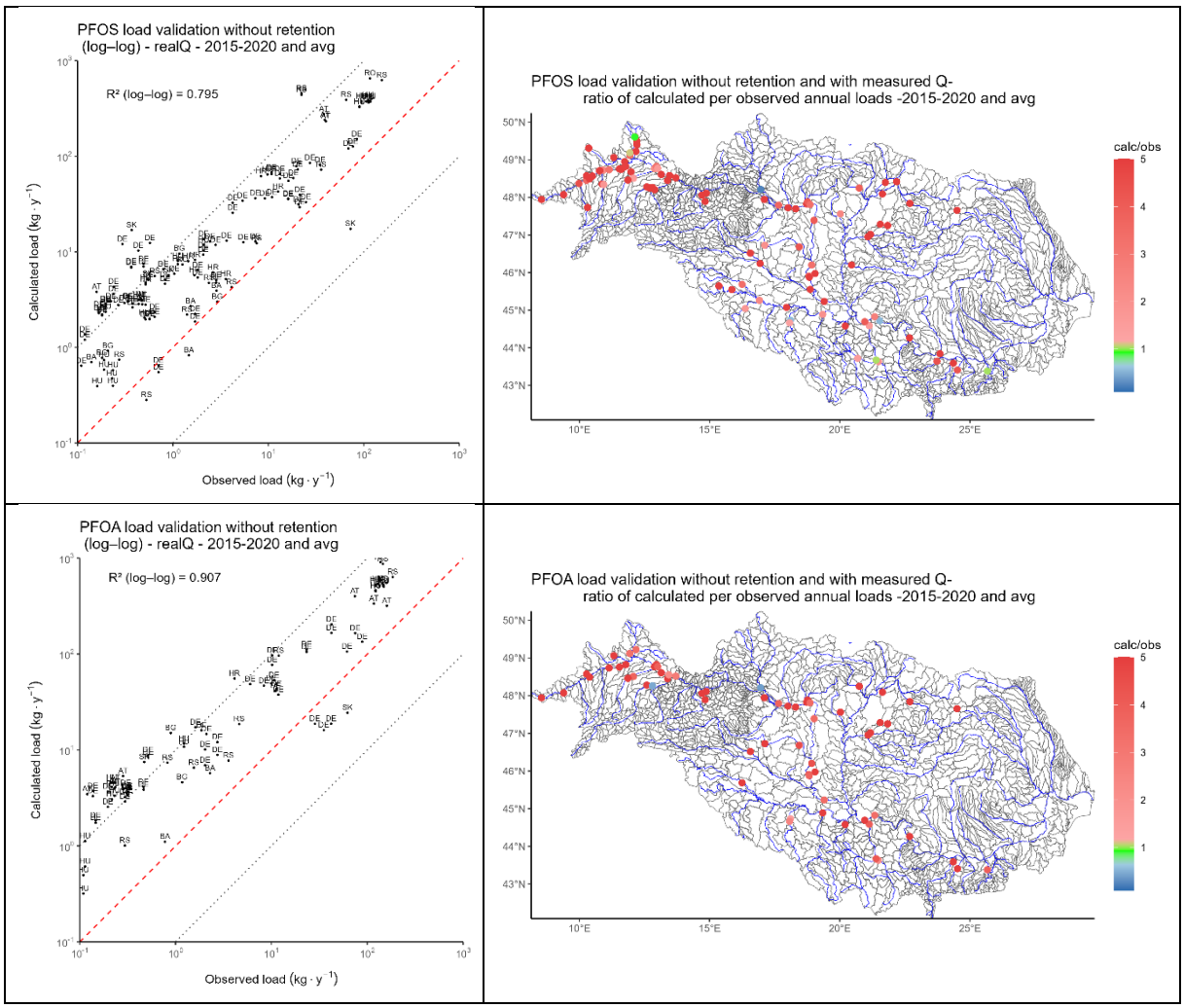


PFAS validation results

The estimation of loads for PFAS substances is much more uncertain than for metals or pharmaceuticals due to the ubiquitous presence of these materials in small concentrations but also present in high concentrations at hot-spot legacy pollution sites. The uneven distribution and scarcity of monitoring data also put a burden on the high-quality validation of the model. Nevertheless, validation of this

substance is possible as it was proved by earlier model applications[17]. The current results (Table 20) show clear overestimation of both modelled substances in a very unbalanced way.

Table 20 - Validation results for PFOS and PFOA for the entire DRB



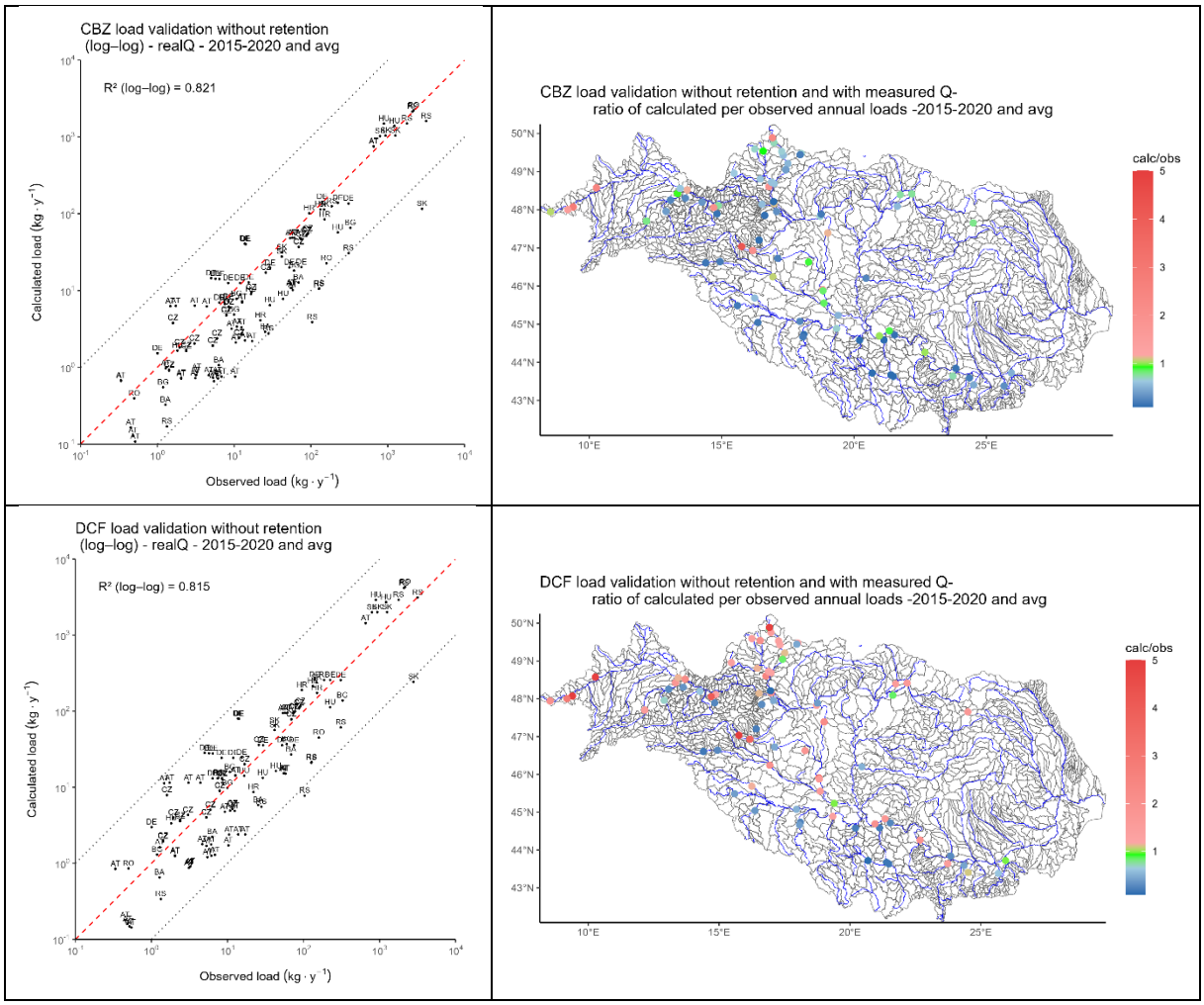
Pharmaceutical validation results

Pharmaceutical compounds are slightly more evident in terms of loads as there are much less pathways (municipal and industrial waste water, and some hot-spots), where these substances can enter into our rivers in significant quantities. The two compounds differ slightly in their behaviour, while *carbamazepine* is a very conservative pollutant, not subject to relevant retention during treatment or in the river systems, *diclophenac* is subject to photodegradation and also some retention during treatment of waste water. Therefore, our current validation result (Table 21) can be interpreted as an underestimation for both chemicals. While the estimation of carbamazepine is very accurate at high loads, at lower load ranges underestimation occurs, especially in the Western Balkan countries, but also slightly in the upper-Danube catchment. *Diclophenac* load estimation also shows an uneven performance. There is a clear underestimation of loads in the Western Balkans, especially in the Bosnian tributaries

[17] Kittlaus, S., Clara, M., van Gils, J., Gabriel, O., Broer, M. B., Hochedlinger, G., Trautvetter, H., Hepp, G., Krampe, J., Zessner, M., & Zoboli, O. (2022). Coupling a pathway-oriented approach with tailor-made monitoring as key to well-performing regionalized modelling of PFAS emissions and river concentrations. Science of The Total Environment, 849, 157764. https://doi.org/https://doi.org/10.1016/j.scitotenv.2022.157764

of the Sava River and the Velika Morava River, but also in the upper Drava, while it is slightly overestimated in the middle and upper section of the Danube, which seems to be in the right order (rate of overestimation is less than 2) considering that retention is not accounted for in this analysis. Spatial differentiation of inhabitant specific emissions or waste water concentrations has to be revised and tested and base concentration values to be revised.

Table 21 - Validation results for carbamazepine and diclophenac for the entire DRB



3 OVERVIEW OF THE RESULTS

3.1 RESULTS OF METALS

3.1.1 Calculated total metal emissions by pathways

Depending on the substance and location, erosion, groundwater, and wastewater plants represent the highest share in the emissions (Figure 17). Besides these, industrial direct emissions and urban systems can also have a substantial role. The amount delivered by surface runoff, and tile drainages is in contrary in most cases minor. The amount delivered by atmospheric deposition is close to zero except for Cd and Pb, where it is still minor.

For As, groundwater is the most important pathway, followed by erosion and wastewater plants. For Cd, the picture is more scattered: besides the previous three pathways, industrial direct emissions also have some role. For Cr, the list is extended by the urban systems. For Cu, urban systems are not so important; the most amount is delivered by erosion (upstream tributaries) or wastewater plants (downstream tributaries). On some catchments (Lower Sava and Timok), the industrial direct emissions are extraordinarily high. For Ni, the picture is similar to that of Cr, but tendentially the share of erosion is lower whereas the share of WWTPs is higher; urban systems don't play a role; besides these two, groundwater is an important pathway and industrial direct emissions also have some, although minor share in the total emissions. Pb mostly originates from erosion, but groundwater, industries and WWTP-s also play some role. For Zn, the picture is complex. The highest amounts are delivered by erosion, groundwater, industries, and wastewater plants, but – except for atmospheric deposition and tile drainages – all pathways come into picture.

A general tendency is, that – as we go from the Upper-Danube to the Lower Danube, the share of point sources decreases whereas that of diffuse sources (in general primarily erosion and groundwater) increases. For some substances (especially Ni) the municipal point sources can have a share as high as 80% in top-most 6 tributaries' catchments (Iller, Lech, Altmühl, Naab, Regen and Isaar). For Zn, the picture is similar, although the share here is 60-70%.

