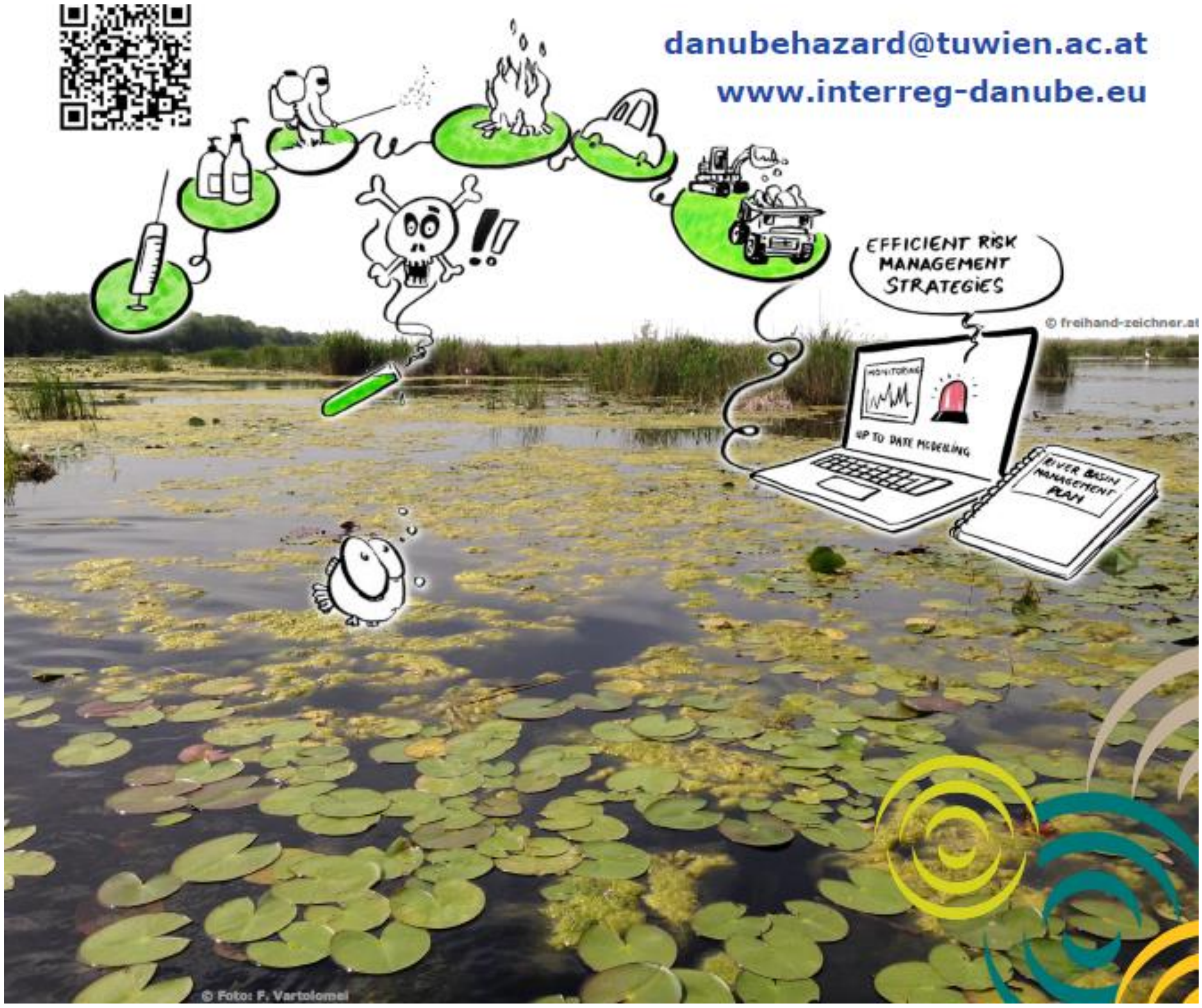
Project Danube Hazard m^{3}c:
Transnational trainings on hazardous substances emission modelling and scenario evaluation



Output T4.4
TRAINING MATERIAL PACKAGES ON MODELLING AND SECENARIO EVALUATION

October 2022

Project co-funded by European Union funds (ERDF, IPA, ENI) and National Funds of the participating countries

PROJECT TITLE: Tackling hazardous substances pollution in the Danube River Basin by Measuring, Modelling-based Management and Capacity building

ACRONYM: Danube Hazard m³c

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AUTHORS AND CONTRIBUTING PARTNERS

Name co-author	Contributing partner
Elvira Marchidan	National Administration Romanian Waters (NARW), RO
Matthias Zessner	TU Wien, AT
Ottavia Zoboli	TU Wien, AT
Steffen Kittlaus	TU Wien, AT
Adrienne Clement	Budapest University of Technology and Economics (BME), HU
Máté Kardos	Budapest University of Technology and Economics (BME), HU
Zsolt Jolánkai	Budapest University of Technology and Economics (BME), HU
Oliver Gabriel	Environment Agency Austria (Umweltbundesamt), AT
Marianne Bertine Broer	Environment Agency Austria (Umweltbundesamt), AT
Jos van Gils	DELTARES
Sibren Loos	DELTARES

Responsible for the Output: Elvira Marchidan (National Administration Romanian Waters)

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Table of contents

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Executive summary

In the frame of Capacity Building work package three transnational training events related to hazardous substances emission modelling and scenario evaluation ware carried out.

The courses took place in Vienna (4-5 October 2022), Budapest (6-7 October 2022) and Bucharest (13-14 October 2022).

These events aimed at effective reaching the specific target groups, which tend to be underrepresented in international platforms.

For the training the project partners developed jointly a learning package that covered the following topics:

1. Topic 1. Emission modelling on catchment scale as a tool to support hazardous substances management
2. MoRE model
3. Danube Hazard model (DHSM) (based on the SOLUTIONS model)
4. DHSM model: Hands-on workshop
5. Workshop (1): Processing of input data
6. Workshop (2): Development and implementation of programmes of measures for scenario analysis
7. Results of MoRE and DHSM models, MoRE vs. DHSM or MoRE and DHSM?

All materials were adapted to specific needs, in order to suit best the current state-of-art in the participating countries and provide high added value for the audience.

The main purposes of the hazardous substances emission modelling and scenario evaluation training course were:

- to improve the understanding of concepts and skills for the modelling of HS emissions and to assist in the development and definition of scenarios and to interpret and assess them appropriately.
- to improve knowledge related to the analysis of significant pollution sources and pathways to help authorities in developing of recommendations at the transnational basin level for effective management interventions/activities.
- to provide educational outcomes and increase competencies in the Danube region in the area of HS modelling.

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Agenda of event

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Tackling hazardous substances pollution in the Danube River Basin by Measuring, Modelling-based Management and Capacity building

Transnational training on hazardous substances emission modelling and scenario evaluation

2022

Agenda

Day 1: 13.10.2022		
09:15	09:30	**Welcome**
09:30	10:15	**Emission modelling on catchment scale as tool to support hazardous substances management** *(Matthias Zessner, TU Wien)* Overview of existing approaches for modelling and scenario analysis (management, climate, ...): scope, potential, limitations and data
10:15	10:40	**Questions and answers**
10:40	11:00	***Coffee break***
11:00	11:45	**MoRE model** *(UBA)* Technical introduction: scope, temporal and spatial scales; data requirements; calculation approaches; technical requirements, conditions and documentation for its use
11:45	12:05	**Questions and answers**
12:05	13:15	***Lunch break***
13:15	14:00	**DHSM model (based on the SOLUTIONS model)** *(Deltares)* Technical introduction: scope, temporal and spatial scales; data requirements; calculation approaches; technical requirements, conditions and documentation for its use
14:00	14:20	**Questions and answers**
14:20	14:40	***Coffee break***
14:40	17:00	**DHSM model: Hands-on workshop** *(Deltares)* Interactive and practical exercise session

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Day 2: 14.10.2022		
9:00	**10:30**	**Workshop (1): Processing of input data** *(BME)*
10:30	**10:50**	***Coffee break***
10:50	**12:10**	**Workshop (2): Development and implementation of programmes of measures for scenario analysis** *(UBA)*
12:10	**13:10**	***Lunch break***
13:10	**14:00**	**Results of MoRE and DHSM models, MoRE vs. DHSM or MoRE amd DHSM?** *TU Wien, Deltares, UBA* Examples of the results in the pilot regions of the Danube Hazard m3c project and for the whole Danube River Basin for different types of hazardous substances. Critical comparison of the two models and disscusion of complementary aspects. Lessons learned in the Danube Hazard m3c project.
14:00	**14:15**	**Questions and answers**
14:15	**14:30**	**Conclusions and feedback of the participants, including filling in the questionnaire**
14:30		**End of the training**

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Training on hazardous substances emission modelling and scenario evaluation

Emission modelling on catchment scale as tool to support hazardous substances management

Vienna, 4th October 2022

Ottavia Zoboli, Matthias Zessner

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Table of contents

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Monitoring versus Modelling for Exposure Assessment

Monitoring versus Modelling for Exposure Assessment

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Monitoring:

- Measurement of site- and time-specific concentration levels in selected places

Modeling:

- Theoretical depiction of interplay between release pattern, partitioning and transformation processes
- local, regional and global models
- assumptions and simplifications

Exposure Assessment via monitoring

Hindsight

Measured environmental concentrations (MEC)

Prerequisites

- Validated analytical tools
- Sufficiently low limit of detection and limit of quantification
- Monitoring campaigns under consideration of regional and temporal variations

Application

- Status assessment for priority substances
- Control of legal standards
- Input data and validation data for of models

Problems

- Available only for known and/or “existing” substances and situations
- Reflect only local conditions at a certain time
- High number of measurements is required to assess spatial and temporal variety of concentrations
- High analytical costs and high number of parameters
- Detection limits sometimes higher than no effect levels (some POPs, some viruses)
- Uncertain quantification at very low concentrations or in specific matrices
- Does not provide information on sources and pathways

Exposure Assessment via modelling

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Calculated ("predicted") environmental concentrations (PEC)

Foresight

Prerequisites

- Good understanding of the system
- Reliable models
- Basic data and information on considered parameters

Application

- (Preliminary) risk assessment
- Identification of sources and pathways
- Assessment of potential developments

Problems

- Reliability of models (classical validation is not possible in many cases)
- Needed basic data and information on considered parameters is not always available
- No consideration of local peculiarities
- Lack on knowledge on formation of metabolites

Monitoring versus Modelling for Exposure Assessment

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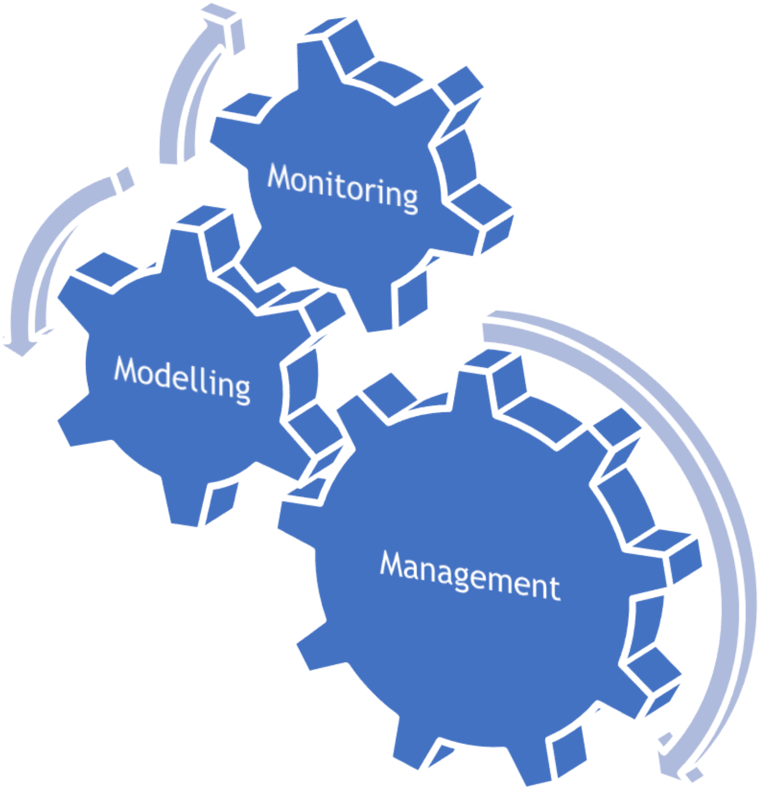

For management purposes a combination should be aspired for development of emission inventories and for the validation of models

Exposure models

Exposure models

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- Selection of processes relevant for the fate of substances (e.g. transport, distribution between environmental compartments, degradation), which can be formalized as mathematical equations
- „Solution" of the models: calculated environmental concentrations as a function of time and space

Goals of exposure models

„realistic" image of the environment

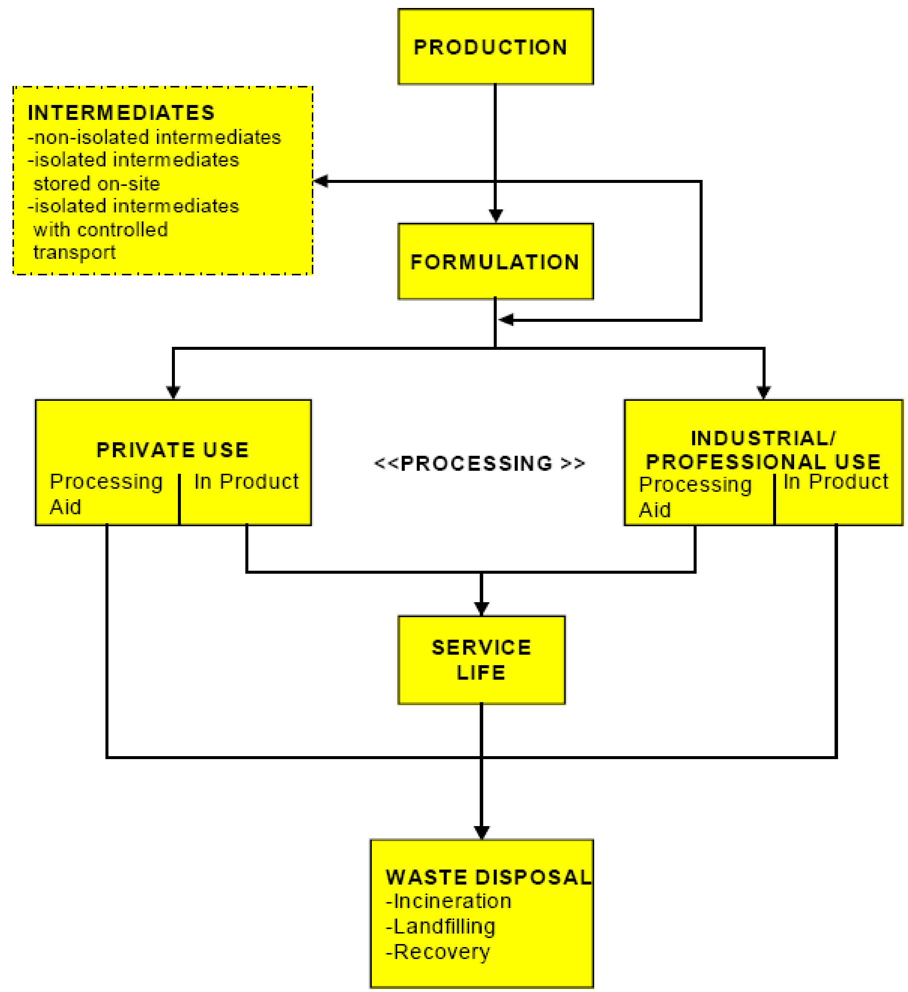
„approximation" of the environment

- understanding of the relevant processes and interactions
- comparative evaluation of chemical fate („*screening*", „*ranking*")
- target endpoints: concentration, spatial pattern, overall persistence, mass flows

Release into the environment

At any stage of the life-cycle of a substance:

- Production of the substance
- Transport and storage
- Formulation into a product
- Private use
  - processing aid
  - in product
- Industrial use
  - processing aid
  - in product
- Service life (releases into the environment of substances from long lasting products by leaching, weathering etc.)
- Waste disposal



Driving forces of release into environment

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Use pattern of a chemical

- mass of substance produced [tonnes / y]
- mass of substance imported [tonnes / y]
- mass of substance exported [tonnes / y]
- use category [-]
  - private/industrial use
- industrial category [-]
  - agricultural industry, chemical industry, electrical/electronic industry, mineral oil and fuel industry etc.
- main category (for existing substances) [-]
  - use in closed systems
  - use resulting in inclusion into or onto a matrix
  - non-dispersive use
  - wide dispersive use

Specific information on the use pattern of the substance

Behaviour in the environment

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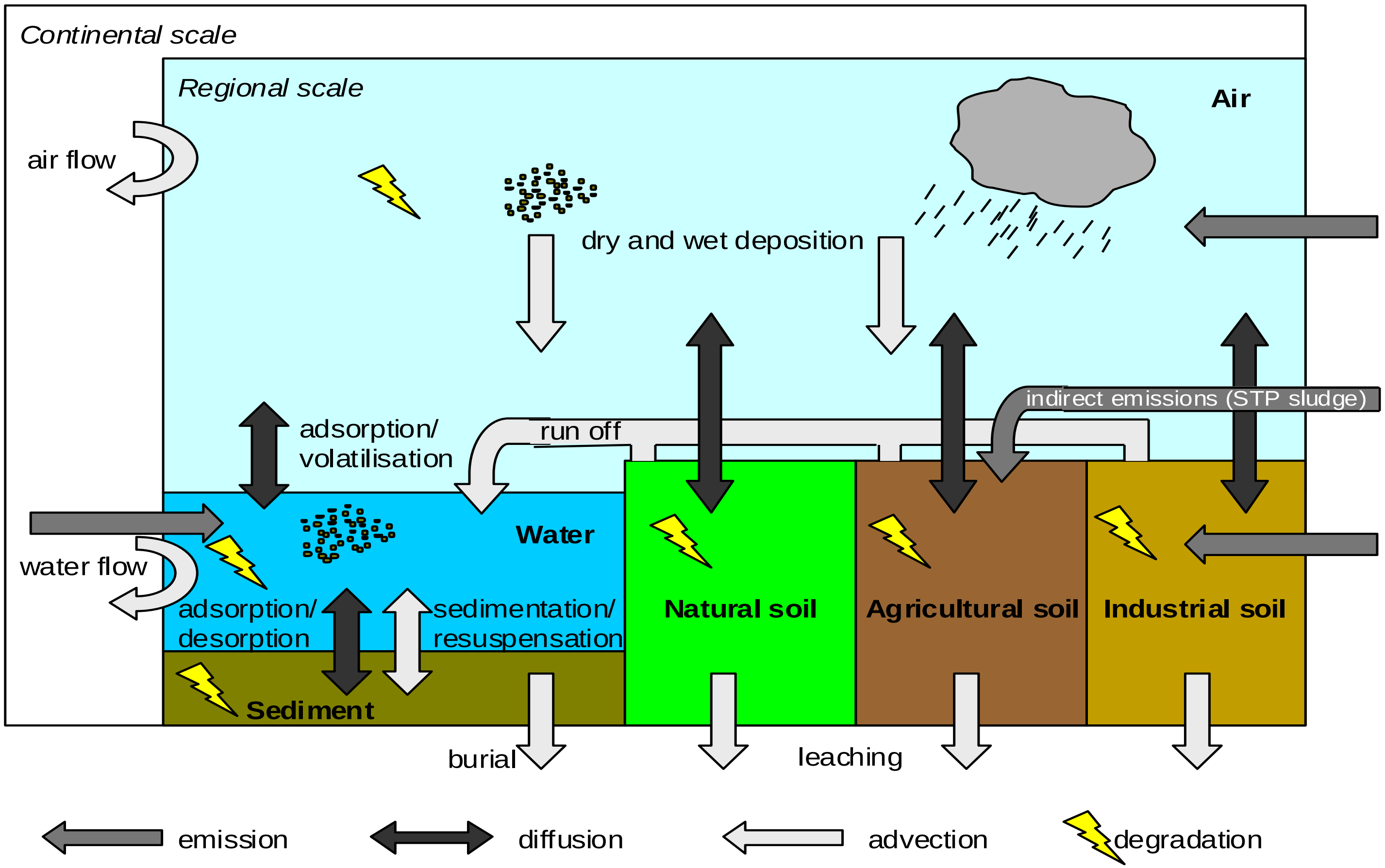

e.g. EUSES (2010) European system for evaluation of substances
http://ecb.jrc.ec.europa.eu/Euses/

Properties for behaviour in the environment

Physico-chemical properties of a chemical (e.g.)

- octanol water partitioning coefficient P_{ow} or K_{ow} [-]
  $K_{ow} = C_o/C_w$; often used $\log K_{ow}$
- organic carbon-water partition coefficient K_{oc} [-]:
  $K_{oc} = C_{oc}/C_w$, often used as $\log K_{oc}$
- soil adsorption coefficient Kd
  $K_d = K_{oc}$ x Organic carbon content in soil
- water solubility [mg/l]
- boiling point (only for some release estimations) [°C]

Abiotic and biotic degradation rates

(e.g. half life time, $T_{1/2}$ [d] or first order rate constant, k [d^{-1}]

$T_{1/2} = \ln 2/k$; $C_t = C_0 * e^{-t*k}$

- hydrolysis
- photolysis in water or air
- biodegradation in waste water treatment plan
- biodegradation in surface waters, soil

Emission models

Emission models as specific type of exposure models

- Emission models focus on inputs of substances into water bodies
- They identify sources and pathways of substances and estimate emission loads release via each of them
- As mass balance models they calculate instream loads and concentrations based on the quantification of emissions
- The accuracy of this type of model can be tested by comparing instream loads and concentrations calculated from emissions with instream loads and concentrations derived from observations
- The spatial boundaries of emissions models must be in line with boundaries of (sub-) catchments
- The (sub-) catchment upstream a monitoring point defines the area responsible for the emissions into the river

Emission Modelling and Emission Inventories

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Legal requirements for emission inventories

According to the Article 5 of the Directive 2008/105/EC (EQS Directive), Member States shall establish an inventory, including maps, if available, of emissions, discharges and losses of all priority substances for each river basin district or part of a river basin district lying within their territory including their concentrations in sediment and biota, as appropriate.

Main objectives of inventorying:

- Obtaining information on the relevance of substances at spatial scale in the river basin
- Enabling compliance check with WFD regarding the reduction of discharges, emissions and losses

Emission Modeling supporting Emission Inventories

Importance of emission modelling in context of emission inventories

- Provides a regionalized system analysis with quantification of pathways and sources and it closes information gaps (e.g. diffuse pollution)
- Avoids high costs and bridges spatial constraints of monitoring
- Shows need for action in catchments where no monitoring has been established
- Significantly contributes to the management cycle (pressures and impact assessment as well as for risk analyses)
- Enables decision makers to be pro-active by the possibility of prognoses
- Supports policy makers in the design of Programs of Measures (by calculating the efficiency and effectiveness of mitigation measures via scenario analyses)

Role of emission models in the WFD management cycle

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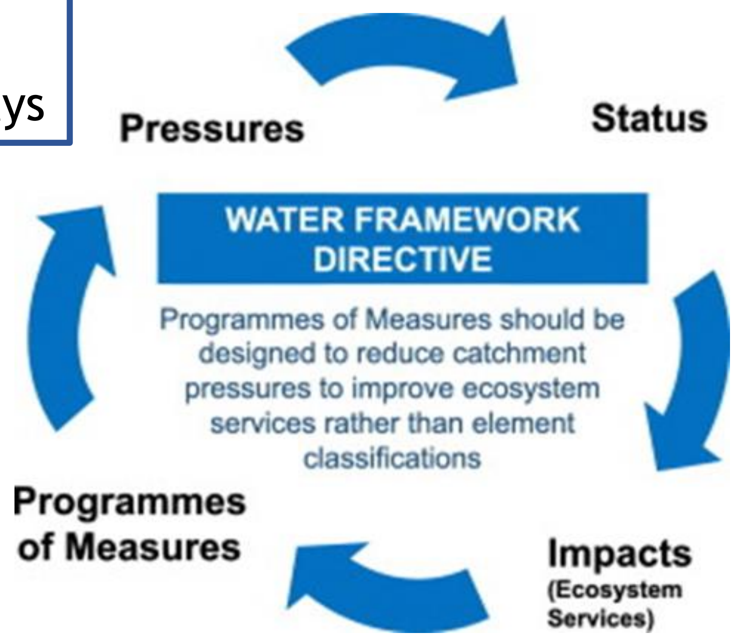
Quantification of significant pressures from different pathways

Completion of more fragmented picture of monitoring



(T. Giakoumis and N. Voulvoulis, 2019)

Gained knowledge:
relevance of pathways
relevance of sources
potential reduction of Measures (scenarios)

Possible risk analyses on scale of modeled Analytical Units

EU-Guidance Document on Inventories

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TIER	BUILDING BLOCKS	EXPECTED OUTPUT	RESULTS FOR THE INVENTORY
STEP 1: ASSESSMENT OF RELEVANCE			
	Information sources identified in Art. 5 of EQS directive, see section I.1	Decision of relevance	List of relevant and less relevant substances
STEP 2: APPROACHES FOR RELEVANT SUBSTANCES			
1. Point source information	• Data on point sources • Emissions factors	• Availability of data • Quality of data • Identification of gaps	• Point source emissions • Listing of identified data gaps
2. Riverine load approach	add: • River concentration • Data on discharge • In stream processes	• Riverine load • Trend information • Proportion of diffuse and point sources • Identification of gaps	• Rough estimation of total lumped diffuse emissions • Verification data for pathway and source orientated approaches • Listing of identified data gaps
3. Pathway orientated approach	add: • Land use data • Data on hydrology • Statistical data • .... •	• Quantification and proportion of pathways • Identification of hotspots • Information on adequacy of POM	• Pathway specific emissions • Additional spatial information on emissions
4. Source orientated approach	add: • Production and use data e.g. from REACH • SFA • Substance specific emission factors • .... •	• Quantification of primary sources • Complete overview about substance cycle • Information on adequacy of POM	• Source specific emissions • Total emissions to environment and proportion to surface waters

Step 1

Step 2

Tier approaches in Step 2

Technical Report - 2012 – 058 Common Implementation Strategy for the Water Framework Directive (2000/60/EC) *Guidance Document No. 28 Technical Guidance on the Preparation of an Inventory of Emissions, Discharges and Losses of Priority and Priority Hazardous Substances*

EU-Guidance Document on Inventories

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3. Pathway orientated approach	Need for emission models		
4. Source orientated approach			

Step 1

Step 2

Tier approaches in Step 2

Technical Report - 2012 – 058 Common Implementation Strategy for the Water Framework Directive (2000/60/EC) *Guidance Document No. 28 Technical Guidance on the Preparation of an Inventory of Emissions, Discharges and Losses of Priority and Priority Hazardous Substances*

Tiers 1-4

Technical Report - 2012 – 058 Common Implementation Strategy for the Water Framework Directive (2000/60/EC) *Guidance Document No. 28 Technical Guidance on the Preparation of an Inventory of Emissions, Discharges and Losses of Priority and Priority Hazardous Substances*

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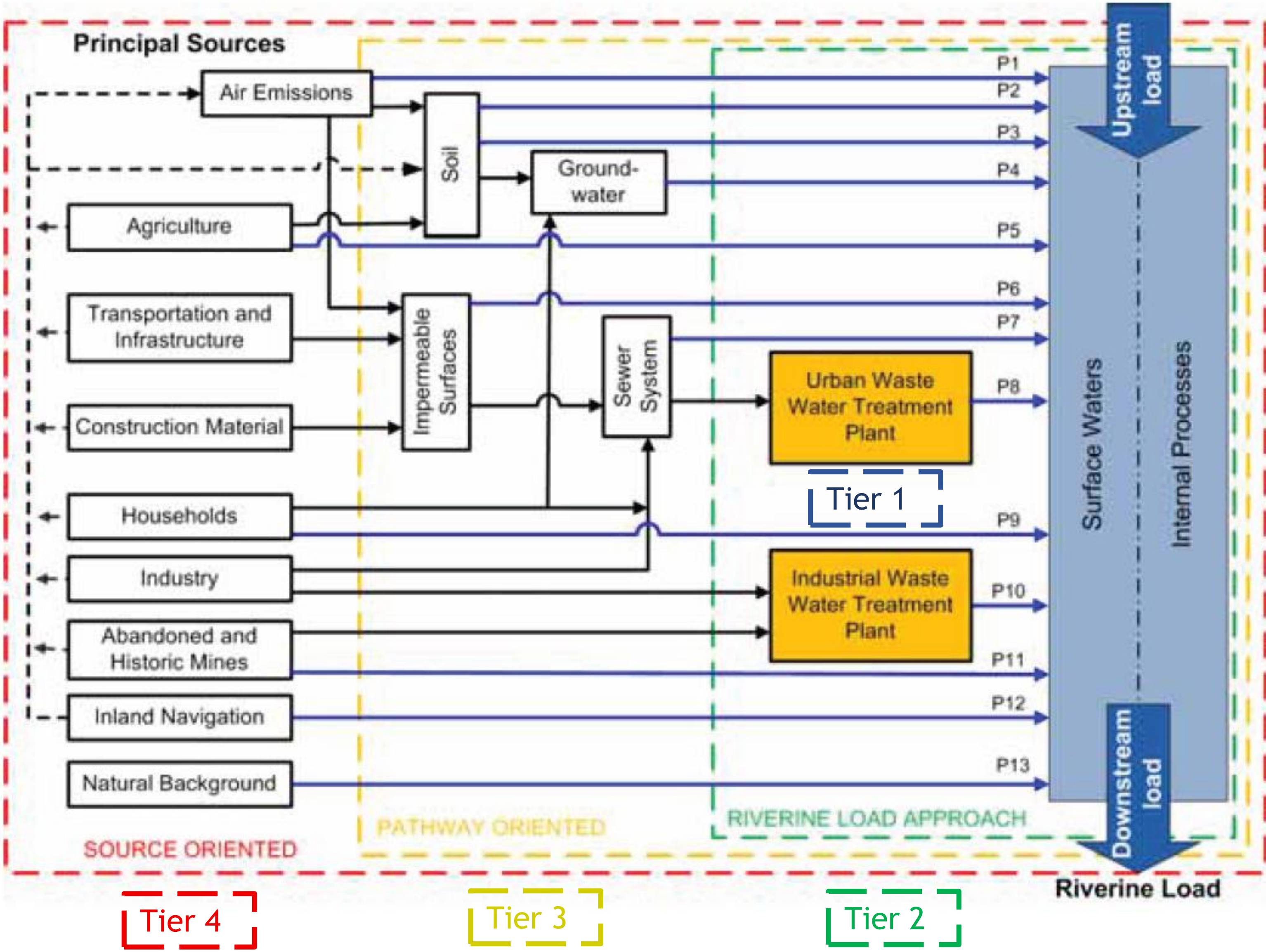

Tier 1: Point source information

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- This tier focuses on point discharges. It uses readily available statistical data regarding discharges from wastewater treatment plants and industries -> it is based on a classical point discharge inventory
- Based on this information, the presence or absence of known point sources can be concluded. The conclusion of absence should be backed up through the analysis of production and use information. If this confirms that the point emission of a substance is negligible, then final confirmation should be provided from the results of emission monitoring, which should be undertaken using appropriate methods.
- This tier is mandatory, as it forms the basis of point and diffuse sources assessment.

Tier 2: Riverine load approach

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- It is based on concentration (water and the suspended solids) and discharge data in rivers considering the basic processes of transport, storage or temporary storage and degradation of substances.
- The resulting riverine load provides information about the recent status of pollution and temporal trends in case of long-term information.
- In combination with the information gained in tier 1 (inventory of point source emissions) it allows estimating which share of loads derive from diffuse emissions -> **first step towards emission model**, with a strongly simplified model for diffuse pollution and retention/degradation
- Results of the riverine load approach indicating high pollutant concentrations, an increasing trend, or a high relevance of diffuse emissions signal the need for a more detailed analysis using the approaches in tiers 3 (pathway oriented) and 4 (source oriented).

Tier 2: Riverine load approach

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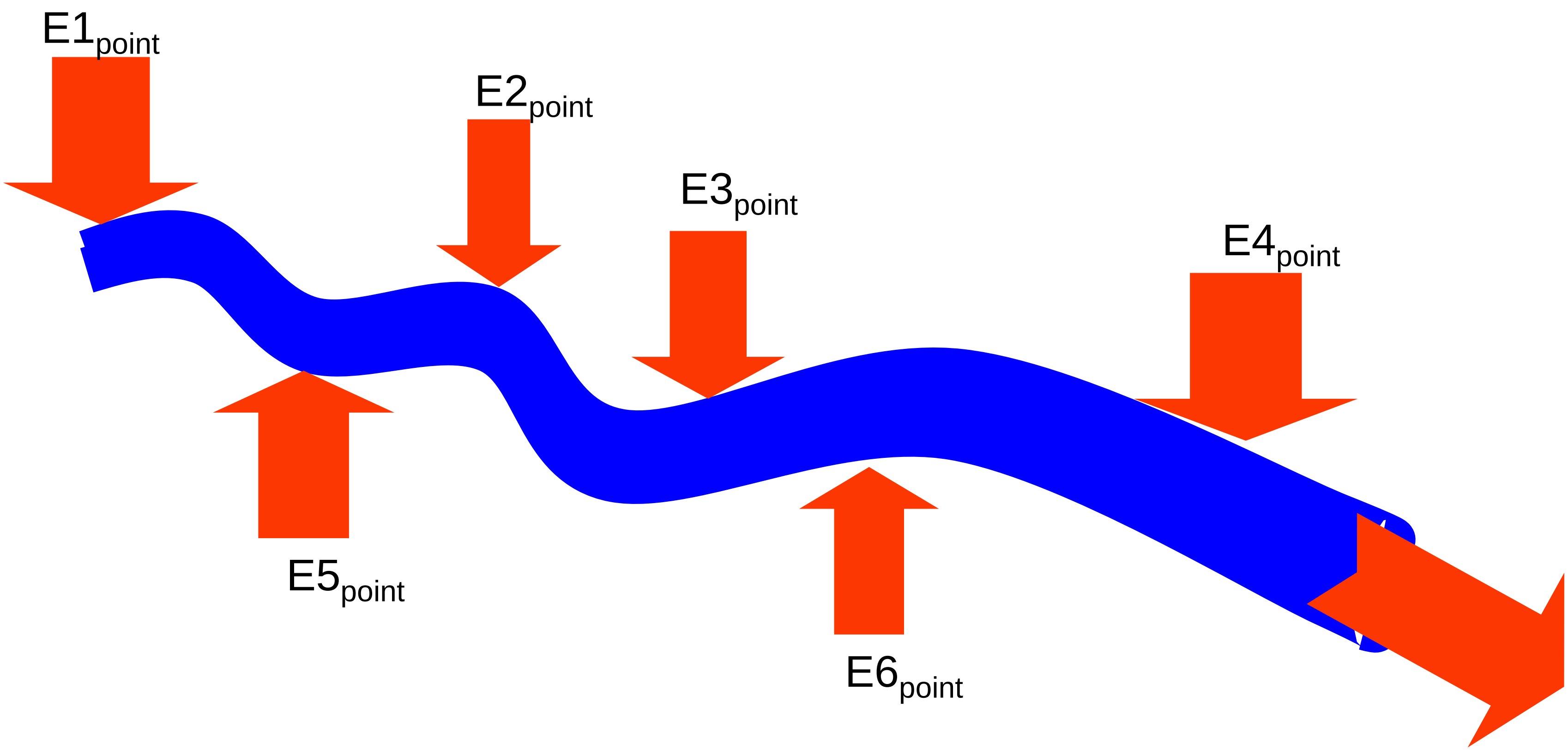

Spatial Level = River from source to monitoring point
Mass balance: $\Sigma E_{diffuse} = I - \Sigma E_{point}$ $(- \Delta - D)$

Tier 3: Pathway oriented approach

- It uses more specific information about land use, hydrology and fate of substances in the environment. The data requirements are higher than for the lower tiers.
- This tier allows identification of the main emission pathways and regional hotspots of emission and provides the quantification of specific emissions (e.g. area specific loads, storm water runoff loads).
- It will, therefore, provide the basis for an accurate inventory.
- For substances following a ubiquitous emission pattern or for which efficient mitigation measures are not available it might be appropriate to enter the next tier (source oriented approach).

For example with the MoRE model used in the project

MoRE Emission model

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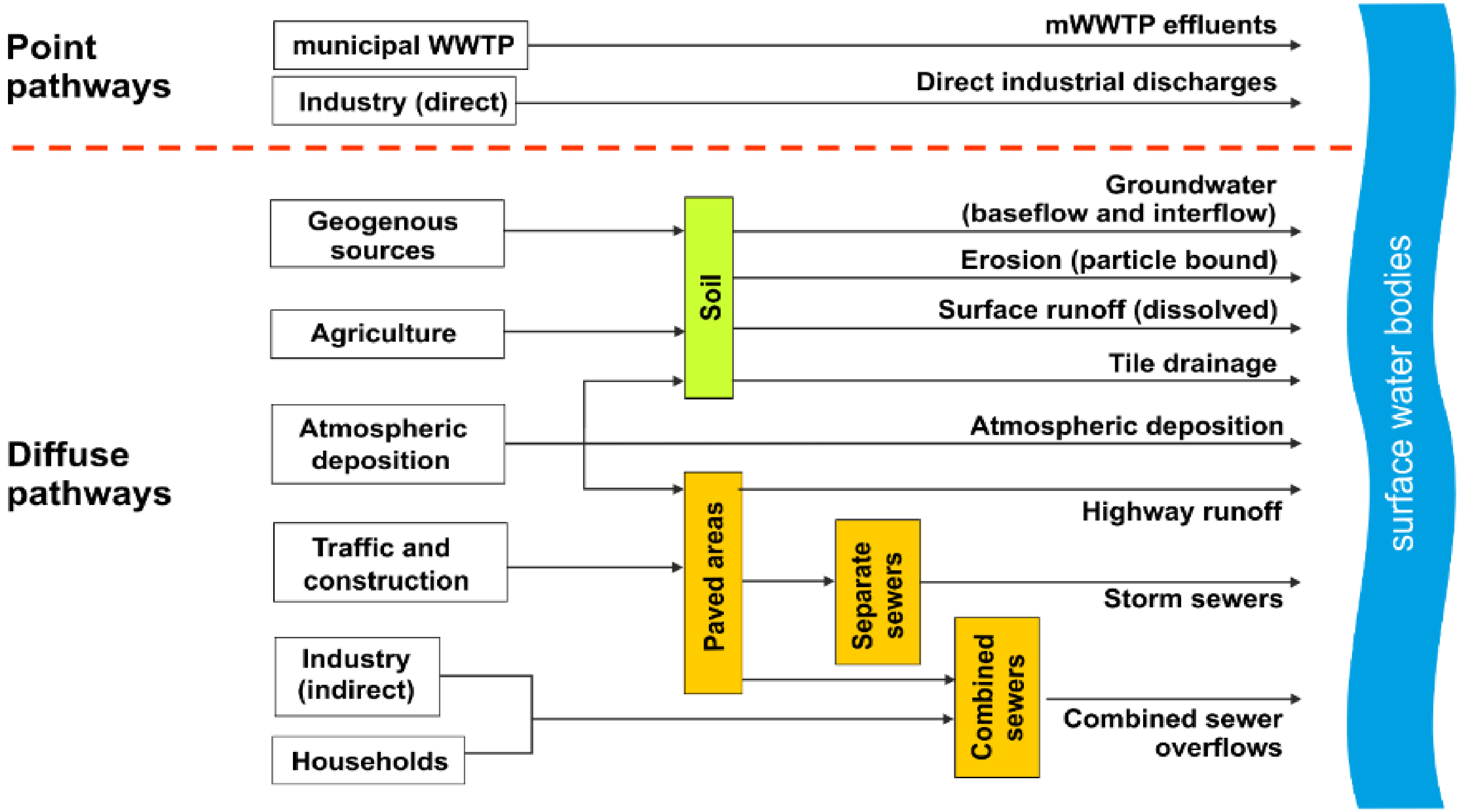

Spatial Level = (Sub-) Catchment

Mass balance model: $I = \Sigma E_{point} + \Sigma E_{diffuse} - \Delta - D$ (chance for validation)

Tier 4: Source oriented approach

- It is based on substance-specific information on production, sales and consumption which to some extent are available e.g. through REACH.
- It allows the drawing of a comprehensive picture of the life cycle of a substance.
- The benefit of this approach is that the information gained is sufficient to implement not only end-of-pipe solutions but also source controls and precautionary measures.