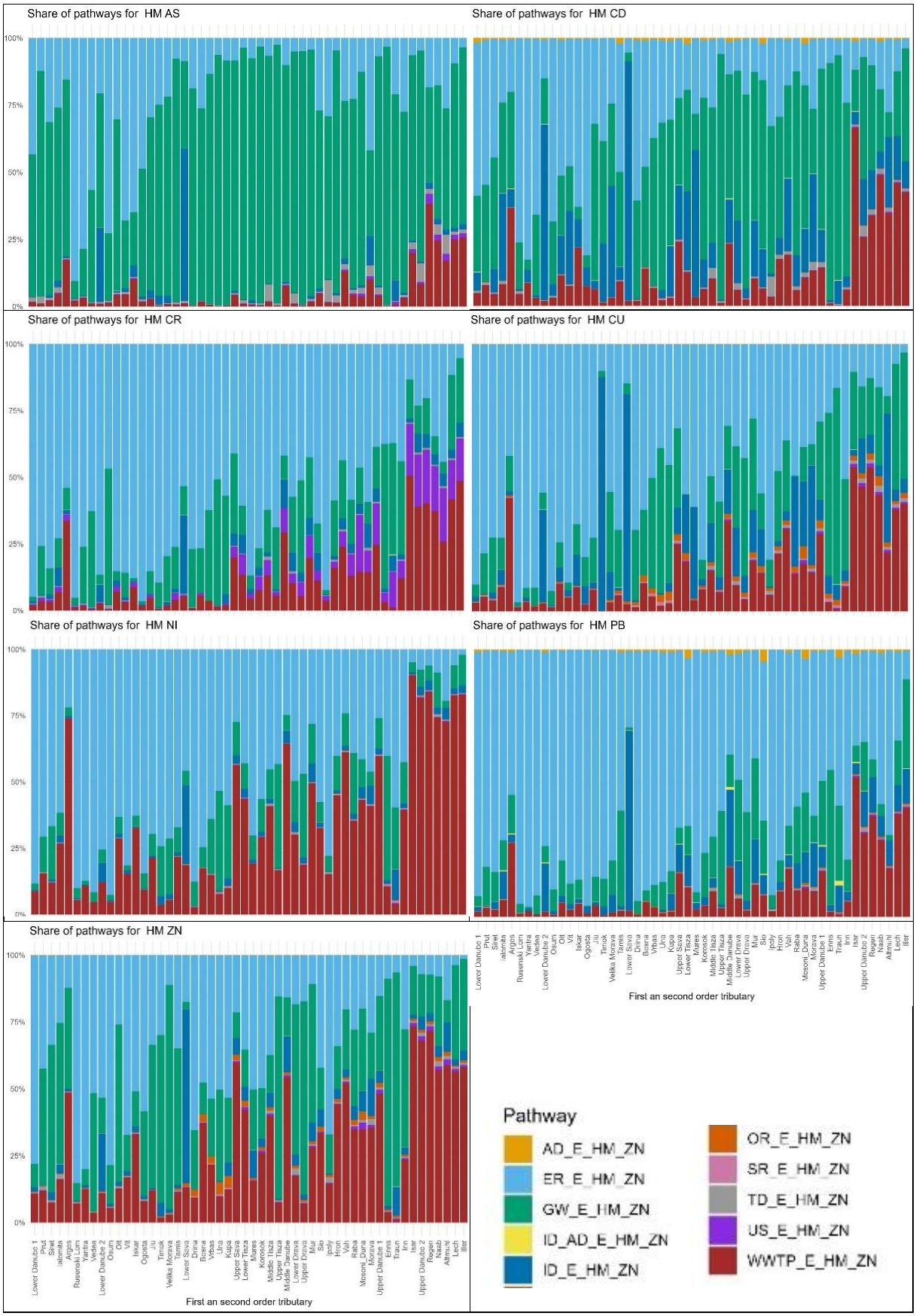


Figure 17 - Share of pathways in the total emissions of the DRB (local emissions) of heavy metals. AA – inputs via groundwater impacted by aerodrome conducting fire-fighting activities; AD – Inputs via atmospheric deposition on water surfaces; ER – Inputs from erosion; GW – Inputs from groundwater; ID – Emissions from industrial direct dischargers; OR – Non-urban roads; SR – Surface runoff; TD – tile drainages; US – urban sewer systems; WWTP – emissions via municipal wastewater treatment plants.

3.1.2 Maps of specific emissions for total metals

Here we report about the geographical pattern in total HM emissions (Figure 18). The dissolved HM emissions indicate similar patterns. Besides the total emissions, maps for the unique pathways were also created and can be found in Annex V.

All seven metals indicated different geographical patterns. For As, the lower Pannonian region as well as the high Alps show higher emissions. For Cd, the effect (emission coming from) the northern Transilvanian mining region can be observed as well as some major towns in the central south: Belgrade and Timisoara. For Cr, Cu and Pb, the Lower Danube, Bulgaria shows higher emissions than most other regions. For Ni, the differences between regions are smaller than for the other metals. For Zn, two regions indicate lower emissions than most of the basin: the North-Austrian part, Bosnia and Herzegovina and the middle and lower Tisa valley.

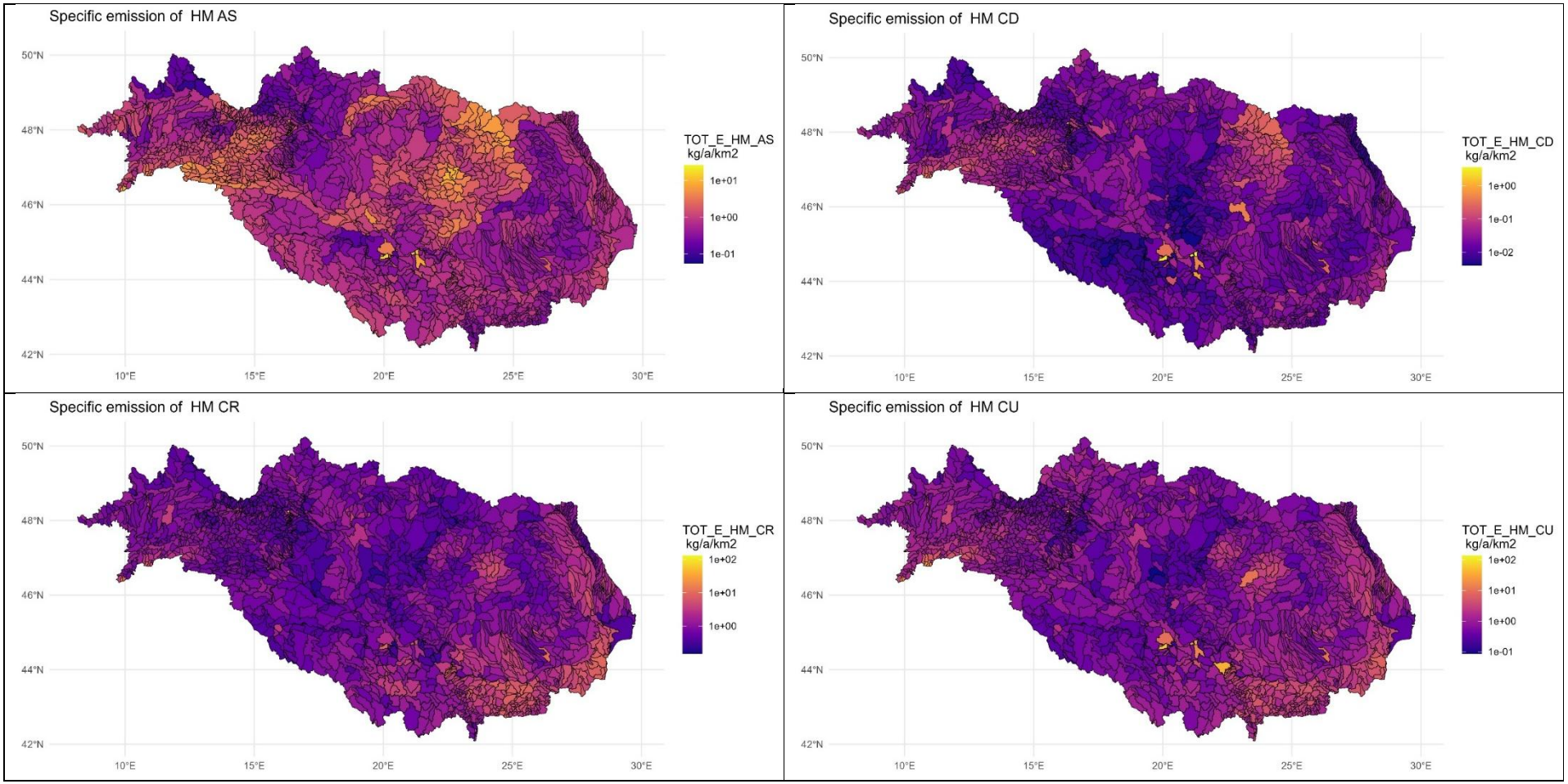


Figure 18 - Total Heavy metal emissions in the Danube River Basin (As, Cd, Cr and Cu).

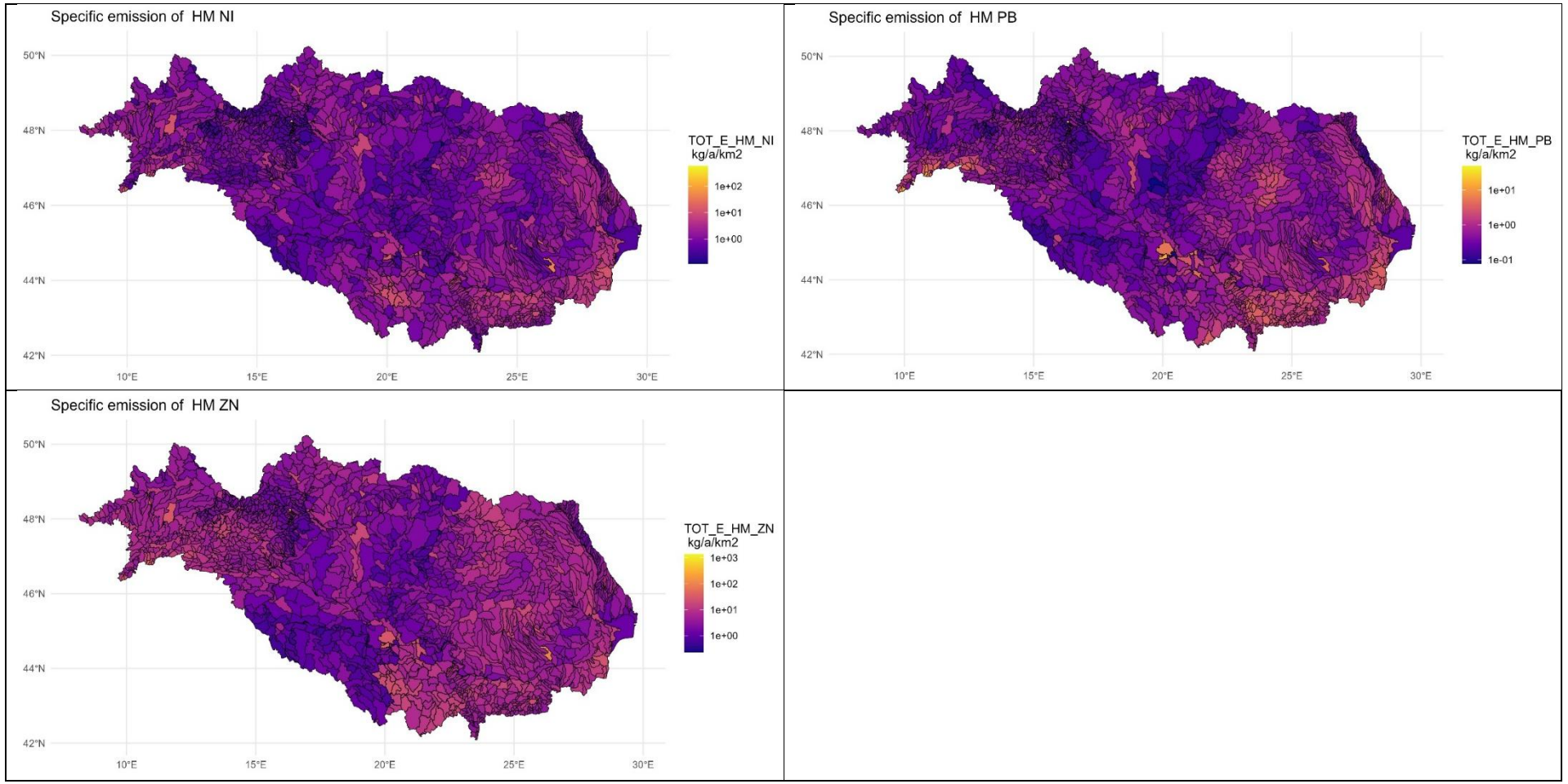


Figure xx. Total Heavy metal emissions in the Danube River Basin (Ni, Pb and Zn).

3.2 RESULTS OF PFAS

3.2.1 Calculated emissions by pathways

Following bar charts visualize the share of the various pathways in the total emissions over the Danube River Basin (Figure 19). The picture is very similar for the two compounds. For both compounds, the two most important pathways are groundwater and wastewater plants, followed by surface runoff. Depending on the location, industries, non-urban roads, tile drainages and urban systems also have share. The only major difference between the two substances is, that for PFOS, aerodromes have some share in the emissions. In contrast to heavy metals, there is no general geographical tendency. The role of wastewaters is very scattered: it varies between 10 and 75%.

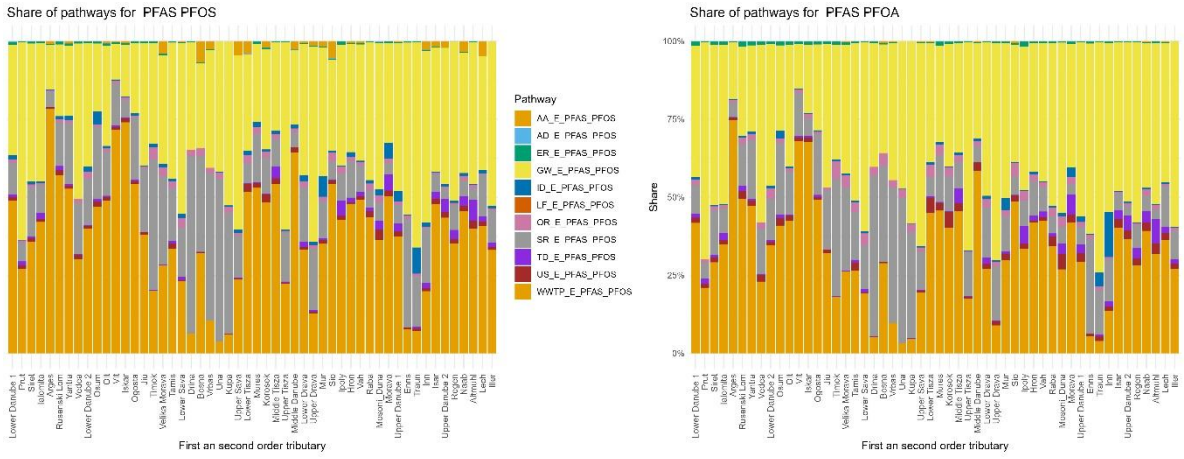


Figure 19 - Share of pathways in the total emissions of the DRB (local emissions) of heavy PFAS. AA – inputs via groundwater impacted by aerodrome conducting fire-fighting activities; AD – Inputs via atmospheric deposition on water surfaces; ER – Inputs from erosion; GW – Inputs from groundwater; ID – Emissions from industrial direct dischargers; OR – Non-urban roads; SR – Surface runoff; TD – tile drainages; US – urban sewer systems; WWTP – emissions via municipal wastewater treatment plants.