Integrated for example within the DHSM model (based on the SOLUTIONS model) used in the project

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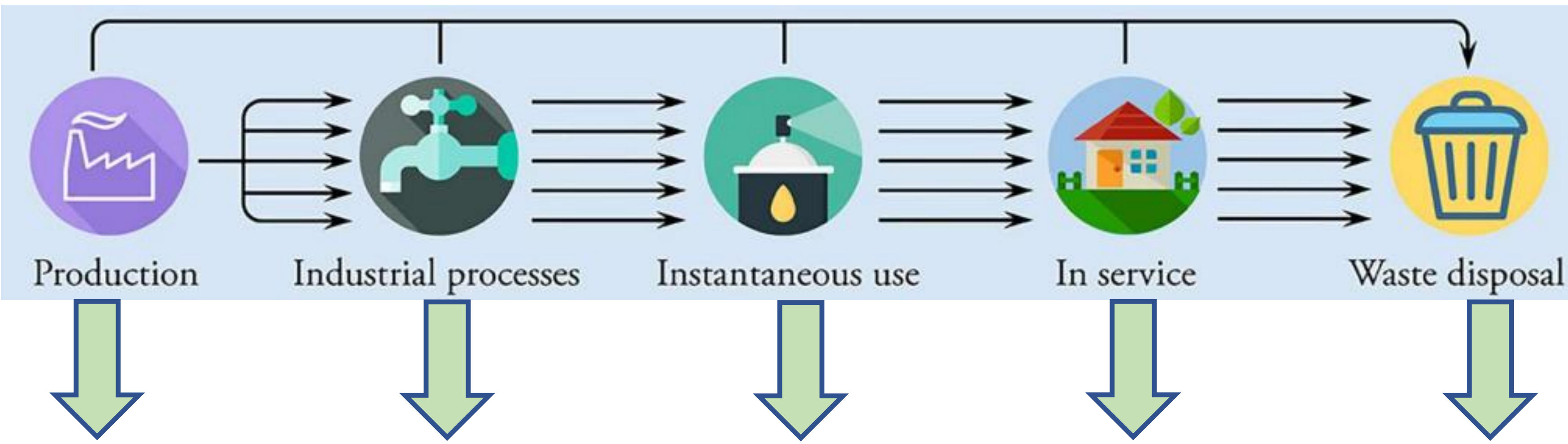
DHSM use of chemicals

Chemicals in the anthroposphere / technosphere

DOI: 10.1289/EHP9372



losses to the environment can be caused by all life-cycle stages:

1. losses from industry
2. losses associated to use
3. losses from wear or aging of products and materials
4. losses from waste management

DHSM stock of chemicals

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- In the Technosphere: products, buildings, infrastructure, waste
- Losses to the environment from these stocks
- Consequences:
  - today's use volume not representative for today's emissions
  - longer time scales: today's emissions dependent on use volumes from past years, decades (depends on product and construction life time, wear and release rates of the chemical)
- Similar issue with stocks in soils
- Solution: use the stock as a source (replace the source by a pathway)
- (also atmospheric deposition is actually a pathway)

DHSM Sources and pathways

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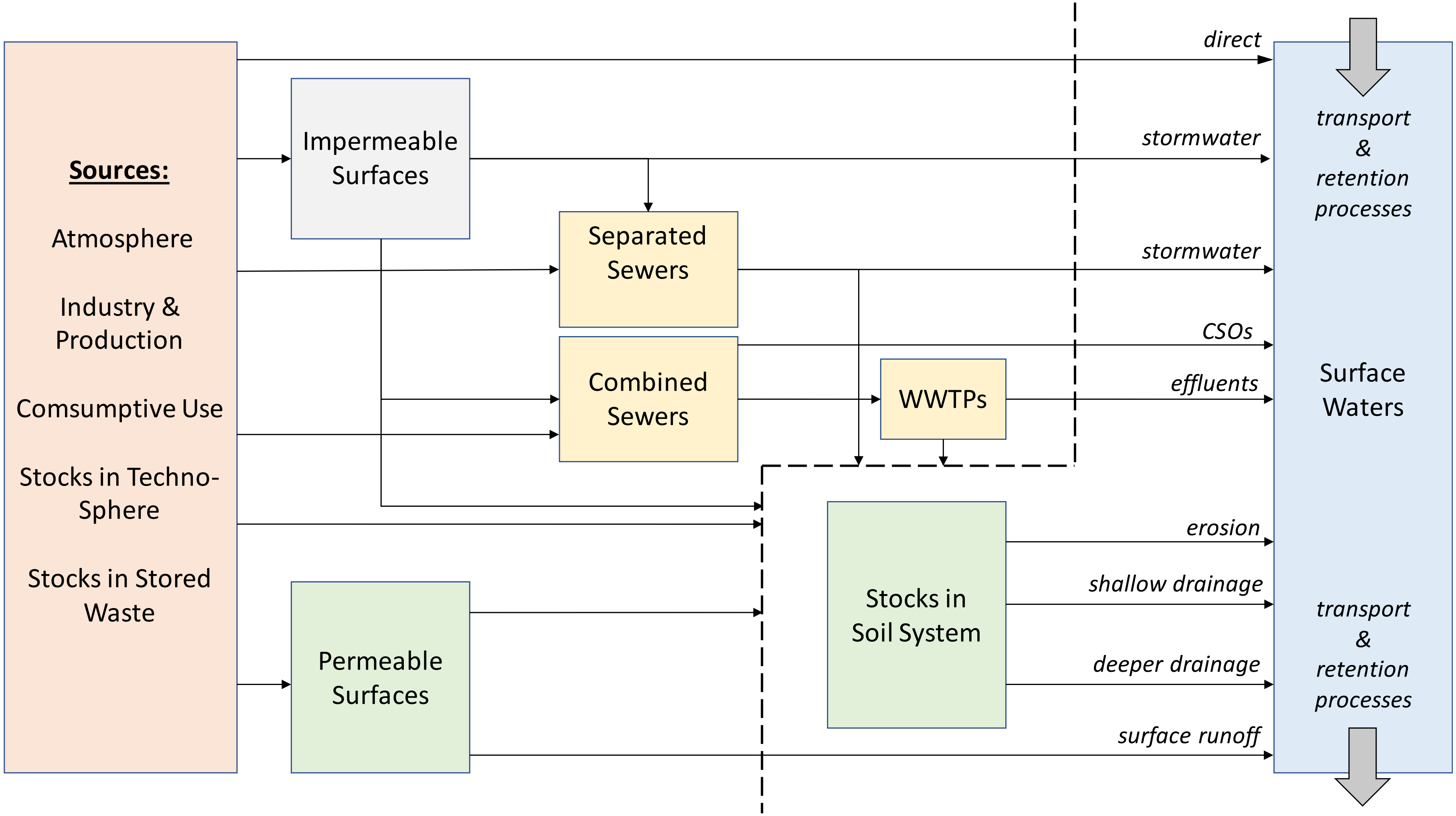

Model outputs (Tier 3 and 4)

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- River loads and concentrations calculated based on emission loads (and storage/degradation) $\Rightarrow$ used for validation against river loads and concentrations from monitoring
- River concentrations for unmonitored rivers to be used for risk assessment (e.g. compared to EQS)
- Regional emission hotspot (sub-catchment scale)
- Relevance of emissions via different pathways or from different sources (sub-catchment scale)
- Expected or potential changes in the system in the future (predictions and scenarios)

Predictions and Scenarios

- Predictions
  - Future developments that will happen with a certain probability.
- Scenarios
  - What would happen if…
- Examples for scenarios
  - Implementation of certain measures or bundles of measures
  - Potential developments (e.g. demography, use of pharmaceuticals, pesticides application)
  - Natural drivers as climate change
- Scenarios can only considered changes that are implemented in the scope of the model (differences between tier 2, 3 and 4)

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Training on hazardous substances emission modelling and scenario evaluation

MoRE model

Vienna, 04.10.2022

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Table of contents

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Scope – MoRE Emission model

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MONERIS:

- IGB-Berlin
- Behrendt et al. 2000
- MOdeling Nutrient Emissions in RIver Systems
- Implemented in MS-Excel

MONERIS for hazardous substances

- Technische Universität Karlsruhe
- Fuchs et al. 2002
- Adaptation of MONERIS to model heavy metals and lindane

Reimplementation: MoRE

- Technische Universität Karlsruhe
- Fuchs et al 2010
- Reimplementation of the MS-Excel-model into a more stable technical framework
- Application for PAHs

Scientific publication of MoRE:

- Karlsruhe Institute of Technology
- Fuchs et al. 2017

Scope – MoRE Emission model

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- Pathway-oriented, conceptual model (**M**odelling **o**f **R**egionalized **E**missions)
- Developed from MONERIS 2.01 model since 2009
- Mainly used to model heavy metals and organic pollutants
- Is built on a PostgreSQL database in order to store the large datasets required for modelling
- Has a flexible structure, enabling adaptations (pathways or pathway modifications) and the implementation of new substances
- Implementation of variants of data sets and of formula possible
- Freely available
- Transparent, comprehensive documentation of input data and approaches

Scope - emission models in the WFD management cycle

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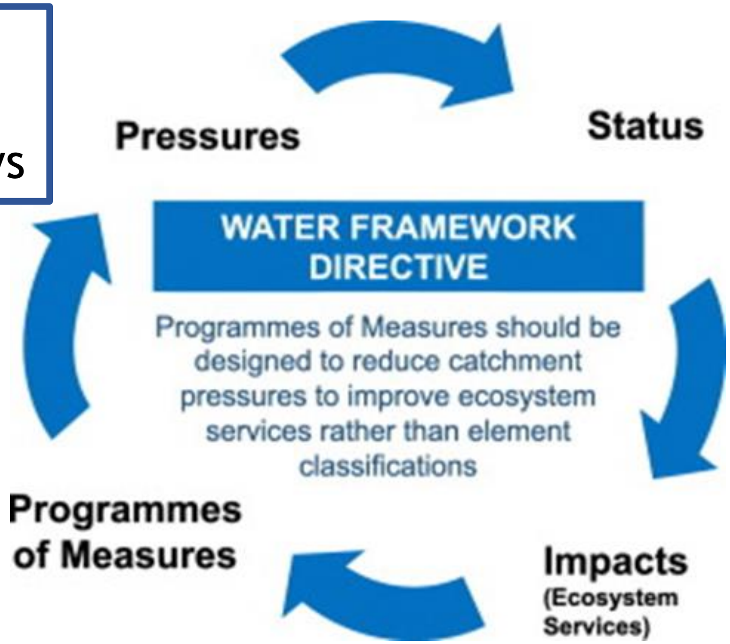
Quantification of significant pressures from different pathways

Completion of more fragmented picture of monitorig



(T. Giakoumis and N. Voulvoulis, 2019)

Gain knowledge:
relevance of pathways
relevance of sources
potential reduction of Measures (by scenarios)

Possible risk analyses on scale of modeled Analytical Units

Scope – pathways

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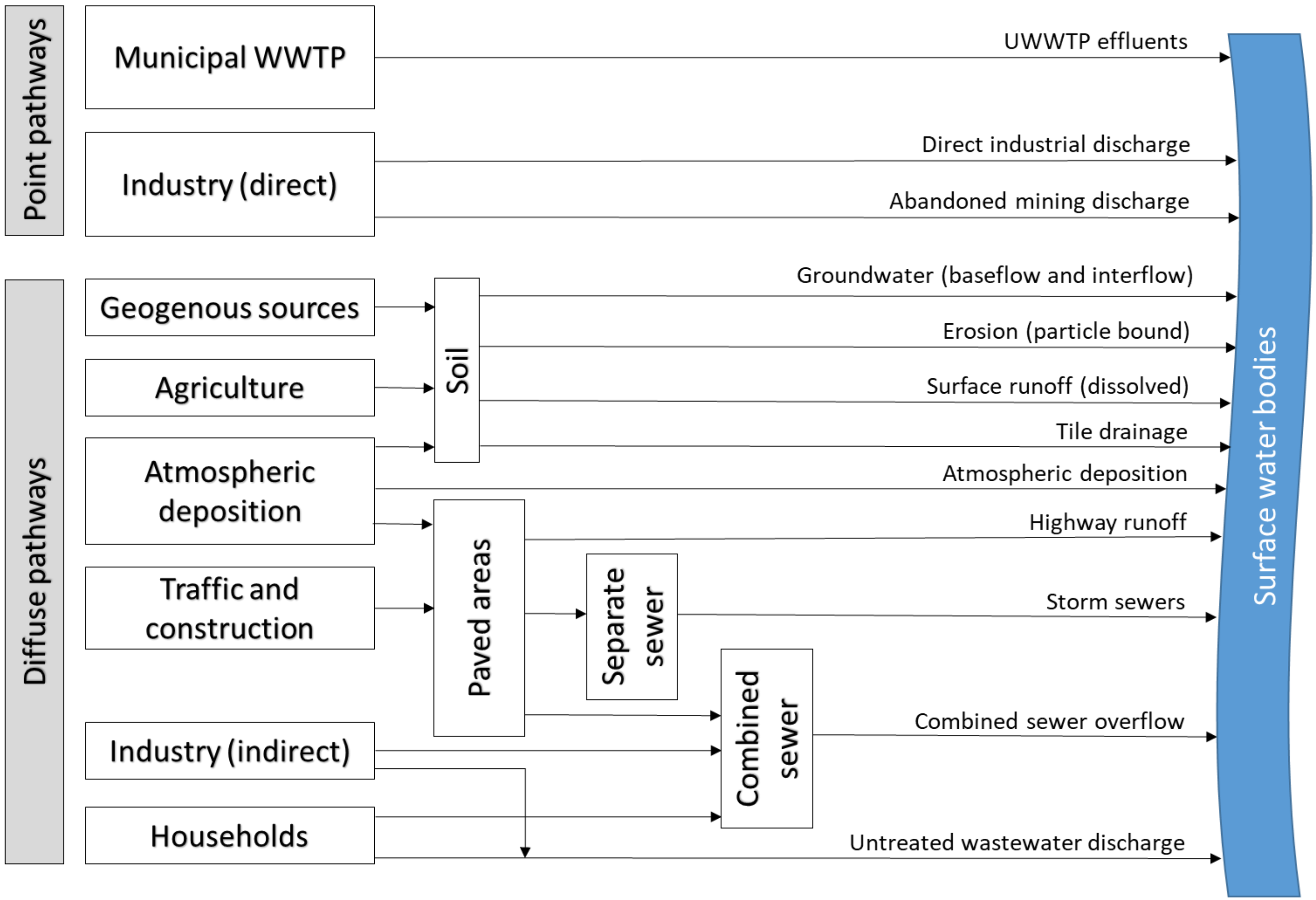

Scope – in the DHm3c project

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Goals

setup the MoRE model in seven pilot regions in four countries well representing the gradient in physical- and economical conditions in the DRB

providing a validated, actual Model adapted to the specific conditions (e.g. status of wastewater treatment and data availability) and a detailed system analysis

Identification of mitigation measures and assessment of their efficiency based on scenario analyses

Benefits

Acting as role model for an assessment of priority substances on EU- and national level

Visualizing crucial system interactions, dominant pathways, sources and gaps; a precondition of a proper management

Give guidance and build capacity to master large parts of the management cycle

Scope – in the DHm3c project

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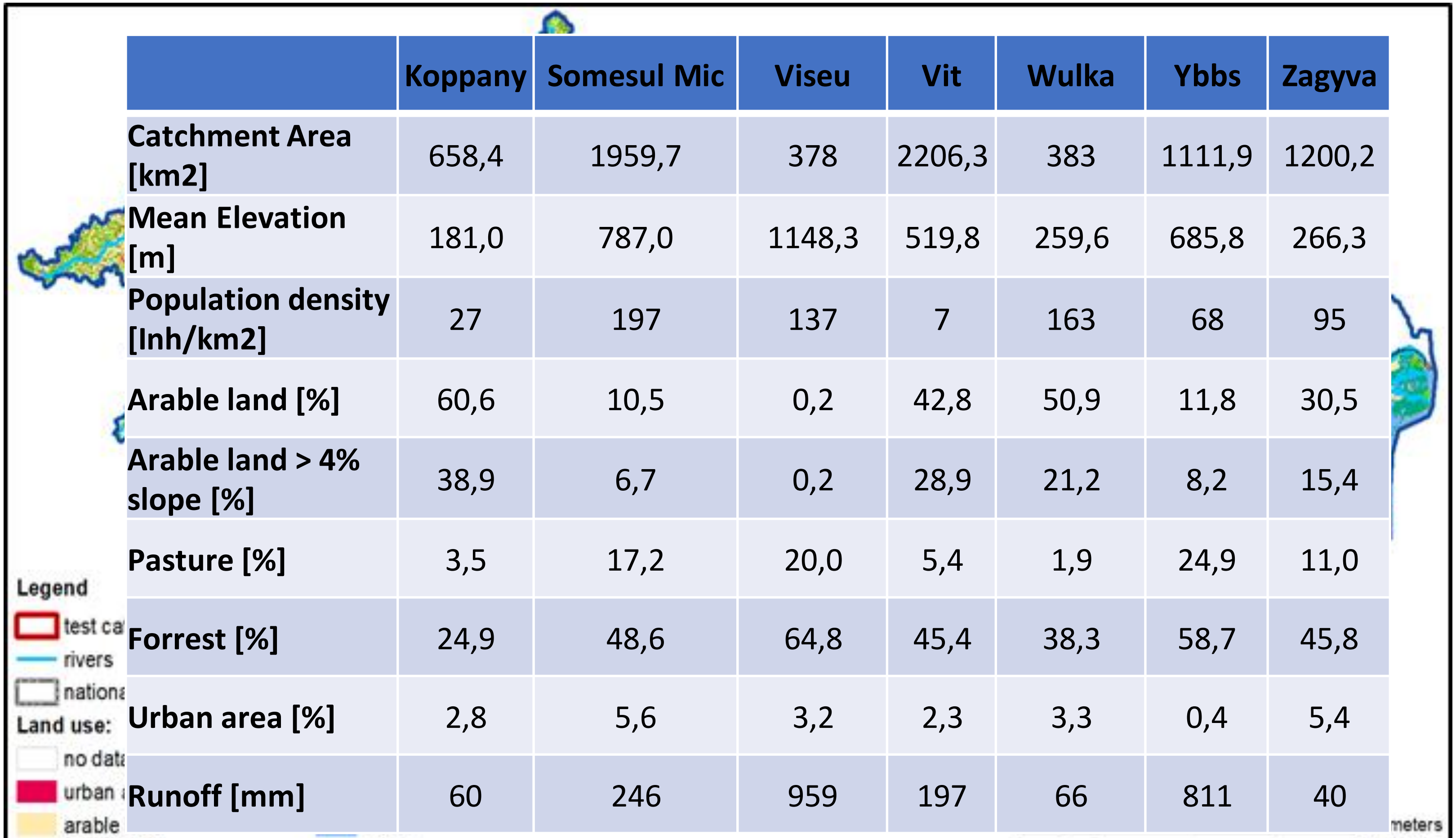
Pilot regions



	Koppany	Somesul Mic	Viseu	Vit	Wulka	Ybbs	Zagyva
Catchment Area [km2]	658,4	1959,7	378	2206,3	383	1111,9	1200,2
Mean Elevation [m]	181,0	787,0	1148,3	519,8	259,6	685,8	266,3
Population density [Inh/km2]	27	197	137	7	163	68	95
Arable land [%]	60,6	10,5	0,2	42,8	50,9	11,8	30,5
Arable land > 4% slope [%]	38,9	6,7	0,2	28,9	21,2	8,2	15,4
Pasture [%]	3,5	17,2	20,0	5,4	1,9	24,9	11,0
Forrest [%]	24,9	48,6	64,8	45,4	38,3	58,7	45,8
Urban area [%]	2,8	5,6	3,2	2,3	3,3	0,4	5,4
Runoff [mm]	60	246	959	197	66	811	40

Temporal scale

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- MoRE operates on annual time steps
- It includes a period of five to six years to minimize the probability to model specific meteorological and hydrological conditions only
- Temporal resolution of relevant input and validation data determine the use of annual or periodic modelling results
- Often reliable monitoring data are available only for few years; in this case it might be reasonable to create transfer functions based on runoff data or suspended solids to estimate loads for other years
- A higher temporal resolution addressing seasonal effects might be helpful, but is not needed for the assessments proceeded with MoRE

Spatial scale

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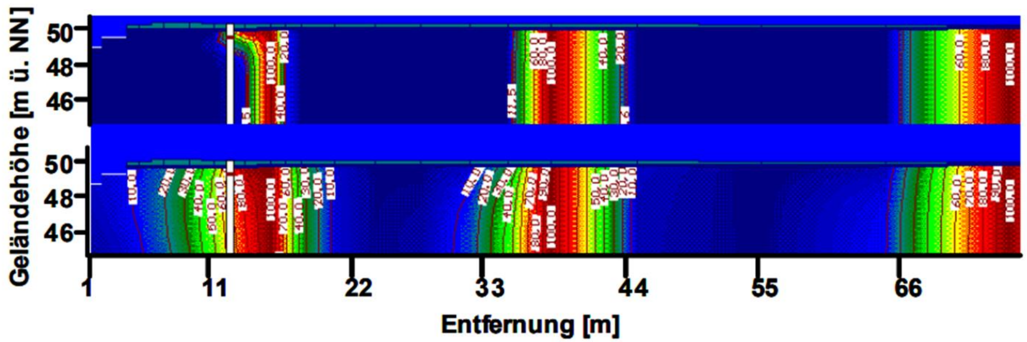
- More operates on catchment scale
- The model is related to the meso scale (catchments with ~50 - >100 km^2)
- Emission modelling with even smaller catchments might work but with growing uncertainty:
  - Semi-empirical approaches implemented in the model are related to the meso-scale
  - Data quality and availability in general decreases with smaller scales
  - Specific conditions might appear that are not represented in the model approaches, describing a generalized process behavior or dependence of various factors
- Less generalized characteristics with specific process behavior of high temporal or spatial resolution could be better addressed by physically-based models

2D Groundwater modelling and substance tracking MODFLOW MT3D (Gabriel, 2011)



Delineation of Subcatchments

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- The delineation of Analytical Units (AU) (~50->100 km^2) is the first crucial step applying the model
- The delineation should be determined by hydrological aspects but also by model specific and strategic aspects
- The technical application can be practiced by using:
  - DEM (raster data)
  - Water network (raster data)
  - Outlet points (vector data)
- Outlet points should/can consider:
  - Hydrological knots, delineating tributaries
  - Quality monitoring stations and/or discharge measuring points
  - Delineated waterbody catchments or clustered water body catchments

  } optimal all aspects!
- Thoroughly plan the delineation in transboundary catchments, inlets from upstream (data!) or boundary rivers

Delineation

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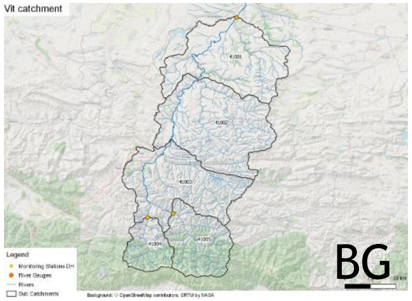
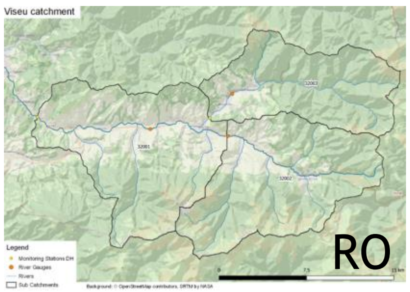
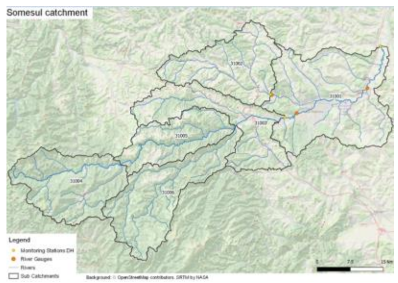
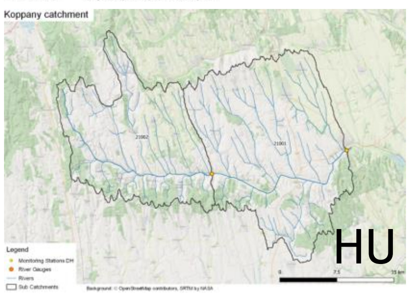
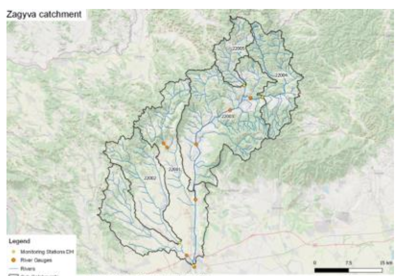


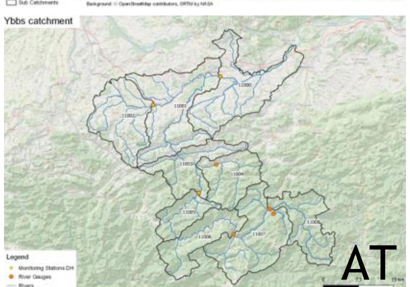
DHm3c
Pilot regions

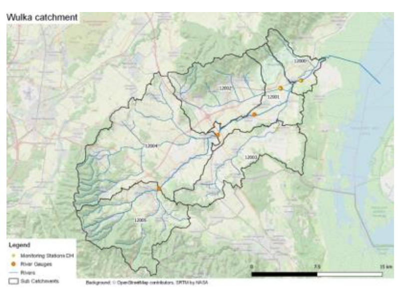


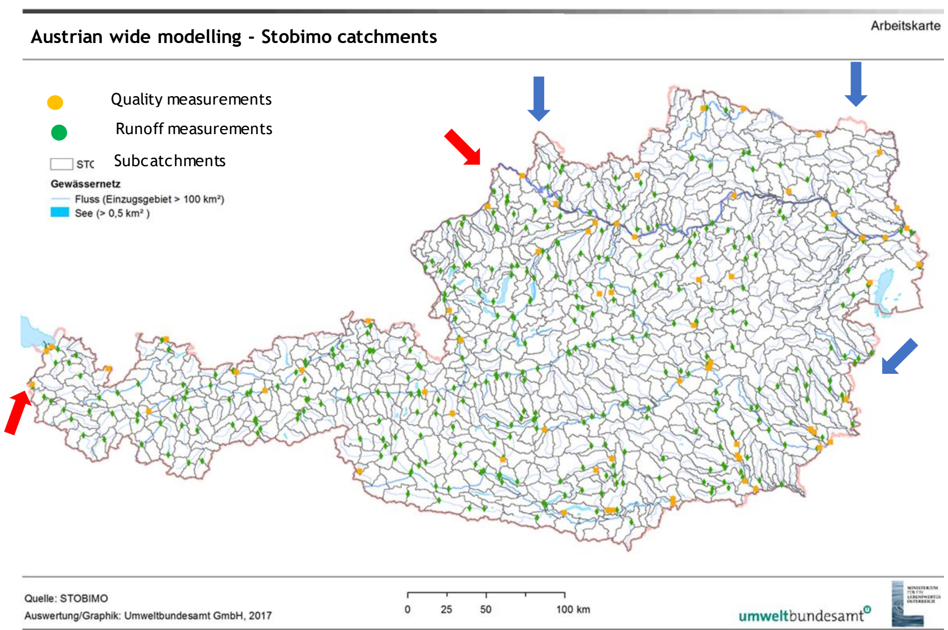












Runoff tree

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- In a second step you have to define the discharge tree
- Discharge tree defines the hydrological hierarchies between the AU (each defined by an ID number)
- Allows calculation of accumulated discharges, loads and consequently of concentrations for each AU at the outlet
- Simple in the DHm3c project with seven pilot regions and a total of 34 AUs but more ambitious in larger approaches, e.g. Austria with 754 catchments
- As mentioned above it should be guaranteed that load and concentration calculation is prepared for regions of strategic interest (assessments, reporting, scientific questions)(like e.g. planning areas, or bioregions)

Data implementation

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➢ Implementation of input data is processed via Excel data input files for different data types, e.g.: “analytical units variables” (e.g.“landuse”); “periodical AU variables”: (precipitation; runoff); “point sources” with metadata description and concentration values

	id point source	year	variable	value	variant	name of input data set	date
2	201	2016	WWTP_ps_Q	2387050	1	National Water Directorate data for 2019	30.03.2022
3	202	2016	WWTP_ps_Q	493060	1	National Water Directorate data for 2019	30.03.2022
4	203	2016	WWTP_ps_Q	41234	1	National Water Directorate data for 2019	30.03.2022
5	204	2016	WWTP_ps_Q	2340	1	National Water Directorate data for 2019	30.03.2022
6	205	2016	WWTP_ps_Q	102076	1	National Water Directorate data for 2019	30.03.2022
7	206	2016	WWTP_ps_Q	72210	1	National Water Directorate data for 2019	30.03.2022
8	207	2016	WWTP_ps_Q	77865	1	National Water Directorate data for 2019	30.03.2022
9	208	2016	WWTP_ps_Q	83210	1	National Water Directorate data for 2019	30.03.2022
10	209	2016	WWTP_ps_Q	2400	1	National Water Directorate data for 2019	30.03.2022
11	210	2016	WWTP_ps_Q	4130	1	National Water Directorate data for 2019	30.03.2022
12	211	2016	WWTP_ps_Q	3084	1	National Water Directorate data for 2019	30.03.2022
13	212	2016	WWTP_ps_Q	10600	1	National Water Directorate data for 2019	30.03.2022
14	213	2016	WWTP_ps_Q	5000	1	National Water Directorate data for 2019	30.03.2022
15	214	2016	WWTP_ps_Q	77500	1	National Water Directorate data for 2019	30.03.2022
16	215	2016	WWTP_ps_Q	11200	1	National Water Directorate data for 2019	30.03.2022
17	216	2016	WWTP_ps_Q	4100	1	National Water Directorate data for 2019	30.03.2022
18	217	2016	WWTP_ps_Q	301178	1	National Water Directorate data for 2019	30.03.2022
19	218	2016	WWTP_ps_Q	123810	1	National Water Directorate data for 2019	30.03.2022
20	219	2016	WWTP_ps_Q	1375811	1	National Water Directorate data for 2019	30.03.2022
21	220	2016	WWTP_ps_Q	81310	1	National Water Directorate data for 2019	30.03.2022

... | point sources | constants | analytical units variables | periodical AU variables | PS dependent variables | **periodical PS variables** | river segm ...

Data implementation

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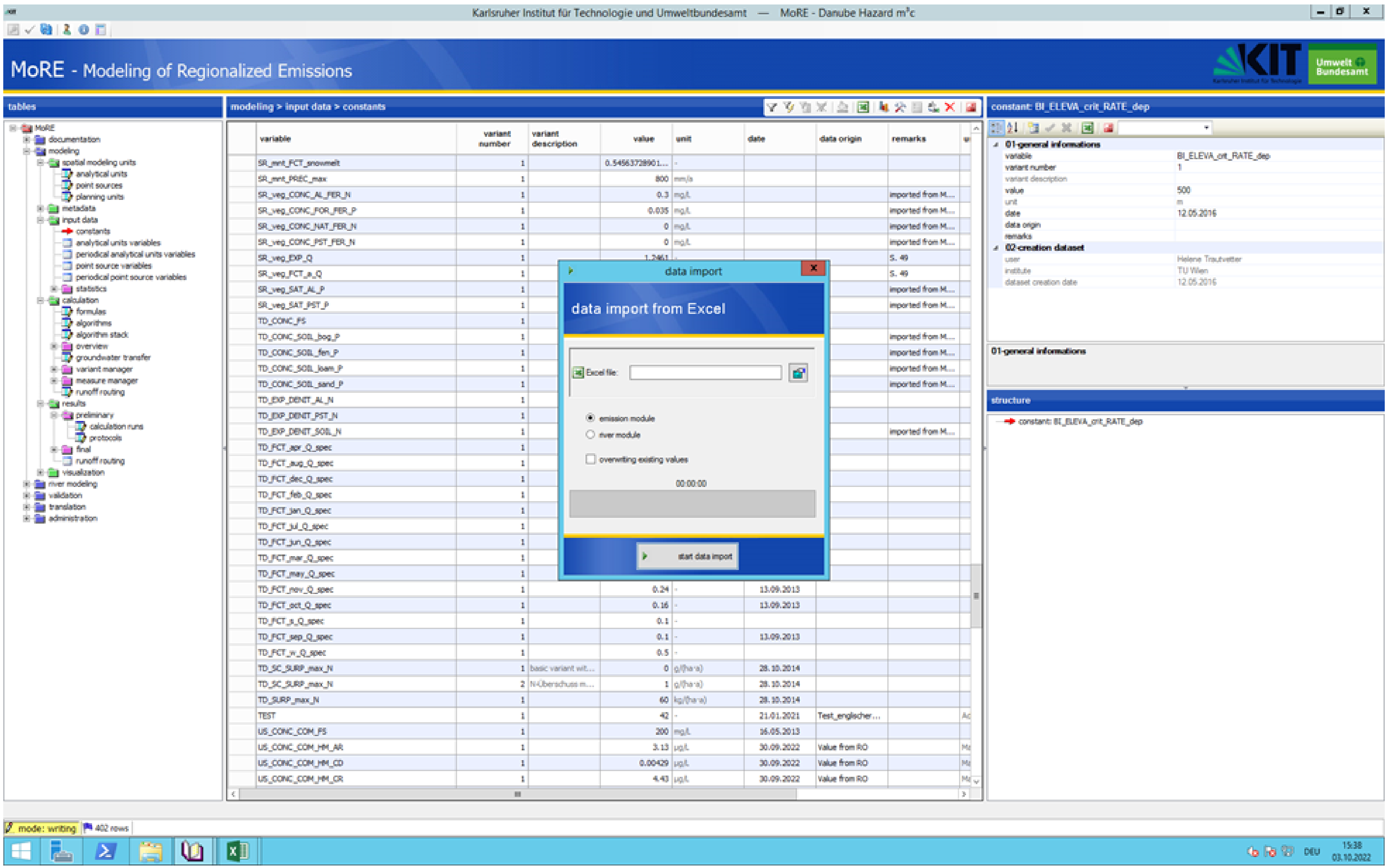

Data requirements

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- In an older EU project "EUROHARP" several model approaches (N,P) of different complexity were compared in catchments all over Europe
- Neither the simple approaches (black models) nor the complex Models (white models) produced unreasonable results "Model limitations were those posed by the simplicity (lacking valuable information), or the data demand of the models"
- The tested MONERIS model (similar to the MoRE approach with respect to data needs) was rated as model with a moderate demand of input data compared to other approaches (i.e. SWAT)
- Nevertheless, even this "moderate" data demand is certainly a challenge for some countries in the Danube region, especially where emission modelling was not yet established

Data requirements

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Basic input data

- GIS or statistical data aggregated to Analytical Units (such as land use)
- Constant spatial data: (e.g. average altitude; average slope)
- Variable spatial data: (e.g. precipitation; discharge)
- Partially easy available data (e.g. landuse), partially data that requires extensive preprocessing (soil loss and soil input using the USLE, the SDR and ER) (Workshop 1)

Data requirements –

Basic input data in pilots

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Input data type	Actual input data code	Name	description	unit	Wulka	Ybbs	Koppany	Zagyva	Vit	Viseu	Somesul Mic
Analytical Unit	BI_A	Area of analytical unit	Area of analytical units	km^2	Available	Available	Available	Available	Available	Available	Available
Topography	BI_ELEVA	Digital Elevation model	mean hights of subcatchments	m	Available	Available	Available	Available	Available	Available	Available
Landuse	BI_A_AL_slope_0-1	arable land	(in 5 slope classes: 0-1; 1-2; 2-4; 4-8; >8 % if possible]	km^2	Available	Available	Available	Available	Available	Available	Available
Landuse	BI_A_PST	pastures		km^2	Available	Available	Available	Available	Available	Available	Available
Landuse	BI_A_WS_mr; BI_A_WS_trib	water surface	main river; tributaries; but also lakes; reservoirs	km^2	Available	Available	Available	Available	Available	Available	Available
Landuse	BI_A_FOR	naturally covered areas	woods; scrubland	km^2	Available	Available	Available	Available	Available	Available	Available
Landuse	BI_A_O	open areas	alpine-mountainous area without vegetation; beaches; dunes	km^2	Available	Available	Available	Available	Available	Available	Available
Landuse	BI_A_OPM	surface mining areas		km^2	Corine (1.3.1)	Corine (1.3.1)	Available	Available	Available	Available	Available
Landuse	BI_A_URB	settlements	total urban areas	km^2	Available	Available	Available	Available	Available	Available	Available
Landuse	BI_A_IMP	impervious urban area	paved areas inside urban areas: settlements; industrial estates; car parks....	km^2	Available	Available	Available	Available	Available	Available	Available
Landuse	BI_A_WL	wetlands		km^2	Available	Available	Available	Available	Available	Available	Available
Landuse	BI_A_OR	country roads	paved road area; not included in settlements	km^2	Available	Available	Available	Available	Available	Available	Available
Landuse	BI_A_REM	other remaining areas	if not very small, please indicate landuse as comment	km^2	Available	Available	Available	Available	Available	Available	Available
Drainages	TD_SHR_a_td_agrl	Tile drained areas	from arable land and pastures	km^2	Available	Available	Available	Available	Not available	Available	Available
Meteorological Data	AD_EVAPO_lt	Evapotranspiration,	mean annual evapotranspiration	mm	Available	Available	Available	Available	Not available	Available	Available
Meteorological Data	(e.g.) BI_PREC_apr	Precipitation	monthly values	mm	Available	Available	Available	Available	Available	Available	Available
Hydrological data	BI_Q_net	Net runoff from	modelling period; annual data on subcatchment level	m^3/s	Available	Available	Available	Available	Available	Available	Available
Erosion	ER_agrl_SL_spec_lt_AL	Soil loss	potential soil loss from arable land (optional from 5 slope classes)	t/(ha·a)	Available	Available	Available	Available	Not available	Available	Available
Erosion	ER_agrl_SL_spect_lt_PST	Soil loss	potential soil loss from pastures	t/(ha·a)	Available	Available	Available	Available	Not available	Available	Available
Sewer sytem	BI_INH	number of inhabitants		inh	Available	Available	Available	Available	Available	Available	Available
Sewer sytem	US_ss_VOL_SST	sedimentation tanks	storage volume of stormwater sedimentation tanks in separate sewer	m^3	Not available	Not available	Available	Available	Available	Available	Available
Sewer sytem	US_cso_VOL_SOT	stormwater overflow	storage volume of stormwater overflow tanks in combined sewer systems	m^3	Not available	Not available	Available	Available	Available	Available	Available
Sewer sytem	US_cso_VOL_spec_SOT	stormwater overflow	storage volume of stormwater overflow tanks in combined sewer systems	m^3/ha	Not available	Not available	Available	Available	Available	Not available	Not available
Sewer sytem	US_L_CS	combined sewers	length of combined sewers	km	Available	Available	Not available	Not available	Available	Available	Available
Sewer sytem	US_L_SS	stormwater sewers	length of stormwater sewers	km	Available	Available	Not available	Not available	Available	Available	Available
Sewer sytem	US_L_WWS	sewage sewers	length of sewage sewers	km	Available	Available	Not available	Not available	Available	Available	Available
Sewer sytem	US_SHR_inh_con_tot	connection rate	percentage of inhabitants that are connected to sewer systems	%	Available	Available	Available	Available	Available	Available	Available
Sewer sytem	US_SHR_inh_conWWTP_tot	connection rate	percentage of inhabitants that are connected to sewer systems and waste	%	Available	Available	Available	Available	Available	Available	Available
Sewer sytem	US_SHR_inh_nss_tot	connection rate	percentage of inhabitants that are not connected to sewer systems	%	Available	Available	Available	Available	Available	Available	Available
Sewer sytem	US_INHC_H2O		inhabitant specific water consumption	l/(inh·d)	Available	Available	Available	Available	Available	Available	Available
Sewer sytem	US_nss_SHR_inhl_towwtp_sept		percentage of inhabitant load that is transported from septic tanks to waste	%	Available	Available	Available	Available	Not available	Not available	Available
Sewer sytem	US_Q_spec_COM		runoff rate for comercial waste water	l/(ha·s)	Not available	Not available	Not available	Not available	Not available	Not available	Not available
Urban wastewater	WWTP_ps_INH_conWWTP	connection rate	number of inhabitants that are connected to sewer systems and waste	inh	Available	Available	Available	Available	Available	Available	Available
Urban wastewater	WWTP_ps_CP	capacity	capacity of the waste water treatment plant (point sources)	PT	Available	Available	Available	Available	Available	Available	Available
Urban wastewater	WWTP_ps_PE	load	nominal load of waste water treatment plant (point sources)	PT	Available	Available	Available	Available	Available	Available	Available
Urban wastewater	WWTP_ps_TS	treatment type	current treatment type of waste water treatment plant (point sources)	-	Available	Available	Available	Available	Available	Available	Available
Urban wastewater	WWTP_ps_Q	discharge	runoff via waste water treatment plant (point sources)	m^3/a	Available	Available	Available	Available	Available	Available	Available
Industrial wastewater	ID_ps_Q	discharge	runoff via industrial direct dischargers	m^3/a	Available	Available	Available	Available	Available	Available	Available

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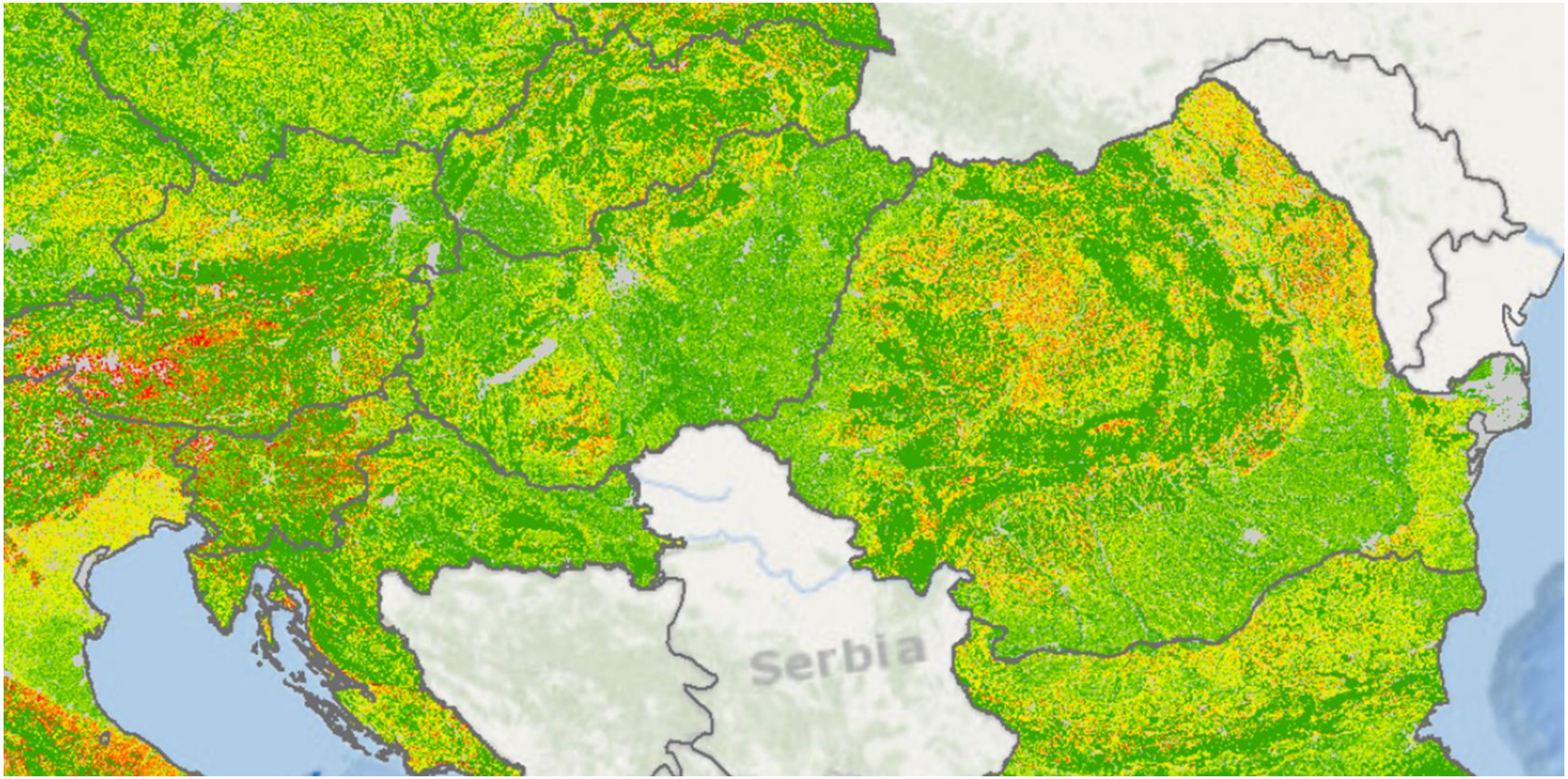
Data requirements-
Examples of alternative data sources

Source: EUROPEAN SOIL DATA CENTRE (ESDAC)JRC



https://esdac.jrc.ec.europa.eu/content/soil-erosion-water-rusle2015

Data requirements-general

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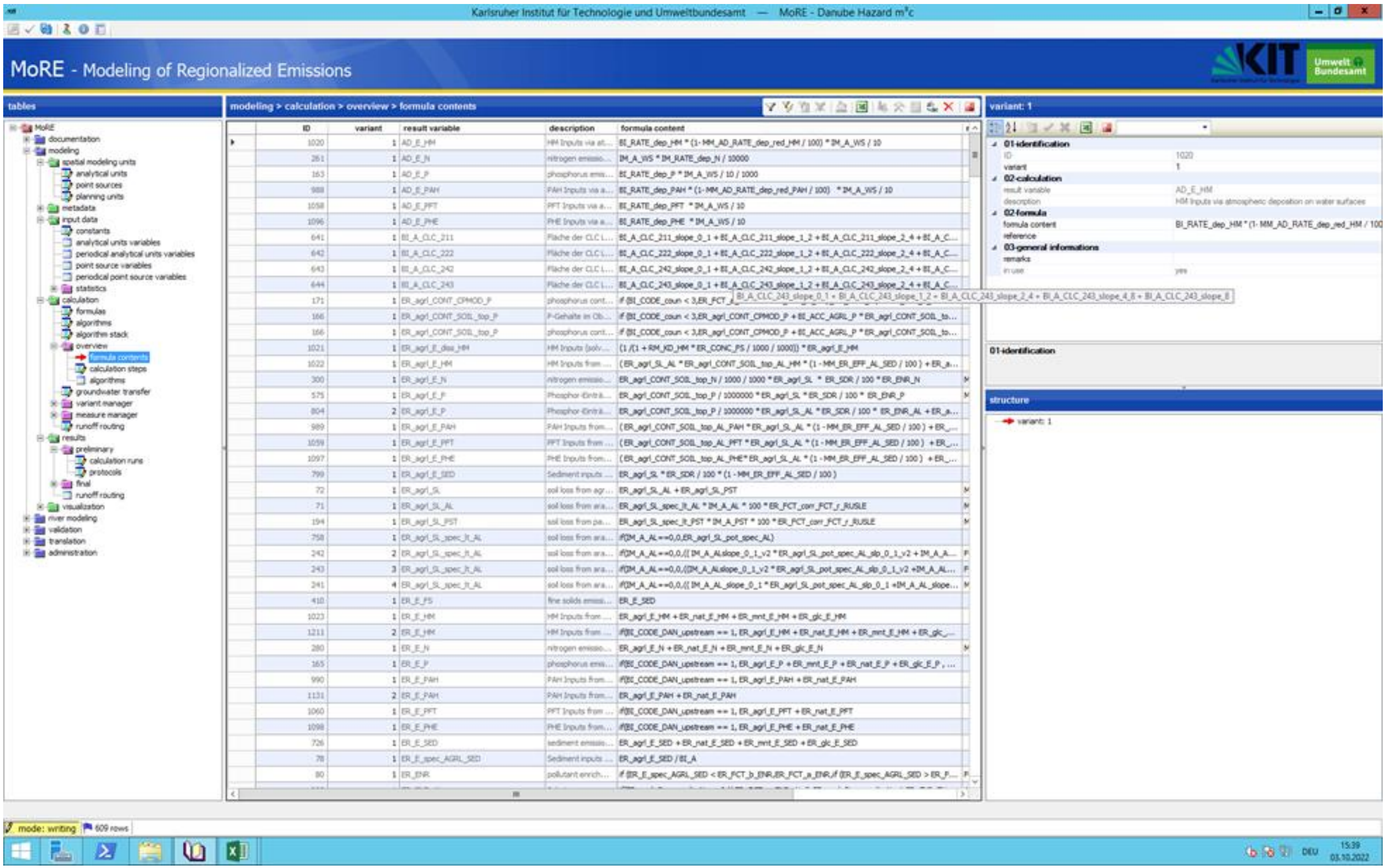
Substance specific input data

- Specific concentration values in different technical or environmental compartments (Workshop 1)
- Often not available or not in that number to create regionalized or generalized datasets by geostatistical methods (e.g. relating soil concentration to geological classes, soil types or landuse)
- Point source data (with the opportunity of detailed meta data description are stored in a specific data base)
- Surface water concentration data and discharges to calculate annual loads or concentrations for model validation

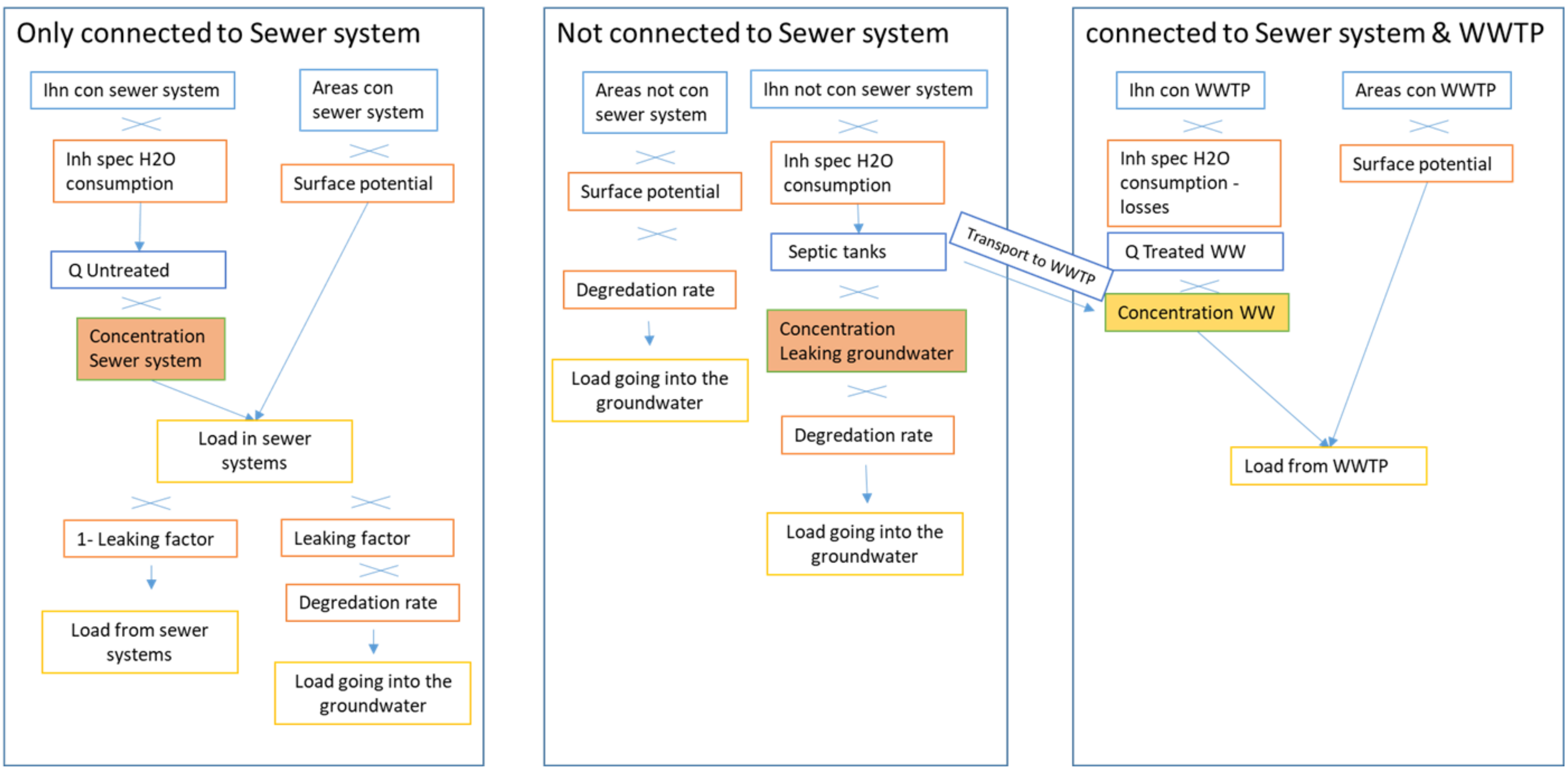
- Strong need of more regionalized and generalized data sets as input parameters for modelling!

Calculation approaches

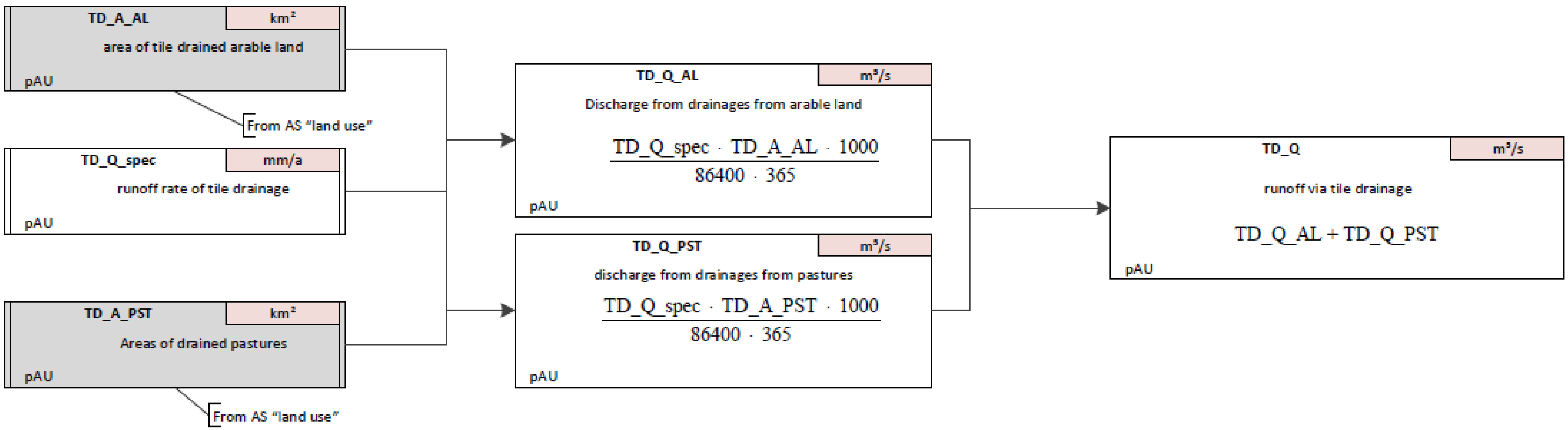


Calculation approaches

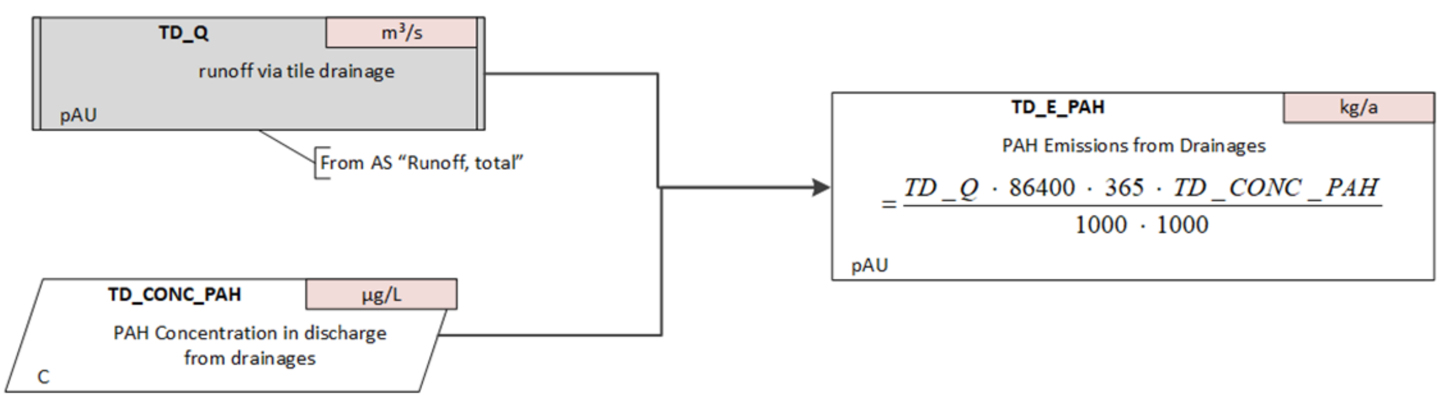
- ➢ Within the pathways calculation approaches can be easily adopted
- ➢ Some approaches simple Q x c load calculations (lack of regionalized data sets for HS) others more complex (actual a high importance of water balance!)



Calculation approaches – simple approaches (Q x conc.)



Emissions > PAH emissions via tile drainage > emissions via tile drainage



Calculation approaches – more complex approaches

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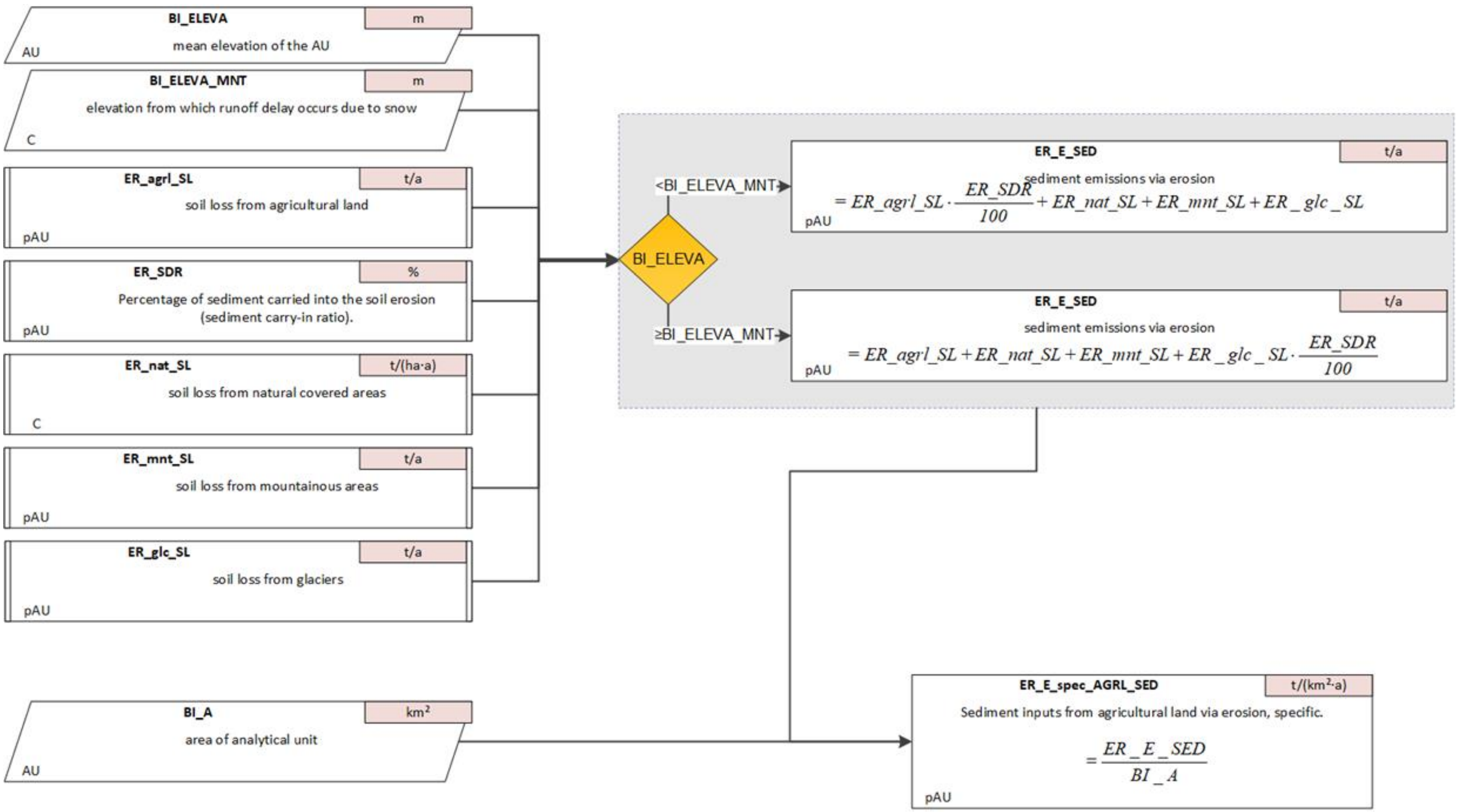

Technical implementation

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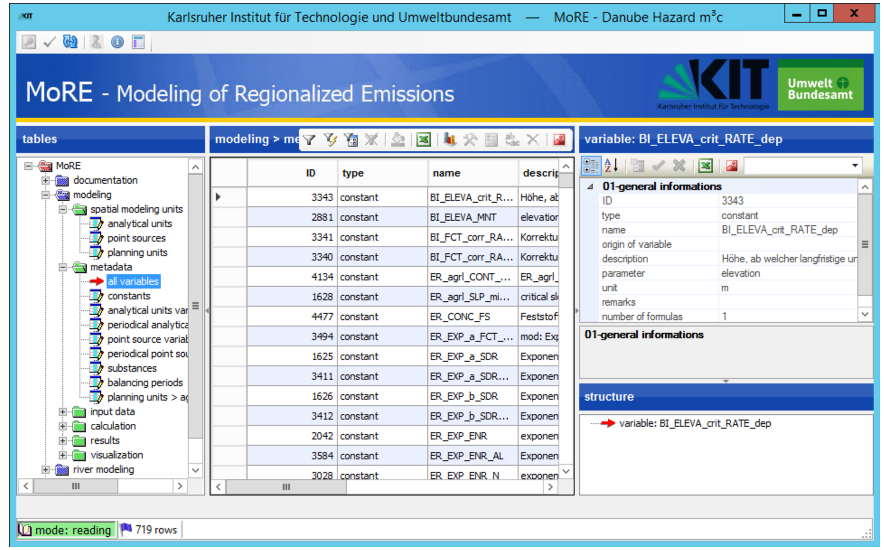
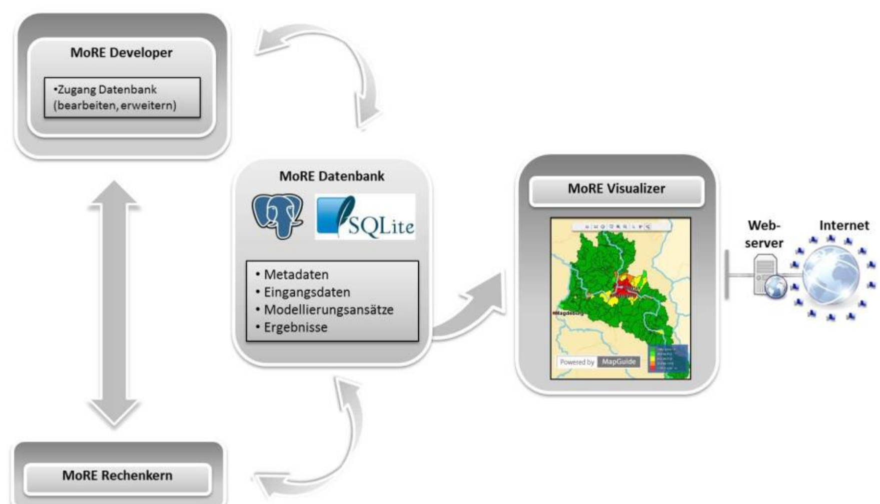
- Database PostgreSQL or SQLite for storage of:
  - Meta data
  - Input data
  - Modeling approaches
  - Result data
- Generic calculation engine:
  - Programmed in C#
  - Reads variables, data and formula for calculation from the data base
- GUI „MoRE Developer“:
  - Tabular based
  - For working on data or modelling approaches
- GUI „MoRE Visualizer“:
  - GIS application in web browser
  - for visualization of final results





Technical requirements

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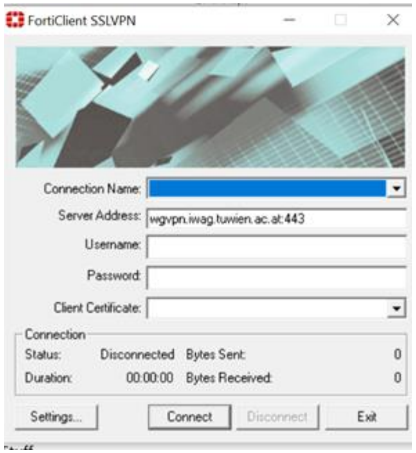
- MoRE "Danube Hazard m3c" version installed on TU-Wien server



- English version provided
- Roles and right of use established (only PP)
- Connection via FortiClient and Remotedesktop

- Planed steps:
- „Clean up" the model structure to establish a clearly arranged basis version
- Maintain a „mother version" with all approaches documented
- Making assessable a reduced SQLite version on the project homepage:

https://www.interreg-danube.eu/approved-projects/danube-hazard-m3c

Technical documentation

- Handbook https://more.iwg.kit.edu/wiki/index.php?title=MoRE_Developer
- Fuchs, S.; Kaiser, M.; Kiemle, L.; Kittlaus, S.; Rothvoß, S.; Toshovski, S.; Wagner, A.; Wander, R.; Weber, T.; Ziegler, S. (2017): Modeling of Regionalized Emissions (MoRE) into Water Bodies: An Open-Source River Basin Management System. Water 2017, 9, 239, doi:10.3390/w9040239. [LINK: https://www.mdpi.com/2073-4441/9/4/239]
- Danube Hazard m3c: Deliverable 2.1.1 “Datasets containing basic input data for pilot regions”
- Danube Hazard m3c: Deliverable 2.1.2 “Technical documentation of the model setup in the pilot regions” with 20 Flowcharts
- Scientific publications and reports

Start calculation engine

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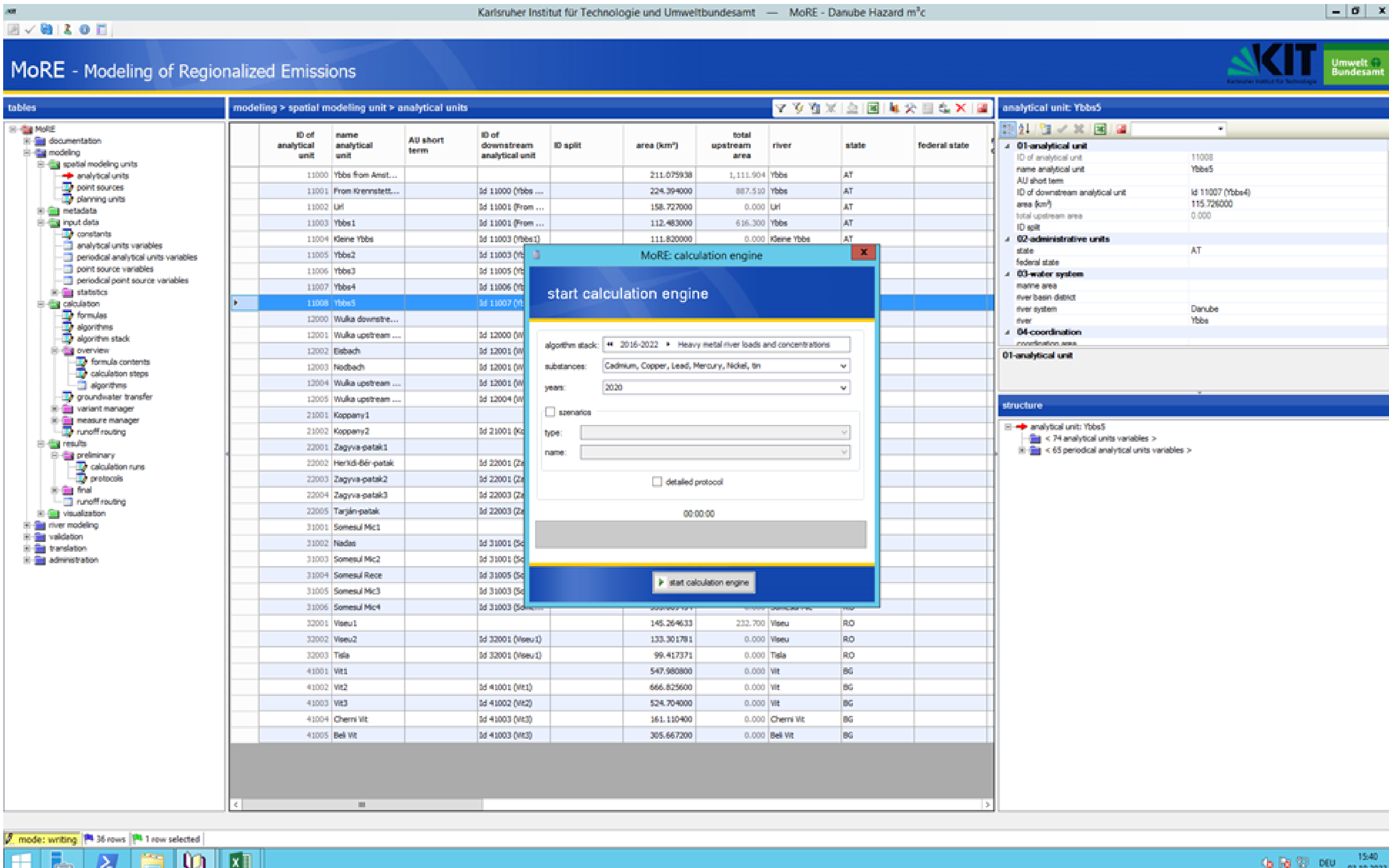

Deltares
Enabling Delta Life

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Danube Hazard m^{3}c
Training on hazardous substances emission modelling & scenario evaluation

DHSM model (based on the SOLUTIONS model)

Vienna, 04.10.2022

Budapest, 06.10.2022

Bucharest, 13.10.2022

Project co-funded by European Union funds (ERDF, IPA, ENI) and National Funds of the participating countries

Introduction to DHSM model

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- Scope, temporal and spatial scales
- Data requirements
- Calculation approaches
  - Approach
  - Evaluation
  - Results
- Using DHSM
  - technical requirements, conditions
  - documentation

Scope, temporal and spatial scales

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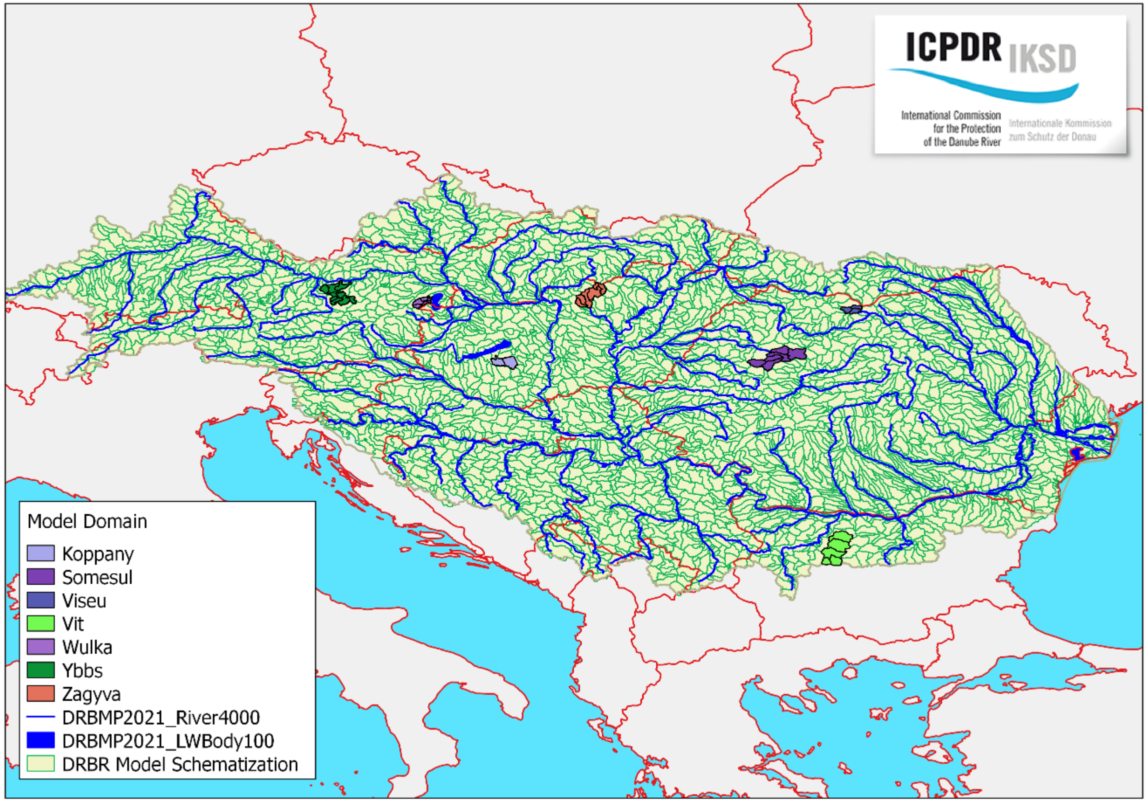
- Scope:
  - ability to support/investigate source controls & precautionary measures for a number of target chemicals
- Model implementation:
  - schematization elements (SE): ~3,500
  - average size SE: ~230 km²
  - Pilot Regions (PR): 7
  - PR's cover: 28 SE's



Target chemicals

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- "What are target chemicals?"
  - Selection criteria: (1) substances representing relevant sources and pathways, (2) substances relevant for ICPDR, national and regional authorities in the basin, (3) substances that can be actually detected and measured, so that data can be expected to be available.

- Metals:
  - arsenic (As), cadmium (Cd), copper (Cu), nickel (Ni), lead (Pb), zinc (Zn) and mercury (Hg).
- PAHs:
  - Polycyclic Aromatic Hydrocarbons (16 so called "EPA PAHs"), among them Benzo[a]pyrene ("BaP").

Target chemicals (continued)

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- PFAS:
  - Per- and polyfluoroalkyl substances: PFOS, PFOA, plus a range of short-chain PFAS (PFPeA, PFHxA, PFHpA, PFNA, PFDA, PFUdA, PFDoA, PFTrDA, PFTeDA, L-PFBS, L-PFHxS).
- Industrial chemicals:
  - with wide dispersive use: 4-tert-octylphenol (“4tO”), nonylphenol (“NP”), bisphenol-A (“BPA”).
- Pesticides:
  - tebuconazole (“Teb”), a fungicide used for wood preservation
  - metolachlor (“Met”), a herbicide in agriculture (including metabolites metolachlor-ESA and metolachlor-OA).
- Pharmaceuticals:
  - diclofenac (“Dic”) and carbamazepine (“Car”).

Source definition for Target chemicals

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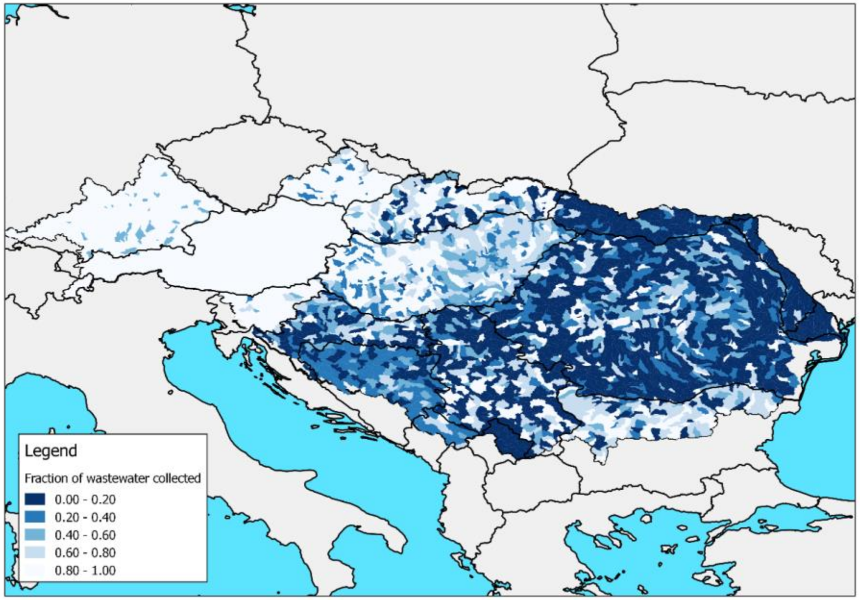
- Preliminary Version and is subject to extension (e.g. mines)
  - *x = accounted for in DHSM*

Target chemical	Atmospheric Deposition	Agriculture	Road Traffic	Built Environment	House-holds	Industry	Mining	Navigation	Natural background
Cadmium	x	x	x		x	x			
Lead	x	x	x	x	x	x			
Copper	x	x	x	x	x	x			
Arsenic	x		x		x	x			
Nickel	x	x	x		x	x			
Mercury	x	x			x	x			
Zinc	x	x	x	x	x	x		x	
Benzo[a]pyrene	x		x		x			x	
PFOS					x				
PFOA					x				
Bisphenol A					x				
Nonylphenol			x		x	x			
4-tert-octylphenol					x	x			
Metolachlor		x			x				
Tebuconazole		x			x				
Carbamezepine					x				
Diclofenac					x				

Data requirements

- General data in support to Emission Modelling
  - Losses (L) of a **pollutant** "p" for a certain **socio-economic activity** "a" are calculated by multiplying an activity rate (AR_a) by an emission factor ($EF_{p,a}$): $L_{p,a} = AR_a \times EF_{p,a}$
- Data used:
  - Population (LandScan (2006)™)
  - Landuse:
    - water surface; agriculture area; (im)permeable surfaces;
  - Hydrology:
    - E-Hype; Hundecha et al., 2016)
  - UWWTD Inventory by ICPDR
    - fraction collected; fraction (un)treated



Quantification of individual sources

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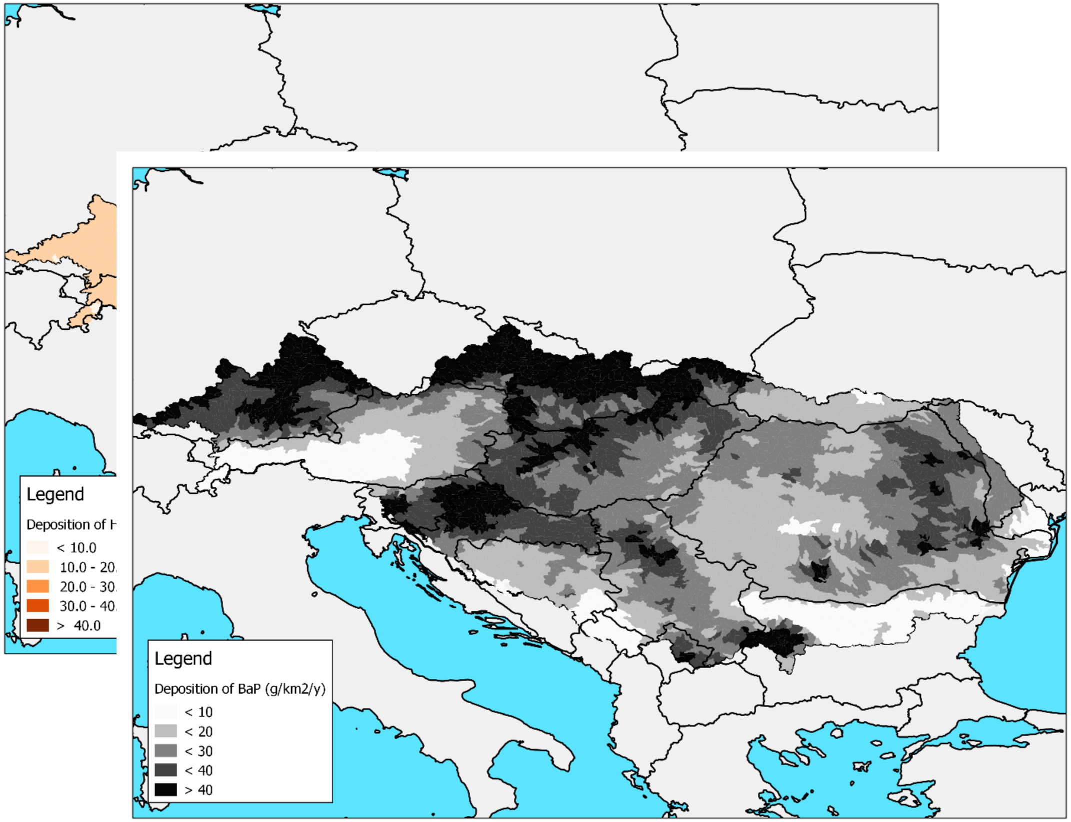
- Atmospheric deposition
  - **E**uropean **M**onitoring & **E**valuation **P**rogramme



Quantification of individual sources

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- Agriculture

  Metals

  - **Activity rate**: agriculture area
  - **Emission factor**: area-specific load (mass/area/time)

  Pesticides

  - **Activity rate**: agriculture area
  - **Emission factor**: area-specific use (mass/area/time)

Quantification of individual sources

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- Road Traffic
  - **Activity rate**: population
  - **Emission factor**: country-specific per capita emission (mass/cap/time), based on factsheets (NL-PRTR*)

	Cars	Buses	Vans	Motorcycles
Tire wear (mg/vkm)	100	300	600	50
Brake wear (mg/vkm)	10	30	40	5
Road surface wear (mg/vkm)	150	700	700	60

Substance	Tire wear (light traffic)	Tire wear (heavy traffic)	Brake wear	Tar-based asphalt	Bitumen-based asphalt	Motor oils
Cd (g/g)	1.00E-06	1.00E-06	0	0	0	5.00E-07
BaP (g/g)	5.40E-06	1.70E-06	0	3.50E-06	7.00E-08	1.20E-05
As (g/g)	1.00E-06	1.00E-06	0	0	0	1.00E-07
Cu (g/g)	5.00E-05	5.00E-05	3.80E-03	0	0	2.60E-05
Pb (g/g)	1.00E-04	1.00E-04	4.20E-04	0	0	2.00E-06
Zn (g/g)	9.50E-03	1.70E-02	1.50E-03	0	0	7.00E-04
Ni (g/g)	5.00E-05	5.00E-05	1.00E-04	0	0	6.00E-06
NP (g/g)	1.00E-05	1.00E-05	0	0	0	0

Country	Cars	Buses	Vans	Motorcycles
Austria	Per capita traffic volume (Mvkm/cap/y)	Per capita traffic volume (Mvkm/cap/y)	Per capita traffic volume (Mvkm/cap/y)	Per capita traffic volume (Mvkm/cap/y)
...	...	...	...	...