3.2.2 Maps of specific emissions

Total PFAS emissions are substantially higher in the upper Danube Basin (primarily Germany) than in most other parts of the Basin (Figure 20). In Upper-Austria, the total emissions can be very significant even in adjacent sub-catchments, which is due to the difference in tile drainage and groundwater emissions. The Northern-Romanian mining regions can also be observed. Economically less developed regions like Moldova, Eastern-Romania and the southern part of the basin indicate lower emissions.

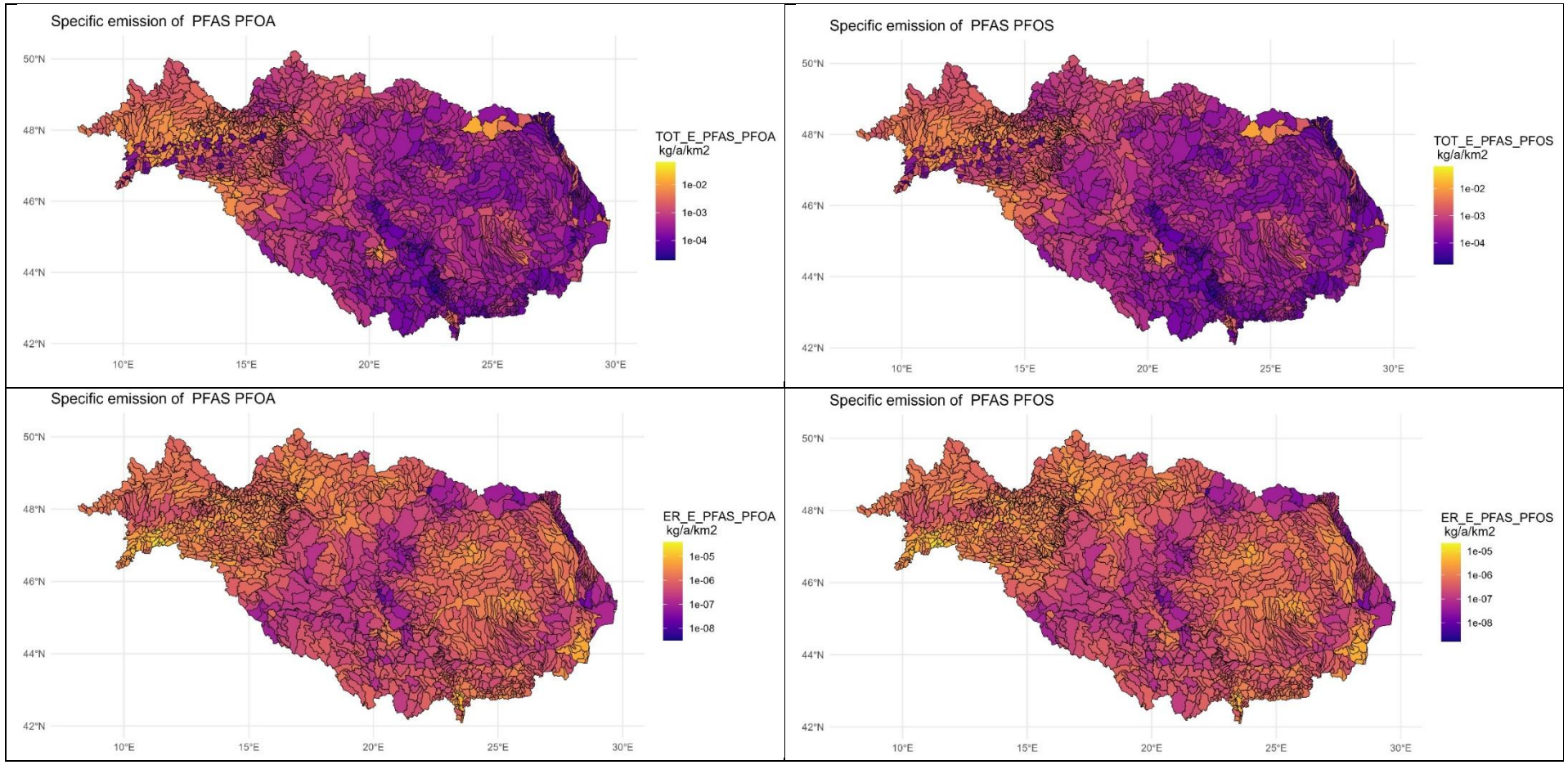


Figure 20 - PFAS emissions in the Danube River Basin: totals (all pathways) and through the erosion pathway.

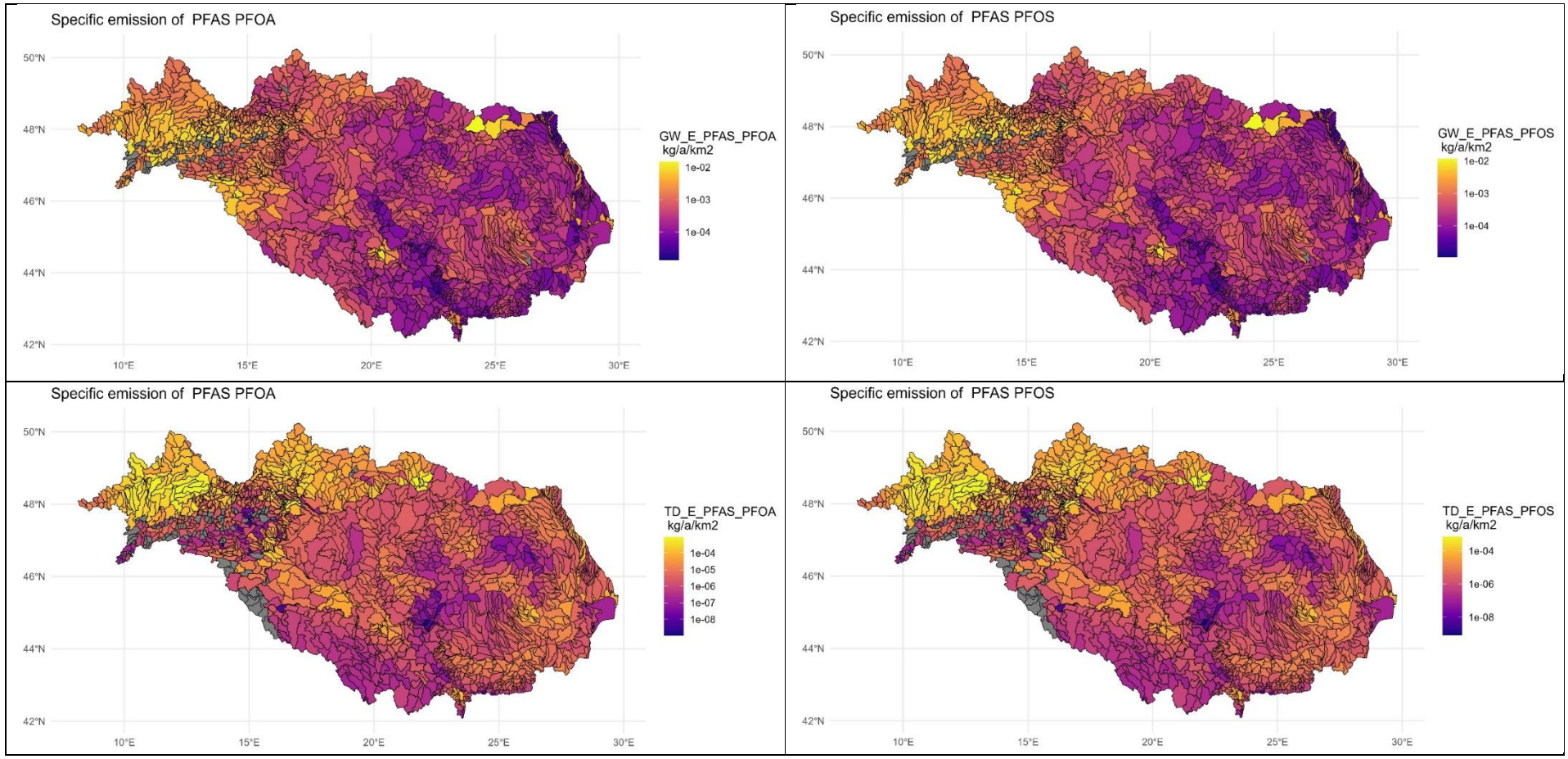


Figure 21 - PFAS emissions in the Danube River Basin through the groundwater and tile drainages pathways.

3.3 RESULTS OF PHARMACEUTICALS

3.3.1 Calculated emissions by pathways

For pharmaceuticals, the picture is simpler compared to the previous substances (Figure 22). Only four pathways play any role in the total emissions: groundwater, industries, urban systems and wastewater plants. The two investigated pharmaceuticals: carbamazepine and diclofenac indicate in general a very similar picture. For both of them, the most important pathway is wastewater plants except for two catchments, where the wastewater share is really low (Traun and Kamp for Carbamazepine and Kamp for Diclofenac). The role of industries is the highest in these two catchments and the Rusenski Lom. The role of urban systems is between 10-20% in most tributaries.

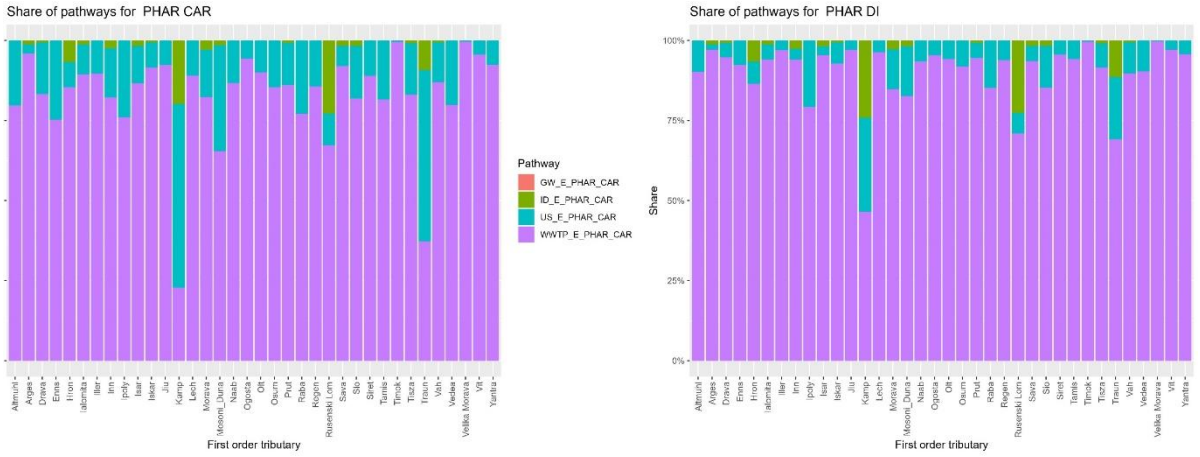
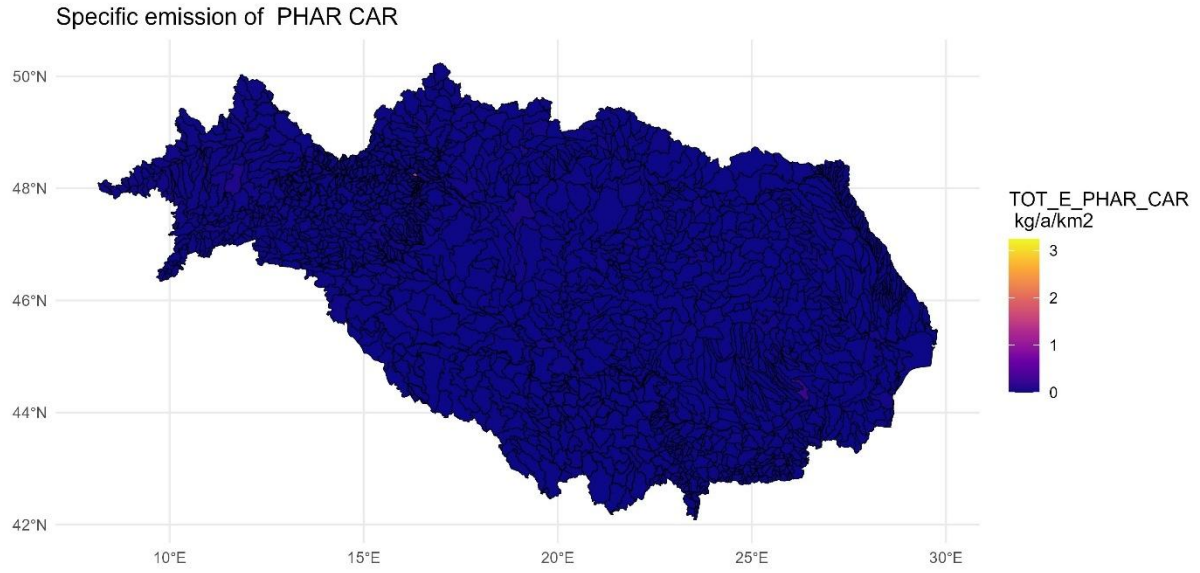


Figure 22 - Share of pathways in the total emissions of the DRB (local emissions) of pharmaceuticals. AA – inputs via groundwater impacted by aerodrome conducting fire-fighting activities; AD – Inputs via atmospheric deposition on water surfaces; ER – Inputs from erosion; GW – Inputs from groundwater; ID – Emissions from industrial direct dischargers; OR – Non-urban roads; SR – Surface runoff; TD – tile drainages; US – urban sewer systems; WWTP – emissions via municipal wastewater treatment plants.