* https://www.emissieregistratie.nl/

Quantification of individual sources

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- Built Environment
  - **Activity rate**: population
  - **Emission factor**: per capita emission (mass/cap/time)

- Provisional EFs in kg/cap/d are:
  - $1.15531^{E\text{-}05}$ for Zn
  - $3.90642^{E\text{-}06}$ for Pb
  - $1.65044^{E\text{-}06}$ for Cu

Quantification of individual sources

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- Households
  - **Activity rate**: population
  - **Emission factor**: per capita emission (mass/cap/time)

Table 4.7: Estimates of per capita emission factors mg/cap/y for target substances

Substance	Fuchs et al. (2010) [1]	NL-PRTR [2]	WWTP data [3]	REACH use volumes [4]
Arsenic		200		
Cadmium	36.5	50	13	
Copper	4626	6540	3146	
Mercury	29.2	18	18	
Nickel	494.4	500	827	
Lead	668	790	424	
Zinc	15794	8993	13171	
Acenaphthene				
Acenaphthylene				
Anthracene		0.71		
Benzo[a]anthracene		2.6		

Quantification of individual sources

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- Industry
  - Larger industrial point sources in the schematization element where their discharge location is.
  - Reported load: E-PRTR Industrial discharges inventory by ICPDR
    - 279 discharge points
    - 38 individual parameters, among them the 7 metals, nonylphenol and 4-tert-octylphenol

Quantification of individual sources

- Navigation
  - **Activity rate:** navigable river length (km)
  - **Emission factor:** emission per unit river length per year (mass/km/time)
  - Supported by factsheets (NL-PRTR)

Table 4.8: Presence of individual PAHs in emissions from coatings and bilge water (Deltares and TNO, 2016).

PAH	Tar coating (% of PAH emission)	Bitumen coating (% of PAH emission)	Bilge water (conc. in oil in mg/kg)
Naphthalene	66.0%		2160
Anthracene	3.2%		300
Phenanthrene	6.5%	14.8%	1500
Fluoranthene	6.5%	10.1%	200
Benzo[*a*]anthracene	3.2%	4.8%	40
Chrysene	3.2%	20.1%	20
Benzo[*b*]fluoranthene			20
Benzo[*k*]fluoranthene	1.6%	10.1%	20
Benzo[*a*]pyrene	3.2%	10.1%	20
Benzo[*g,h,i*]perylene	3.2%	20.1%	0.7
Indeno[*1,2,3-cd*]pyrene	3.2%	10.1%	20

\+ translated into emissions per ship to the DRB waterways

Quantification of individual sources

- Mining (to be implemented)
  - Use of TMF's

- Natural Background
  - realistic concentrations in soils and rocks can be provided for metals

Calculation approaches: Methodology

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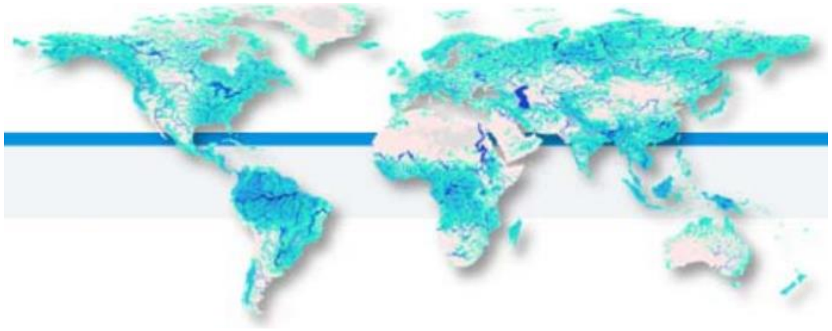
- The SOLUTIONS project
  - Emerging pollutants

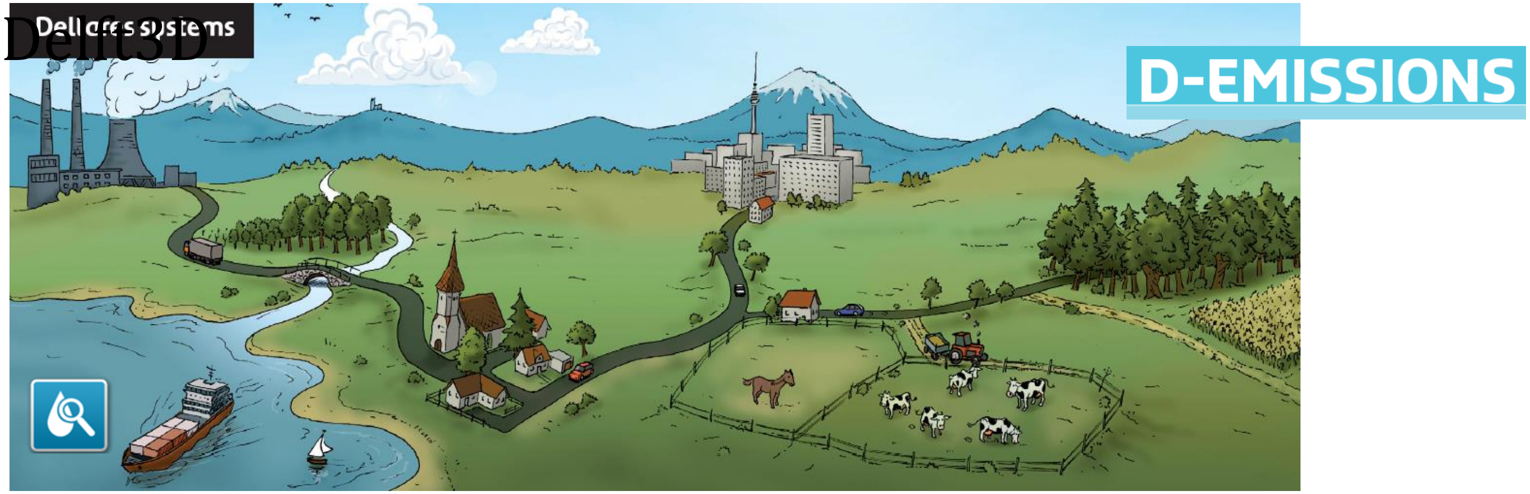
    Brack, W., Altenburger, R., Schüürmann, G., Krauss, M., Herráez, D. L., van Gils, J., … & de Aragão Umbuzeiro, G. (2015). The SOLUTIONS project: challenges and responses for present and future emerging pollutants in land and water resources management. Science of The Total Environment, 503, 22-31.

- E-HYPE (Europe)
  - World-Wide Hydrological Predictions by SMHI (Swedish Meteorological and Hydrological Institute)



DHSM: Emissions + Fate & Transport

- generic open source water quality modelling software
  Delft3D



DHSM: Source oriented approach

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TIER	BUILDING BLOCKS	EXPECTED OUTPUT	RESULTS FOR THE INVENTORY
STEP 1: ASSESSMENT OF RELEVANCE			
	Information sources identified in Art. 5 of EQS directive, see section I.1	Decision of relevance	List of relevant and less relevant substances
STEP 2: APPROACHES FOR RELEVANT SUBSTANCES			
1. Point source information	• Data on point sources • Emissions factors	• Availability of data • Quality of data • Identification of gaps	• Point source emissions • Listing of identified data gaps
2. Riverine load approach	add: • River concentration • Data on discharge • In stream processes	• Riverine load • Trend information • Proportion of diffuse and point sources • Identification of gaps	• Rough estimation of total lumped diffuse emissions • Verification data for pathway and source orientated approaches • Listing of identified data gaps
3. Pathway orientated approach			
4. Source orientated approach	Need for emission models		

Step 1

Step 2

- Source specific emissions
- Proportion to surface waters

Tier approaches in Step 2

Technical Report - 2012 – 058 Common Implementation Strategy for the Water Framework Directive (2000/60/EC) *Guidance Document No. 28 Technical Guidance on the Preparation of an Inventory of Emissions, Discharges and Losses of Priority and Priority Hazardous Substances*

Source oriented

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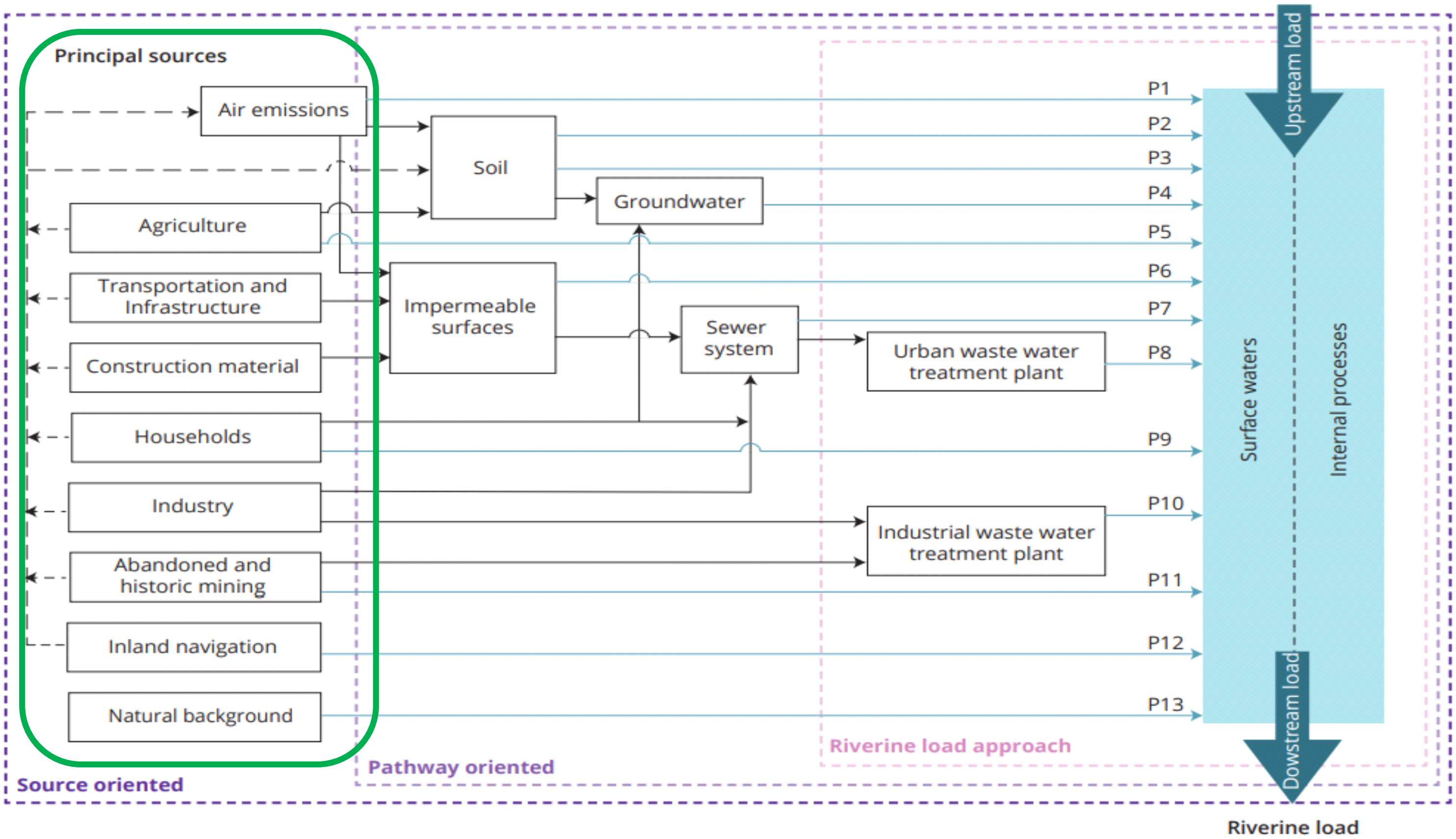
- sources as defined in WFD-CIS Guidance
  (Common Implementation Strategy; European Comm., 2012).

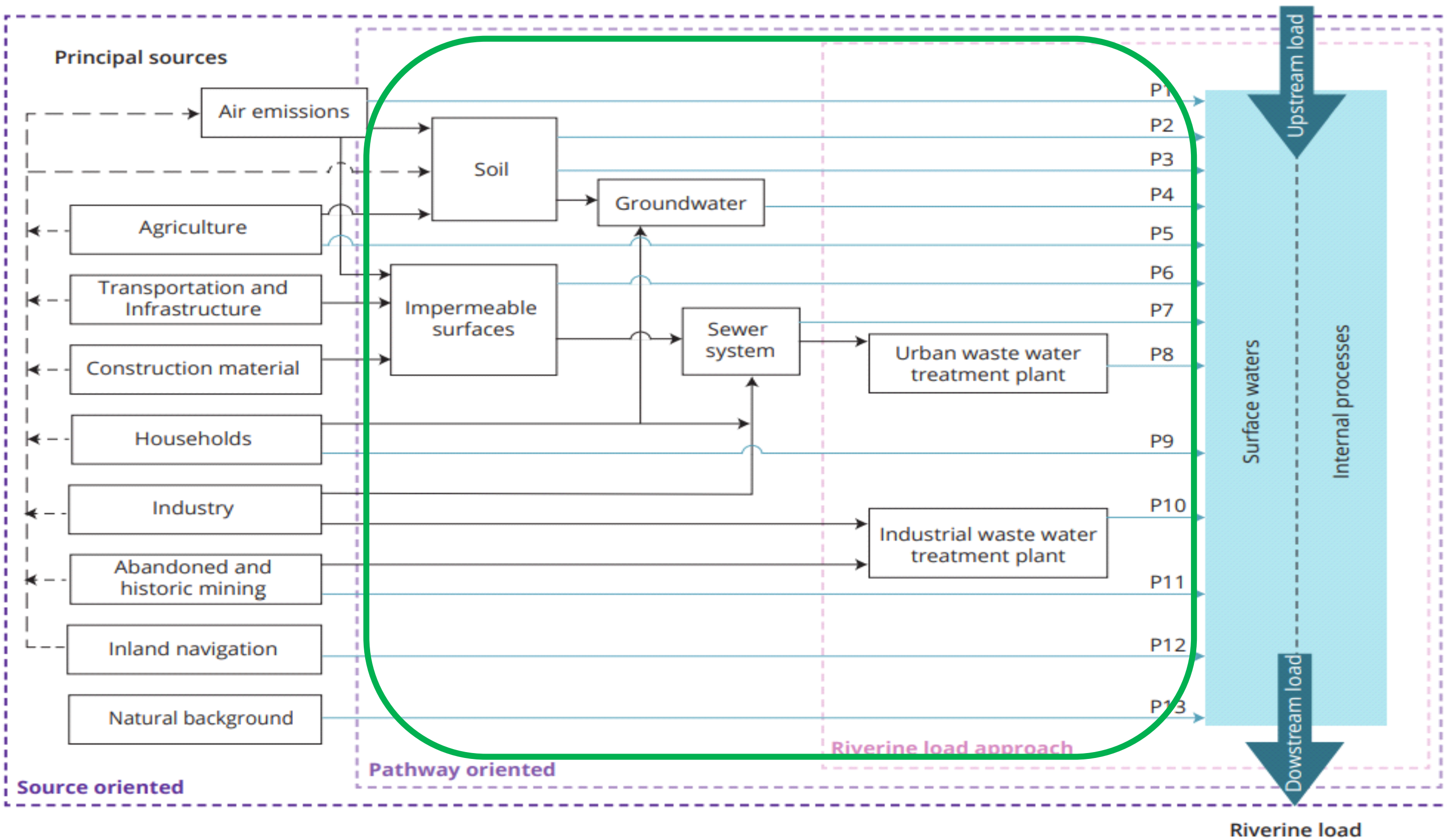
- Losses of polutants distributed in space



scheme from: European Commission (2012), in this form copied from EEA (2018)

Pathways … from source to river

- comprehensive pathways, equivalent to MONERIS for N, P
- transport hydrology driven: built-up stock in dry conditions



scheme from: European Commission (2012), in this form copied from EEA (2018)

Pathways … zooming in

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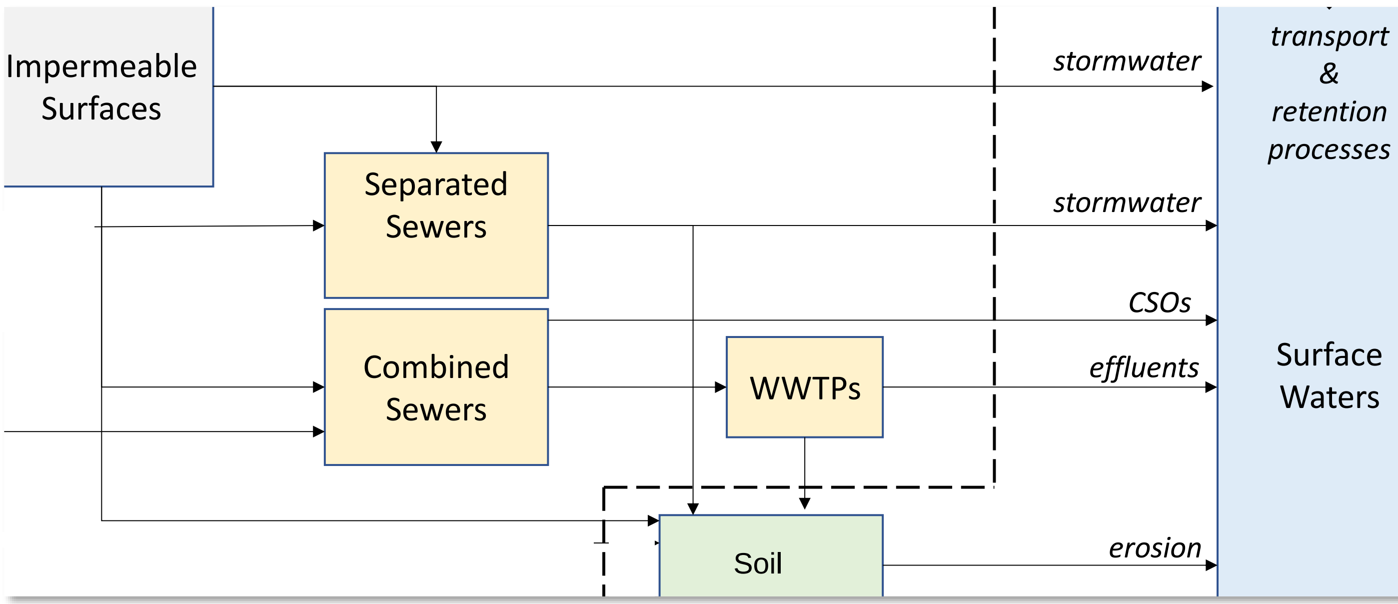
- From Impermeable Surfaces to Surface Waters:



Model Scheme

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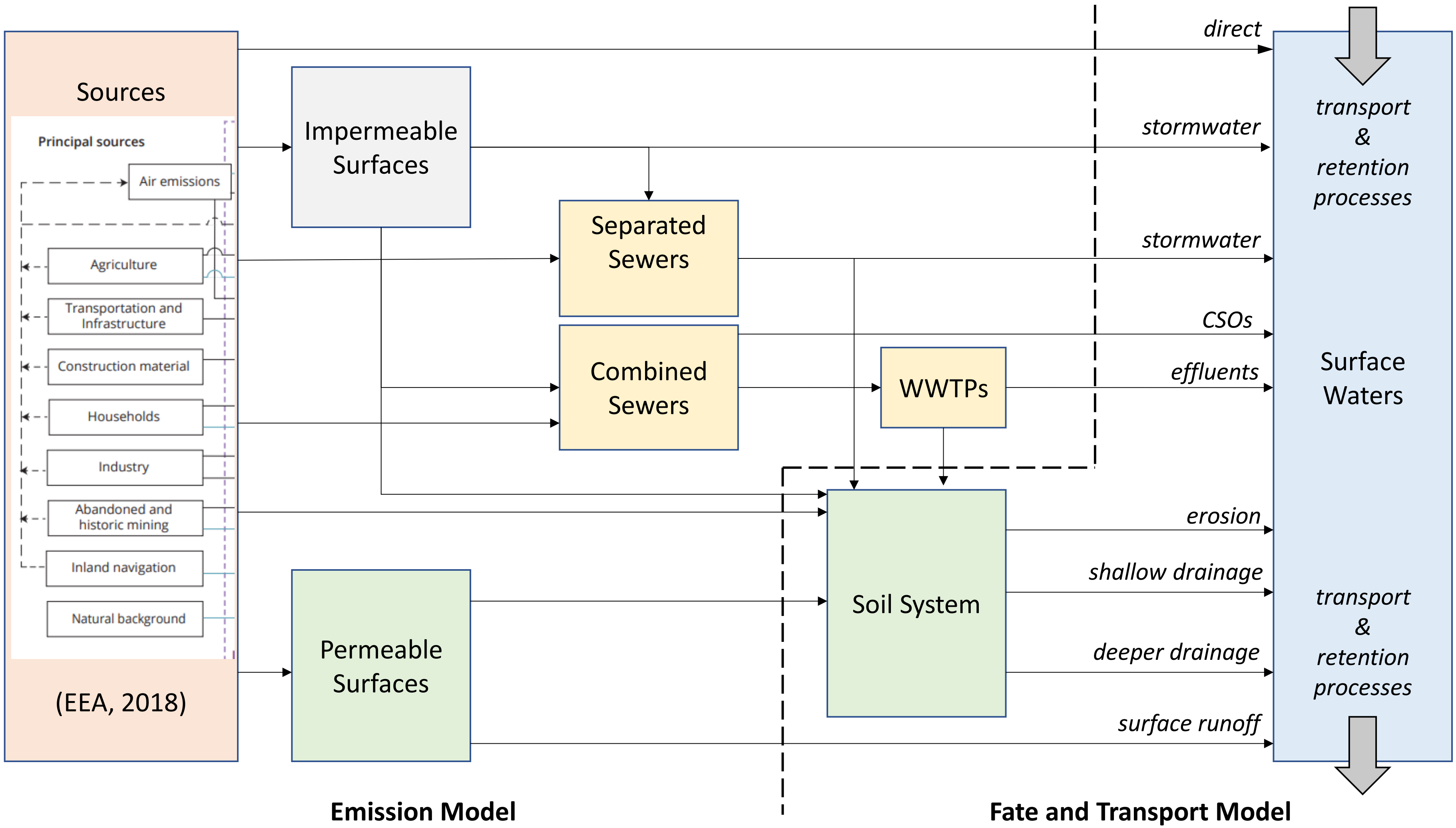


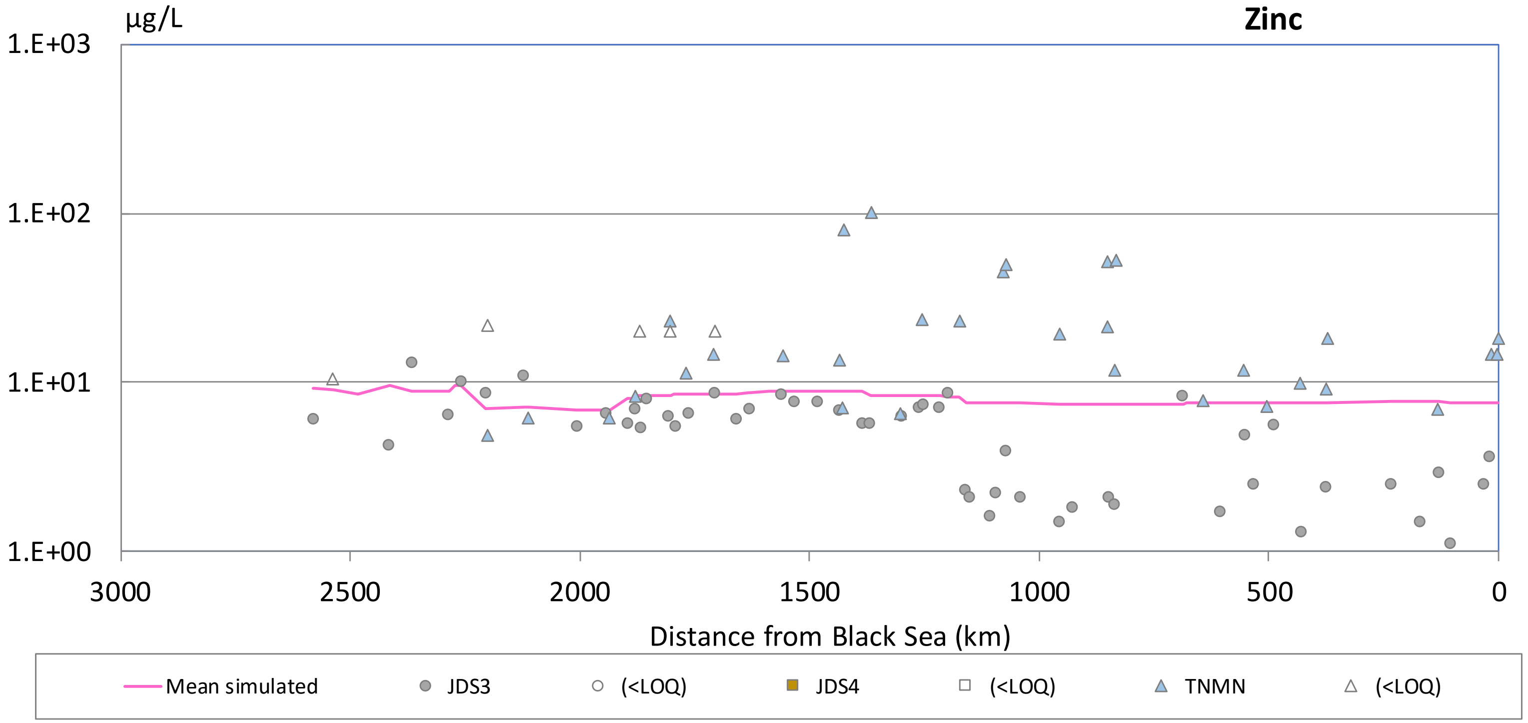
Calculation approaches: evaluation

… in the same range as observations?

- Monitoring data obtained from
  - Transnational Monitoring Network (TNMN)
  - Joint Danube Surveys JDS3 (2013) and JDS4 (2019)
  - Differences between surveys for metals and organic chemicals
- Comparison
  - 14 out of the 17 simulated substances,
    insufficient data for “BaP” (PAHs), “4tO”, “NP” (Industrial chemicals)

… in the same range as observations?

- Metals:
  - good fit (order of magnitude),
    Pb somewhat higher, As somewhat lower



longitudinal profiles plot

... in the same range as observations?

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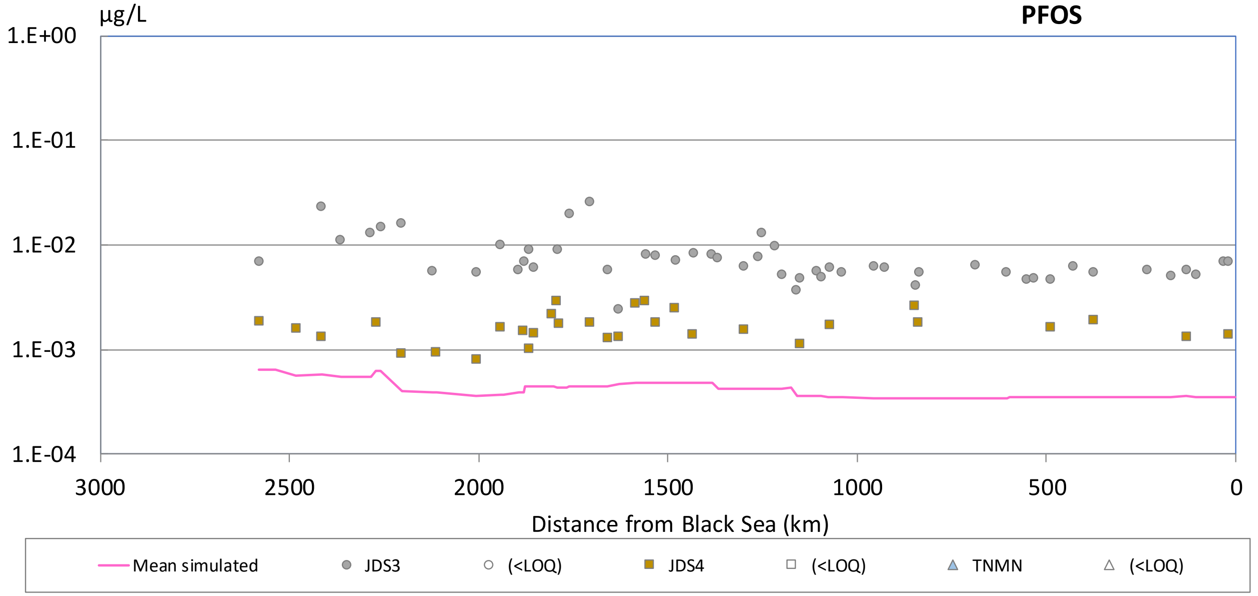
- PFOS, PFOA:
  - “missing relevant sources or processes”



longitudinal profiles plot

- Pesticides & pharma’s:
  - lack of regionalized use data
    - “Met” & carbamazepine underestimated, “Teb” & diclofenac overestimated

Calculation approaches: results

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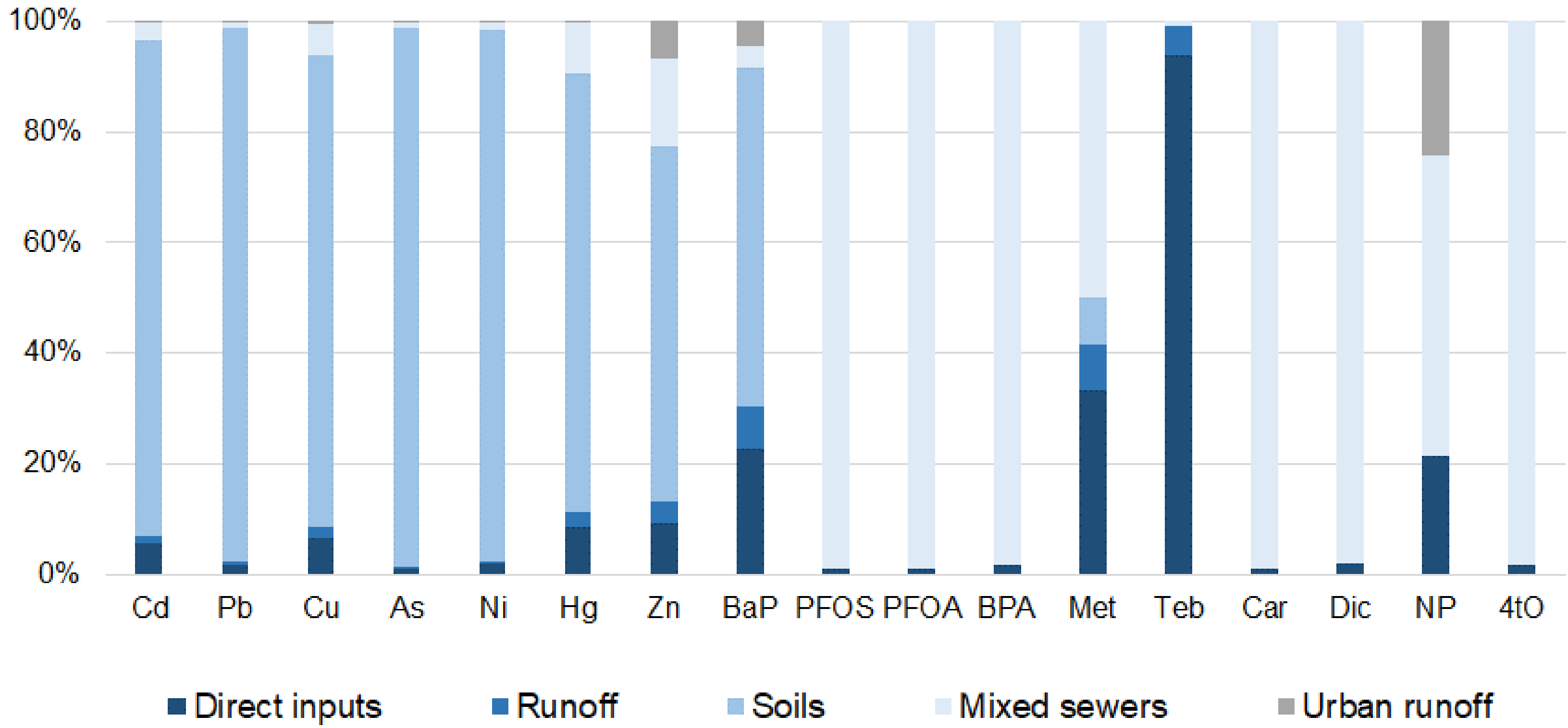
- Section 6.1 of the report:
  - absolute (kg/y) & relative (%) emission data

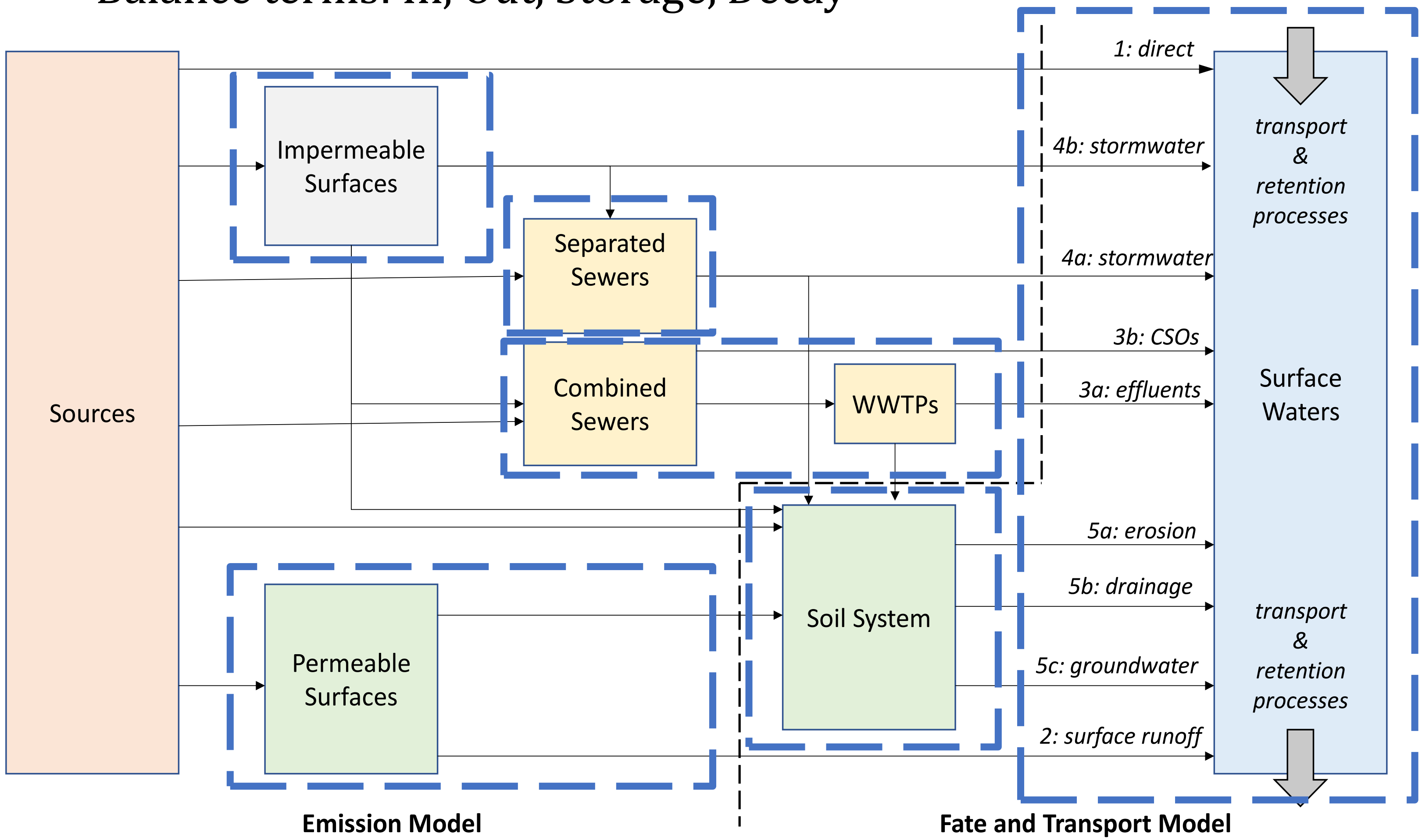


As: arsenic, Cd: cadmium, Cu: copper, Ni: nickel, Pb: lead, Zn: zinc, Hg: mercury, BaP: benzo[a]pyrene, Dic: diclofenac, Car: carbamazepine, 4tO: 4-tert-octylphenol, NP: nonylphenol, BPA: bisphenol-A, PFOS: perfluorooctanesulfonic acid, PFOA: perfluorooctanoic acid, Teb: tebuconazole, Met: metolachlor.