3.3.2 Maps of specific emissions

Maps of total emissions of pharmaceuticals don't indicate a too visible pattern, except that the largest cities (Vienna and Bucharest) draw out (Figure 23).



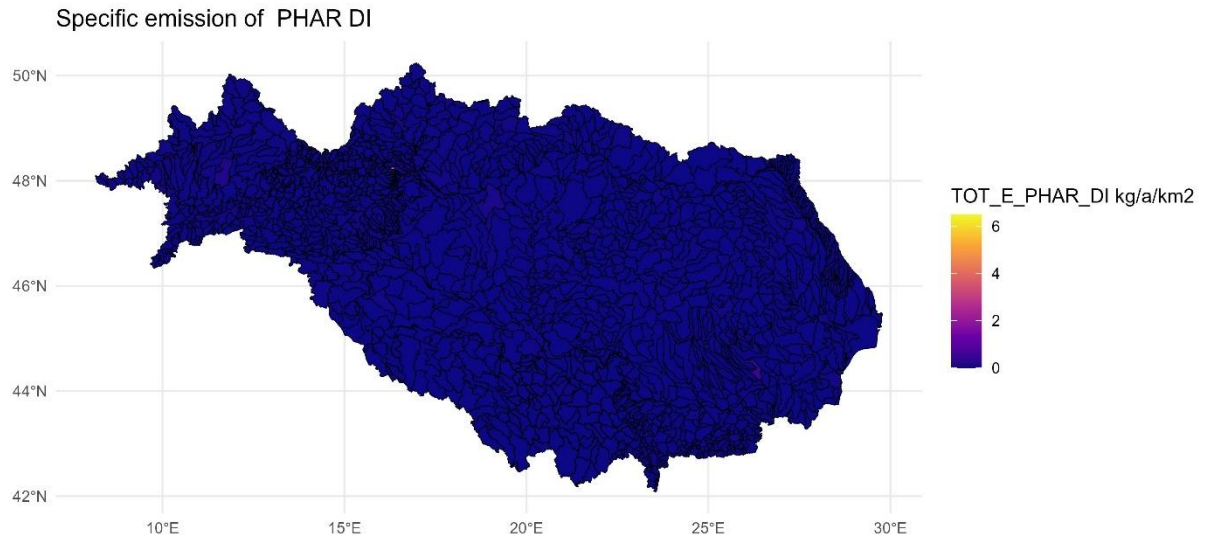


Figure 23 - Pharmaceutical emissions in the Danube River Basin: sum of all pathways.

4 TECHNICAL IMPLEMENTATION OF THE SCENARIOS WITHIN THE MODEL

Scenarios can be implemented in multiple ways in the MoRE model.

One of the most convenient ways is through variants, which are a set of input parameters that represent one type of input data set, for example in case of climate scenarios, multiple runoff data sets can be implemented with different variant names: e.g. Current condition, future condition.

Scenarios can be also implemented by specific built-in variables, such as variables for measures. These can be used for emission reduction scenarios. In the current model version, there are measure variables (highlighted in bold) present for the CSO and SS pathways of urban systems:

US_cso_E_HM = if(BI_CODE_coun=>100, 0,US_cso_Q * US_cso_CONC_FUN * (1- (**MM_US_cso_EFF_FS** /100 * US_KD_FUN / 1000 * US_cso_CONC_FS / 1000) / (1 + US_KD_FUN / 1000 * US_cso_CONC_FS / 1000)) /1000 /1000)

US_ss_E_HM = if(BI_CODE_coun=>100,0,US_ss_Q * US_ss_CONC_HM * (1- (**MM_US_ss_EFF_FS** /100 * US_KD_HM / 1000 * US_ss_CONC_FS / 1000) / (1 + US_KD_HM / 1000 * US_ss_CONC_FS / 1000))/1000 /1000)

Pollution reduction scenario for atmospheric deposition is also available (MM_AD_RATE_dep_red_HM) that influences multiple pathways, atmospheric deposition (AD), surface runoff (SR) and open road runoff (OR):

SR_E_HM = SR_Q * 86400 * 365 * SR_CONC_HM * (1- **MM_AD_RATE_dep_red_HM** /100) / 1000 / 1000

OR_E_HM = (OR_SFL_HM - MM_AD_RATE_dep_red_HM /100 * BI_RATE_dep_HM) * IM_A_OR_qsr / 10

AD_E_HM = BI_RATE_dep_HM * (1- **MM_AD_RATE_dep_red_HM** / 100) * IM_A_WS / 10

Erosion control can be also implemented this way, unless we implement a different set of C factors in the model.

ER_agrl_E_HM = (ER_agrl_SL_AL * ER_agrl_CONT_SOIL_top_AL_HM * (1 - **MM_ER_EFF_AL_SED** / 100) + ER_agrl_SL_PST * ER_agrl_CONT_SOIL_top_PST_HM) * ER_SDR * 0.01 * ER_ENR_AL / 1000

The last way to implement a scenario is to introduce calculation of alternatives. In the current model, such alternative is present for a lot of pathways, for example, the estimation of wastewater loads, where loads can be calculated based on single concentration values (variant 2), or by wastewater plant treatment stages (variant 3):

variant	formula content
1	if(WWTP_ps_CP >= MM_WWTP_CP_min_TS4, WWTP_CONC_HM * (1 - MM_WWTP_EFF_HM / 100), WWTP_CONC_HM)
2	WWTP_ps_Q * WWTP_CONC_HM/1000000
3	if(WWTP_treatment_type=0,WWTP_ps_Q*WWTP_CONC_NOTREAT_HM*10^-6,if(WWTP_treatment_type = 1,WWTP_ps_Q*WWTP_CONC_PRIM_HM*10^-6,if(WWTP_treatment_type = 2,

Figure 24 – Example of formula variants to implement scenarios

5 ANNEXES

5.1 ANNEX 1 - DESCRIPTION OF MODEL ALGORITHMS

5.1.1 Analytical units, runoff routing

The MoRE model calculates emissions for analytical units (AU), these are the units of aggregation in the model, variables within this unit is constant, therefore the resolution of the model outputs will be equal of the resolution of the AUs. Most data is defined for these units in the preprocessing steps, e.g. the soil concentration for an AU is determined from base soil concentration maps with finer resolution by statistical methods (mean, median or quantiles in most cases). The sizes of the analytical units of the Danube River Basin (DRB) varies country by country with smallest sizes in Austria and larges sizes in Hungary, Romania and the countries in the western Balkans (Figure 25). The Danube River Basin contains 1727 units in total. The average area of the units is 468.6 km^2, while the median value is 322 km^2.

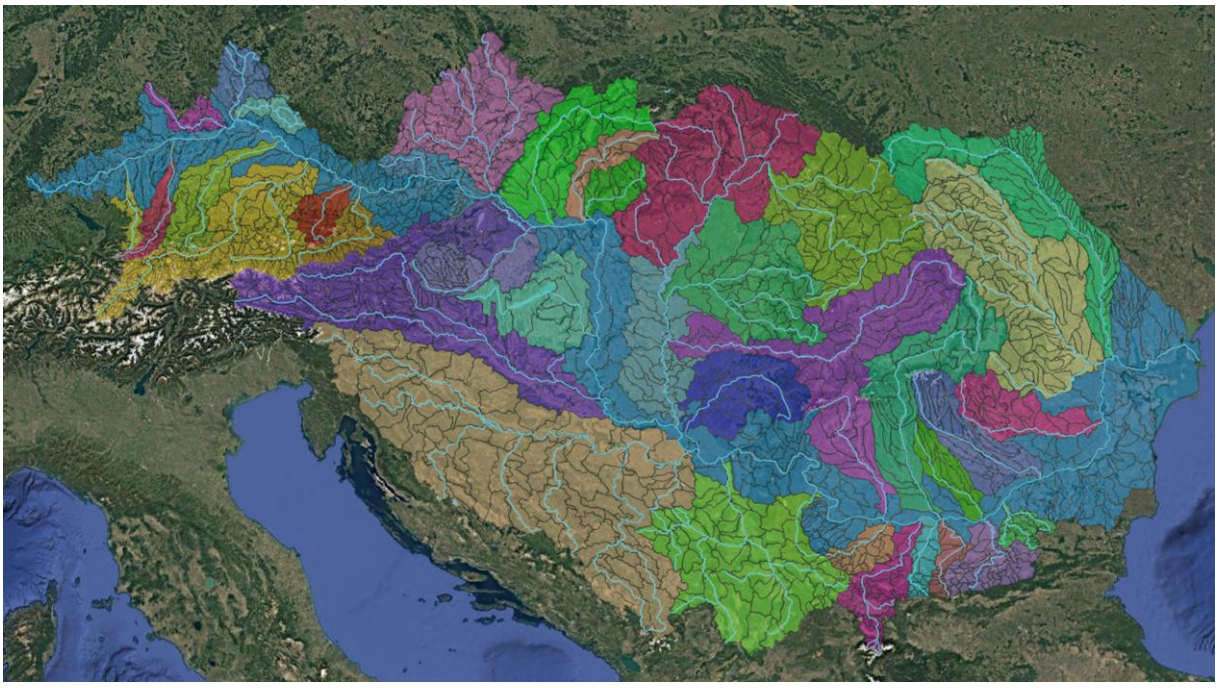


Figure 25 – Analytical units in the DRB for the MoRE model in the Tethys project. Colouring refer to separate subbasins.

Runoff and river loads are aggregated in the model by a built-in aggregation scheme of the MoRE model, called *more_rl_upstr*, which follows the hydrological tree by the defined downstream id variable (input data).

An example is shown below, where total runoff is aggregated:

TOT_FNE_Q = more_rl_upstr(TOT_FNE_Q) + if(IM_Q < 0, BI_Q_net, IM_Q)

The function is preparing the hydrological tree for each Aus and aggregate the loads, then adds the total runoff from the AU itself (BI_Q_net).

There is a testing scheme in the model, where this runoff hierarchy is built, which also checks if the input data is correct or not. This function is called the runoff routing, which can be utilized for the selected analytical units by clicking the tools option (Figure 26).

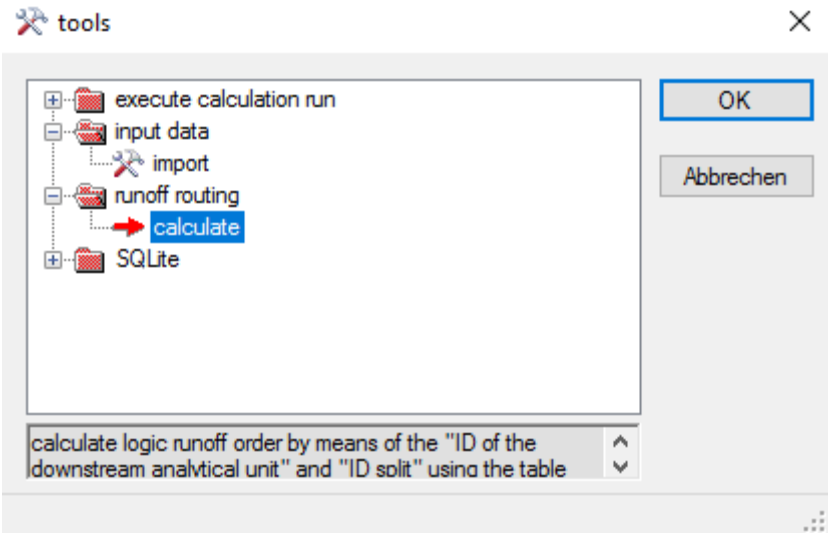


Figure 26 – pop-up window in the MoRE model GUI to start model calculations

5.1.2 Calculation of land use balance

Proper land use information is important as the areas associated with the specific pathways are primary information in the model calculations. Apart from primary input data, such as area of agricultural land, or water surfaces, secondary or intermediate information has to be calculated. In the model this preprocessing step can be done using the algorithm building tool of the model (MoRE user manual[18], Figure 27,Figure 28 Figure 28, Figure 29), in which a sequential calculation of defined algorithms takes place.

[18] Fuchs, S., Wander, R., Rogozina, T., & Hilgert, S. (2011). Modeling of Regionalized Emissions (MoRE) - Developer and Visualizer user interfaces - Manual.

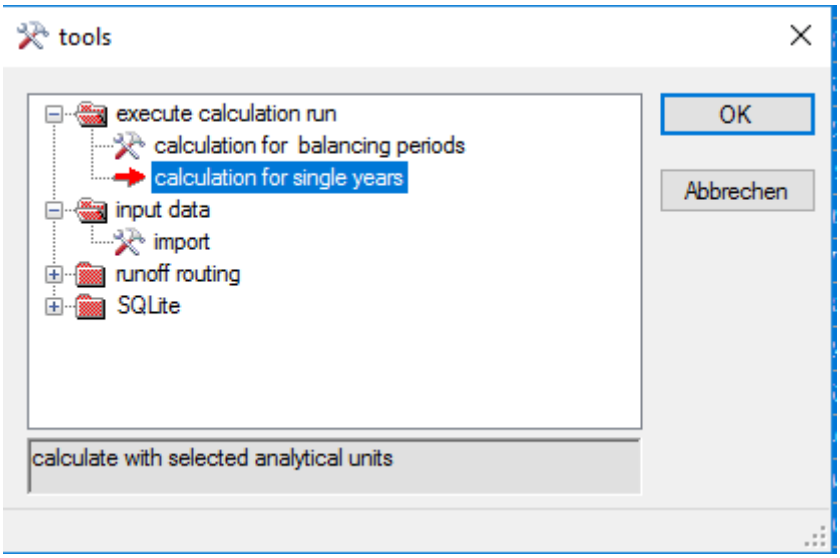


Figure 27 – The prompt to start the model calculation within the MoRE toolbox pop-up windos.