Figure 30: Relative proportion of the emission pathways of the target compounds

Calculation approaches: results

- Zooming in: detailed balances for compartments
  - Balance terms: In, Out, Storage, Decay



Calculation approaches: results

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Danube Hazard m³c

Basin-wide simulation results

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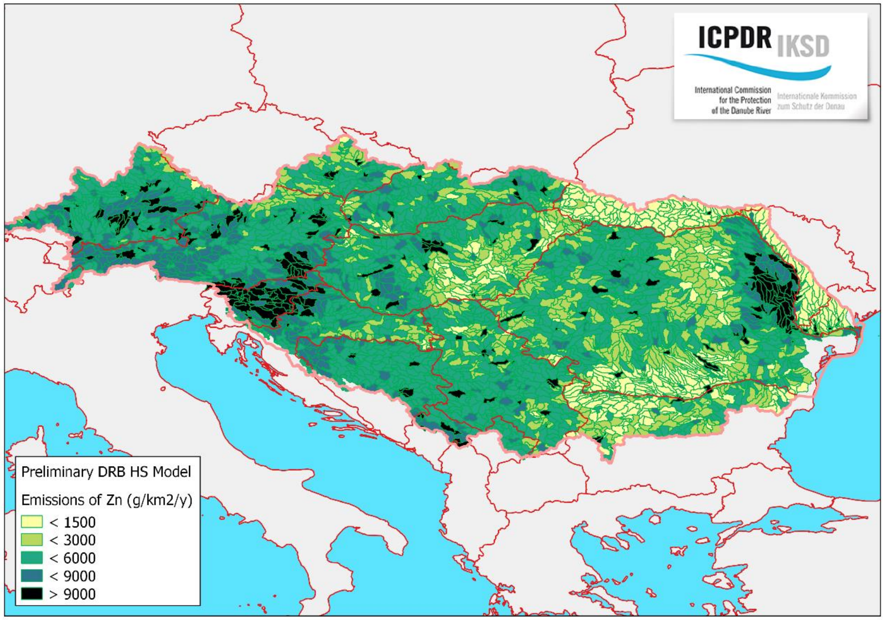
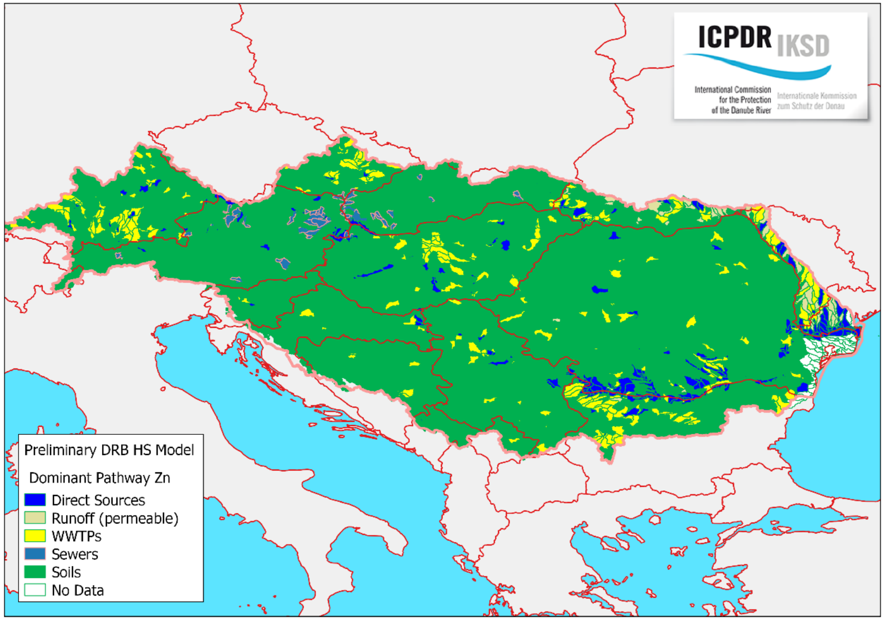
- Metals
  - In most places the soil related pathways are dominant (60% or more). Contributions > 10% occur for industry discharges (Cu, 29%) and mixed sewers (Zn, 16%)
  - Locally, direct sources (industry, deposition on lakes, WWTPs) are dominant

Emission



Dominant Pathway



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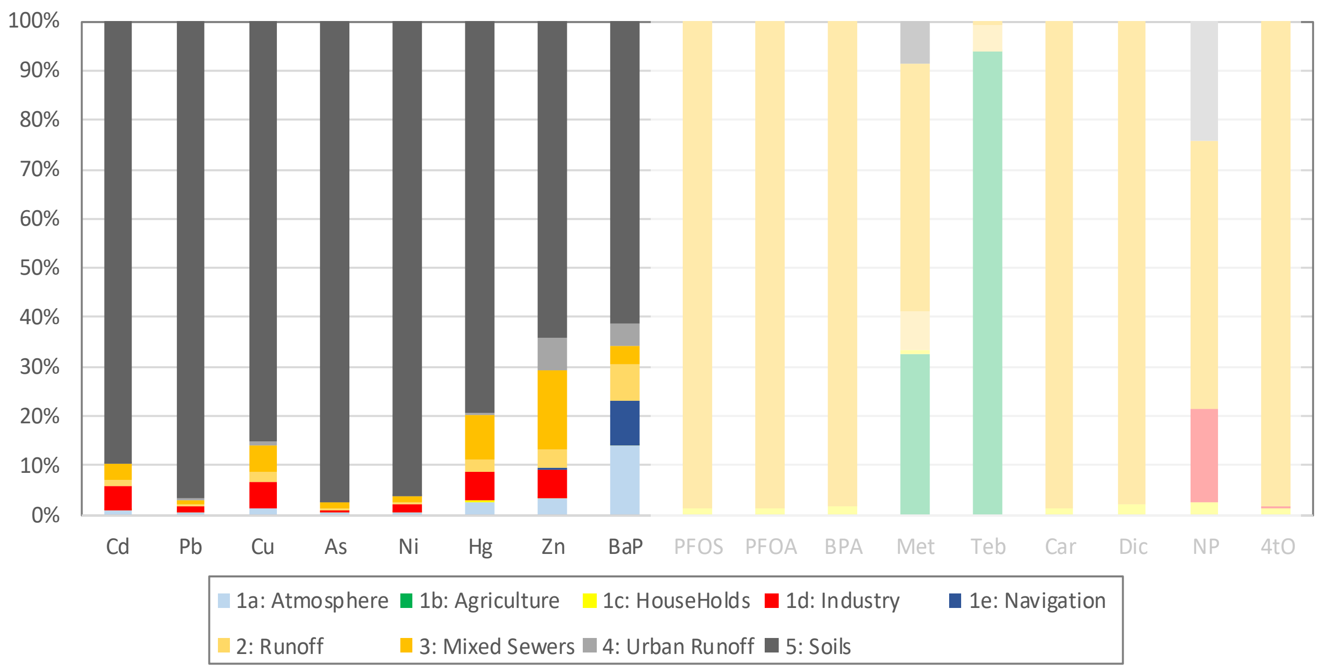

Basin-wide simulation results

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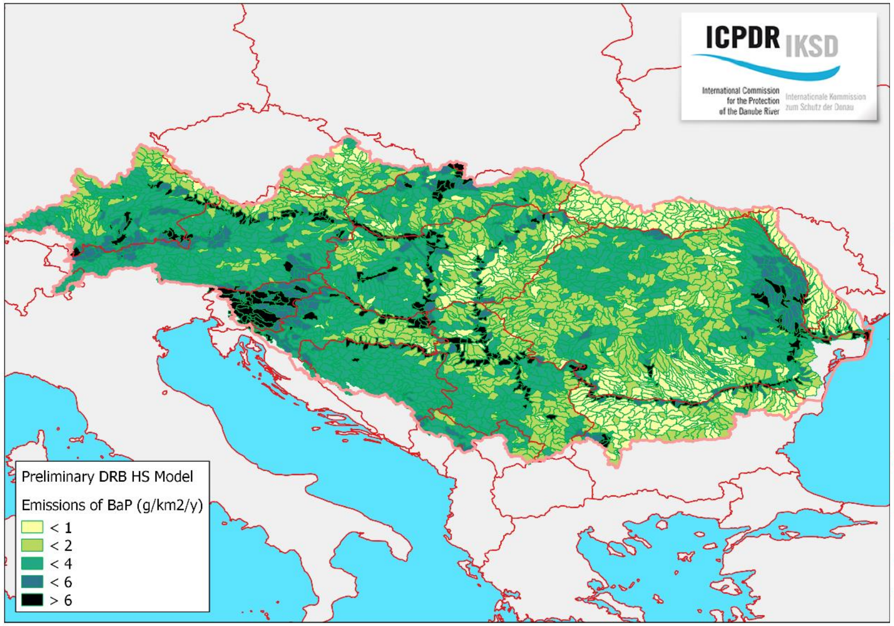
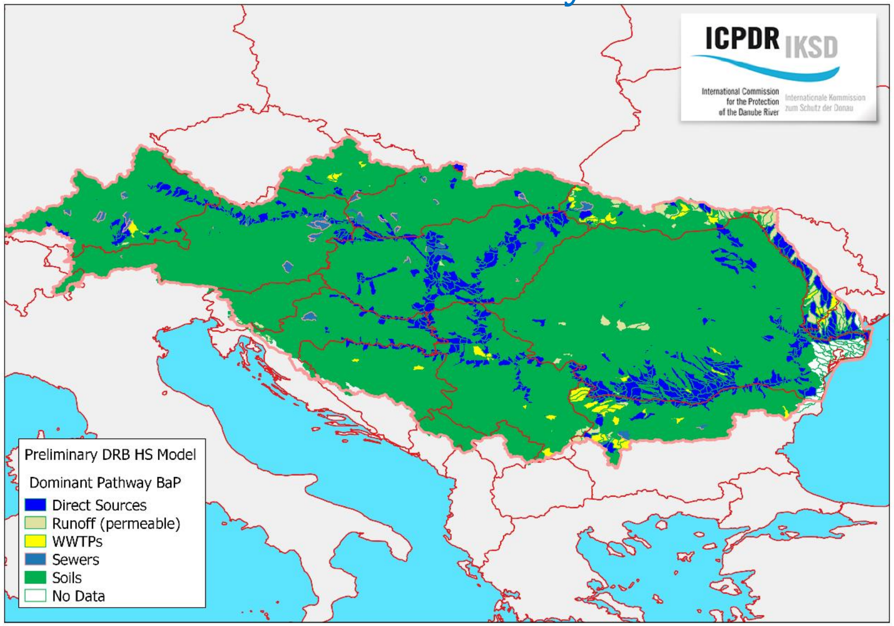
- PAHs:
  - benzo[a]pyrene: largest contribution from soils (61%, indirect atmospheric deposition), with noticeable contributions from direct atmospheric deposition (14%), navigation, runoff, WWTPs and sewers (all < 10%).

Emission



Dominant Pathway



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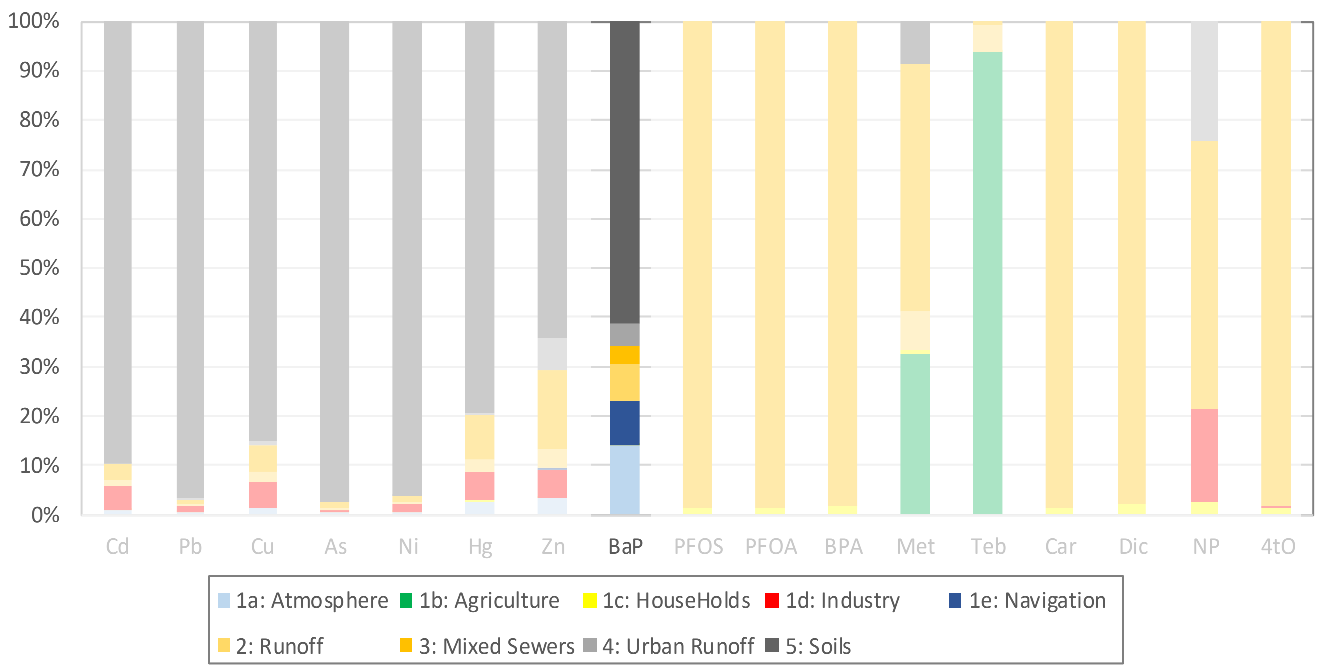
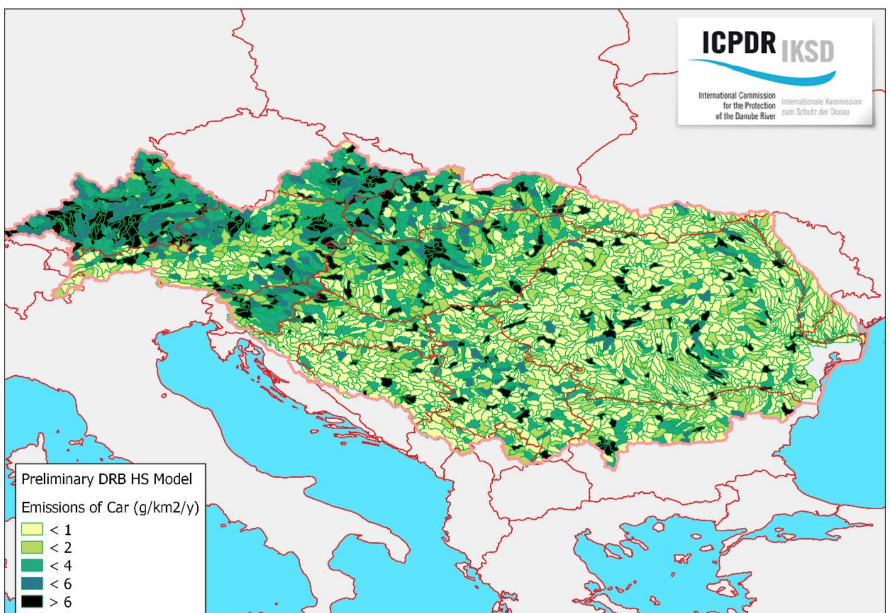


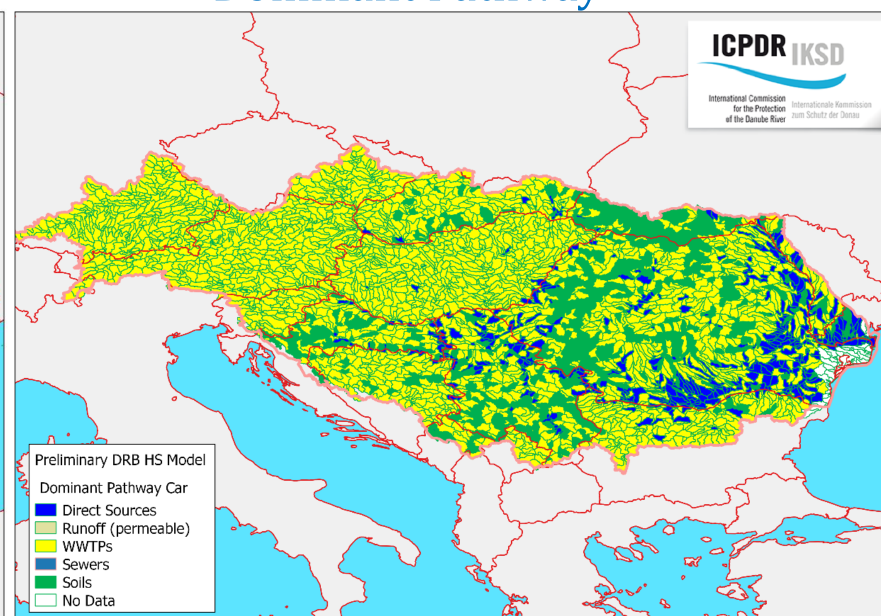
Basin-wide simulation results

- Pharmaceuticals:
  - only contributions from households (mixed sewer systems >98%)
  - Carbamazepine: WWTPs dominant (high population and high connection rate to sewers)

Emission



Dominant Pathway



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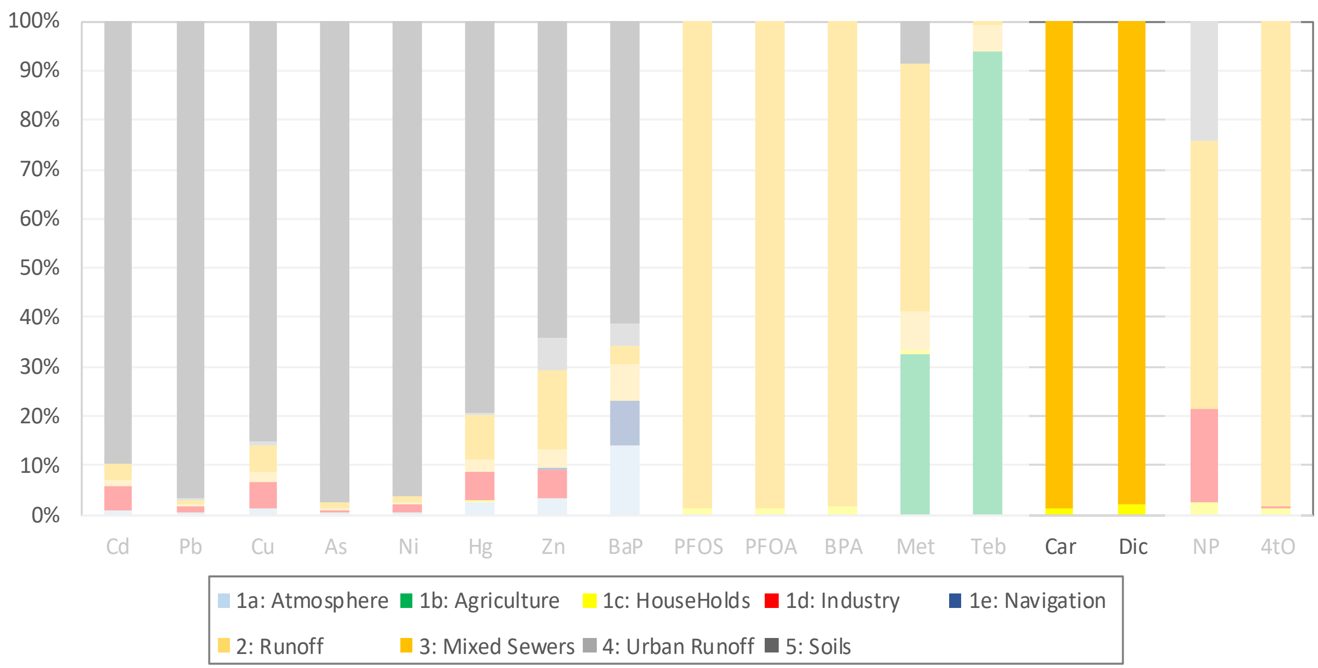

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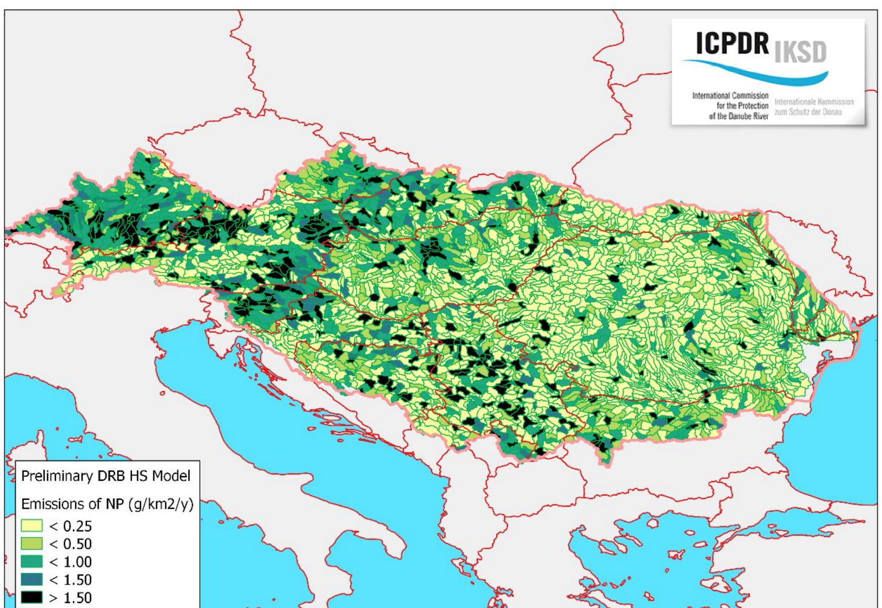
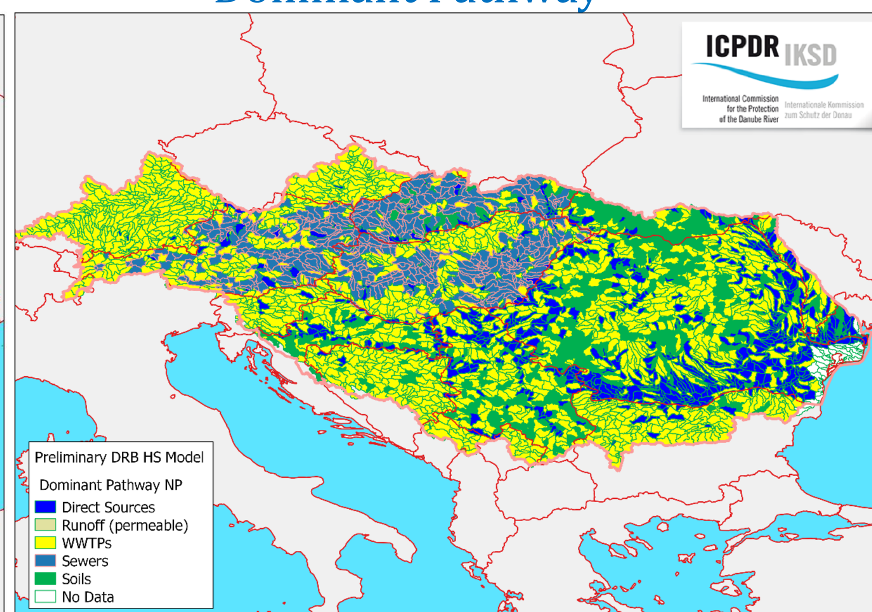
Basin-wide simulation results

- Industrial chemicals:
  - nonylphenol (NP): spatial distribution of the emission follows the population distribution and traffic intensity
  - Other chemicals: only households defined (lack of information)

Emission



Dominant Pathway



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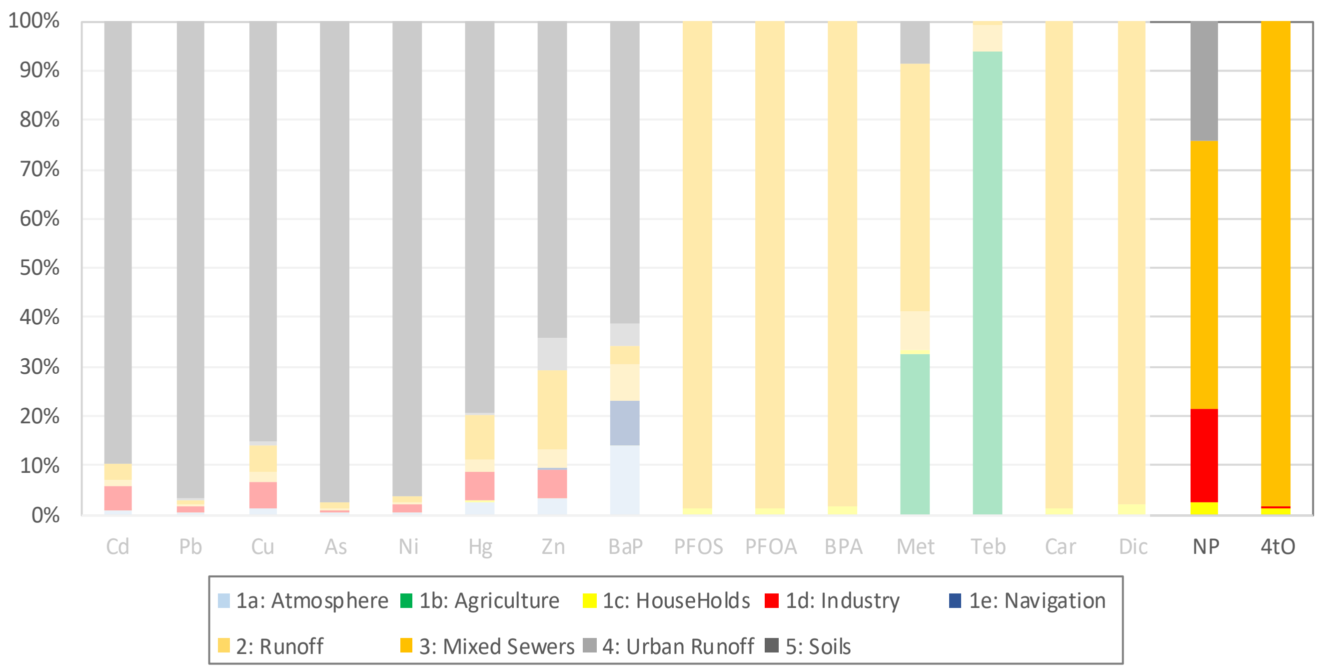
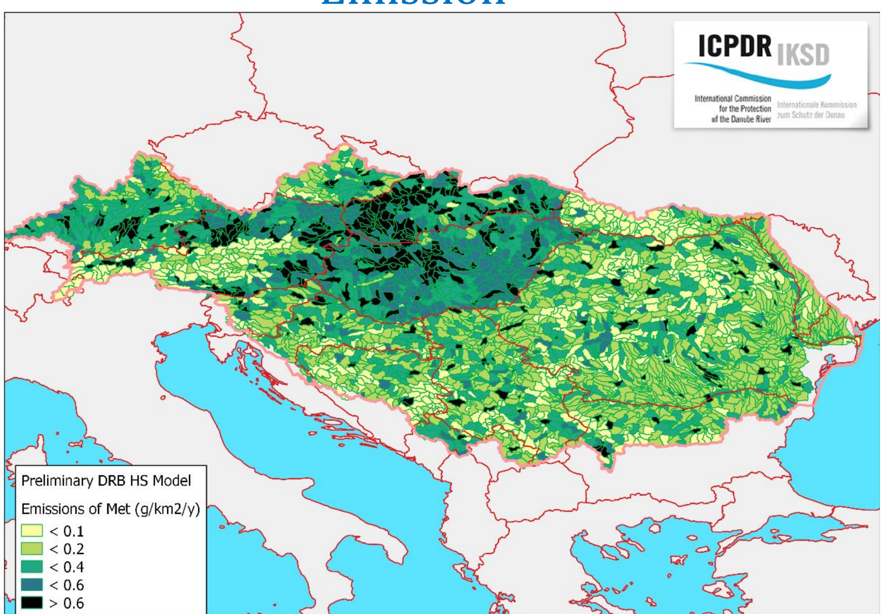


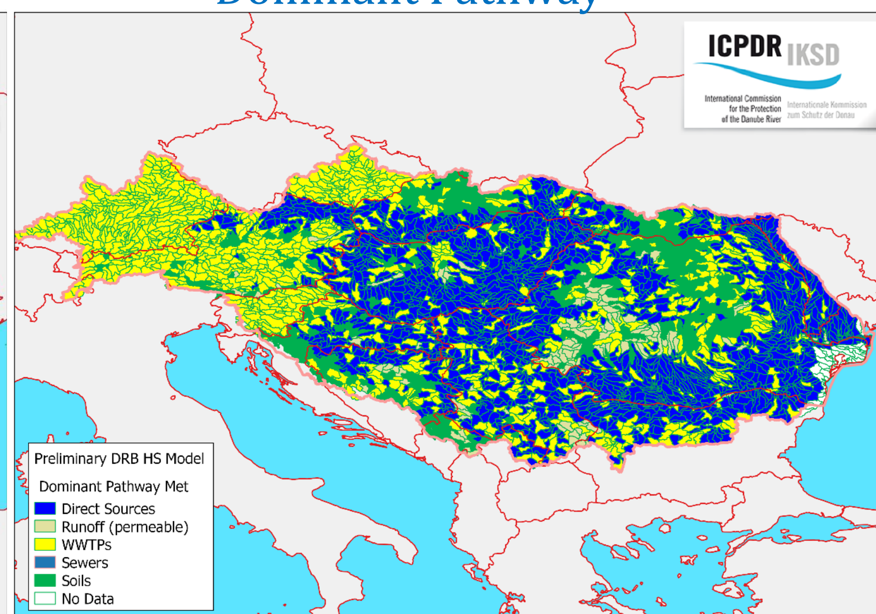
Basin-wide simulation results

- Pesticides:
  - Tebuconazole: dominated by direct losses
  - Metolachlor: significant contribution via wastewater (mixed sewers, 50%) (probably not correct, under revision)
  - Differences: sorption properties and current quantification of sources

Emission



Dominant Pathway



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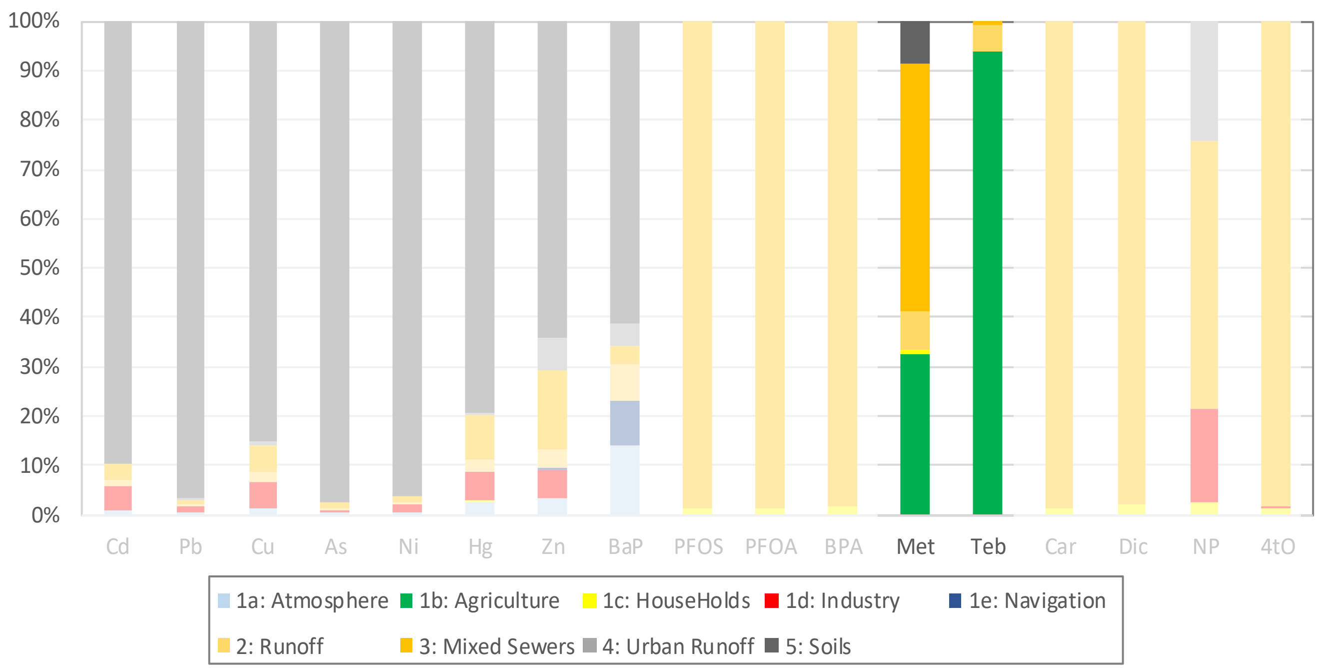

Basin-wide simulation results

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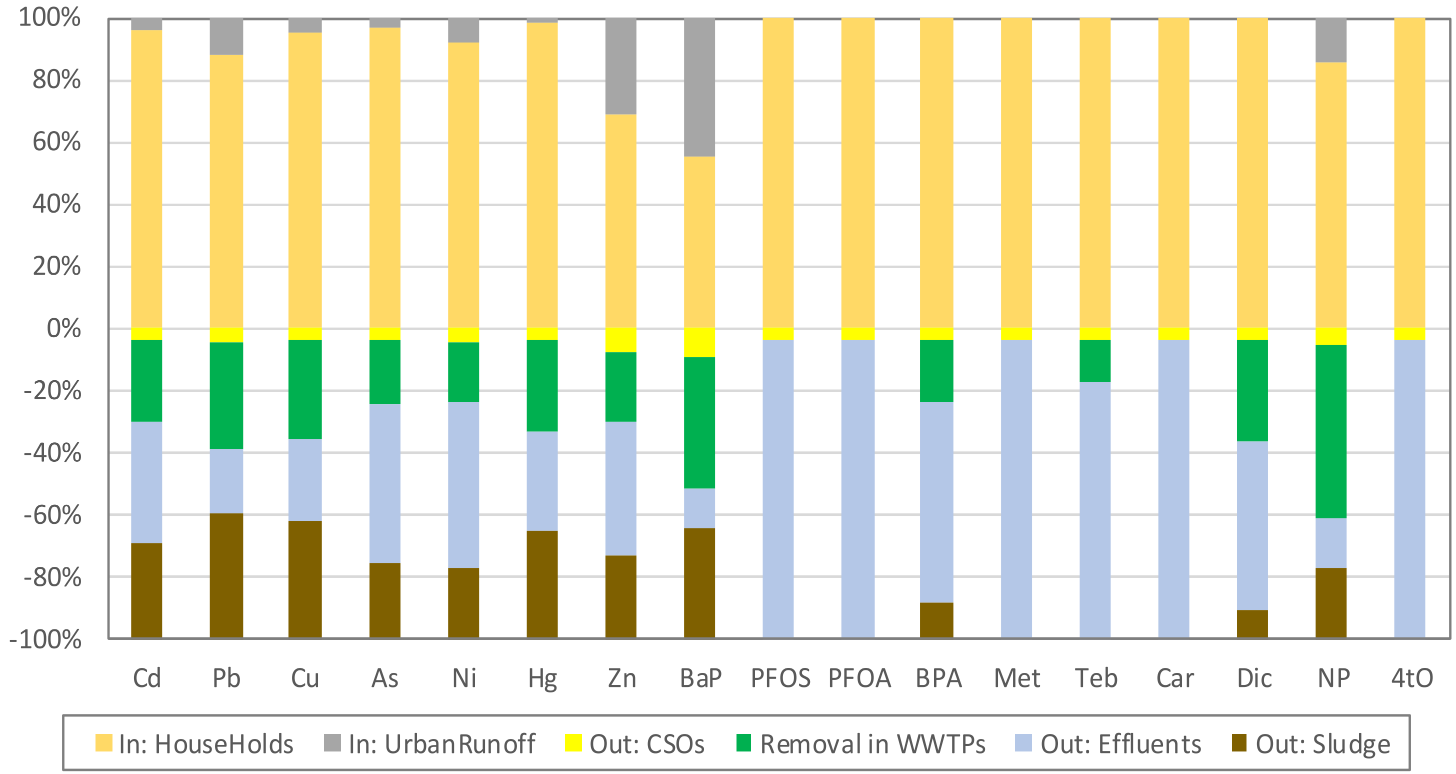
- Compartment:
  - Combined sewers and WWTPs: Inflow and outflows



Support/investigate source controls & precautionary measures

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- Management tool: capability for scenario implementation
  - Changes of sources
    - e.g. use of chemicals,
    - stocks of legacy chemicals
  - Changes of management practices affecting pathways
    - e.g. wastewater collection and treatment,
    - sludge re-use,
    - stormwater collection and management

Technical requirements

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- Requirements DHSM:
  - Windows based PC (OS Windows 10, 8GB RAM, 20-40 GB storage).
- Availability DHSM after project completion (March 2023):
  - compiled software + data via ICPDR
- Source code of the software used:
  - opensource (https://oss.deltares.nl/web/delft3d)

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Documentation

- general user guide (https://oss.deltares.nl/web/delft3d)
- input file description (https://oss.deltares.nl/web/delft3d)
- Mass balances output (delivered to ICPDR)
- Emission Modelling plug in (delivered to ICPDR)
- Model description and validation (Danube Hazard m3c Deliverable)
  - after project completion (March 2023)

Questions?

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Deltares
Enabling Delta Life

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Training on hazardous substances emission modelling and scenario evaluation

DHSM model: Hands-on workshop

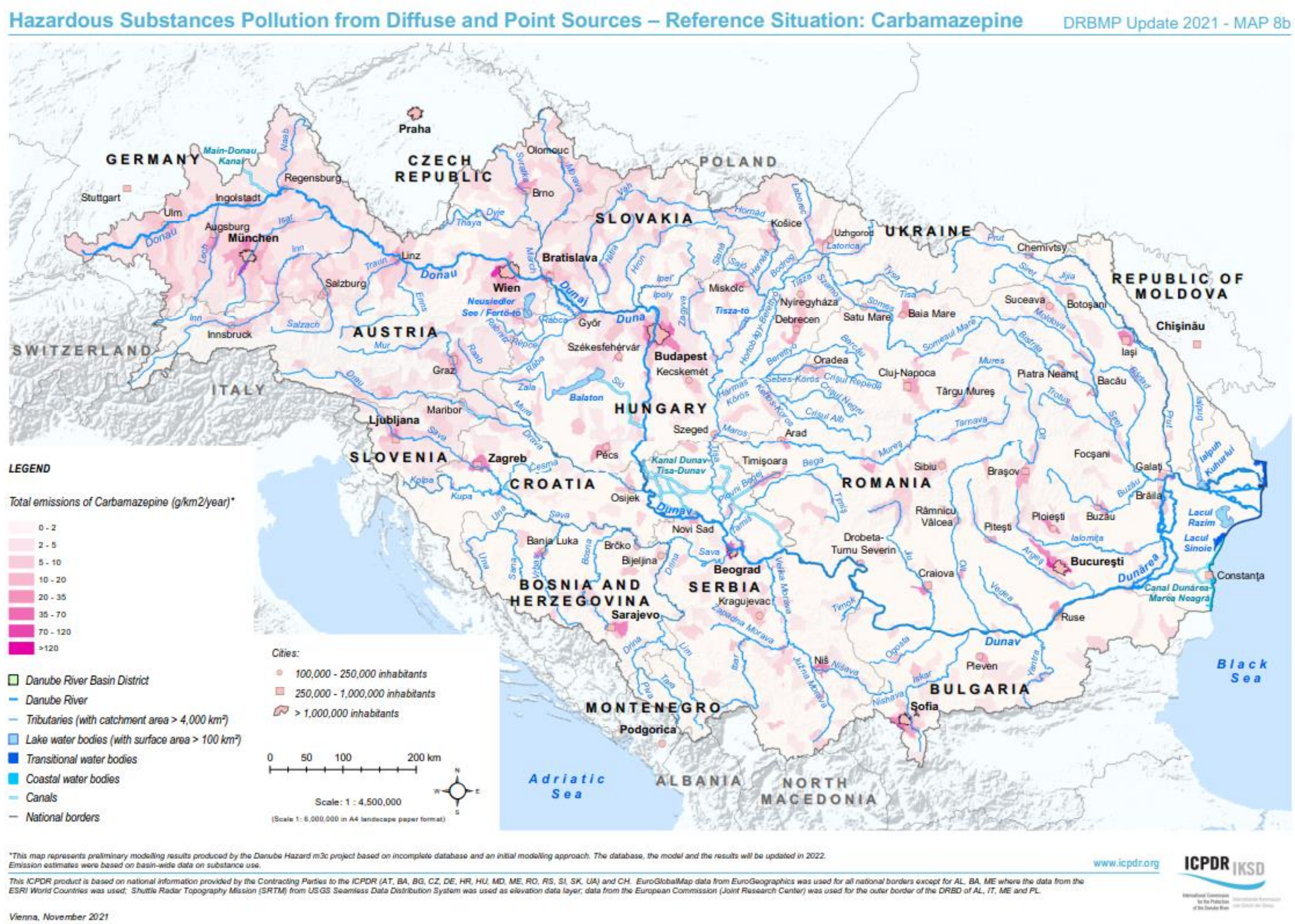
Vienna 4 October
Budapest 6 October
Bucharest 13 October

Project co-funded by European Union funds (ERDF, IPA, ENI) and National Funds of the participating countries

Contents

How it was made?