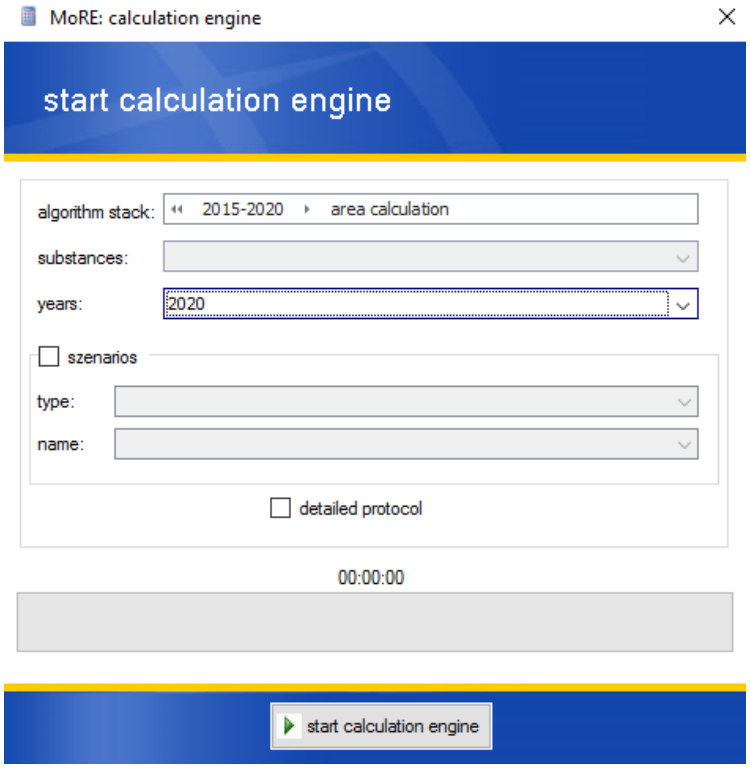


Figure 28 – Setting up the calculation in the model.

step	algorithm
01	areas > land use (variant 1)
02	Areas > Agricultural areas > Agricultural areas (variant 1)
03	areas > tile drained areas > tile drained areas (variant 1)
04	Areas > Urban impervious areas > Urban impervious areas, total (variant 1)
05	Areas > Areas contributing to the formation of surface runoff > Areas contributing to the formation ...
06	Areas > Areas contributing to groundwater recharge > Areas contributing to groundwater recharge...

Figure 29 – Algorithm stack for the area balance calculation

As shown in Figure 29, there are 6 calculation algorithms within this stack: Land use (Table 22), Agricultural areas (Table 23), tile drained areas (Table 24), total impervious areas (Table 25), Areas contributing to the formation of surface runoff (Table 26) and areas contributing to groundwater recharge (Table 27).

Table 22 - Preprocessing calculation of land uses for further use in the model

step	formula	formula content
01	IM_A_AL_slope_0_1 (variant 3)	BI_A_AL_slope_0_1
02	IM_A_AL_slope_1_2 (variant 3)	BI_A_AL_slope_1_2
03	IM_A_AL_slope_2_4 (variant 3)	BI_A_AL_slope_2_4
04	IM_A_AL_slope_4_8 (variant 3)	BI_A_AL_slope_4_8
05	IM_A_AL_slope_8 (variant 3)	BI_A_AL_slope_8
06	IM_A_AL (variant 3)	IM_A_AL_slope_0_1 + IM_A_AL_slope_1_2 + IM_A_AL_slope_2_4 + IM_A_AL_slope_4_8 + IM_A_AL_slope_8
07	IM_A_PST_agrl (variant 2)	BI_A_PST
08	IM_A_PST (variant 4)	IM_A_PST_agrl
09	IM_A_AGRL (variant 1)	IM_A_AL + IM_A_PST
10	IM_A_NAT (variant 4)	BI_A_FOR
11	IM_A_GLC (variant 3)	BI_A_GLC
12	IM_A_O (variant 4)	BI_A_O
13	IM_A_MNT (variant 4)	BI_A_MNT
14	IM_A_OPM (variant 4)	BI_A_OPM
15	IM_A_URB (variant 4)	BI_A_IMP + BI_A_URB
16	IM_A_OR_qsr (variant 2)	BI_A_OR * OR_SHR_a_or_qsr_tot /100
17	IM_A_OR_qgw (variant 2)	BI_A_OR * (1 - OR_SHR_a_or_qsr_tot / 100)
18	IM_A_OR (variant 1)	IM_A_OR_qsr + IM_A_OR_qgw
19	IM_A_WS (variant 2)	BI_A_WS_sat
20	IM_A_WL (variant 3)	BI_A_WL
21	IM_A_REM (variant 1)	BI_A_REM
22	IM_A_calc (variant 1)	IM_A_AGRL + IM_A_NAT + IM_A_O + IM_A_GLC + IM_A_MNT + IM_A_OPM + IM_A_URB + IM_A_WL + IM_A_WS + IM_A_OR + IM_A_REM
23	IM_A_diff (variant 1)	IM_A_calc - BI_A

Table 23 – caclulation of arable land share in the AUs

step	active	formula	formula content
02	TRUE	ER_SHR_a_al_tot (variant 1)	IM_A_AL / BI_A * 100

Table 24 – calculation of tile drained areas

step	active	formula	formula content
01	TRUE	TD_A_AL (variant 1)	IM_A_AL * (TD_SHR_a_td_agrl / 100)

02	TRUE	TD_A_PST (variant 1)	IM_A_PST_agrl * (TD_SHR_a_td_agrl / 100)
03	TRUE	IM_A_TDA (variant 1)	TD_A_AL + TD_A_PST

Table 25 – calculation of total urban impervious areas in the model

step	active	formula	formula content
01	TRUE	US_A_IMP (variant 1)	BI_A_IMP
02	TRUE	IM_A_URB_imp (variant 1)	if(BI_A_IMP > IM_A_URB , IM_A_URB , BI_A_IMP)
03	FALSE	US_SHR_a_imp_urb (variant 2)	if (IM_A_URB == 0, 0,US_A_IMP / IM_A_URB*100)

Table 26 - calculation of surface runoff in the model

step	active	formula	formula content
01	TRUE	IM_A_SR_cont (variant 3)	IM_A_AGRL + IM_A_NAT + IM_A_O + IM_A_URB - IM_A_URB_imp + IM_A_OR_qsr
02	TRUE	SR_veg_A_NONIMP (variant 1)	IM_A_AGRL + IM_A_NAT + IM_A_O

Table 27 – calculation of areas contributing to groundwater recharge

step	active	formula	formula content
01	TRUE	GW_A_rech (variant 1)	if ((BI_A - IM_A_WS - IM_A_URB_imp - IM_A_TDA - IM_A_OPM - IM_A_OR_qsr) <= 0, 0.001, BI_A - IM_A_WS - IM_A_URB_imp - IM_A_TDA - IM_A_OPM - IM_A_OR_qsr)
02	TRUE	GW_A_rech_NAT (variant 1)	if (GW_A_rech - (IM_A_AGRL - IM_A_TDA) <= 0, 0.001, GW_A_rech - (IM_A_AGRL - IM_A_TDA))

5.1.3 Calculation of water balance

Water balance is also calculated by a set of model algorithms. Each pathway is calculated by multiple steps.

Surface runoff:

Surface runoff is a product of mountainous runoff and runoff from vegetated land, which are calculated based on empiric equations as stated in Table 13.

Table 28-algorithm to calculate surface runoff from unsealed areas

step	active	formula	formula content
01	TRUE	SR_mnt_Q_spec (variant 1)	if (IM_PREC_yr > SR_mnt_PREC_max , SR_mnt_FCT_a_Q_uncor * (IM_PREC_yr - SR_mnt_PREC_max)^ SR_mnt_EXP_Q_uncor , 0)

02	TRUE	SR_mnt_Q_uncorr (variant 1)	(IM_A_MNT + IM_A_GLC) * SR_mnt_Q_spec * 1000 / 86400 / 365
03	TRUE	SR_mnt_Q (variant 1)	if (BI_Q_net * SR_mnt_FCT_snowmelt < SR_mnt_Q_uncorr, BI_Q_net * SR_mnt_FCT_snowmelt, SR_mnt_Q_uncorr)
04	TRUE	IM_Q_spec (variant 3)	((BI_Q_net*365*86400)-WWTP_Q)/1000/BI_A
05	TRUE	SR_veg_Q_spec (variant 1)	if(IM_Q_spec <= 0, 0, SR_veg_FCT_a_Q * IM_Q_spec ^ SR_veg_EXP_Q)
06	TRUE	SR_veg_Q (variant 3)	SR_veg_Q_spec / 86.4 / 365 * BI_A
07	TRUE	SR_Q (variant 1)	SR_veg_Q + SR_mnt_Q

Runoff from non-urban roads is calculated from the product of annual precipitation (IM_PREC_yr) and runoff coefficients (OR_RC which is set to 0.95) (Table 29).

Table 29 – Algoritm to calculate runoff from roads outside urban areas.

step	active	formula	formula content
01	IGAZ	OR_Q (variant 1)	IM_A_OR_qsr * IM_PREC_yr * OR_RC * 1000 /365 / 86400

Runoff from water surfaces is calculated according to the original Moneris formula (Table 30), which requires monthly precipitation and long term average evapotranspiration values. This latter has been derived from CWATM model output netcdf time series data.

Table 30 – Tethys Danube MoRE algorithm to calculate runoff from water surfaces

step	active	formula	formula content	formula reference
01	IGAZ	IM_PREC_yr (variant 1)	BI_PREC_jan + BI_PREC_feb + BI_PREC_mar + BI_PREC_apr + BI_PREC_may + BI_PREC_june + BI_PREC_july + BI_PREC_aug + BI_PREC_sept + BI_PREC_oct + BI_PREC_nov + BI_PREC_dec	
02	IGAZ	IM_PREC_s (variant 1)	BI_PREC_may + BI_PREC_june + BI_PREC_july + BI_PREC_aug + BI_PREC_sept + BI_PREC_oct	
03	IGAZ	IM_Q_WS (variant 1)	if ((IM_PREC_yr - AD_EVAPO_lt) < 0,0,(IM_PREC_yr - AD_EVAPO_lt) * (IM_A_WS / (86.4 * 365)))	MONERIS V 2.01 (2009)
04	IGAZ	IM_Q_prec (variant 1)	IM_PREC_yr * BI_A / 365 / 86400 * 1000	

Runoff from urban systems (US) is calculated by three set of equations The first set is to estimate runoff via sewer system that is not connected to treatment plants (only sewer systems – OSS, Table 31). Here runoff from inhabitants (INH), impervious areas (IMP) and commercial areas (COM) are calculated. The second set of equations estimate runoff from areas and inhabitants, which are not con-

nected to sewer systems (Table 32). The third set is a complete calculation of runoff from sewer systems (Table 33) including all types, that is storm sewers (SS), combined sewers (CSO) and sewers not connected to treatment plants (OSS).

Table 31 – algorithm to calculate runoff from inhabitants, impervious and commercial areas only connected to sewer systems

step	active	formula	formula content
01	IGAZ	US_oss_A_IMP (variant 2)	IM_A_URB*US_SHR_inh_oss_tot/100
02	IGAZ	US_RC (variant 1)	US_FCT_a_RC + US_FCT_b_RC * (US_SHR_a_imp_urb / 100)
03	IGAZ	US_oss_Q_IMP (variant 2)	US_oss_A_IMP*IM_PREC_yr* US_RC* 1000
04	IGAZ	IM_INH_oss (variant 1)	US_SHR_inh_oss_tot / 100 * BI_INH
05	IGAZ	US_oss_Q_INH (variant 2)	IM_INH_oss*365*US_INHC_H2O/1000
06	IGAZ	US_Q_COM (variant 1)	US_Q_spec_COM * 100 * 86400 * 365 / 1000 * US_DUR_q_COM / 24 * US_A_IMP * US_SHR_a_com_tot / 100
07	IGAZ	US_oss_Q (variant 2)	(US_oss_Q_INH+US_oss_Q_IMP+US_Q_COM)*US_LEAK_oss
08	IGAZ	US_oss_Q_GW (variant 3)	(US_oss_Q_INH+US_oss_Q_IMP+US_oss_Q_COM)*(1-US_LEAK_oss)

Table 32 – algorithm to calculate runoff from inhabitants, impervious areas not connected to sewer systems

step	active	formula	formula content
01	TRUE	IM_INH_nss (variant 1)	US_SHR_inh_nss_tot / 100 * BI_INH
02	TRUE	US_nss_A_IMP (variant 2)	IM_A_URB*US_SHR_inh_nss_tot/100
04	TRUE	US_nss_Q_INH (variant 1)	IM_INH_nss*365*(US_INHC_H2O/1000)
05	TRUE	US_SHR_a_imp_urb (variant 2)	if (IM_A_URB == 0, 0, US_A_IMP / IM_A_URB*100)
06	TRUE	US_RC (variant 1)	US_FCT_a_RC + US_FCT_b_RC * (US_SHR_a_imp_urb / 100)
07	TRUE	US_nss_Q_IMP (variant 1)	US_nss_A_IMP * IM_PREC_yr * US_RC * 1000
08	TRUE	US_nss_Q (variant 1)	US_nss_Q_INH+US_nss_Q_IMP

Table 33– algorithm to calculate runoff via sewer systems (combined – CSO- and storm sewers - SS)

step	active	formula	formula content
01	True	US_A_IMP (variant 1)	BI_A_IMP
02	True	US_A_IMP_com (variant 2)	US_A_IMP_com_dlm
04	True	US_cso_A_IMP (variant 1)	if(BI_INH==0, 0, (US_SHR_a_cs_tss / 100) * US_A_IMP * (US_SHR_inh_conWWTP_tot / 100))
05	True	US_cso_A_IMP_com (variant 1)	(US_SHR_a_cs_tss / 100) * US_A_IMP_com * (US_SHR_inh_conWWTP_tot / 100)
06	True	US_cso_SHR_q_cso_css_IMP (variant 1)	((4000 + 25 * US_cso_Q_spec_CSS_RAIN) / (0.551 + US_cso_Q_spec_CSS_RAIN)) / (US_cso_SHR_vol_real_tot_STO/ 100* US_cso_VOL_spec_STO_100p + ((36.8 + 13.5 *

			US_cso_Q_spec_CSS_RAIN) / (0.5 + US_cso_Q_spec_CSS_RAIN))) - 6 + ((IM_PREC_yr - 800) / 40)
07	True	IM_INH_conWWTP (variant 1)	US_SHR_inh_conWWTP_tot / 100 * BI_INH
08	True	US_cso_Q_CSS_COM (variant 1)	US_Q_spec_COM * 100 * 86400 * 365 / 1000 * US_cso_A_IMP_com * US_DUR_q_COM / 24
09	True	US_cso_Q_CSS_IMP (variant 1)	US_cso_A_IMP * IM_PREC_yr * US_RC * 1000
10	True	US_cso_Q_CSS_INH (variant 1)	if(US_A_IMP <= 0 ,0,IM_INH_conWWTP * US_cso_A_IMP / US_A_IMP * US_INHC_H2O * 365 / 1000)
11	True	US_cso_Q_INH (variant 1)	US_cso_Q_CSS_INH * US_cso_DUR / 365
12	True	US_cso_Q_IMP (variant 1)	US_cso_Q_CSS_IMP * US_cso_SHR_q_cso_css_IMP / 100
13	True	US_cso_Q_COM (variant 1)	US_cso_Q_CSS_COM * US_cso_DUR / 365
14	True	US_cso_Q_calc (variant 1)	US_cso_Q_IMP + US_cso_Q_INH+US_cso_Q_COM
16	True	US_cso_Q (variant 2)	US_cso_Q_calc
17	True	US_ss_A_IMP (variant 1)	if(BI_INH==0,0,(1 - (US_SHR_a_cs_tss / 100)) * US_A_IMP * (US_SHR_inh_conWWTP_tot / 100))
18	True	US_ss_Q_calc (variant 2)	US_ss_A_IMP*IM_PREC_yr* US_RC* 1000
19	True	US_ss_Q (variant 1)	US_ss_Q_calc
20	True	US_Q (variant 4)	(US_ss_Q + US_cso_Q + US_oss_Q) / (86400 * 365)

Calculation of tile drain flow

Tile drain flow is calculated by multiplying monthly precipitation with empirical monthly factors for specific tile drain flow (TD_FCT_month_Q_spec, Table 34). These factors vary between 0.08 (August) and 0.69 (January). These factors are derived from earlier applications, and might be not accurate for each regions of the basin, however no major differences is expected due to similar vegetation periods across the basin.

Table 34 - algorithm for the calculation of tile drain flow

step	active	formula	formula content
			(BI_PREC_jan * TD_FCT_jan_Q_spec) + (BI_PREC_feb * TD_FCT_feb_Q_spec) + (BI_PREC_mar* TD_FCT_mar_Q_spec) + (BI_PREC_apr * TD_FCT_apr_Q_spec) + (BI_PREC_may * TD_FCT_may_Q_spec) + (BI_PREC_june * TD_FCT_jun_Q_spec) + (BI_PREC_july * TD_FCT_jul_Q_spec) + (BI_PREC_aug * TD_FCT_aug_Q_spec) + (BI_PREC_sept * TD_FCT_sep_Q_spec) + (BI_PREC_oct * TD_FCT_oct_Q_spec) + (BI_PREC_nov * TD_FCT_nov_Q_spec) + (BI_PREC_dec * TD_FCT_dec_Q_spec)
01	TRUE	TD_Q_spec (variant 2)	
02	TRUE	TD_Q_AL (variant 1)	(TD_Q_spec * TD_A_AL * 1000) / (86400 * 365)
03	TRUE	TD_Q_PST (variant 1)	(TD_Q_spec * TD_A_PST * 1000) / (86400 * 365)
04	TRUE	TD_Q (variant 1)	TD_Q_AL + TD_Q_PST

Calculation of groundwater flow

In the Moneris approach, the water balance is set up in a way that first the surface runoff from unsealed areas, urban systems, open roads, tile drain flow is estimated, then these are subtracted from annual total runoff (BI_Q_net), which is an input data to the model. The resulting water balance difference gives the specific groundwater flow, from which subsequently the groundwater flow is calculated (Table 35).

Table 35 – algorithm for the calculation of groundwater flow

step	active	formula	formula content	formula reference
03	FLASE	GW_Q_spec_uncorr (variant 1)	if (GW_A_rech == 0.001, 1, ((BI_Q_net - IM_Q_WS - SR_Q - TD_Q - US_Q - OR_Q) * 86400 * 365 - WWTP_Q - ID_Q) / GW_A_rech /1000)	MONERIS V 2.01 (2009)
04	TRUE	GW_Q_spec (variant 7)	if (GW_A_rech <= 0.001 || ((BI_Q_net - IM_Q_WS - SR_Q - TD_Q - US_Q - OR_Q) * 86400 * 365 - WWTP_Q) <= 0 , 0, ((BI_Q_net - IM_Q_WS - SR_Q - TD_Q - US_Q - OR_Q) * 86400 * 365 - WWTP_Q) / GW_A_rech / 1000)	Zessner et al. (2011) [Application in alpine catchments in Austria]
05	TRUE	GW_Q (variant 1)	(GW_Q_spec * GW_A_rech) / (86.4 * 365)	MONERIS V 2.01 (2009)

Checking runoff balance and aggregating flow

The first two step of the algorithm (Table 36) refers to the check of modelled water balance and total runoff. The steps from 3 to 6 refer to the check of total runoff at locations, where measured Q data is included.

Table 36 – algorithms to check water balance and total runoff

step	active	formula	formula content
01	TRUE	IM_Q (variant 3)	TD_Q + IM_Q_WS + US_Q + SR_Q + GW_Q + OR_Q + (WWTP_Q) / 86400 / 365
02	TRUE	IM_Q_diff (variant 1)	BI_Q_net - IM_Q
03	TRUE	TOT_FNE_Q (variant 2)	more_rl_upstr(TOT_FNE_Q) + if (IM_Q < 0, BI_Q_net, IM_Q)
04	TRUE	TOT_FNE_Q_outlet (variant 2)	(more_rl_upstr(TOT_FNE_Q) + if(IM_Q < 0, BI_Q_net , IM_Q)) * (1 - RM_FCT_Q_SPLIT)
05	TRUE	IM_Q_diff_obs_calc (variant 1)	if(TOT_FNE_Q_obs > 0, TOT_FNE_Q_obs - TOT_FNE_Q_outlet , 0)
06	TRUE	IM_Q_net_diff_obs_calc (variant 1)	if(TOT_FNE_Q_obs > 0, IM_Q_diff_obs_calc / (1 - RM_FCT_Q_SPLIT) + BI_Q_net ,0)

5.1.4 Soil erosion and fine solids transport

Erosion (ER) calculation (Table 37) is following the original Moneris approach, where soil loss (SL) is calculated for 5 agricultural categories, based on slope classes (slp = <1,1-2,2-4,4-8,>8%), pastures (PST) and natural vegetation (NAT). Beside this in the MoRE model erosion is also calculated for alpine areas including mountainous areas (MNT) and glaciers (GLC). Calculated erosion is corrected for each year by multiplying the long-term values with the correction factor (ER_FCT_corr_RUSLE) for the rainfall erosivity (USLE R factor). The correction method is a revised method for alpine areas[19]. R factor correction might be different for the different parts of the Danube River Basin, therefore these empirical formulas would need revision.

Table 37 – algorithm to calculate erosion for agricultural land, natural land, glaciers and mountains

step	active	formula	formula content
01	TRUE	ER_FCT_r_RUSLE_alp (variant 1)	if(IM_PREC_s < 0,1,(IM_PREC_s * ER_FCT_a_FCT_r_RUSLE_alp)^ ER_EXP_a_FCT_r_RUSLE_alp - ER_FCT_b_FCT_r_RUSLE_alp)
02	TRUE	ER_FCT_r_lt_RUSLE_lt (variant 1)	if(ER_PREC_s_lt < 0, 1,(ER_PREC_s_lt * ER_FCT_a_FCT_r_RUSLE_alp)^ ER_EXP_a_FCT_r_RUSLE_alp - ER_FCT_b_FCT_r_RUSLE_alp)
03	TRUE	ER_FCT_corr_FCT_r_RUSLE (variant 1)	ER_FCT_r_RUSLE_alp / ER_FCT_r_lt_RUSLE_lt
04	TRUE	ER_agrl_SL_spec_lt_AL (variant 4)	if(IM_A_AL==0,0, ((IM_A_AL_slope_0_1 * ER_agrl_SL_pot_spec_AL_slp_0_1 + IM_A_AL_slope_1_2 * ER_agrl_SL_pot_spec_AL_slp_1_2 + IM_A_AL_slope_2_4 * ER_agrl_SL_pot_spec_AL_slp_2_4 + IM_A_AL_slope_4_8 * ER_agrl_SL_pot_spec_AL_slp_4_8 + IM_A_AL_slope_8 * ER_agrl_SL_pot_spec_AL_slp_8) / IM_A_AL))
05	TRUE	ER_agrl_SL_AL (variant 1)	ER_agrl_SL_spec_lt_AL * IM_A_AL * 100 * ER_FCT_corr_FCT_r_RUSLE
06	TRUE	ER_agrl_SL_PST (variant 1)	ER_agrl_SL_spec_lt_PST * IM_A_PST * 100 * ER_FCT_corr_FCT_r_RUSLE
07	TRUE	ER_agrl_SL (variant 1)	ER_agrl_SL_AL + ER_agrl_SL_PST
08	TRUE	ER_SDR (variant 1)	if (BI_SLP > ER_agrl_SLP_min_SDR, ER_FCT_a_SDR * (BI_SLP + ER_FCT_d_SDR)^ ER_EXP_a_SDR * (ER_SHR_a_al_tot + ER_FCT_e_SDR)^ ER_EXP_b_SDR, 0)
09	TRUE	ER_agrl_E_SED (variant 2)	ER_agrl_SL * ER_SDR / 100
10	TRUE	ER_E_spec_AGRL_SED (variant 1)	ER_agrl_E_SED / BI_A
11	TRUE	ER_nat_SDR (variant 1)	ER_FCT_SDR_nat * exp(BI_SLP * ER_EXP_SDR_nat) * 100

[19] Zessner, M., Kovacs, A., Schilling, C., Hochedlinger, G., Gabriel, O., Natho, S., Thaler, S., & Windhofer, G. (2011). Enhancement of the MONERIS Model for Application in Alpine Catchments in Austria. International Review of Hydrobiology, 96(5), 541–560. https://doi.org/https://doi.org/10.1002/iroh.201111278

12	TRUE	ER_NAT_E_SED_max (variant 1)	IM_A_NAT*100*0.2
13	TRUE	ER_nat_E_SED (variant 4)	if(ER_CODE_method_nat> 10, ER_NAT_E_SED_max, ER_nat_SL_AU * 100 * ER_nat_SDR / 100 * IM_A_NAT * ER_FCT_corr_FCT_r_RUSLE)
14	TRUE	ER_mnt_E_SED (variant 2)	IM_A_MNT*100*0.2
15	TRUE	ER_glc_E_SED (variant 1)	ER_glc_E_spec_lt_SED * 100 * IM_A_GLC
16	TRUE	ER_E_SED (variant 1)	ER_agrl_E_SED + ER_nat_E_SED + ER_mnt_E_SED + ER_glc_E_SED
17	TRUE	ER_ENR_AL (variant 1)	if(ER_agrl_SL_spec_lt_AL <=0 || ER_FCT_a_ENR_AL * ER_agrl_SL_spec_lt_AL ^ ER_EXP_ENR_AL < 1,1, if(ER_FCT_a_ENR_AL * ER_agrl_SL_spec_lt_AL ^ ER_EXP_ENR_AL > 4.5, 4.5,ER_FCT_a_ENR_AL * ER_agrl_SL_spec_lt_AL ^ ER_EXP_ENR_AL))
18	TRUE	ER_FCT_r_RUSLE_alp (variant 1)	if(IM_PREC_s < 0, 1, (IM_PREC_s * ER_FCT_a_FCT_r_RUSLE_alp)^ ER_EXP_a_FCT_r_RUSLE_alp - ER_FCT_b_FCT_r_RUSLE_alp)

Fine sediment calculation from urban systems, tile drain systems and waste water treatment plants.

An empirical estimation (Table 38) is used for calculation sewer loads that was set up in earlier model applications. Key input variables are the concentration of fine solids in combined sewer systems (US_cso_CONC_FS) and storm sewer systems (US_ss_CONC_FS). These values came also for model applications as constant values. Values have not been revised in the current application as no specific data is available at partner institutions, nor in literature. The same applies for tile drain calculations and WWTPs (Table 39, Table 40). These estimates are very rough and serves as an order of magnitude estimate.