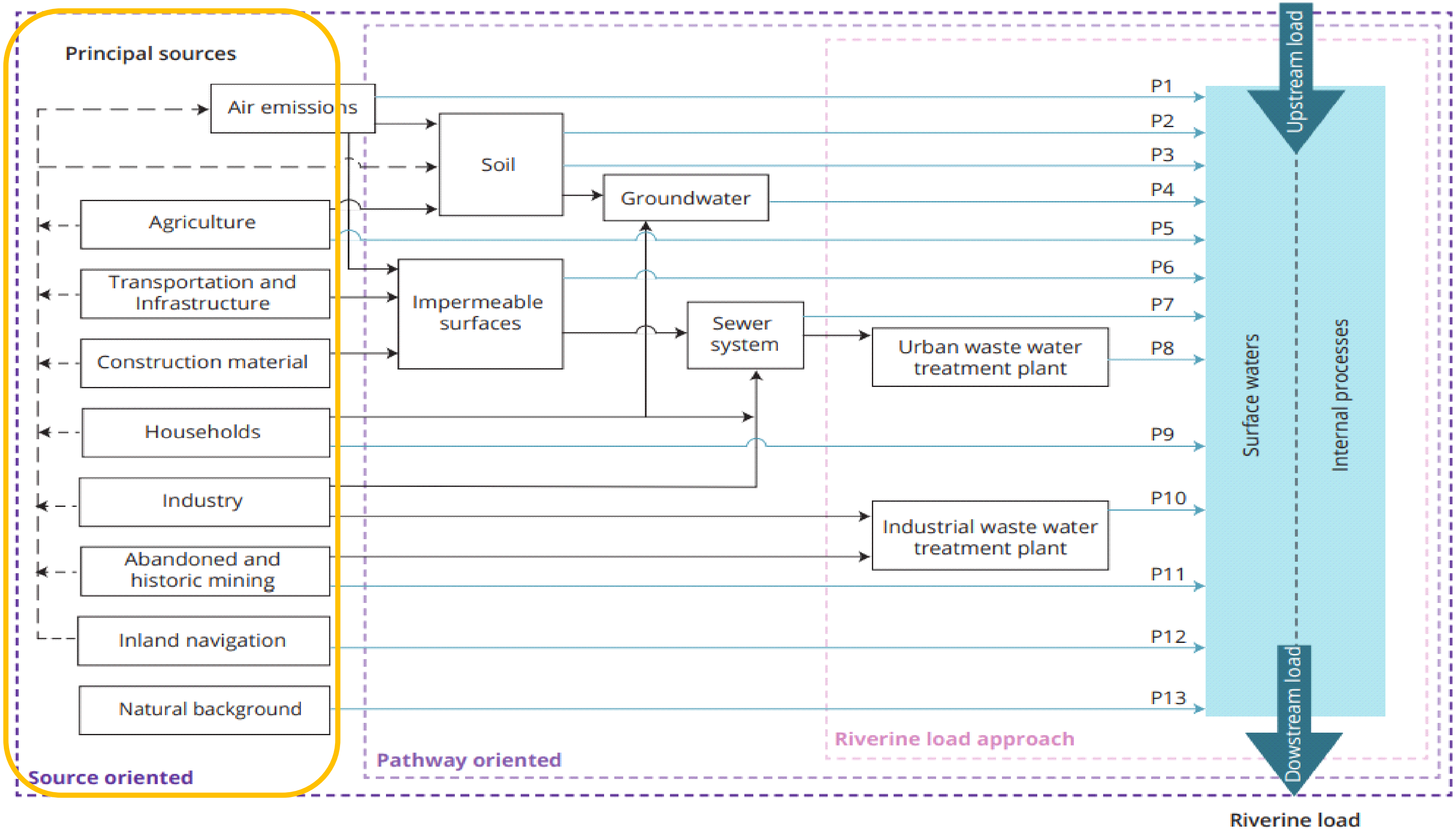
The emission estimates included in the DRBMP 2021 Update



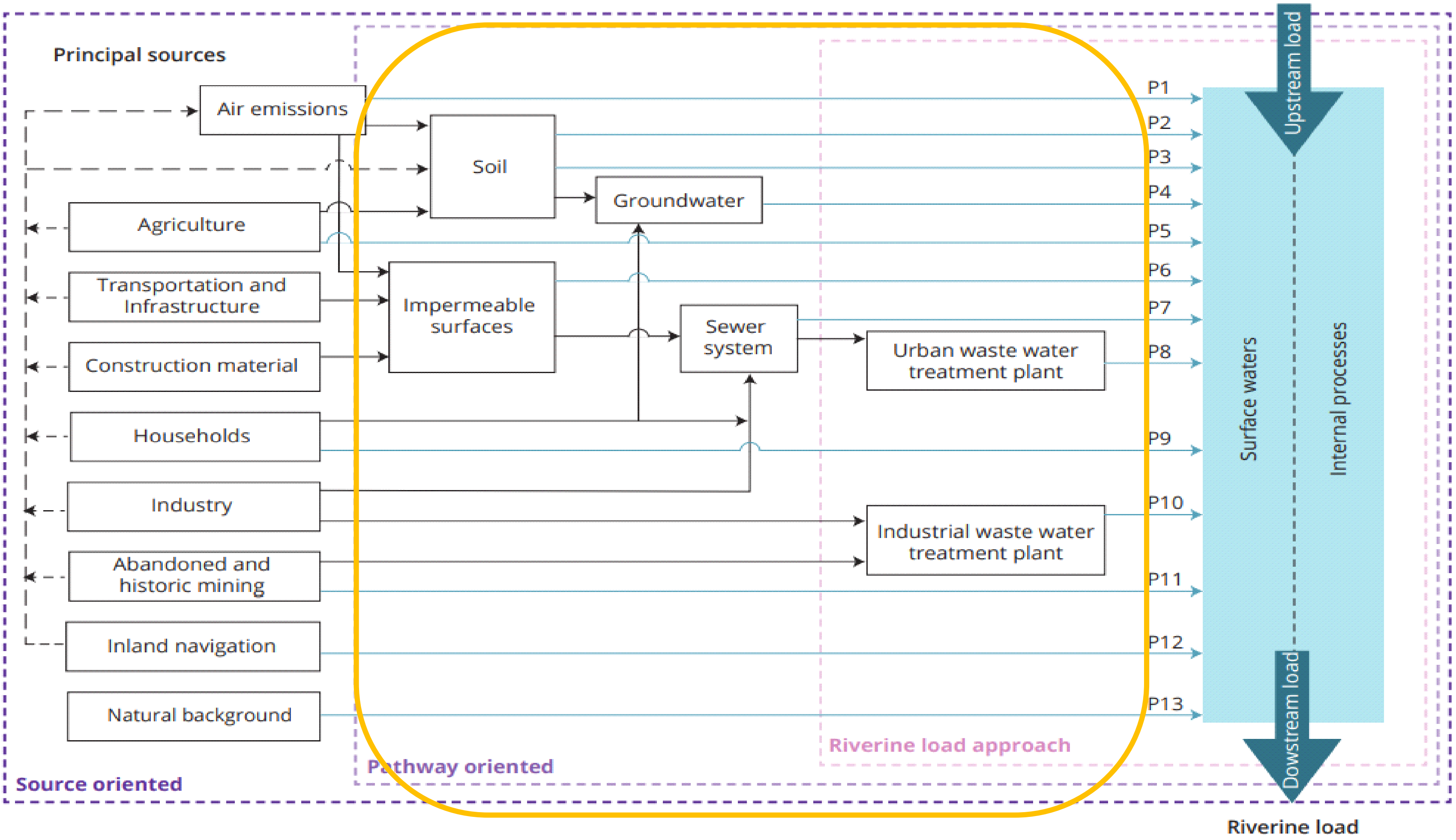
Managing expectations

- The DHSM is not designed to be used by non-experts
  - there no graphical user interfaces for pre- and postprocessing
  - there is no guidance in the form of a guided workflow
- At the same time it is not very complicated to use
  - we will give it a try
  - do not be afraid, the worst that can happen is that you make the model crash
- The objective:
  - that you get a feeling for how these things work
  - in the wider perspective of understanding what the models can and what they cannot achieve

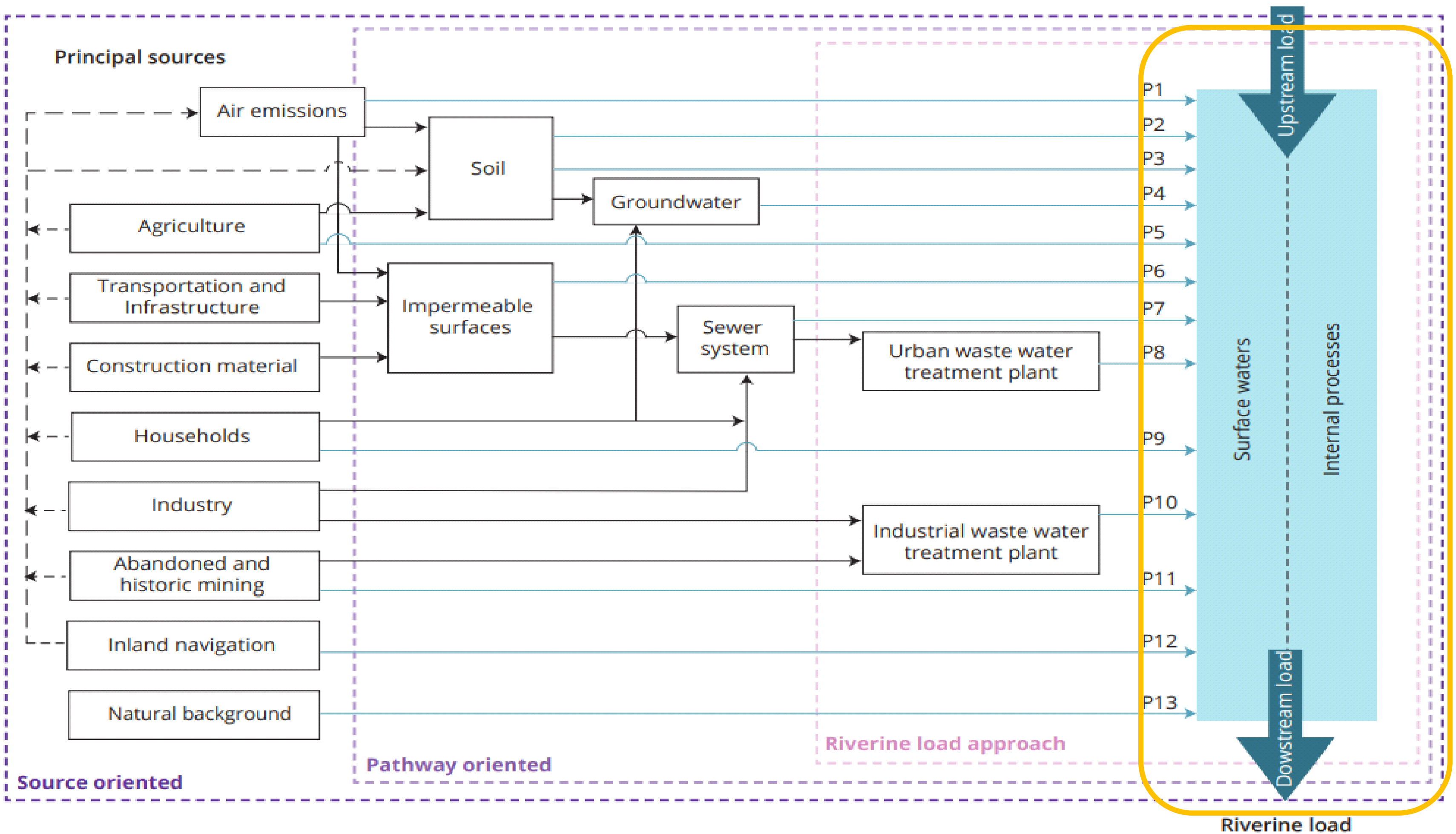
Points to remember



Points to remember



Points to remember



The model system lay-out

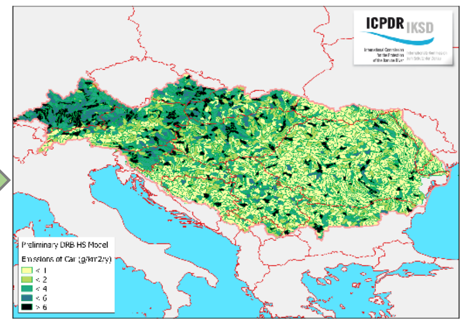
input data (x,y)
- sources
- pathways

stored data (x,y,t)

hydrology

sediment

emission model



water quality model

Output (x,y,t)

masses/ concentrations

mass balances

The software we use

- Delft3D-WAQ (aka DELWAQ)
- Why? It offers the functionality we need:
  - flexible input of data
  - numerical solution of mass balance equation / advection-diffusion equation
  - automatic facilities to produce mass balances (developed in *daNUbs* (!))
  - option to add functionality (definition of supporting variables, source term in mass balance equation
- Source code can be freely downloaded
- Compliation is required and complicated, Deltares provides a compiled version to ICPDR

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The software we use

Documentation:

- general user guide (https://oss.deltares.nl/web/delft3d)
- input file description (https://oss.deltares.nl/web/delft3d)
- Mass balances output (delivered to ICPDR)
- Emission Modelling plug in (delivered to ICPDR)
- Model decsription and validation (Danube Hazard m3c Deliverable)

Files and folders

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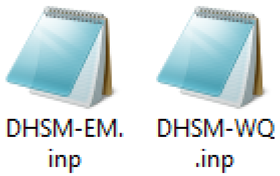
AR_Maps	“activity rate” maps
DHSM__Carbamazepine	files for modelling a substance
GIS_Maps	some maps for GIS presentations
H_Danube	stored schematization, hydrology and sediment data
Programs	DELWAQ programme and supporting tools
WW_Man	maps related to wastewater and stormwater management

Files and folders (2)

input_subs	substance-specific input
output	final output
present	presentations of results
run	(folder where actual calculations take place)
system	(definition of workflows)
step1-em.bat Type: Windows Batch File	run step 1: emission model (< 1 minute)
step2-wq.bat Type: Windows Batch File	run step 2: water quality model (20-30 minutes)
step3-pp.bat Type: Windows Batch File	run postprocessing steps

Run folder



- step 1 and step 2 main input files

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Input file conventions

- blanks as separator
- use new line freely
- place DHSM related input anywhere between #6 and #7
- use “;” to add comments
- use keyword INCLUDE to include the contents of an external text file, to keep the main input file compact

Relevant input forms

- Input items need to be defined by a prefined name (use manuals)

- An input item with a constant alue:

```
CONSTANTS Item DATA value
```

- A spatially variable constant alue:

```
PARAMETERS Item ALL DATA
3477 values for all schematizaion elements
```

Schematization elements (SEs)

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Input processing

- Preparation of spatial data is kept separate from the software (using map of SE's, GIS expertise needed)
- E.g. waste water management data (\WW_Man\wwman.inc)

Lister - [p:\11204121-002-danubehazardm3c\modelv3_HandsOn\WW_Man\wwman.inc]

File Edit Options Encoding Help 0 %

;	fSew	fSep	fDCTP	fTr0	fTr1	fTr2	fSldInc	fComSew		Danube	SUBID	Country
	0.60	0.00	0.40	0.00	0.00	1.00	0.20	0.50	;	1	9000145	Ukraine
	1.00	0.00	0.00	0.00	0.00	1.00	0.65	0.70	;	2	9000229	Germany
	0.60	0.00	0.40	0.00	0.00	1.00	0.65	0.70	;	3	9000233	Germany
	1.00	0.00	0.00	0.00	0.00	1.00	0.65	0.70	;	4	9000235	Germany
	1.00	0.00	0.00	0.00	0.00	1.00	0.65	0.70	;	5	9000236	Germany
	0.13	0.00	0.87	0.83	0.00	0.17	0.20	0.50	;	6	9000306	Ukraine
	1.00	0.00	0.00	0.00	0.00	1.00	0.56	0.28	;	7	9000385	Austria
	0.79	0.00	0.21	1.00	0.00	0.00	0.20	0.60	;	8	9000400	Moldova
	0.88	0.00	0.12	0.00	0.00	1.00	0.18	0.50	;	9	9000665	Hungary
	0.95	0.00	0.05	0.00	0.00	1.00	0.18	0.50	;	10	9000669	Hungary
	0.99	0.01	0.00	0.00	0.00	1.00	0.56	0.28	;	11	9000674	Austria
	0.00	0.00	1.00	1.00	0.00	0.00	0.10	0.10	;	12	9000678	Slovakia
	0.74	0.00	0.26	0.00	0.00	1.00	0.11	0.85	;	13	9000684	Czech_Rep.

Input processing

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- Substance specific input follows conventions as discussed
- Input item names to be derived from manuals
- Preparation of files per source follows algorithms as layed out in the project report
  - often by simple excel processing using tabulated properties of the SE's like land use, country, surface area, population, etc.
- Look for yourself
  (but do not be disappointed ...)

Files and folders (2)

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input_subs	substance-specific input
output	final output
present	presentations of results
run	(folder where actual calculations take place)
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step3-pp.bat Type: Windows Batch File	run postprocessing steps

Substance specific input data

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AR_Industr.inc Type: Include File	activity rate source industry
AR_Navig.inc Type: Include File	activity rate source navigation
drydep.inc Type: Include File	dry deposition rate
EF_agr.inc Type: Include File	emission factor agriculture
EF_built.inc Type: Include File	emission factor built environment
EF_HouseH.inc Type: Include File	emission factor households
EF_roadtr.inc Type: Include File	emission factor road traffic
parameters.inc Type: Include File	fate and transport model parameters
S1_init.inc Type: Include File	initial concentrations in top soils
treatment.inc Type: Include File	treatment efficiency

Calculation steps

- Step 1: emissions (done in a few seconds)
- Step 2: water quality (20-30 minutes)

Specific postprocessing

- maps of input items: output\spatial-EM.csv
- overall mass balances: output\balance-all.csv
- river concentrations: output\river-conc.csv
- mapped emissions: output\maps-EM.csv

Presentation of data

- QGis project for
  - maps of input items
  - maps of emissions
- Excel for
  - overall mass balances
  - river concentrations

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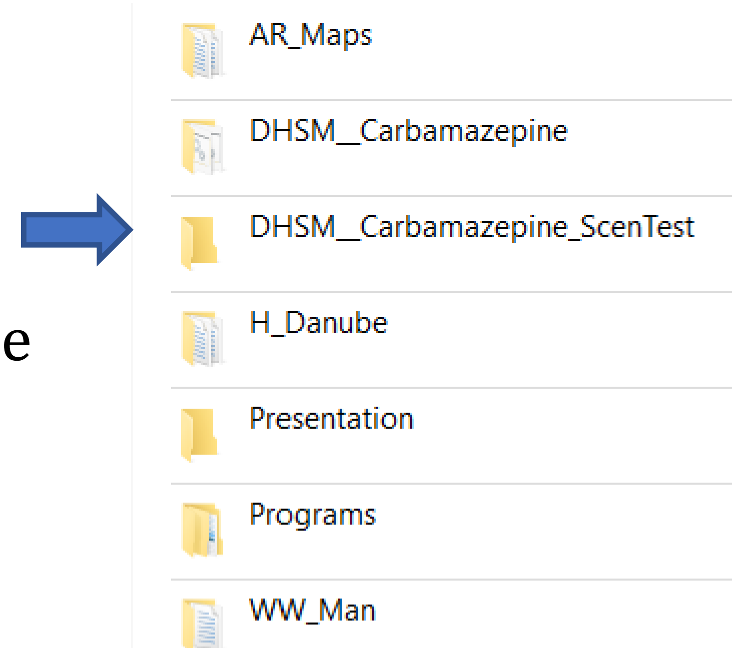
For the daredevils …

- Try your own scenario
- Create a new folder
- Copy the contents of DHSM_Carbamazepine there
- Change the input
- Run
- See *Steps for a few simple scenario simulations.docx*



Deltares

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Thank you for attendance

We acknowledge the support from ICPDR

We acknowledge the contribution of all Danube Hazard m3c partners to the work presented here

Hydrology data were provided by SMHI (Sweden)

Project co-funded by European Union funds (ERDF, IPA, ENI) and National Funds of the participating countries

Logo of hosting partner/speakers organisation (not wider/higher than EU flag)

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Danube Hazard m³c
Training on hazardous substances emission modelling and scenario evaluation

Workshop on input data preparation
[Venue], [Date]

Project co-funded by European Union funds (ERDF, IPA, ENI) and National Funds of the participating countries

Table of contents

- Temporal data (30-40 minutes)
  - Overview (type of temporal data, precipitation, concentration and riverflow, high frequency data from sensors, low-flow/high-flow)
  - Time series processing for load calculation (three methods intercomparison)
  - Issues with HS data (LOQ, LOD, quantification)
- Spatial data (50-60 minutes)
  - Type of spatial data
    - Interpolation of point data (e.g. precipitation)
    - Modelled data using geostatistical methods (krieging, runoff, erosion, soil parameters)
    - Modelled data from other sources (EMEP)
    - Calculated spatial data based on balance approach (surplus)

Table of contents

- Spatial data (50-60 minutes)
  - Type of spatial data
    - Substance specific data
      - Literature data (per soil types, point sources)
      - Administrative data (sales data, farmers diaries)
      - Measured data (actual stock)
- Uncertainties of data types
  - Temporal data (fequencies vs accuracy, source data accuracy)
  - Spatial data (interpolation accuracy, source data accuracy)

Substance-specific data requirements of the MoRE model – point sources

Type of pathway	Pathway	Input data	Spatial scale	Temporal scale
Point	Municipal WWTP effluent	Effluent loads OR water amount and effluent concentration	For each plant or lumped over AU	Annual average
Point	Industrial WWTP effluent or direct industrial discharge	Effluent loads OR water amount and effluent concentration	For each plant or lumped over AU	Annual average
Point	Abandoned mining site	Effluent loads OR water amount and effluent concentration	For each site or lumped over AU	Annual average

Substance-specific data requirements of the MoRE model – point sources

Type of pathway	Pathway	Input data	Spatial scale	Temporal scale
Diffuse	Agricultural erosion	Soil content in agricultural land	Lumped over AU	Current conc. level
Diffuse	Erosion from natural soils	Soil content in natural covered land	Lumped over AU	Current conc. level
Diffuse	Surface runoff from pervious soils	Concentration in surface runoff from pervious land	Lumped over AU	Annual average
Diffuse	Tile drainage	Concentration in tile drainage discharge	Lumped over AU	Annual average
Diffuse	Groundwater	Concentration in groundwater	Lumped over AU	Annual average
Diffuse	Atmospheric deposition	Deposition rate	Lumped over AU	Annual average
Diffuse	Atmospheric deposition	Concentration in rain water	Lumped over AU	Annual average
Diffuse	Discharge through combined sewer overflows	Concentration in combined sewer overflows	Lumped over AU	Annual average
Diffuse	Discharge through storm sewer outlets	Concentration in storm sewer outlets	Lumped over AU	Annual average
Diffuse	Inland navigation	Emissions loads of PAH via steel construction for hydraulic engineering	Lumped over AU	Annual average
Diffuse	Inland navigation	Emissions loads of PAH via motor boat exhaust	Lumped over AU	Annual average

Substance-specific data requirements for the SOLUTIONS model

Type of pathway	Pathway	Input data	Spatial scale	Temporal scale
Point & Diffuse	Wastewater	Use volume and use type of chemical, population density map, waste water management maps (connection to sewers, treatment level)	Lumped per SC, use volume optional per country or even on EU level	Annual average
Point & Diffuse	Stormwater	Use volume and use type of chemical, population density map, paved area map, combined-/separated sewers map	Lumped per SC, use volume optional per country or even on EU level	Annual average
Point	Abandoned mining site	Effluent loads OR water amount and effluent concentration		Annual average
Diffuse	Agricultural emissions (pesticides)	Amount used	Country level or finer if available	Annual average
Diffuse	Atmospheric deposition	Deposition rate	Lumped per SC	Annual average
Diffuse	Inland navigation	Emissions via steel construction for hydraulic engineering	Lumped per SC	Annual average
Diffuse	Inland navigation	Emissions via motor boats	Lumped per SC	Annual average

Intermediate results of the SOLUTIONS model, for which validation data are required.

Type of pathway	Pathway	Validation data	Spatial scale	Temporal scale
Point	Municipal WWTP effluent	Effluent loads OR water amount and effluent concentration	For each plant or lumped over AU	Annual average
Point	Industrial WWTP effluent or direct industrial discharge	Effluent loads OR water amount and effluent concentration	For each plant or lumped over AU	Annual average
Diffuse	Agricultural erosion	Soil content in agricultural land	Lumped over AU	Current conc. level
Diffuse	Erosion from natural soils	Soil content in natural covered land	Lumped over AU	Current conc. level
Diffuse	Surface runoff from pervious soils	Concentration in surface runoff from pervious land	Lumped over AU	Annual average
Diffuse	Tile drainage	Concentration in tile drainage discharge	Lumped over AU	Annual average
Diffuse	Groundwater	Concentration in groundwater	Lumped over AU	Annual average
Diffuse	Discharge through combined sewer overflows	Concentration in combined sewer overflows	Lumped over AU	Annual average
Diffuse	Discharge through storm sewer outlets	Concentration in storm sewer outlets	Lumped over AU	Annual average

Meteorological & atmospheric data

Precipitation (& temperature)

- Usual determined ear morning (7:00), refers to the previous 24 hours
- Month totals (averages) more than enough for the models

Atmospheric deposition

- Wet on / dry on / bulk
- NOT air concentration!!!
- Location: background vs. urban, …

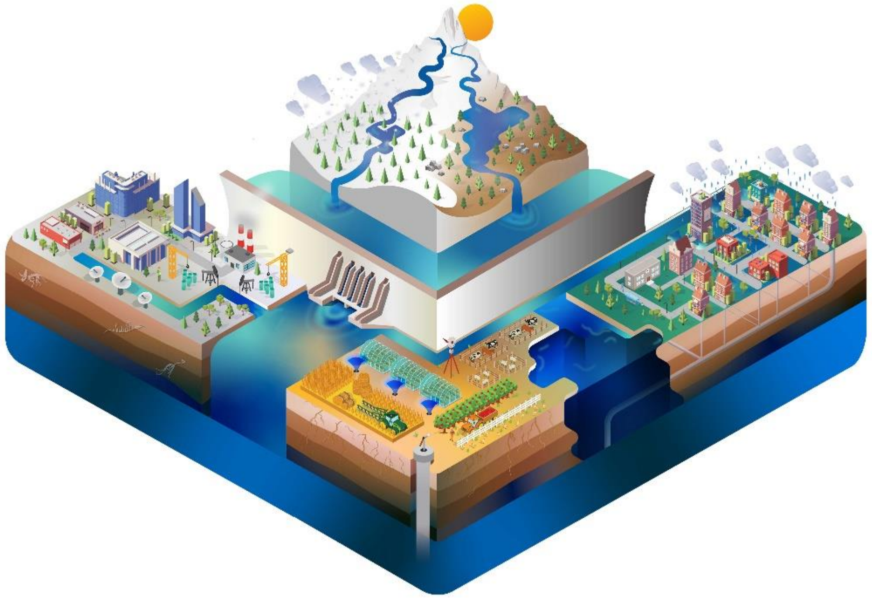
Data sources (meteorology)

	Spatial coverage	Spatial resolution	Time coverage	Temporal resolution	Data format
National meteo. service	Country	?	Far past - present	?	Time series. Radar data?
ForeSEE 4.0	Danube basin	0.1°	1950 - 2020	Day	NetCDF / ASCII (grid)
E-OBS	Europe	0.1°/0.25°	1950 - present	Day	NetCDF-4
ERA5 - Land	Global	0.1°	1950 - present	Month, Day, Hour	GRIB (binary grid)
CarpatClim	44-50°N 17-27°E	0.1°	1961 - 2010	Day	Gridded data
Climate Forecast System Rean. CFSR	Global	0.5°	1979 - 2017	Day, Month	GRIB
European Climate Assessment and Dataset	Global		1755 - 2020	Day, Month	Point data (CSV)
GPCP	Global	2.5° 1.0°	1979 - present 1996 - present	Month Day	NetCDF4
Precip f. satellite microwave obs.	Global	1.0°	2000 - 2017	Month, Day	NetCDF4

Hydrological data types & sources

Water level & **river flow**

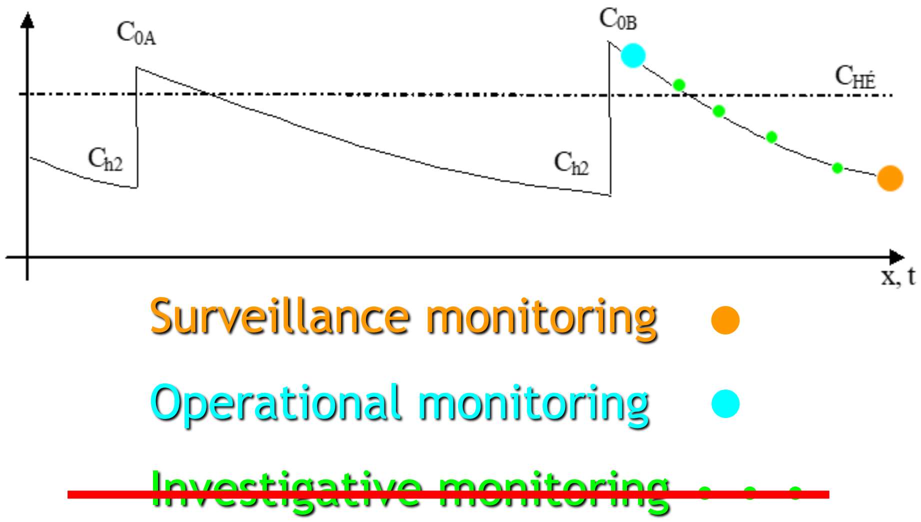
- Measured by local water authorities @ specific locations
- Usual measure water level, use rating curve…
- Important for the calculation of loads



Alternative sources: **modelled data**

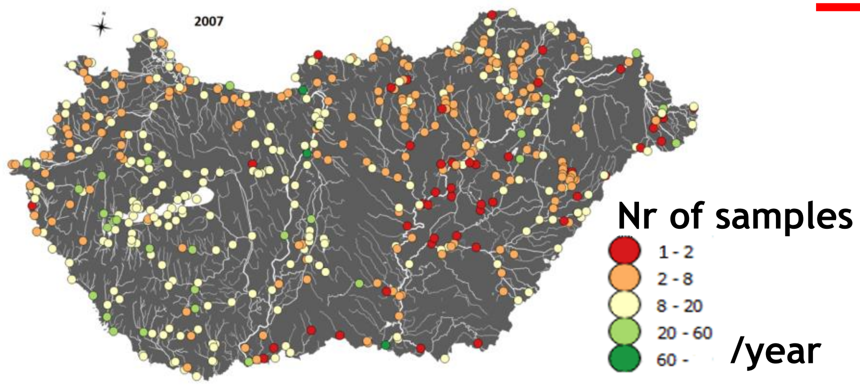
- Does the local authority use a water balance model (e.g. HEC-HMS, HEC-RAS, etc.)?
- European models: E-hype, CWATM, LISFLOOD, …

Water quality (concentrations)



Regular measurements: government /water authorities

- Usual according to WFD
- 1/year…50/year + rotation of locations
- Data accessibility?
- Coincident water gage!



Alternative sources:

- EEA WISE
- ICPDR TNMN (few stations but free)
- Data from scientific / management projects

Water quality – continuous measurements

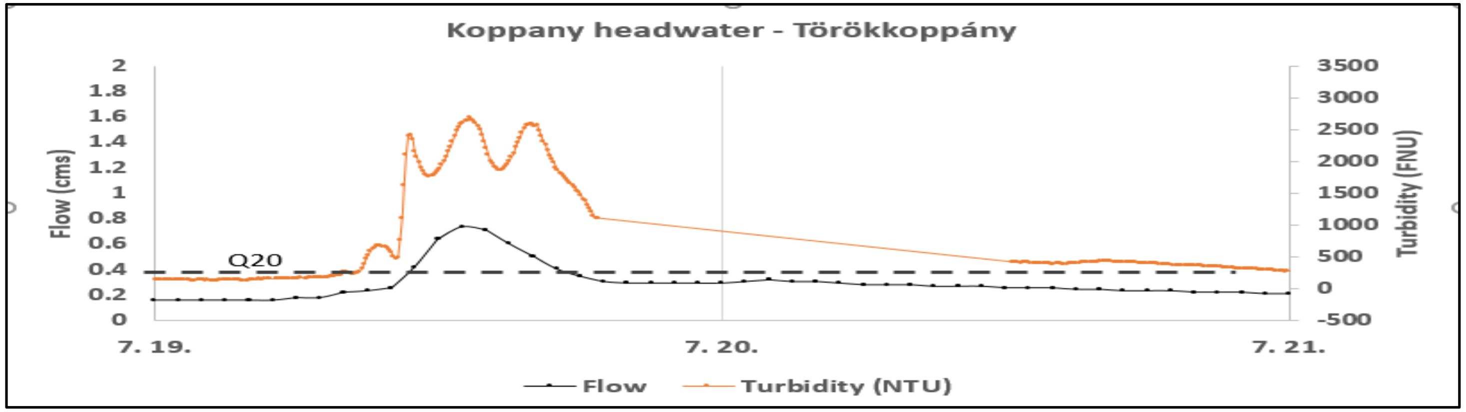
Limited number of locations

Limited number of parameters

- (temperature), **conductivity, turbidity**, oxygen, **pH, redox**, (some nutrients, …)

Data screening & processing important!

- Is the data calibrated? For the particular location?
- Outliers, missing periods, …



A special case: targeted sampling in the DH m³c project

Low and mindflow conditions:

week spot sampling,

8 samples (2 months) = 1 composite

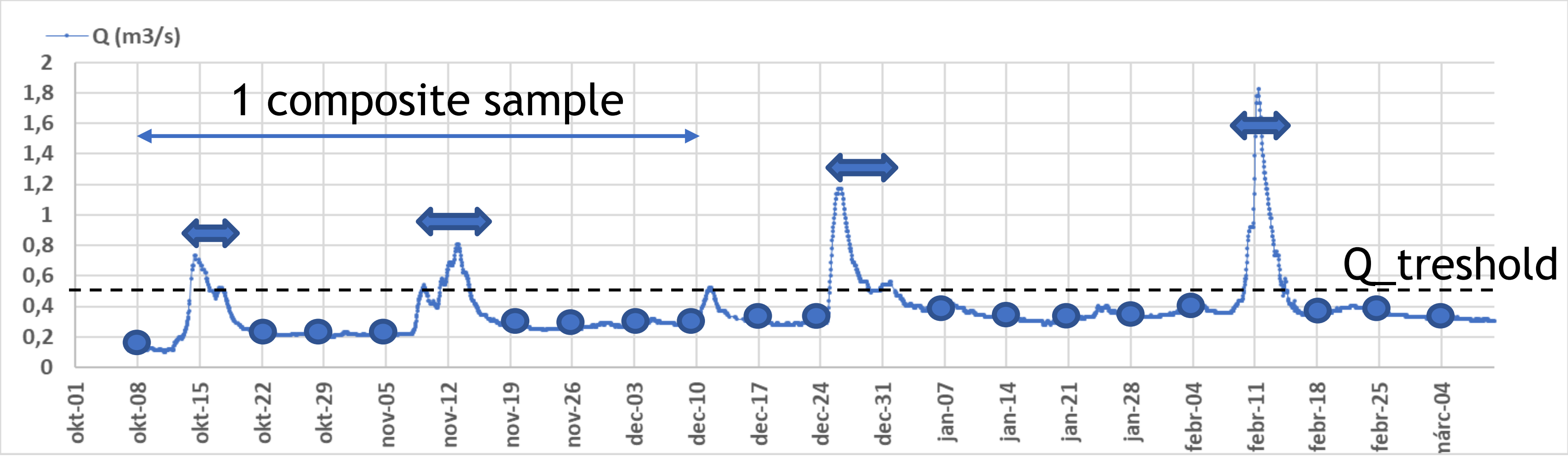
High flow events:

flow proportional sampling

with autosamplers

+ continuous online measurement of indicator parameters:

- turbidity
- conductivity



Point sources outlets

Inflow or outflow? ☺ **Outflow** from plant, inflow into the river

Urban systems (w or w/o industrial)

WW treatment: / Channel system:	Not present	Present
Not present	-	
Combined	Channel system outflows (~same category as CSOs)	CSOs, WWTP effluents
Separated	Storm water channel effluents, Sewage channel effluents	Storm water channel effluents, WWTP effluents

\+ Industrial direct dischargers

Collection system

Type of system: combined / separated

Length of the different types

Number of inhabitants connected

Number of inhabitants not connected → treatment type for them

Treatment system

Stormwater sedimentation tank (volume m^3)

WWTP capacity, connected inhabitants

Treatment technology (primary, secondary, other)

Data sources for WW systems

Data from the respective national authority

- Self-control measurements of plants
- Usual not free available
- Hungary: "water utility online data processing system"

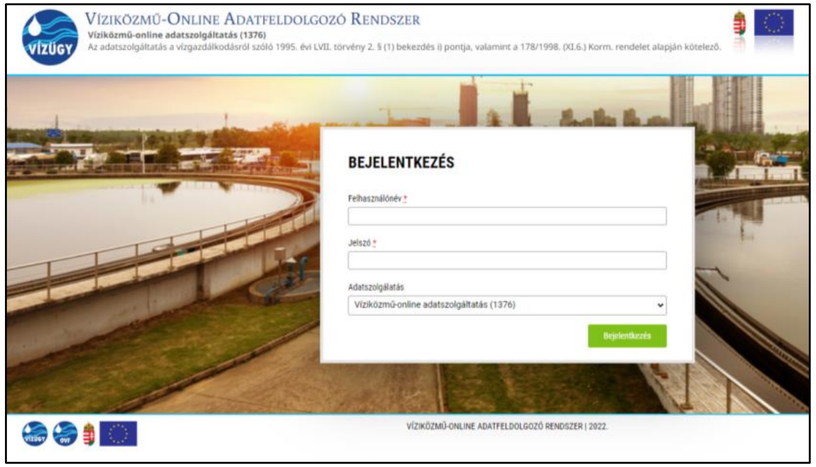
EEA UWWTD data ("Waterbase")

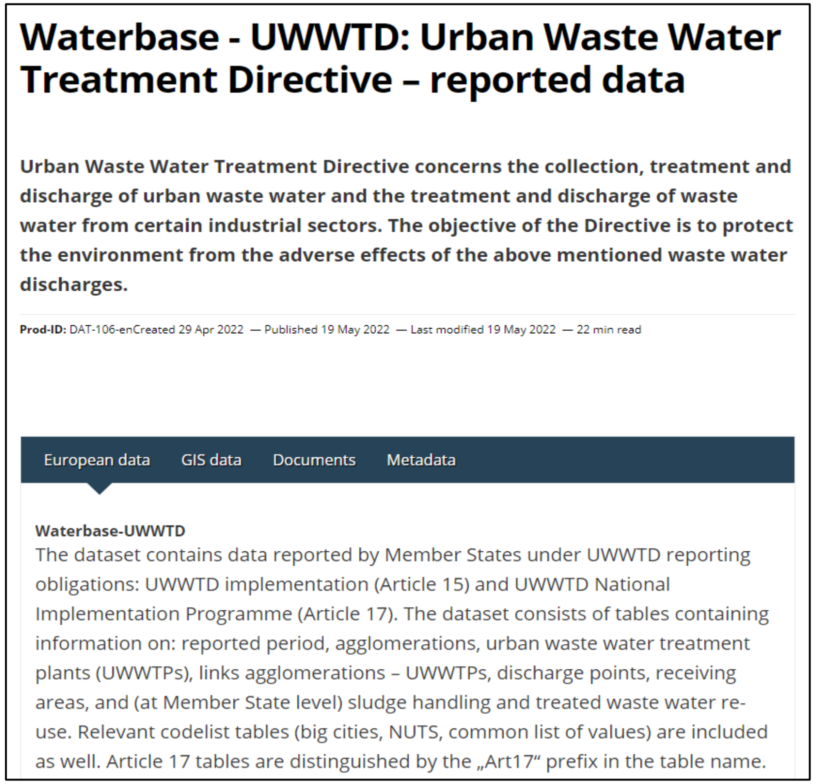
- Levels: Agglomerations, Plants, Discharge points
- Basic water quality + treatment technology

E-PRTR

- On large municipal and industrial direct dischargers –
- no discharge data, on concentrations

Projects…





Waterbase - UWWTD: Urban Waste Water Treatment Directive – reported data

Urban Waste Water Treatment Directive concerns the collection, treatment and discharge of urban waste water and the treatment and discharge of waste water from certain industrial sectors. The objective of the Directive is to protect the environment from the adverse effects of the above mentioned waste water discharges.

Prod-ID: DAT-106-enCreated 29 Apr 2022 — Published 19 May 2022 — Last modified 19 May 2022 — 22 min read

European data | GIS data | Documents | Metadata

Waterbase-UWWTD

The dataset contains data reported by Member States under UWWTD reporting obligations: UWWTD implementation (Article 15) and UWWTD National Implementation Programme (Article 17). The dataset consists of tables containing information on: reported period, agglomerations, urban waste water treatment plants (UWWTPs), links agglomerations – UWWTPs, discharge points, receiving areas, and (at Member State level) sludge handling and treated waste water re-use. Relevant codelist tables (big cities, NUTS, common list of values) are included as well. Article 17 tables are distinguished by the „Art17" prefix in the table name.

Mining facilities

Tailings management facilities

Important: periods of operation / decanting

Very specific for the mining activity

Treated / untreated

Data sources:

- Self control data
- Project data

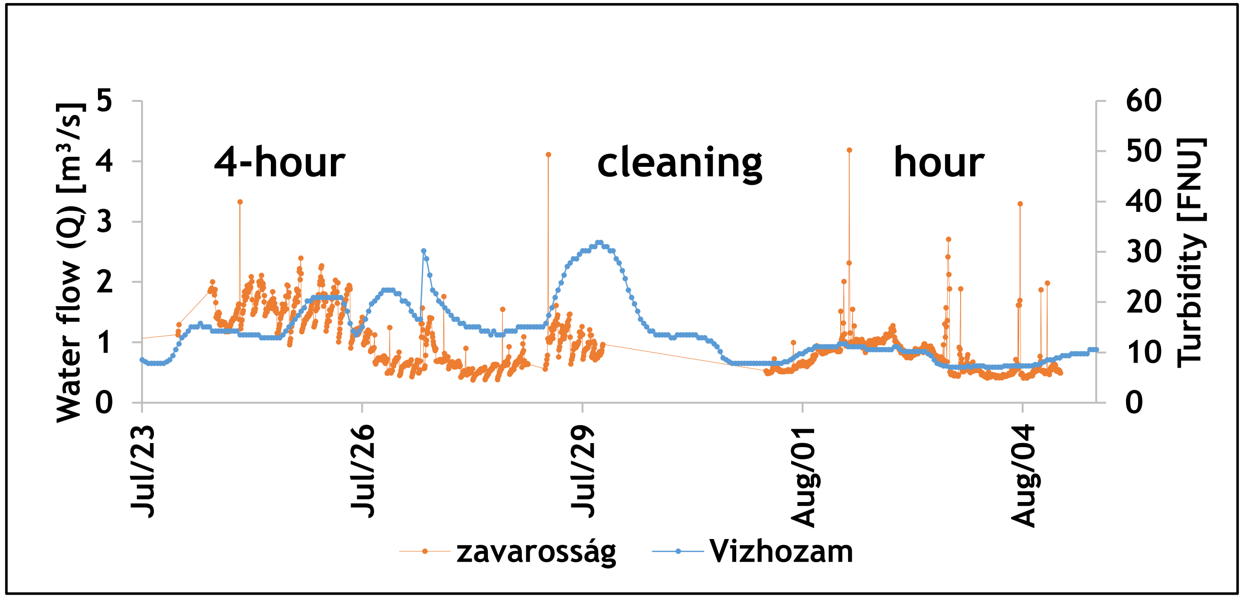
Quality check & screening

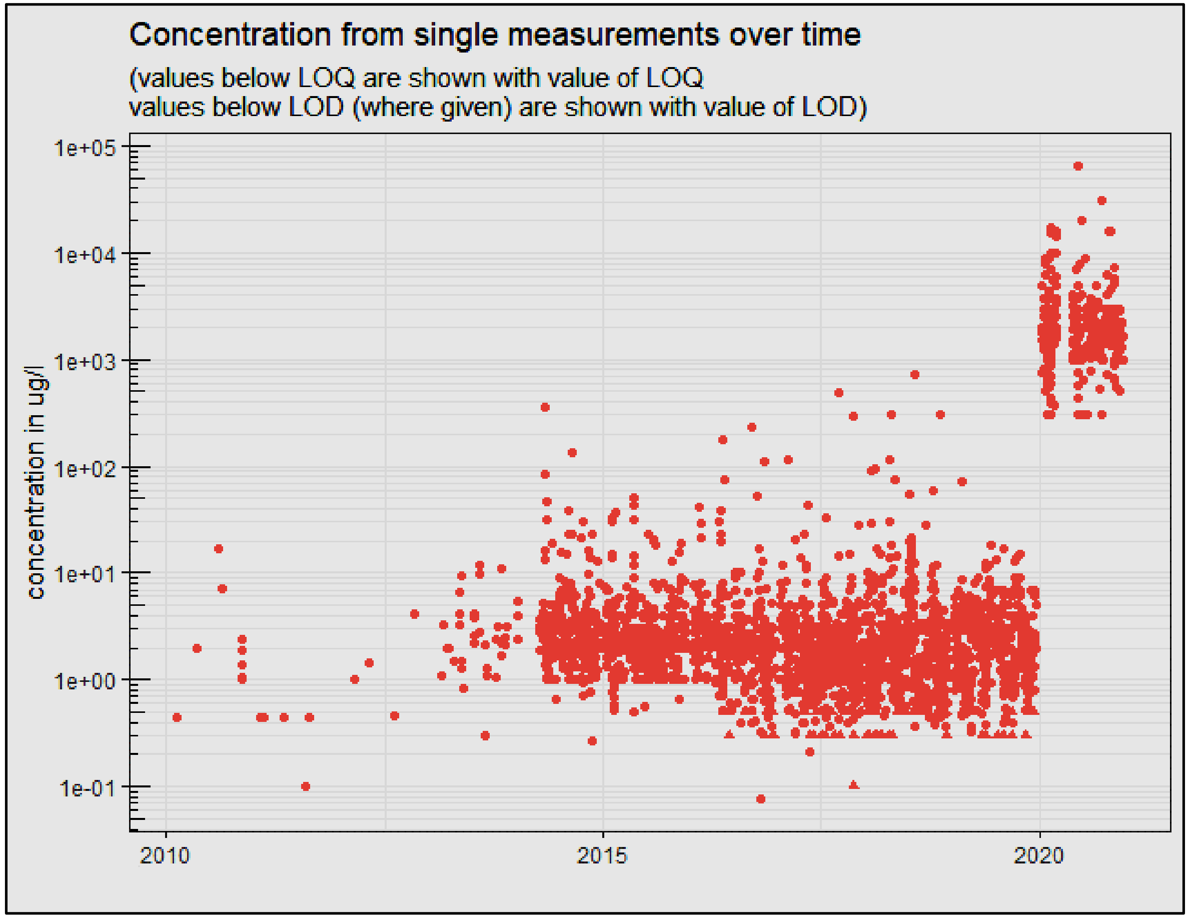
Local knowledge & expertise – protocols

Visual check

Manual check of outliers

Never delete values… Flagging!





Load calculation - basics

$$L(t) = \int_0^t Q(t) \cdot C(t)\, dt$$

Methods:

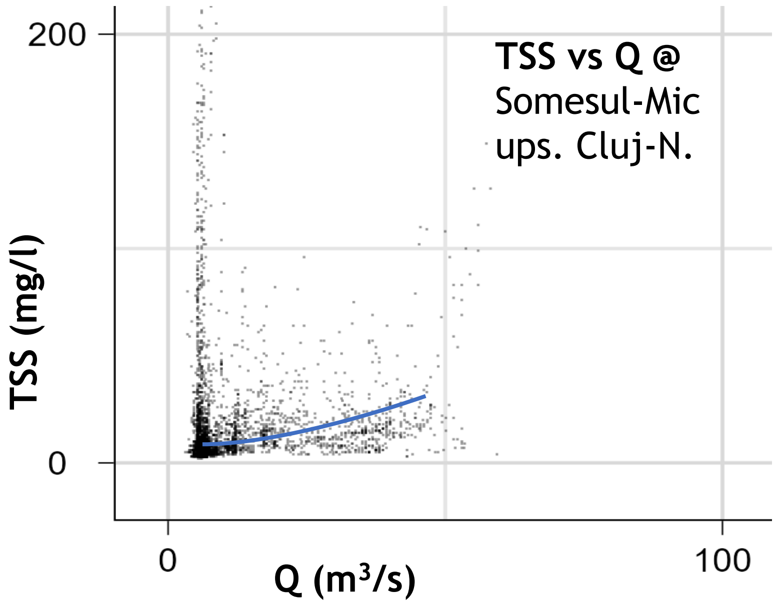
- Averaging ~ interpolation
- Proportion estimation
- Regression

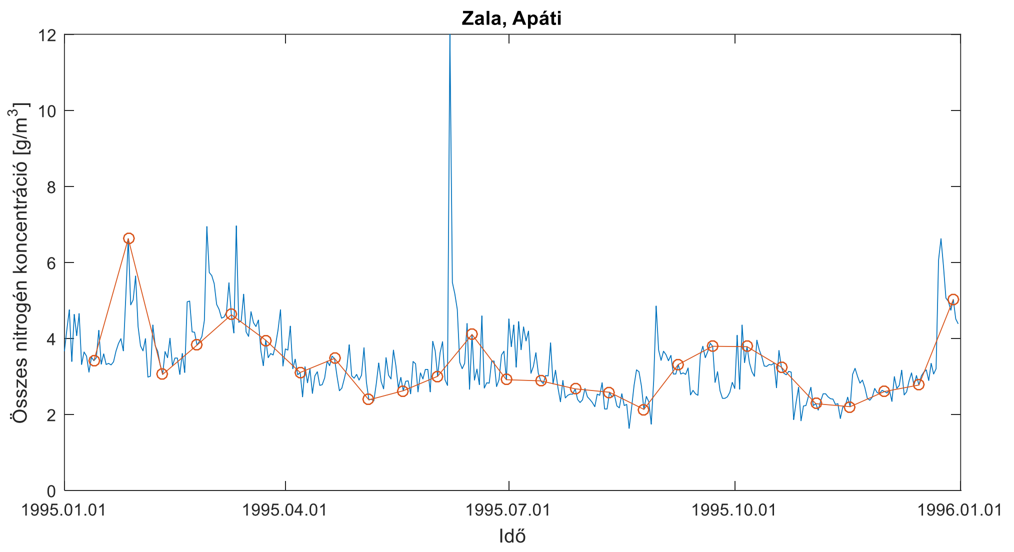
$$L \approx \bar{q} \cdot \bar{c}$$

$$L \approx \overline{q \cdot c}$$

$$L \approx \bar{Q} \cdot \bar{c}$$

$$L \approx \frac{\bar{Q}}{\bar{q}} \cdot \overline{q \cdot c}$$





Load calculation: stratification

Stratificaiton

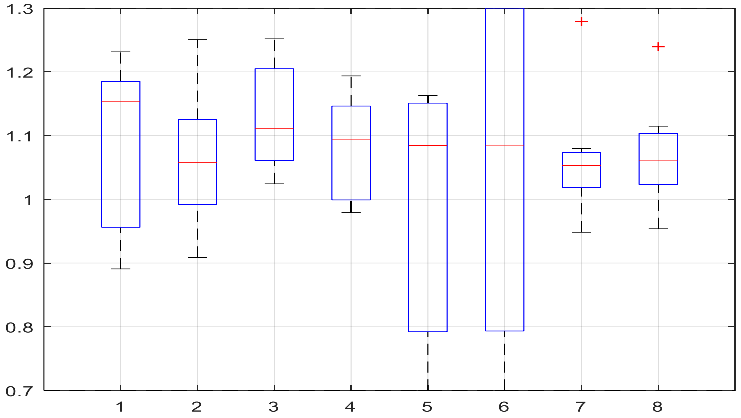
- By time (month / seasonal)
- Low flow – high flow periods
- Rising / falling limb

Applicable to every method

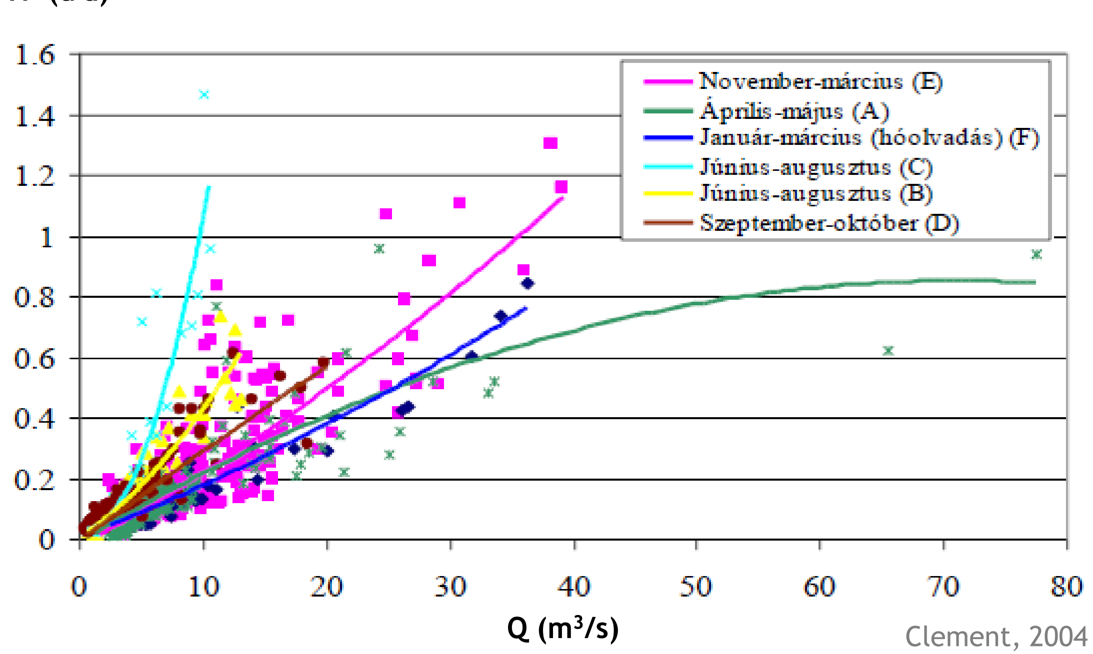
$$L \approx \frac{365}{12} \sum_{m=1}^{12} \frac{\sum_i Q_{im}}{N_m} \cdot \frac{\sum_i c_{im}}{n_m}$$

$$L \approx \frac{365}{4} \sum_{h=1}^{4} \frac{\sum_i Q_{ih}}{N_h} \cdot \frac{\sum_i c_{ih}}{n_h}$$

Comparison of 8 regression methods



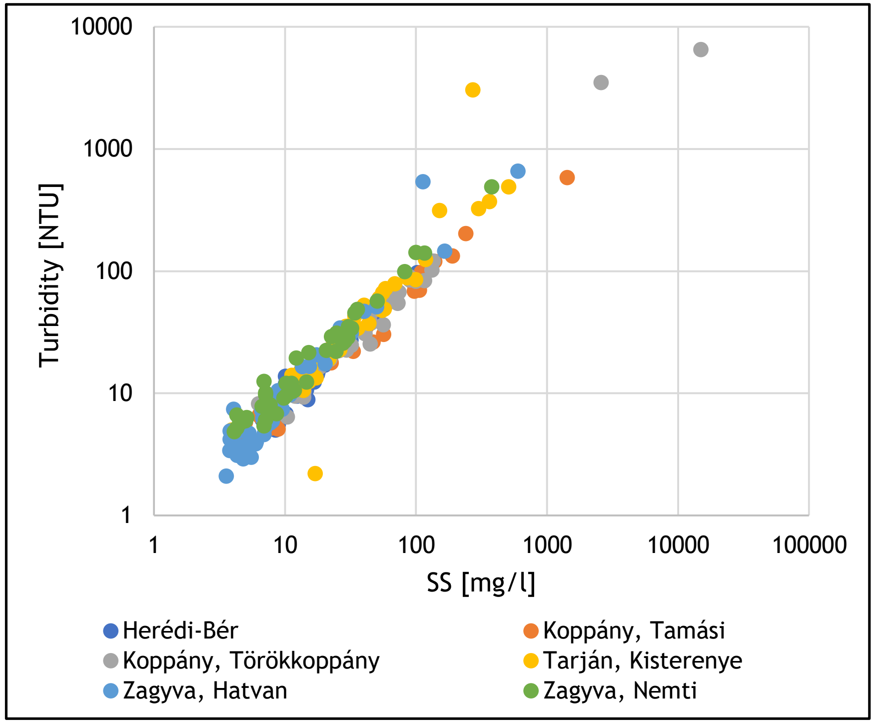
Stratified regression

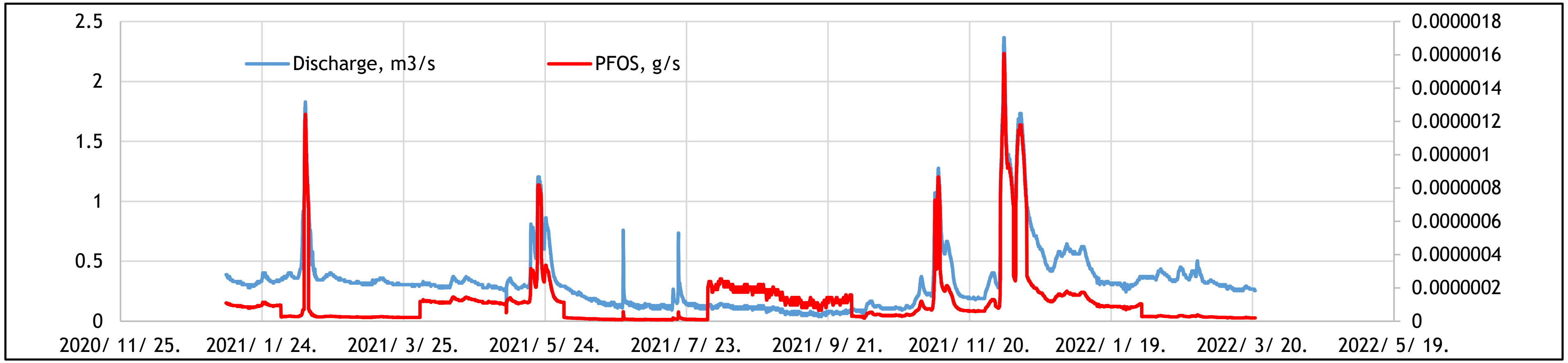


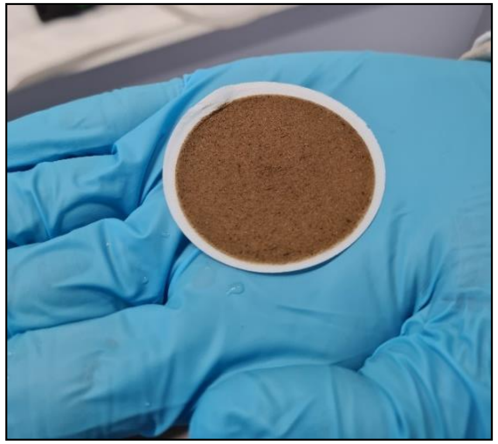
Clement, 2004

Load calculation

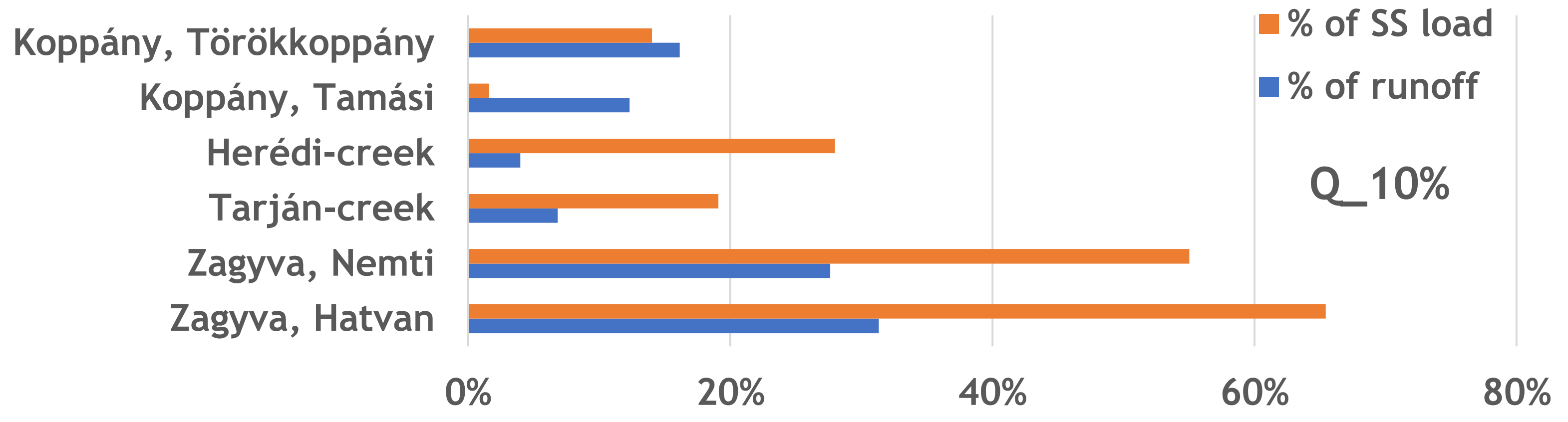
1. Establish the turbidity TSS relationship
   (or check the built-in formula of the device)
2. Relate the particular contaminant to the TSS
   try many methods
3. Calculate year load amounts via many methods
   and compare them







Calculation of SS and pollutant loads based on stratified river sampling



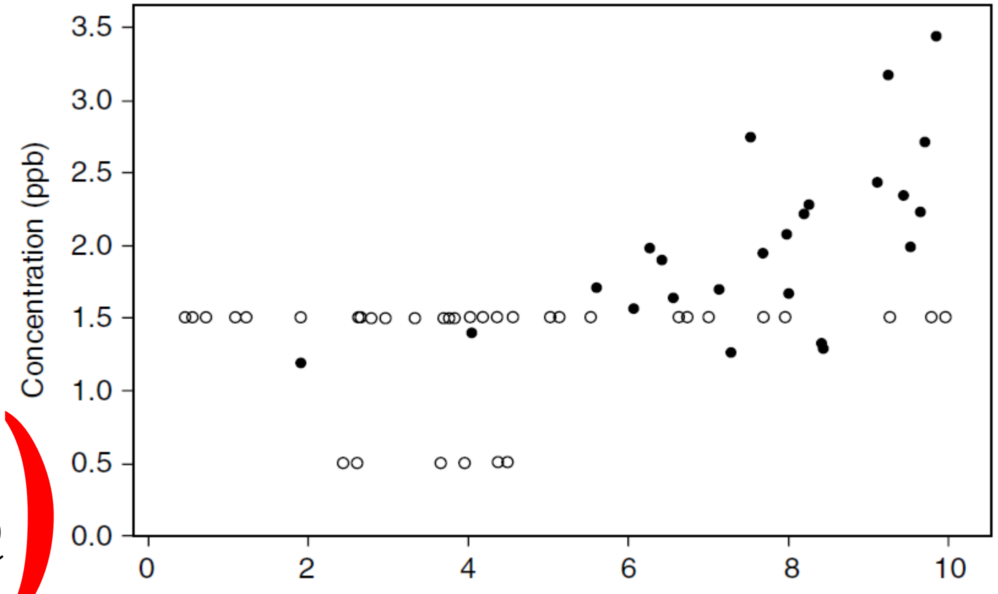
Contribution of high flow events to the total runoff and SS load

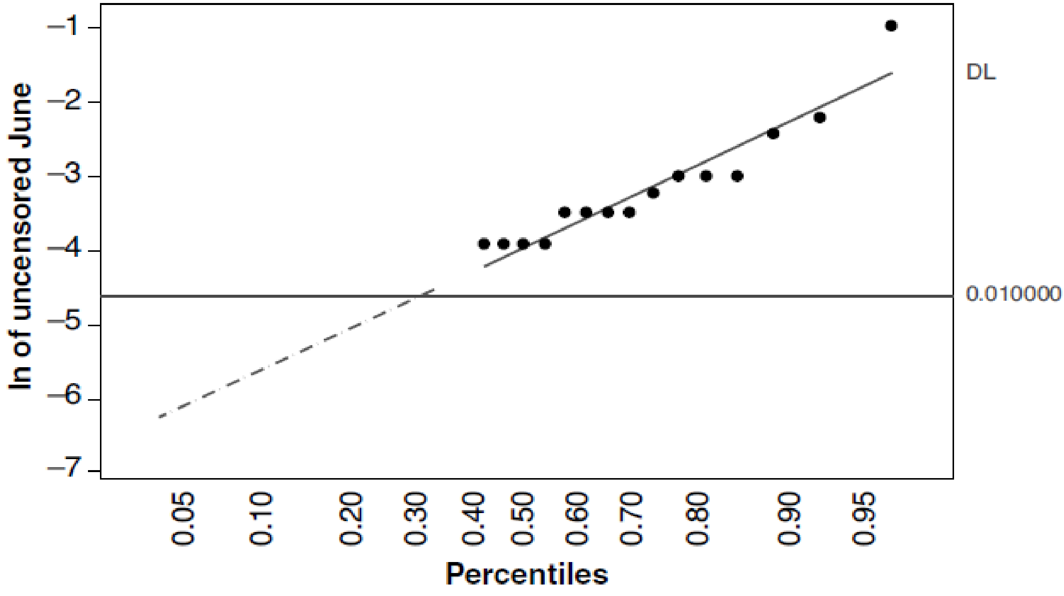
	Q5%		Q10%		Q30%	
	% of runoff	% of SS load	% of runoff	% of SS load	% of runoff	% of SS load
Zagyva, Hatvan	19%	53%	31%	65%	49%	77%
Zagyva, Nemti	16%	45%	28%	55%	58%	86%
Tarján-creek	4%	12%	7%	19%	40%	49%
Herédi-creek	4%	27%	4%	28%	6%	31%
Koppány, Tamási	5%	0%	12%	2%	60%	11%
Koppány, Törökkoppány	10%	7%	16%	14%	33%	46%

Censored data (<LOD, <LOQ)

- LOQ ≷ EQS
- ~~Ignoring~~
- Substitution
  - Most common: substitution of LOQ/2 or 0.71*LOQ → OK for status assessment
- Imputation
  - Estimate the distribution
  - Regression on order statistics

It has to be dealt with!!

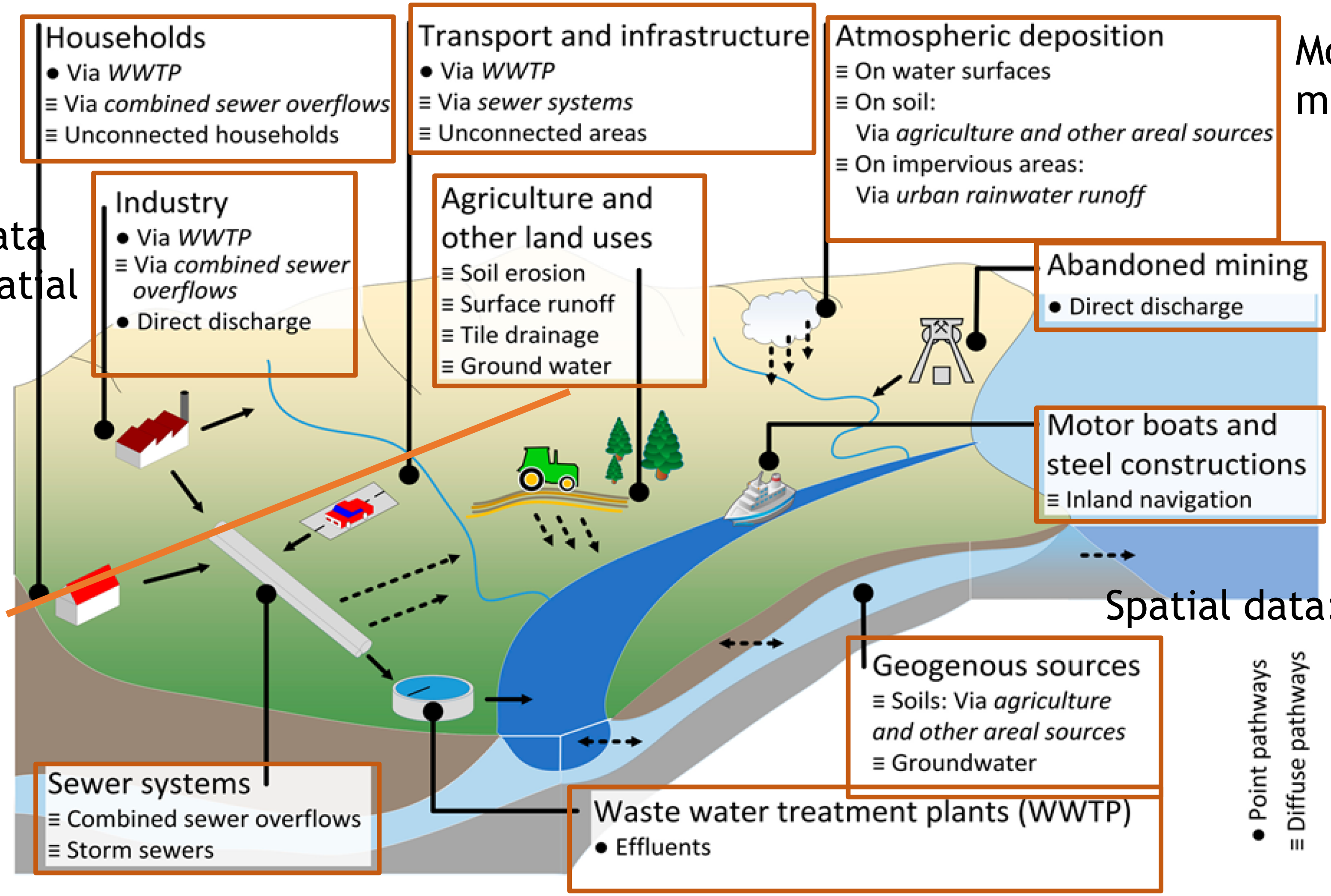




Helsel 2012: Statistics for Censored Environmental Data Using Minitab and R

Emission pathways and related data types

Statistical data linked to spatial units



Statistical data linked to spatial units

Statistical data linked to spatial units

Spatial data:
soil maps
Land use maps
erosion maps
Substance budgets
Water balance maps

Modelled emissions maps

Land use maps
Mining statistical data

Statistical data:
Country scale navigation data

Spatial data: geological maps

Statistical data linked to spatial units

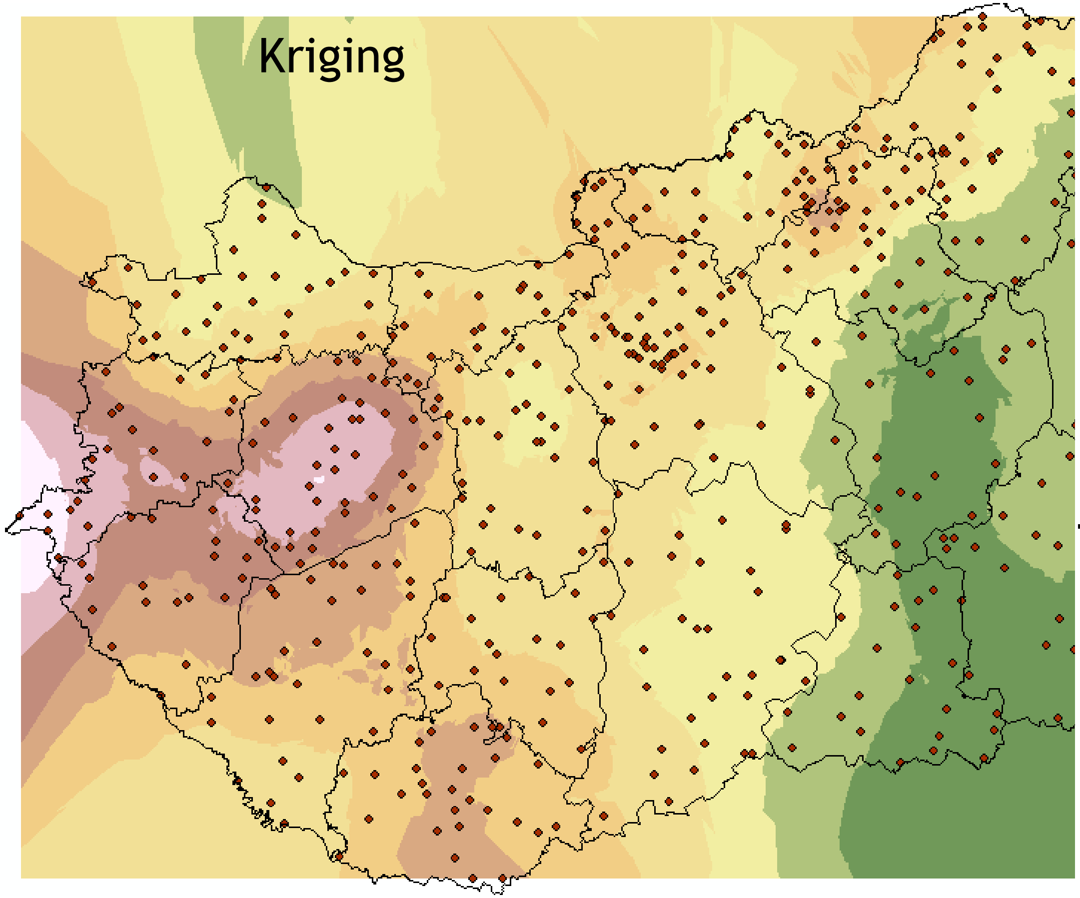
Statistical data linked to spatial units

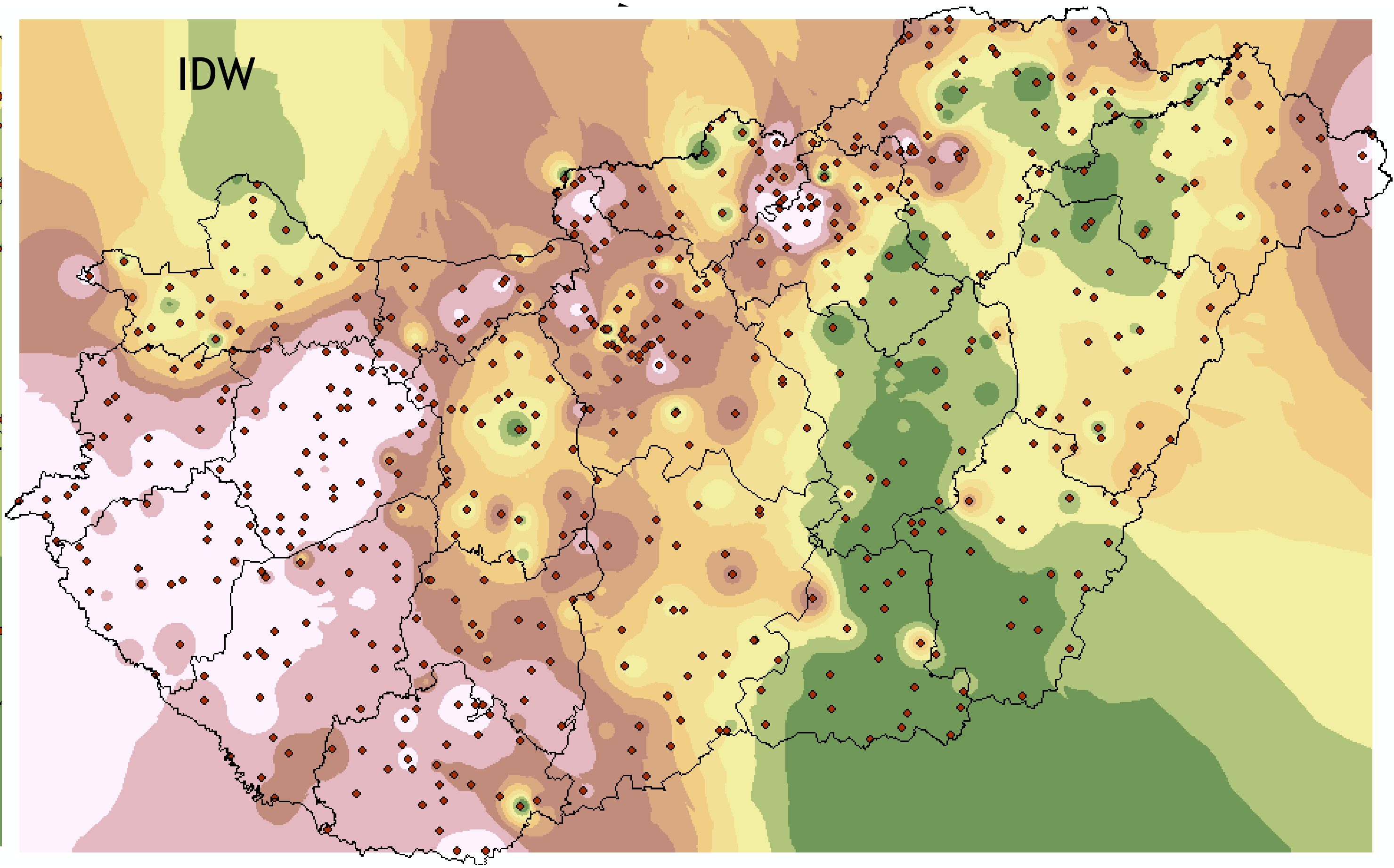
Fuchs et al. (2017) Modeling of Regionalized Emissions (MoRE) into Water Bodies: An Open-Source River Basin Management System. Water, 9(4), 239

Spatial data source type: point data

Source: spatial point data

Data processing: spatial interpolation and zonal/spatial statistics



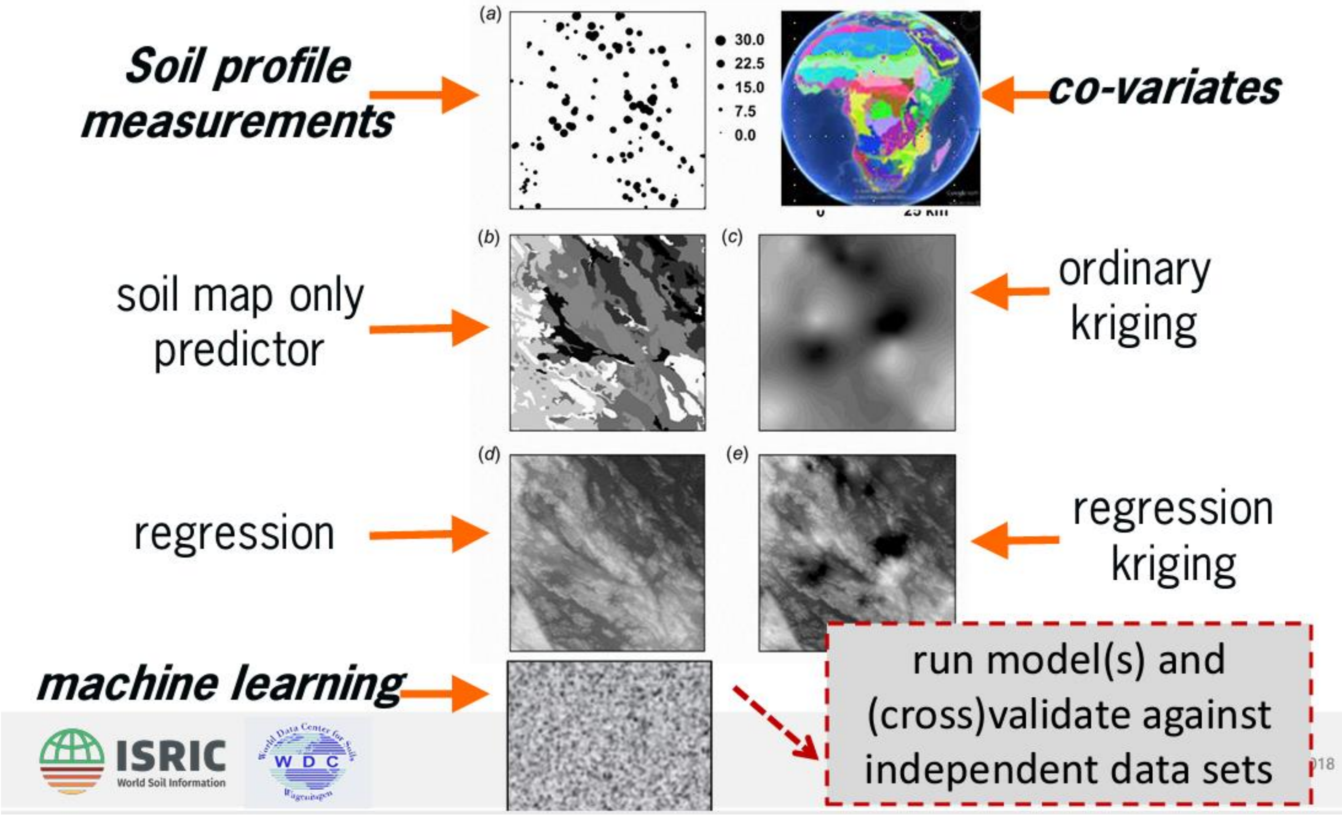


Spatial data source type: Modelled data

1. Input from a deterministic emission model
   - Examples:
     - atmospheric deposition
     - Runoff from hydrological model
     - Soil loss ratio maps (USLE)
2. Input from a stochastical derived dataset
   - Based on point dataset (e.g. soil profiles)
   - Spatial interpolation techniques
   - Machine learning methods

Some techniques are using environmental variables as co-variets (e.g. land use, climate, terrain morphology)

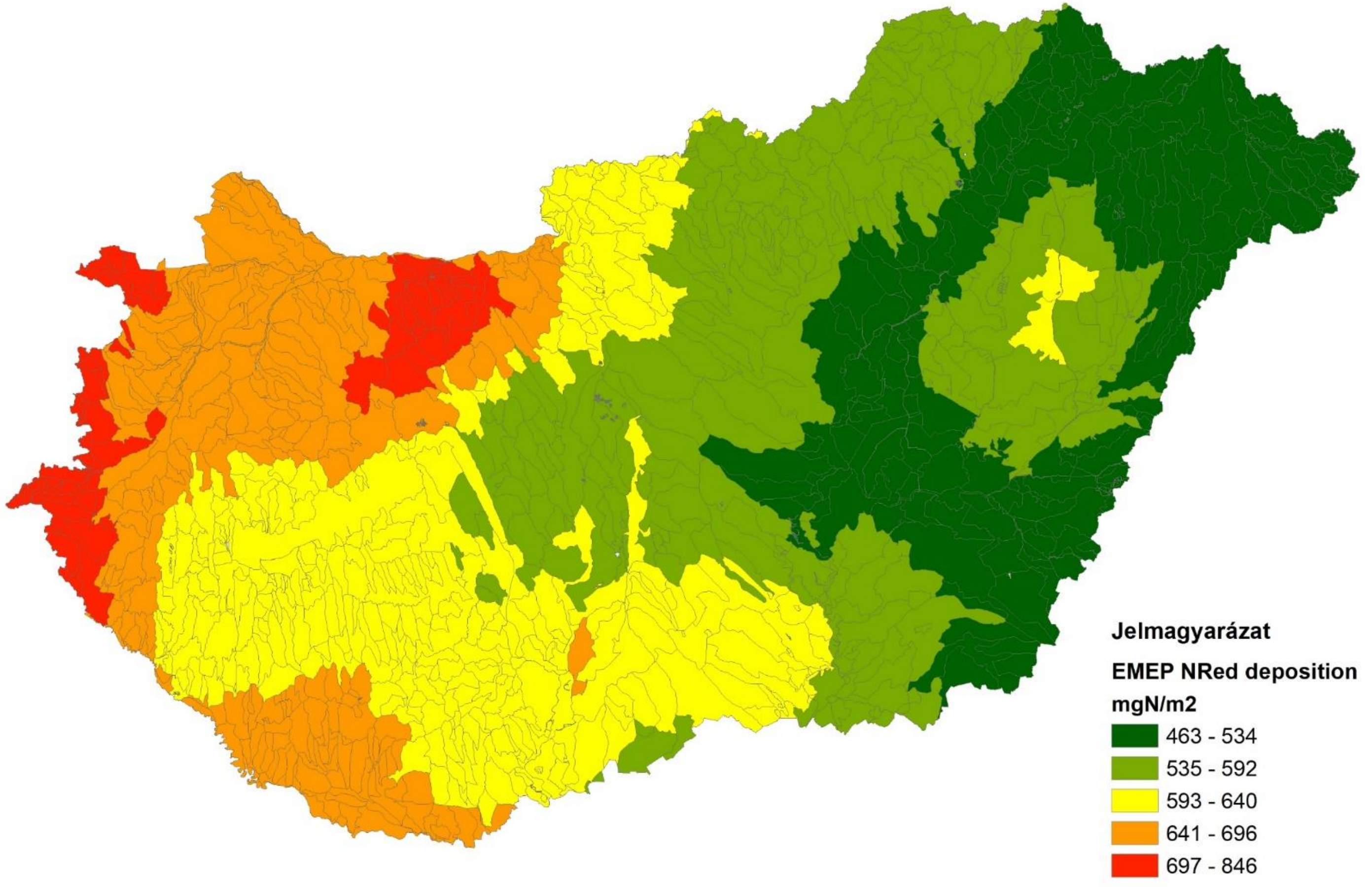
//www.isric.org/sites/default/files/2018_Batjes_Bonares_Conference.pdf