Table 38 - algorithm to calculate fine solids emission via urban systems

step	active	formula	formula content
01	TRUE	US_cso_E_FS (variant 1)	US_cso_Q * US_cso_CONC_FS * (1- (MM_US_cso_EFF_FS /100)) / (1000 * 1000)
02	TRUE	US_ss_E_FS (variant 1)	US_ss_CONC_FS * (1- (MM_US_ss_EFF_FS /100))* US_ss_Q / (1000*1000)
03	TRUE	US_E_FS (variant 1)	US_ss_E_FS + US_cso_E_FS

Table 39 - algorithm to calculate fine solids emission via tile drain systems

step	active	formula	formula content
01	IGAZ	TD_E_FS (variant 1)	TD_Q * 86400 * 365 * TD_CONC_FS / (1000 * 1000)

Table 40 - algorithm to calculate fine solids emission via waste water treatment plants

step	active	formula	formula content
01	IGAZ	WWTP_E_FS (variant 1)	more_psaggrau(WWTP_ps_Q) * WWTP_CONC_FS / (1000 * 1000)

Summing up the fine sediment loads

Total loads are the result of the aggregation of the four pathways described above (Table 41). Aggregation along the flow tree uses the more_rl_upstr function of the MoRE model.

Table 41 - algorithm to aggregate fine sediment loads

step	active	formula	formula content
01	IGAZ	TOT_E_FS (variant 1)	TD_E_FS + ER_E_SED + US_E_FS + WWTP_E_FS
02	IGAZ	TOT_FNE_E_FS (variant 1)	more_rl_upstr(TOT_FNE_E_FS) + TOT_E_FS

5.1.5 Calculation of point sources

Direct municipal

The calculation has three different approaches in the model (Table 42, see O.2.1 section 4.1.1). The first option is to calculate loads based on treatment technologies (step 01), where NOTREAT, PRIM (primary), SEC (secondary), TERT (tertiary), QUART (quarternary) are referring to the highest treatment stage of a given plant. Each treatment stage has a separate concentration value. This option has an advantage in terms of scenario calculations of urban policies (e.g. UWWTD recast[20]), which needs the reset of the treatment stages. The second option is the differentiation between waste water treatment plants by their capacities. The third option is to calculate waste water emissions from inhabitant specific loads, which is an available option for the estimation of pharmaceutical loads via municipal waste water pathway.

Table 42 – algorithm to calculate HM point source loads from WWTPs

step	active	formula	formula content
01	TRUE	WWTP_ps_E_HM (variant 3)	if(WWTP_treatment_type=0, WWTP_ps_Q*WWTP_CONC_NOTREAT_HM*10^-6,if(WWTP_treatment_type = 1, WWTP_ps_Q*WWTP_CONC_PRIM_HM*10^-6,if(WWTP_treatment_type = 2, WWTP_ps_Q*WWTP_CONC_SEC_HM*10^-6, if(WWTP_treatment_type = 3, WWTP_ps_Q*WWTP_CONC_TERT_HM*10^-6, WWTP_ps_Q*WWTP_CONC_QUART_HM*10^-6))))
02	TRUE	WWTP_small_E_HM (variant 1)	WWTP_s_CONC_HM * WWTP_small_Q / 1000 / 1000
03	TRUE	WWTP_E_HM (variant 1)	more_psaggrau(WWTP_ps_E_HM) + WWTP_small_E_HM
04	TRUE	WWTP_E_diss_HM (variant 1)	(1 /(1 + RM_KD_HM * WWTP_CONC_FS / 1000 / 1000))* WWTP_E_HM

Table 43– algorithm to calculate PFAS point source loads from WWTPs

step	active	formula	formula content

[20] Kardos, M. K., Patziger, M., Jolánkai, Z., & Clement, A. (2025). The new urban wastewater treatment directive from the perspective of the receiving rivers' quality. Environmental Sciences Europe, 37(1), 10. https://doi.org/10.1186/s12302-024-01040-2

01	TRUE	WWTP_ps_E_PFAS (variant 4)	if(WWTP_treatment_type=0, WWTP_ps_Q*WWTP_CONC_NOTREAT_PFAS/1000000, if(WWTP_treatment_type = 1, WWTP_ps_Q*WWTP_CONC_PRIM_PFAS/1000000, if(WWTP_treatment_type = 2, WWTP_ps_Q*WWTP_CONC_SEC_PFAS/1000000, if(WWTP_treatment_type = 3, WWTP_ps_Q*WWTP_CONC_TERT_PFAS/1000000, WWTP_ps_Q*WWTP_CONC_QUART_PFAS/1000000))))
02	FALSE	WWTP_ps_EF_inh_PFAS (variant 2)	if(WWTP_ps_PE == -9999, -9999, WWTP_ps_E_PFAS / WWTP_ps_PE * 1000 * 1000 * 1000)
03	TRUE	WWTP_small_E_PFAS (variant 2)	WWTP_s_CONC_PFAS * WWTP_small_Q / 1000 / 1000
04	TRUE	WWTP_E_PFAS (variant 1)	more_psaggrau(WWTP_ps_E_PFAS) + WWTP_small_E_PFAS

Table 44– algorithm to calculate PHAR point source loads from WWTPs

step	active	formula	formula content
01	TRUE	WWTP_ps_E_PHAR (variant 2)	if(WWTP_treatment_type=0, WWTP_ps_Q*WWTP_CONC_NOTREAT_PHAR/(1000*1000), if(WWTP_treatment_type = 1, WWTP_ps_Q*WWTP_CONC_PRIM_PHAR/(1000*1000), if(WWTP_treatment_type = 2, WWTP_ps_Q*WWTP_CONC_SEC_PHAR/(1000*1000), if(WWTP_treatment_type = 3, WWTP_ps_Q*WWTP_CONC_TERT_PHAR/(1000*1000), WWTP_ps_Q*WWTP_CONC_QUART_PHAR/(1000*1000)))))
02	TRUE	WWTP_small_E_PHAR (variant 1)	WWTP_s_CONC_PHAR * WWTP_small_Q / 1000 / 1000
03	TRUE	WWTP_E_PHAR (variant 1)	more_psaggrau(WWTP_ps_E_PHAR) + WWTP_small_E_PHAR
03_var2	FALSE	WWTP_E_PHAR (variant 1)	WWTP_INH_LOAD_PHAR * BI_INH * US_SHR_inh_con_tot/100

Direct industrial

In the current model application the calculation of direct emission loads from direct dischargers are calculated outside the model, therefore it receives AU emissions directly as point source emissions (ID_ps_E_HM), only the aggregation of these is done in the model using the aggregation function of the MoRE model (Table 45).

Table 45 – load aggregation of point source industrial direct dischargers

step	active	formula	formula content
01	TRUE	ID_E_HM (variant 1)	more_psaggrau(ID_ps_E_HM)

Urban systems – population connected only to sewer system (no WWTP)

This pathway can be calculated both as point source loads or as diffuse pathways. In this section the point source description is introduced. This kind of description can only be used, if waste water collection data is available for cities or agglomerations. As ICPDR provided such data, this method can be applied at several parts of the Danube River Basin.

The calculation equals to the WWTP point source emission calculation method according to the variant of treatment stages. WWTP concentration values of NOTREAT apply to the emissions via this pathway.

Legacy hot spots

This pathway is created to account for sites, where known groundwater contamination is present. There have been many sites all over Europe, where the soil and groundwater have been contaminated with metals or PFAS compounds and sometimes also with pharmaceuticals. Most of these sites have been rehabilitated, but there are still sites with existing contamination. Data of contaminated sites can be loaded in the model from national databases. Emissions from legacy hot spots are calculated by using a concentration x discharge approach as shown in Table 47.

Table 46– calculation algorithm of PFAS via groundwater from legacy hot spot sources.

step	active	formula	formula content
01	TRUE	AA_ps_Q (variant 1)	if(BI_PREC_AA_lt > AD_EVAPO_AA_lt,AA_A_GW/10 * (BI_PREC_AA_lt - AD_EVAPO_AA_lt)/86.4/365,0)
02	TRUE	AA_ps_E_PFAS (variant 1)	AA_ps_Q * AA_CONC_PFAS * 86400*365/1000/1000/1000
03	TRUE	AA_E_PFAS (variant 2)	more_psaggrau(AA_ps_E_PFAS)
04	FALSE	AA_FNE_E_PFAS (variant 1)	more_fne_tot(AA_E_PFAS)

Aerodromes

As there is numerous evidence about the fact that groundwater is contaminated below airports with PFAS substances, we have introduced this pathway based on earlier application in the Promisces project[21] (Table 47). The estimation is simply comprising of the multiplication of an estimated average concentration (see O.2.1, section 2.4.8) with an initial calculation of the annual recharge at the site premises; for which the area of the airport is used, which is divided by a factor of 10, as a rough initial estimate of the area of the training facilities at airports (possibly overestimating the real size). Recharge is calculated from the difference of annual precipitation (BI_PREC_AA) and long term evapotranspiration (AD_EVAPO_AA_lt).

Table 47– calculation algorithm of PFAS via groundwater from Aerodromes hot spot sources.

step	active	formula	formula content

[21] Liu, M., Saracevic, E., Oudega, T. J., Obeid, A. A. A., Nagy-Kovács, Z., László, B., Kittlaus, S., Zoboli, O., Krampe, J., Derx, J., & Zessner, M. (2025). Investigating the extent of PFAS contamination in the Upper Danube Basin across environmental compartments. Environmental Sciences Europe, 37(1), 99. https://doi.org/10.1186/s12302-025-01141-6

01	TRUE	AA_ps_Q (variant 1)	if(BI_PREC_AA_lt > AD_EVAPO_AA_lt, AA_A_GW/10 * (BI_PREC_AA_lt - AD_EVAPO_AA_lt)/86.4/365,0)
02	TRUE	AA_ps_E_PFAS (variant 1)	AA_ps_Q * AA_CONC_PFAS * 86400*365/1000/1000/1000
03	TRUE	AA_E_PFAS (variant 2)	more_psaggrau(AA_ps_E_PFAS)
04	FALSE	AA_FNE_E_PFAS (variant 1)	more_fne_tot(AA_E_PFAS)

Landfill sites

Landfills are relevant point source hot-spots for each substance group of our analysis. The approach is similar to airodromes and other legacy hot-spots. Concentrations below landfills are difficult to estimate however. Most reported values refer to leachate concentrations and not actual groundwater levels. Concentrations may also change in a very wide range, but this is discussed in the 2.3.9 chapter. Table 48 shows the algorithm to calculate pharmaceutical emissions for AUs starting with the calculation of point source discharge (LF_ps_Q), then point source emission (LF_ps_E_PHAR) and finishing with the aggregation of point source discharges for AUs, which produces AU level emission values (LF_E_PHAR).

Table 48 – calculation algorithm of pharmaceuticals via groundwater from landfill sites.

step	active	formula	formula content
01	TRUE	LF_ps_Q (variant 1)	if((BI_PREC_LF_lt - AD_EVAPO_LF_lt)<0,0, BI_A_LF/10 * (BI_PREC_LF_lt - AD_EVAPO_LF_lt)/86.4/365)
02	TRUE	LF_ps_E_PHAR (variant 1)	LF_ps_Q * LF_ps_CONC_PHAR / 1000 / 1000 * (100-MM_DI_PHAR)/100
03	TRUE	LF_E_PHAR (variant 1)	more_psaggrau(LF_ps_E_PHAR)

5.1.6 Calculation of diffuse sources

Emissions via groundwater

In the current model set up the groundwater is calculated for a simple Q*concentration approach for heavy metals Table 49. In the case of PFAS, the calculation starts with the estimation of groundwater concentrations, then the emissions are calculated similarly to heavy metals Table 50.

Table 49 – calculation of groundwater HM emission and related variables

step	active	formula	formula content
01	TRUE	GW_E_HM (variant 1)	(GW_Q * 86400 * 365 * GW_CONC_HM) / (1000 * 1000)
02	TRUE	GW_FNE_CONC_HM (variant 1)	if(more_fne_all(GW_Q)==0,0,more_fne_all(GW_E_HM) * 1000 * 1000 / more_fne_all(GW_Q)/ 86400 / 365)

Table 50 - calculation of groundwater PFAS emission and related variables

step	active	formula	formula content
01	TRUE	GW_CONC_PFAS (variant 1)	GW_FCT_CALIB_PFAS*ER_agrl_CONT_SOIL_top_AL_PFAS/ KD_OC_PFAS/GW_CONC_CALC_FOC_PFAS
02	TRUE	GW_E_PFAS (variant 1)	(GW_Q * 86400 * 365 * GW_CONC_PFAS) / (1000 * 1000)

Emissions via tile drainage

In the case of tile drainage the difference between HM and PFAS calculation is that for HM the emissions are based on concentration of groundwater (Table 51) which is transferred to tile drain concentration with a conversion factor, while in the case of PFAS, the tile drain concentration is calculated from soil concentrations (Table 52).

Table 51 – calculation of HM loads via tile drainge

step	active	formula	formula content
01	TRUE	TD_E_HM (variant 1)	(TD_Q * 86400 * 365 * GW_CONC_HM) / (1000 * 1000)*TD_FCT_GW_CONC_RATE_HM

Table 52 – calculation of PFAS loads via tile drainge

step	active	formula	formula content
01	TRUE	TD_CONC_PFAS (variant 1)	TD_FCT_CALIB_PFAS*ER_agrl_CONT_SOIL_top_AL_PFAS/ KD_OC_PFAS/ GW_CONC_CALC_FOC_PFAS
02	TRUE	TD_E_PFAS (variant 1)	(TD_Q * 86400 * 365 * TD_CONC_PFAS) / (1000 * 1000)

Emissions via surface runoff

Surface runoff for both HM and PFAS substance groups are calculated similarly. The only differenc is that in the case of HM the concentration of HM in surface runoff is estimated using distribution coefficients between soil and water phase directly (Table 53), while for PFOA this estimation is based on the organic carbon fraction of the soil (Table 54). In both case the starting point is the concentration of the substances in the agricultural topsoil.

Table 53 – calculation of HM loads via surface runoff

step	active	formula	formula content
01	TRUE	SR_CONC_CALC_HM (variant 1)	ER_agrl_CONT_SOIL_top_AL_HM/ KD_SOIL_WATER_HM
02	TRUE	SR_E_HM (variant 2)	SR_Q*86400*365*SR_CONC_CALC_HM/1000/1000

Table 54 – calculation of PFAS loads via surface runoff

step	active	formula	formula content
01	TRUE	SR_CONC_CALC_PFAS (variant 1)	ER_agrl_CONT_SOIL_top_AL_PFAS/ KD_OC_PFAS/GW_CONC_CALC_FOC_PFAS*SR_FCT_CALIB_PFAS
02	TRUE	SR_E_PFAS (variant 1)	SR_Q * 86400 * 365 * SR_CONC_PFAS / 1000 / 1000

Emissions via erosion

Erosion is calculated from several lad use types in the model; therefore, pollutant emissions are also related to these sub-pathways. In the case of HM, this pathways are agricultural lands, glaciers, mountainous lands and natural areas (Table 55). For PFAS, this is more simple as only agricultural and natural lands can be differentiated based on available concentration data (Table 56).

Table 55 – calculation of HM loads via erosion

step	active	formula	formula content
01	TRUE	ER_ENR_HM (variant 1)	if(ER_E_spec_AGRL_SED < 1 ,ER_FCT_a_ENR_HM ,if(ER_FCT_a_ENR_HM * ER_E_spec_AGRL_SED ^ ER_EXP_ENR_HM < 1 ,1 ,ER_FCT_a_ENR_HM * ER_E_spec_AGRL_SED ^ ER_EXP_ENR_HM))
02	TRUE	ER_agrl_E_HM (variant 1)	(ER_agrl_SL_AL * ER_agrl_CONT_SOIL_top_AL_HM * (1 - MM_ER_EFF_AL_SED / 100) + ER_agrl_SL_PST * ER_agrl_CONT_SOIL_top_PST_HM) * ER_SDR * 0.01 * ER_ENR_AL / 1000
03	TRUE	ER_agrl_E_diss_HM (variant 1)	(1 /(1 + RM_KD_HM * ER_CONC_FS / 1000 / 1000)) * ER_agrl_E_HM
04	TRUE	ER_glc_E_HM (variant 1)	ER_glc_E_SED * ER_CONT_ROCK_HM / 1000
05	TRUE	ER_mnt_E_HM (variant 1)	ER_mnt_E_SED * ER_CONT_ROCK_HM / 1000
06	TRUE	ER_nat_E_HM (variant 1)	ER_nat_E_SED * ER_nat_CONT_SOIL_HM / 1000
07	TRUE	ER_nat_E_diss_HM (variant 1)	(1 /(1 + RM_KD_HM * ER_CONC_FS / 1000 / 1000)) * ER_nat_E_HM
08	TRUE	ER_E_HM (variant 1)	ER_agrl_E_HM + ER_nat_E_HM + ER_mnt_E_HM + ER_glc_E_HM

Table 56 – calculation of PFAS loads via erosion

step	active	formula	formula content
01	TRUE	ER_agrl_E_PFAS (variant 1)	(ER_agrl_CONT_SOIL_top_AL_PFAS * ER_agrl_SL_AL * (1 - MM_ER_EFF_AL_SED / 100) + ER_agrl_CONT_SOIL_top_PST_PFAS * ER_agrl_SL_PST) * ER_SDR / 100 /1000/1000

02	TRUE	ER_nat_E_PFAS (variant 1)	ER_nat_E_SED * ER_nat_CONT_SOIL_PFAS / 1000/1000
03	TRUE	ER_E_PFAS (variant 2)	ER_agrl_E_PFAS + ER_nat_E_PFAS

Emissions via roads outside of settlements

This pathway is very specific for road transport, which is primarily related to HM elements, but PFAS is also present on road surfaces, therefore this pathway is also accounted for in the model. In the case of HM, the estimation is based on the surface deposition potential, from which the deposition by 'background' is subtracted (Table 57). In the case of PFAS this is simplified as deposition values from background is uncertain (Table 58).

Table 57 - calculation of HM loads via roads outside of settlements

step	active	formula	formula content
01	TRUE	OR_E_HM (variant 1)	(OR_SFL_HM - MM_AD_RATE_dep_red_HM /100 * BI_RATE_dep_HM) * IM_A_OR_qsr / 10
02	TRUE	OR_E_diss_HM (variant 1)	(1 /(1 + US_KD_HM * OR_CONC_FS / 1000 / 1000)) * OR_E_HM

Table 58 - calculation of PFAS loads via roads outside of settlements

step	active	formula	formula content
01	TRUE	OR_E_PFAS (variant 1)	OR_SFL_PFAS * IM_A_OR_qsr / 10

Emissions via atmospheric deposition into water surfaces

Atmospheric deposition calculation for HM is simply based on the deposition rate (BI_RATE_dep_HM) for each substance, which is multiplied with the water surface (IM_A_WS) within the AU (Table 60). For PFAS, the deposition rate is estimated in the first step, based on soil concentrations in pastures (resulting higher loads than agricultural lands) multiplied by a conversion rate (AD_SOIL_RATE_PFAS) and the water surface (Table 61).

Table 59 - calculation of HM loads via atmospheric deposition on water surfaces

step	active	formula	formula content
01	TRUE	AD_E_HM (variant 1)	BI_RATE_dep_HM * (1-MM_AD_RATE_dep_red_HM / 100) * IM_A_WS / 10

Table 60 - calculation of PFAS loads via atmospheric deposition on water surfaces

step	active	formula	formula content
01	TRUE	BI_RATE_dep_PFAS (variant 1)	ER_agrl_CONT_SOIL_top_PST_PFAS * AD_SOIL_RATE_PFAS * 10^-9 * IM_PREC_yr * 10^4 * 10^-3

02	TRUE	AD_E_PFAS (variant 1)	BI_RATE_dep_PFAS * IM_A_WS / 10

5.1.7 Calculation of the total emissions, retention and river load

Total emissions for each analytical unit is calculated by summing up emissions from all pathways, which is introduced below for heavy metals (Table 61), pharmaceuticals (Table 62) and PFAS substances (Table 63). River load calculation has different options in the model.

1. Simple aggregation of the loads from AUs are done if emissions are calculated without retention (Table 65).
2. If accounting for riverine retention, then the first step is to calculate retention in tributaries and main rivers of each Aus. The calculation of river retention has also two options: the original approach follows the method described in Table 64 and Table 66. The alternative approach is based on the empirical formulas that are under development and subject to further calibration of the retention parameters.

Both total and dissolved river loads are calculated in the same way.

Table 61 - calculation of the total emissions for heavy metals

step	active	formula	formula content
01	TRUE	TOT_E_HM (variant 1)	ID_E_HM + WWTP_E_HM + AD_E_HM + TD_E_HM + AM_E_HM + ER_E_HM + US_E_HM + SR_E_HM + GW_E_HM + OR_E_HM + ID_AD_E_HM
02	FALSE	TOT_FNE_E_HM (variant 1)	more_rl_upstr(TOT_FNE_E_HM) + TOT_E_HM

Table 62 - calculation of the total emissions for pharmaceuticals

step	active	formula	formula content
01	TRUE	TOT_E_PHAR (variant 1)	ID_E_PHAR + WWTP_E_PHAR + US_E_PHAR

Table 63 - calculation of the total emissions for PFAS

step	active	formula	formula content
01	TRUE	TOT_E_PFAS (variant 2)	ID_E_PFAS + WWTP_E_PFAS + AD_E_PFAS + TD_E_PFAS + ER_E_PFAS + US_E_PFAS + SR_E_PFAS + GW_E_PFAS + OR_E_PFAS + AA_E_PFAS + LF_E_PFAS
02	FALSE	TOT_EF_inh_PFAS (variant 1)	TOT_E_PFAS / if(BI_INH == 0 , 1 , BI_INH) * 1000 * 1000 * 1000
03	FLASE	TOT_FNE_E_PFAS (variant 1)	more_rl_upstr(TOT_FNE_E_PFAS) + TOT_E_PFAS

Table 64 - calculation of river retention according to the original Moneris method

step	active	formula	formula content
01	TRUE	RM_FCT_ret_method_q_TRIB (variant 1)	1 / (1 + RM_FCT_a_method_q * (BI_Q_net / BI_A * 1000)^ RM_EXP_a_method_q)
02	TRUE	RM_HL_TRIB (variant 1)	if (BI_A_WS_trib + BI_A_WS_lakes_trib <= 0, 100 * 1000 * 1000, (BI_Q_net * 365 * 86400) /

			((BI_A_WS_trib + BI_A_WS_lakes_trib) * 1000 * 1000))
03	TRUE	RM_FCT_ret_method_hl_TRIB (variant 1)	1 / (1 + RM_FCT_a_method_hl * RM_HL_TRIB ^ RM_EXP_a_method_hl)
04	TRUE	RM_FCT_ret_TRIB (variant 1)	(RM_FCT_ret_method_hl_TRIB + RM_FCT_ret_method_q_TRIB) / 2
05	TRUE	TOT_FNE_Q (variant 1)	if(more_rl_upstr(TOT_FNE_Q) < 0 , 0 , more_rl_upstr(TOT_FNE_Q)) + if(IM_Q < 0, if(BI_Q_net < 0 , 0 , BI_Q_net), IM_Q)
06	TRUE	RM_HL_MR (variant 2)	if((BI_A_WS_mr + BI_A_WS_lakes_mr)<=0, 100*1000*1000, TOT_FNE_Q * 365 * 86400 / ((BI_A_WS_mr + BI_A_WS_lakes_mr) * 1000 * 1000))
07	TRUE	RM_FCT_ret_method_hl_MR (variant 1)	1 / (1 + RM_FCT_a_method_hl * RM_HL_MR ^ RM_EXP_a_method_hl)

River loads

The calculation of river loads without retention is simply consist of two steps, aggregating the river loads of upstream Aus, then adding the river load of the given AU to the total upstream loads (Table 65). In the case, when retention calculation is used (original equations, Table 66), the point source loads and urban CSO loads are subtracted from total loads, as it is anticipated that most point source loads are emitted to the main river and not into the tributaries. The retention factors for tributaries (_ret_TRIB) are than applied for these tributary loads. For main rivers (MR) the retention factor for main rivers is applied (RM_FCT_ret_method_hl_MR). In the last step, the upstream river load of main river, the tributary loads and the point source loads are summed up. River load estimation for dissolved loads can be calculated similarly (Table 67).

Table 65 – calculation of aggregated river loads of heavy metals without retention

step	active	formula	formula content
01	TRUE	RM_RL_upstr_HM (variant 2)	more_rl_upstr(RM_RL_HM)
02	TRUE	RM_RL_HM (variant 3)	RM_RL_upstr_HM+TOT_E_HM

Table 66 – calculation of aggregated total river loads of heavy metals with retention

step	active	formula	formula content
01	TRUE	RM_E_diff_HM (variant 1)	TOT_E_HM - WWTP_E_HM - ID_E_HM - AM_E_HM - US_cso_E_HM
02	TRUE	RM_RL_TRIB_HM (variant 1)	RM_E_diff_HM * RM_FCT_ret_TRIB
03	TRUE	RM_RL_upstr_HM (variant 1)	RM_FCT_ret_method_hl_MR * more_rl_upstr(RM_RL_HM)
04	TRUE	RM_RL_HM (variant 1)	RM_RL_upstr_HM + RM_RL_TRIB_HM + WWTP_E_HM + ID_E_HM + AM_E_HM + US_cso_E_HM
05	TRUE	RM_CONC_HM (variant 1)	RM_RL_HM * 1000 * 1000 /(TOT_FNE_Q * 86400 * 365)

Table 67 - calculation of aggregated dissolved river loads of heavy metals with retention

step	active	formula	formula content
01	TRUE	RM_E_diff_diss_HM (variant 1)	TOT_E_HM - ER_E_HM - US_E_HM - WWTP_E_HM - ID_E_HM - AM_E_HM - OR_E_HM + ER_agrl_E_diss_HM + ER_nat_E_diss_HM + US_ss_E_diss_HM + OR_E_diss_HM +US_oss_E_diss_HM
02	TRUE	RM_RL_diss_TRIB_HM (variant 1)	RM_E_diff_diss_HM * RM_FCT_ret_TRIB
03	TRUE	RM_RL_diss_up-str_HM (variant 1)	RM_FCT_ret_ANSATZ_hl_MR * more_rl_upstr(RM_RL_diss_HM)
04	TRUE	RM_RL_diss_HM (variant 1)	RM_RL_diss_upstr_HM + RM_RL_diss_TRIB_HM + WWTP_E_diss_HM + ID_E_HM + AM_E_HM + US_cso_E_diss_HM
05	TRUE	RM_CONC_diss_HM (variant 1)	RM_RL_diss_HM * 1000 * 1000 /(TOT_FNE_Q * 86400 * 365)

5.2 ANNEX 2 – R VERSION

5.3 ANNEX 3 – MORE IMPORT FILES

5.4 ANNEX 4 – MORE RESULTS (OUTPUT FILES)

5.5 ANNEX 5 – MORE RESULT FIGURES (BAR CHARTS AND MAPS)