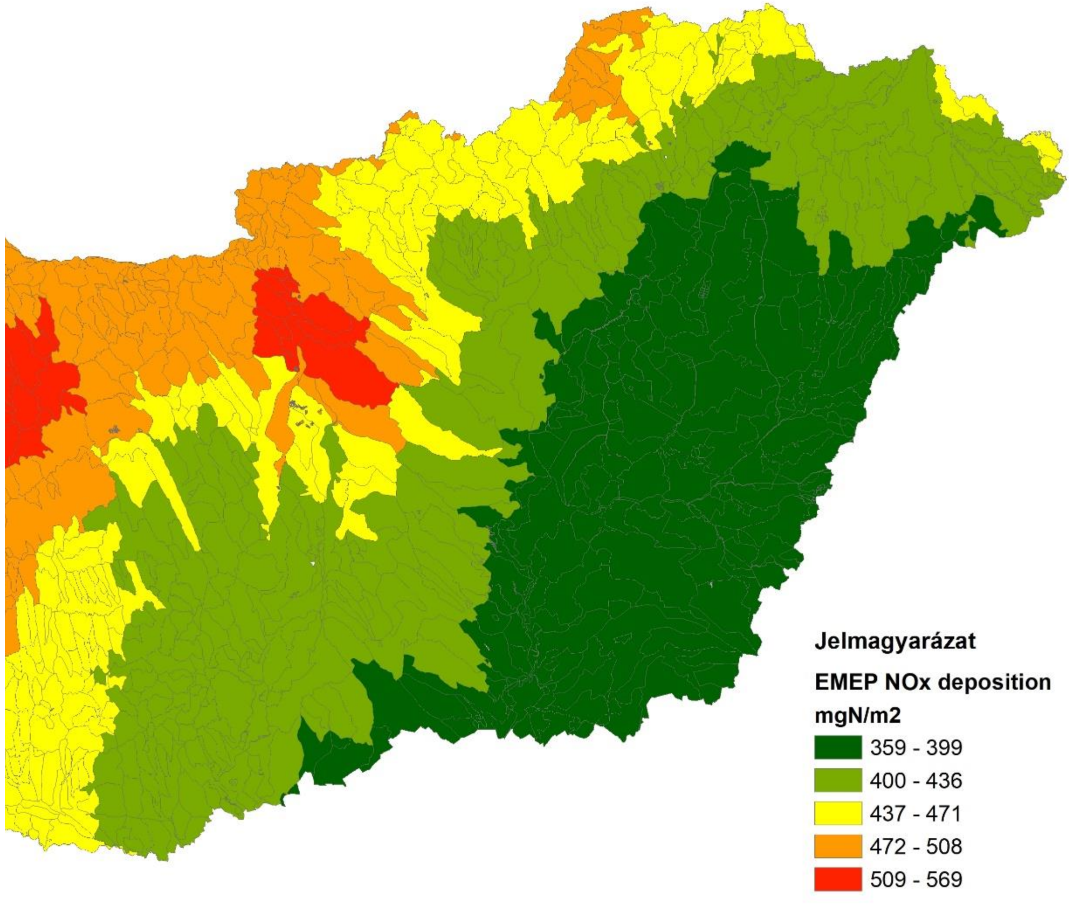
Modelled spatial data

Deterministical derived data
Example: EMEP atmospheric deposition (EMEP: European Monitoring and Evaluation Programme for Long-range Transboundary Air Pollution)

Deposition of reduced nitrogen forms

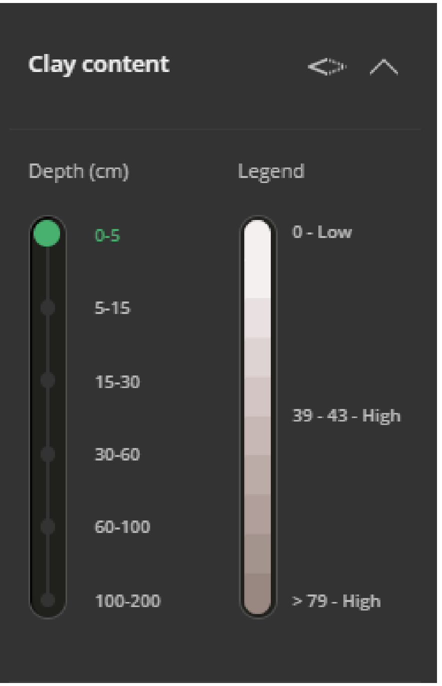


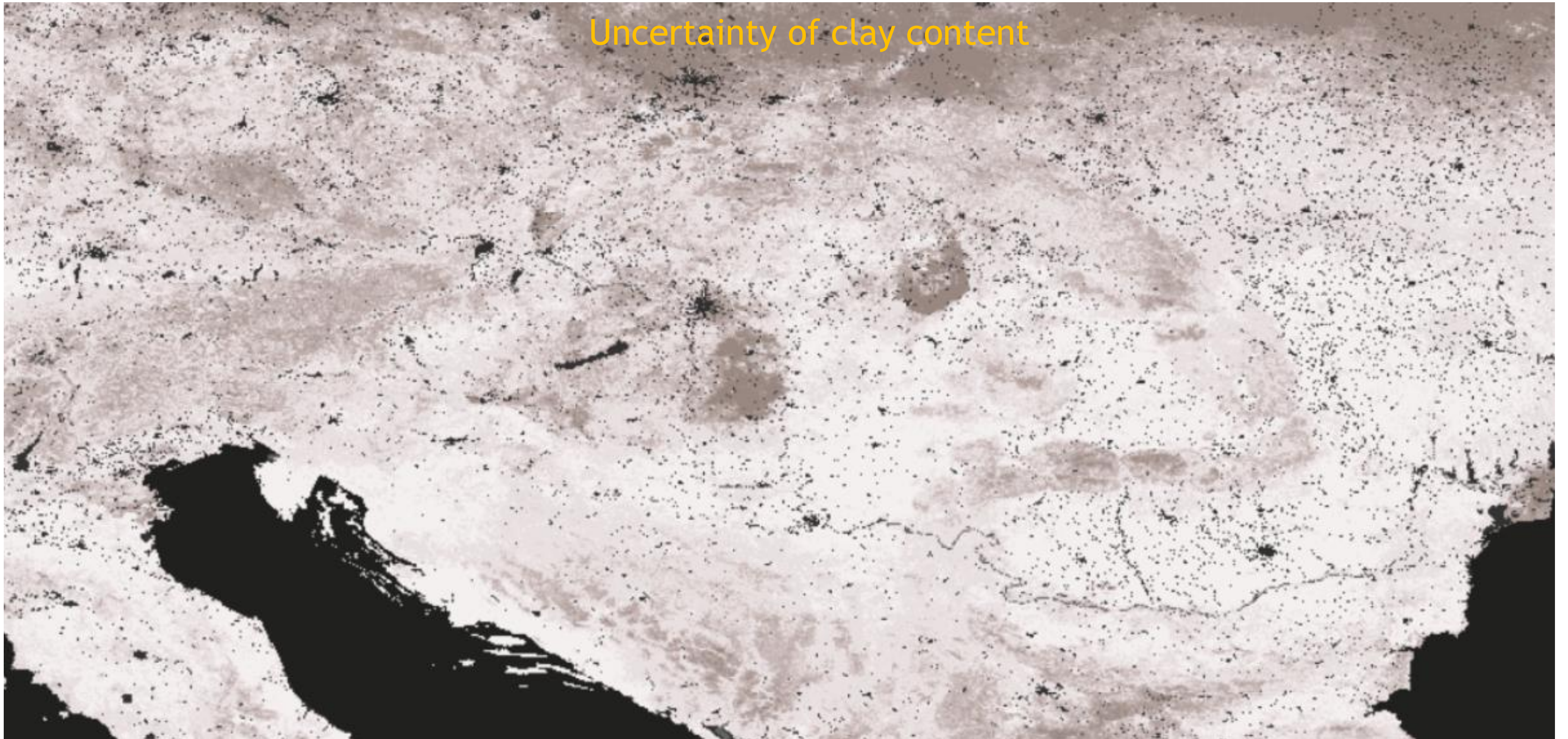
Deposition of oxidized nitrogen forms



Modelled spatial data

Stochastical derived data
Example: Gridded soil datasets
SoilGrids (https://soilgrids.org/)

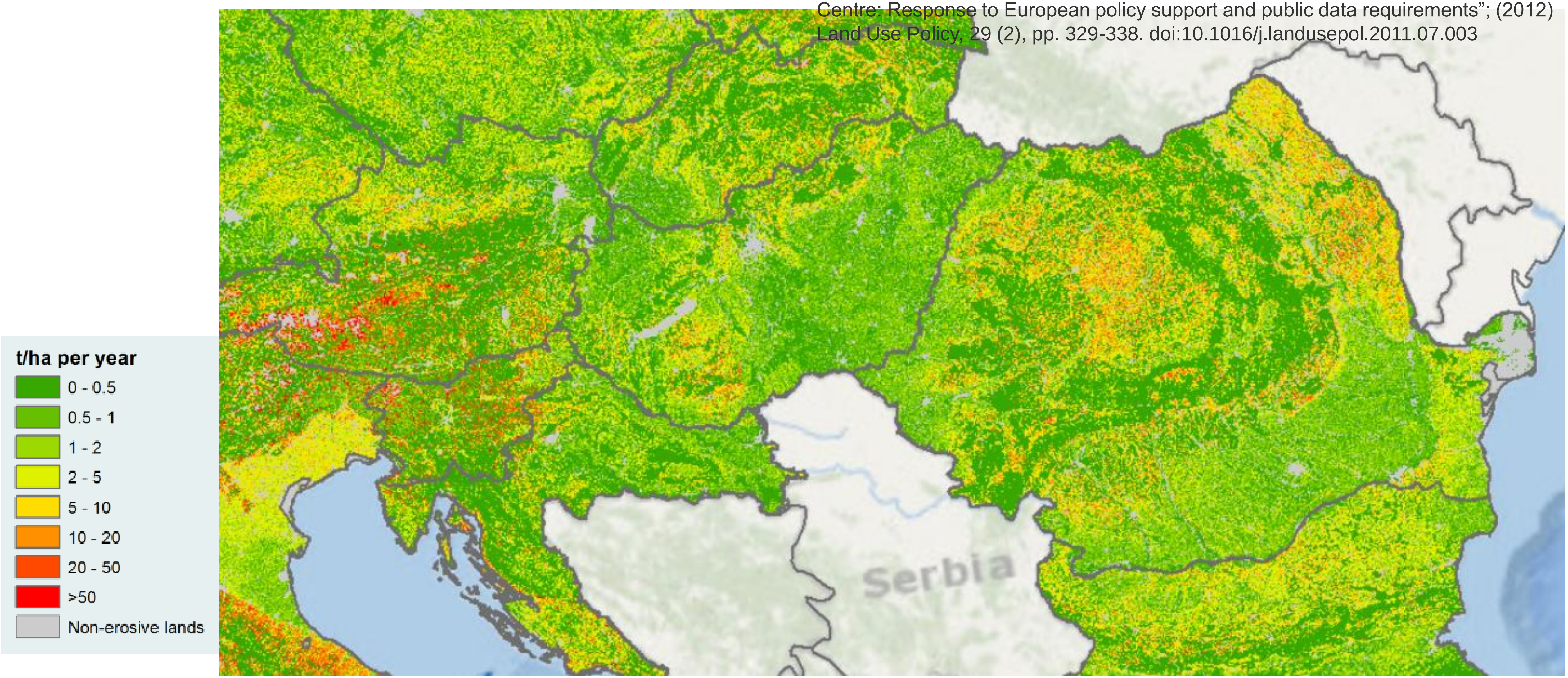




Modelled spatial data – Soil loss

Source: e.g. European scale map from JRC

•Panagos P., Van Liedekerke M., Jones A., Montanarella L., “European Soil Data Centre: Response to European policy support and public data requirements”; (2012) Land Use Policy, 29 (2), pp. 329-338. doi:10.1016/j.landusepol.2011.07.003



Modelled spatial data – Soil loss

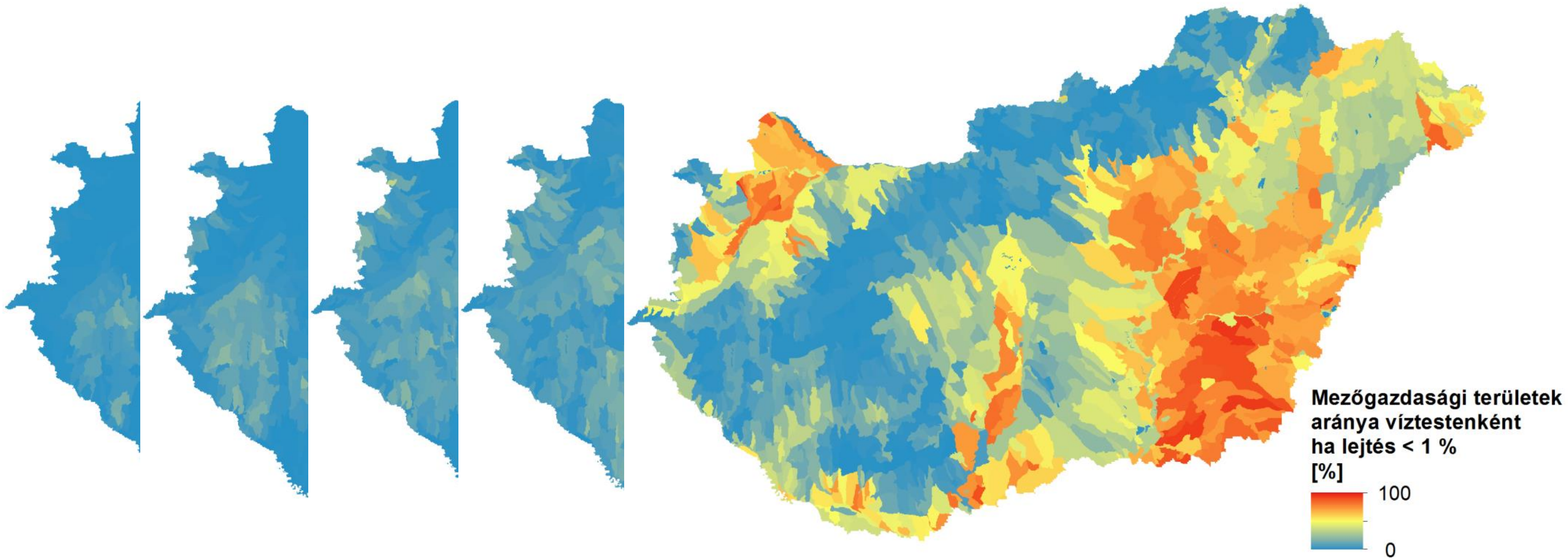
- Soil loss data is general determined by the USLE modell, developed by the USGS (Wischmeyer, 1978)
- SL = R*K*C*S*L*P (R-rainfall, K-soil erodibility, C-vegetation cover, S – slope, L – slope length, P – erosion reduction practices)
- It is a model that was developed to **determine long term average** soil loss on agricultural plots by sheet and rill erosion
- Sources of error: when used for short term calculations it can cause significant errors as the actual erosion is driven by **actual rainfall erosivity** and **runoff**.
- Annual rainfall erosivity (R factor)estimation methods:
  - Annual precipitation
  - Modified Furnier Index
  - Etc

Modelled spatial data – Soil loss

Data preprocessing using GIS methods

e.g. - Spatial aggregation using conditions

- raster calculations
- zonal statistics



Spatial data source type: Spatial budgets

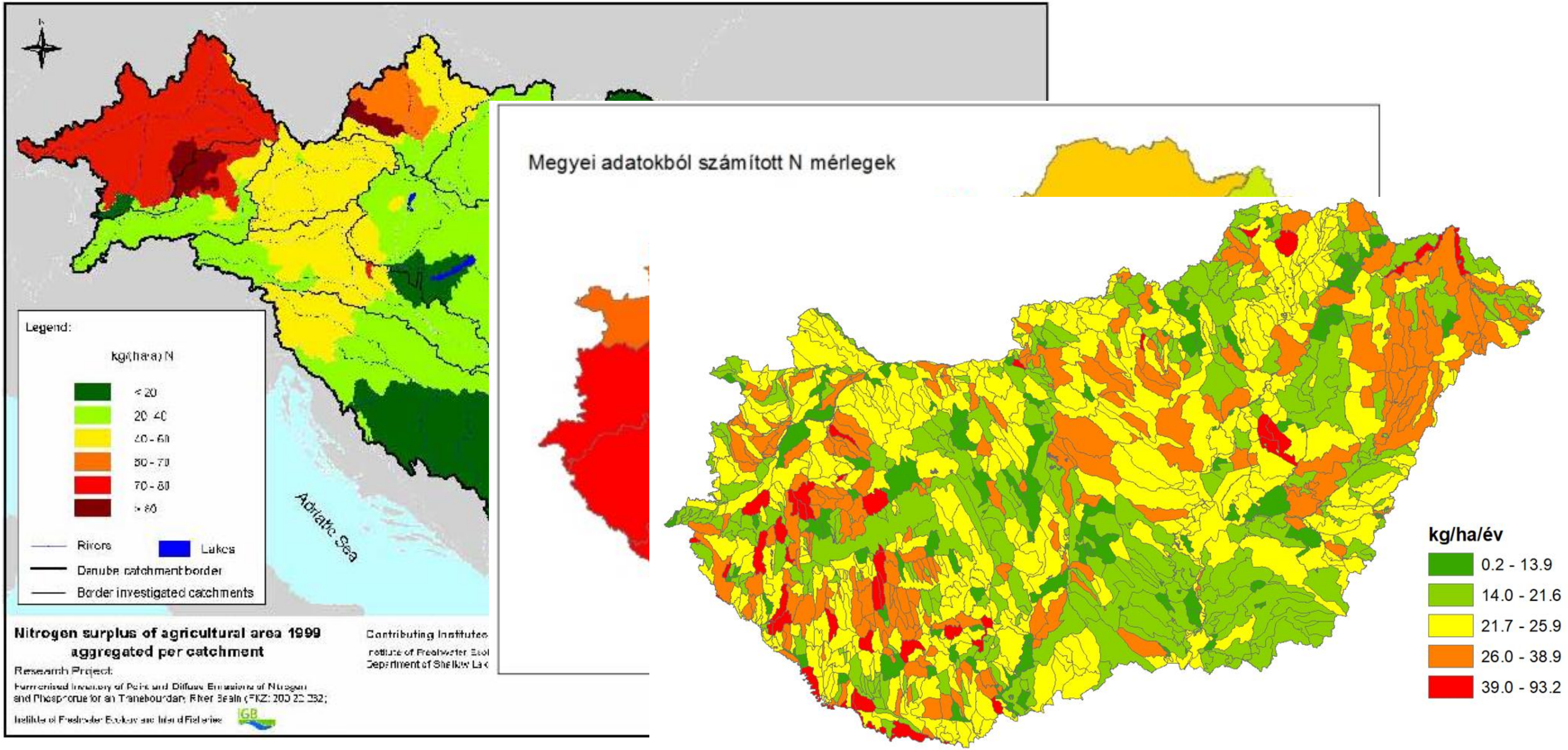
- Stock = Input – Output (year or multi annual scale)
- Primary use in agriculture
- Agronomical and environmental budgets: slight different approach
- Farm gate budgets, soil surface budgets, land budgets etc.
- Most well known environmental budget estimation: OECD Nutrient budget Manual
- Data quality is determined by the spatial resolution of statistical data
  - NUTS1 → NUTS2 → NUTS3 → country scale finer datasets
- Ways to transfer plot scale budgets to larger units
  - Transfer with plant production data
  - Simple zonal statistics

Example:nutrient budgets

	Input			Output			Surplus		
	Farm	Land	Soil	Farm	Land	Soil	Farm	Land	Soil
Animal products (meat, milk, etc.)				x					
Sold crop products				x	x	x			
Fodder[a]					x	x			
Mineral fertilizer	x	x	x						
Feed (concentrates)	x								
External organic nitrogen sources[b]	x	x	x						
Net manure import/export, and withdrawals[c]	x	x							
Manure excretion		x							
Manure application[d]			x						
Crop residues					x	x			
Crop residues returned to/left on the soil		x	x						
Biological N fixation	x	x	x						
Atmospheric deposition	x	x	x						
Soil N-stock changes[e]						x	x	x	
N-gas emissions before manure application[f]							x	x	
Leaching and run-off before manure appl.							x	x	
N-gas emissions from soil[f]							x	x	x
Leaching and run-off from soils							x	x	x

Source: OECD manual, 2013

Input data: nitrogen surplus scales and resolution



Spatial data source type: application rates

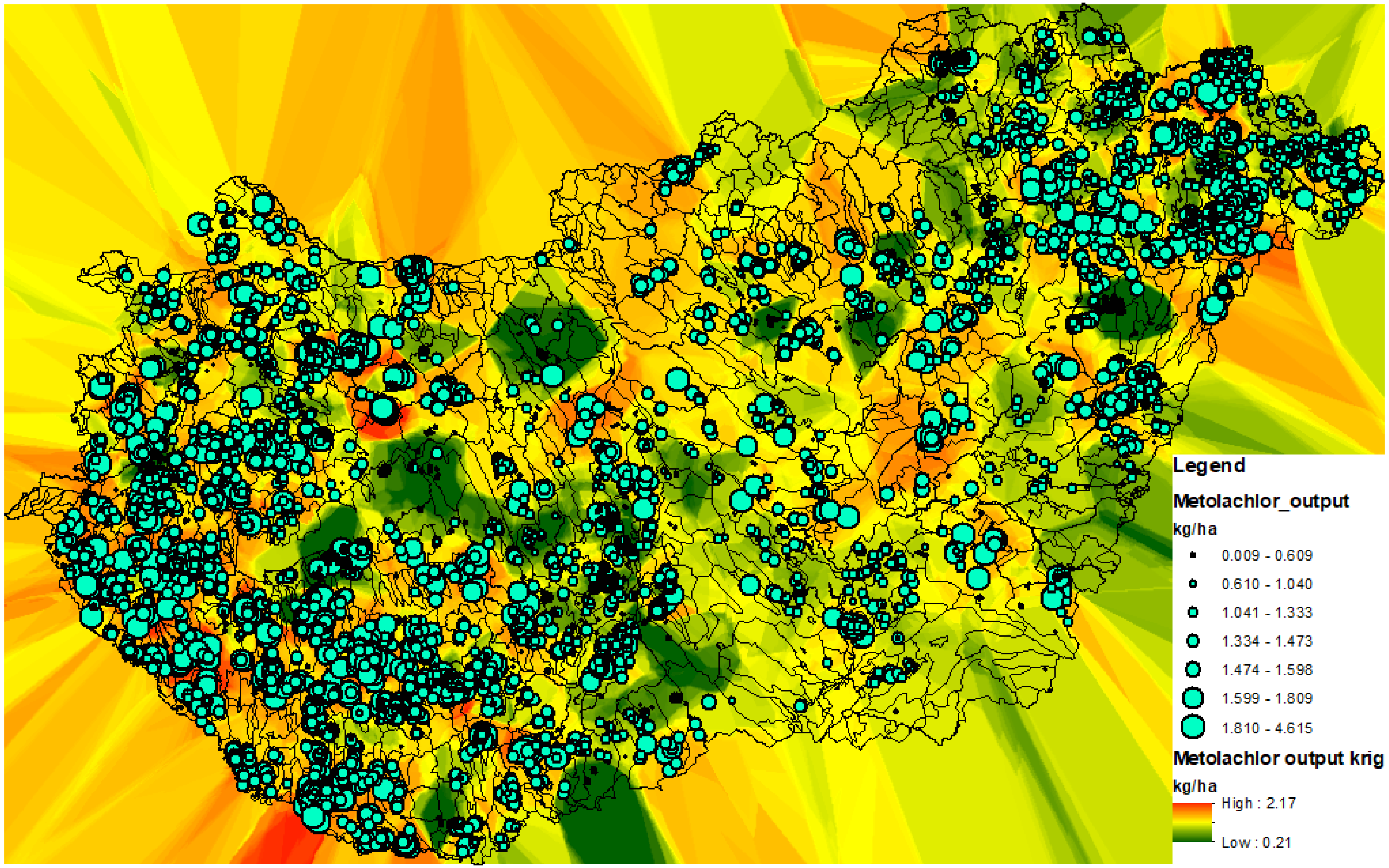
Peszticide use data

→ direct use to create map

→ Link information to plant

Production data

→create emission factor



Urban emissions

- Statistical data:
  - population, connected to sewer systems
  - sewer system data: CSO volumes, Storm sewers, sedimentation tanks
  - Water consumption
  - Share of impervious area
- Land use data
  - Impervious area
  - Road surfaces
- Calculated data
  - Runoff rate of waste water (l/s/ha)

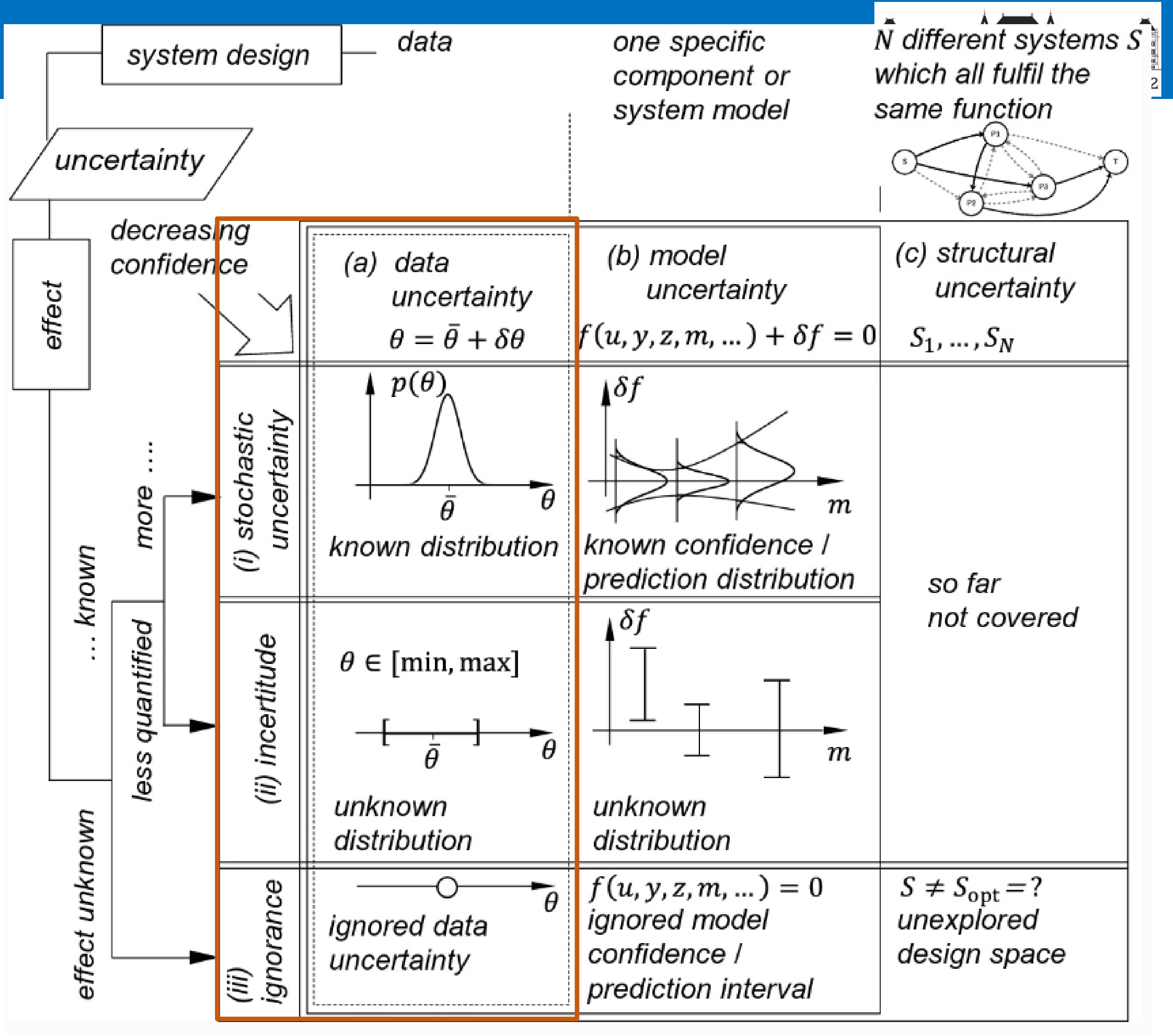
Data uncertainty

State variables

- Precpitation
- Temperature
- Land cover
- Population

Model parameters

- Parameters to estimate sediment delivery ratio
- Emission factor for metal emissions from soils



Source: Pelz et al, 2021 (https://doi.org/10.1007/978-3-030-78354-9_2)

Data uncertainty

Aleatoric uncertainty
- natural variability of the variable
- Irreducable or random data noise

Epistemic uncertainty
Reducable uncertainty
- Caused by ignorance, knowledge gaps or insufficient data
- E.g. measurment error of satellite data
- Estimation errors due to wrong approaches during data processing

Stochastic approach:
Random variable and it's distribution can be assumed
- Parametric
- Non-parametric

Incertitude:
Propability is unknown
Fuzzy set theory can be applied

Source: Pelz et al, 2021 (https://doi.org/10.1007/978-3-030-78354-9_2)

Input data – time variant data

name	description	unit	parameter
Climate Data			
Evapotranspiration	yearly values	mm	evapotranspiratior
Precipitation	monthly values	mm	precipitation

Input data – population, canalization & point sources

name	description	unit	parameter
Statistical Data about inhabitants and waste water system			
number of inhabitants	Resolution, in time and space?	inh	number of inhabita
US_ss_VOL_SST	storage volume of stormwater sedimentation tanks in separate sewer systems	m^3	storage volume
US_cso_VOL_SOT	storage volume of stormwater overflow tanks in combined sewer systems	m^3	storage volume
US_cso_VOL_spec_SOT	storage volume of stormwater overflow tanks in combined sewer systems, area-specific	m^3/ha	storage volume, sp
US_L_CS	length of combined sewers	km	length
US_L_SS	length of stormwater sewers	km	length
US_L_WWS	length of sewage sewers	km	length
US_SHR_inh_con_tot	percentage of inhabitants that are connected to sewer systems	%	percentage
US_SHR_inh_conWWTP_tot	percentage of inhabitants that are connected to sewer systems and waste water treatment plants	%	percentage
US_SHR_inh_nss_tot	percentage of inhabitants that are not connected to sewer systems	%	percentage
US_INHC_H2O	inhabitant specific water consumption	l/(inh·d)	water consumptior
US_nss_SHR_inhl_towwtp_sept	percentage of inhabitant load that is transported from septic tanks to waste water treatment plants	%	percentage
US_Q_spec_COM	runoff rate for comercial waste water	l/(ha·s)	runoff rate
Point source data			
WWTP_ps_INH_conWWTP	number of inhabitants that are connected to sewer systems and waste water treatment plants (point sources)	inh	
WWTP_ps_CP	capacity of the waste water treatment plant (point sources)	PT	
WWTP_ps_PE	nominal load of waste water treatment plant (point sources)	PT	
WWTP_ps_TS	current treatment type of waste water treatment plant (point sources)	-	
WWTP_ps_Q	runoff via waste water treatment plant (point sources)	m^3/a	

Input data – spatial:
landuse; topography; tile drained areas; soil loss

name	description	unit	parameter
Topography			
Digital Elevation model	Which Resolution is available?	m	elevation
Landuse			
Landuse data set	Which categories are included? MoRE uses currently the following aggregated categories:	km²	area
	arable land		
	pastures		
	water surface		
	naturally covered areas (including woods)		
	open areas (alpine, beaches, dunes)		
	surface mining areas		
	settlements		
	wetlands		
	others		
Tile drained areas	from arable land and pastures	km²	area
Impervious areas	Resolution?		
Climate Data			
Evapotranspiration	yearly values	mm	evapotranspiratior
Precipitation	monthly values	mm	precipitation
Hydrology			
Net runoff from catchments	if available, otherwise to be calculated from climate parameters and runoff at gauging stations		
Soil loss	potential soil loss from arable land	t/(ha·a)	soil loss, specific
	potential soil loss from pastures	t/(ha·a)	soil loss, specific
	if data about soil loss isn't available, more data about agricultural practices (cultures, measures against soil loss …) is needed to calculate soil loss with the USLE		

Computational units

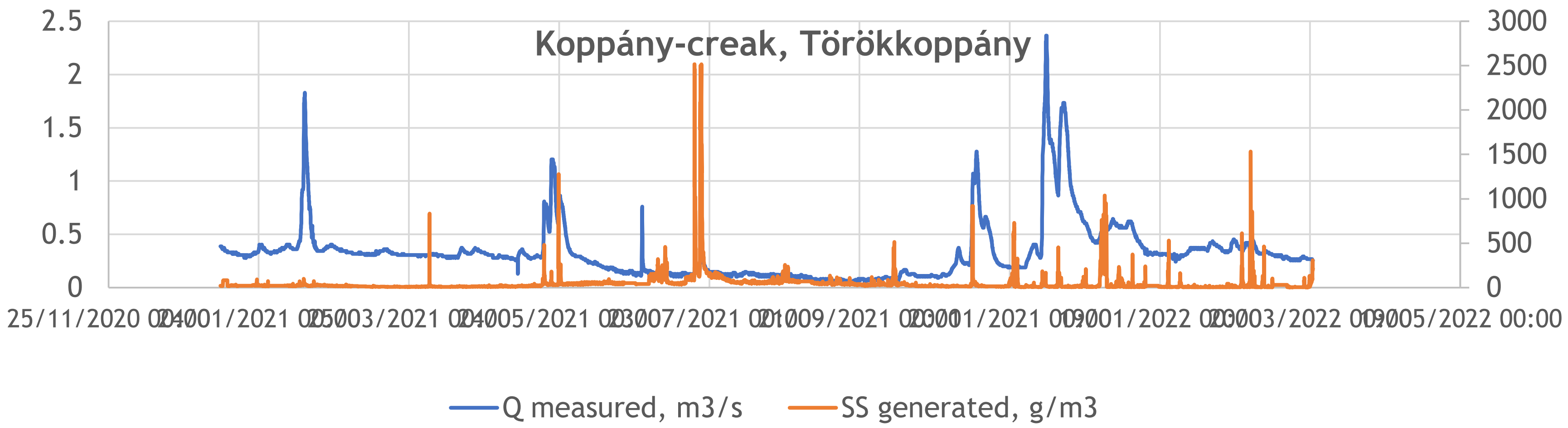
MoRE: “anatical units” (AUs and Sub Aus)

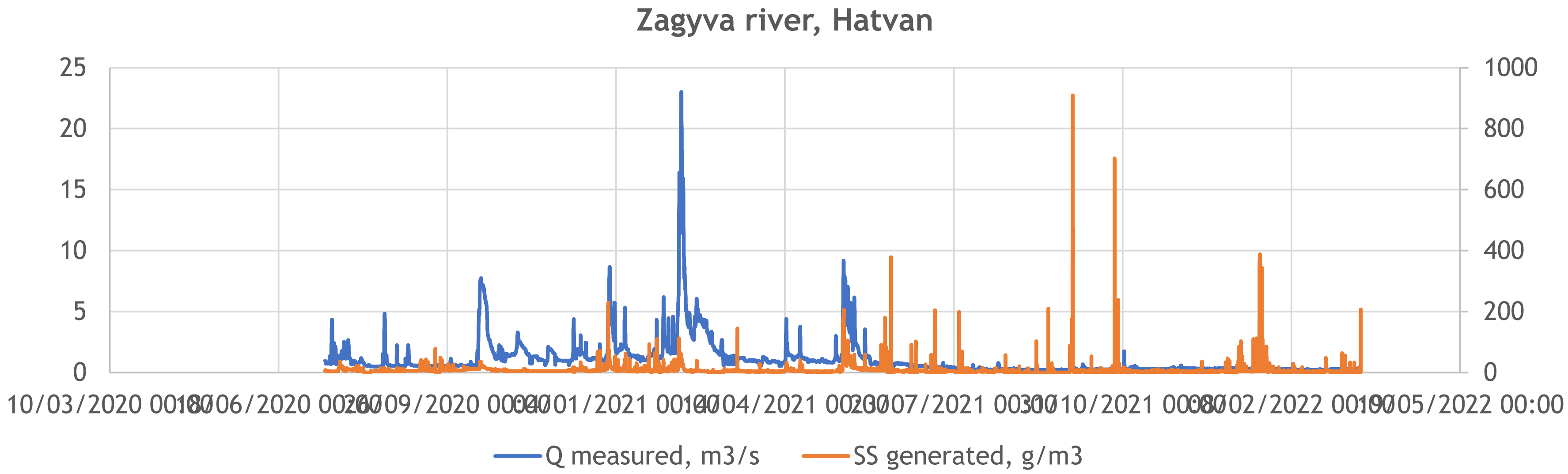
SOLUTIONS: “schematization elements”

Data needs:

- high resolution digital elevation model
- hydrographic network
- quality monitoring stations
- discharge monitoring station

Calculation of SS and pollutant loads based on stratified river sampling

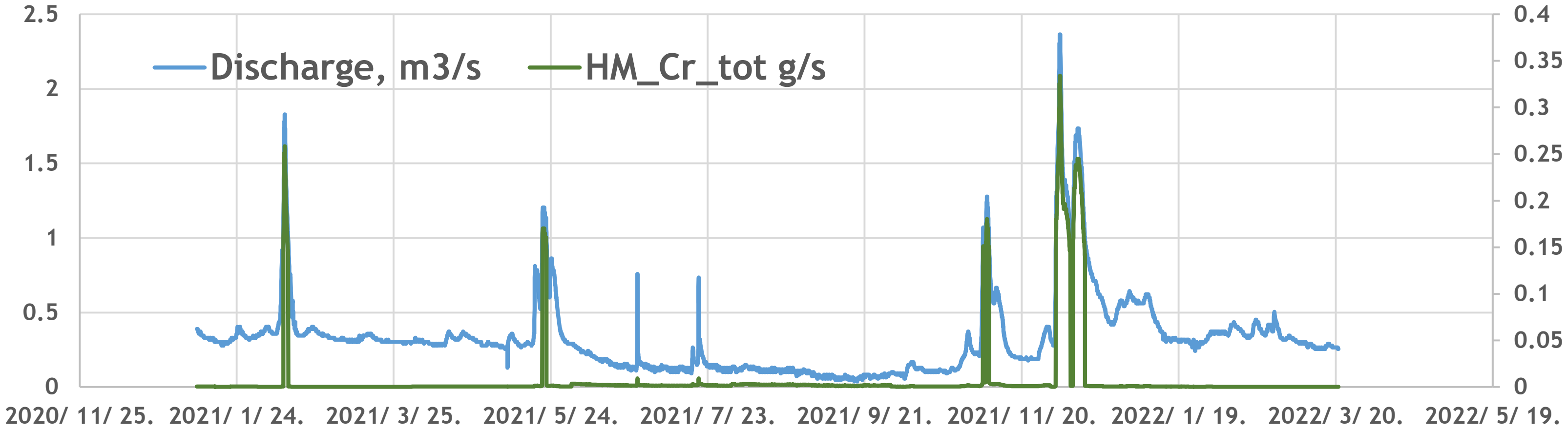


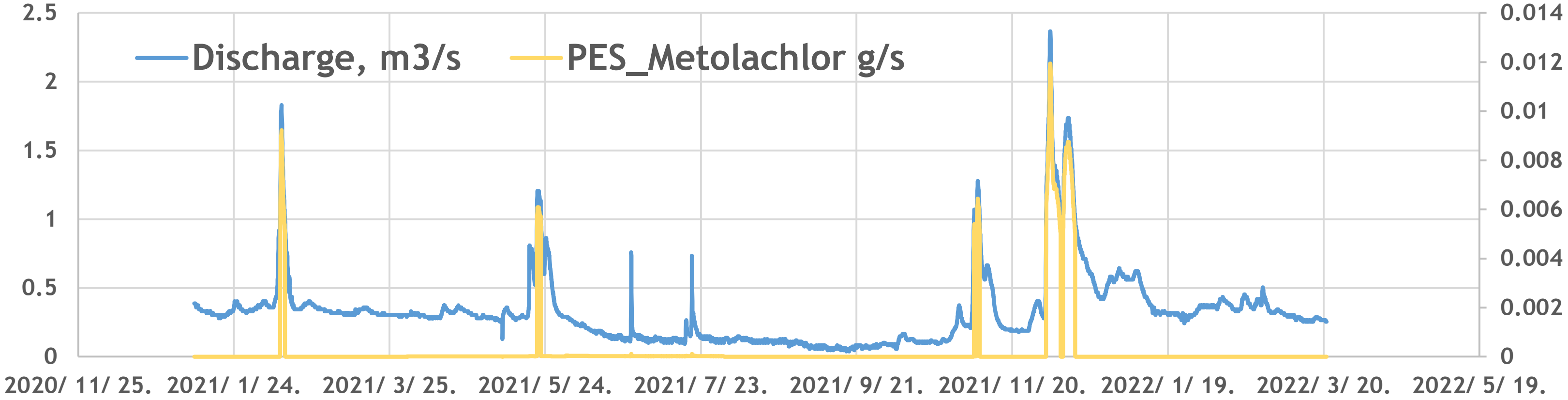


Data evaluation: calculation of SS and pollutant loads based on the stratified river sampling

If $Q < Q_{10\%}$ $L_{lowflow} = \Sigma\ (Qi * C\_composite)$

If $Q > Q_{10\%}$ $L_{highflow} = \Sigma\ (Qi * C\_flow\ event's\ average)$

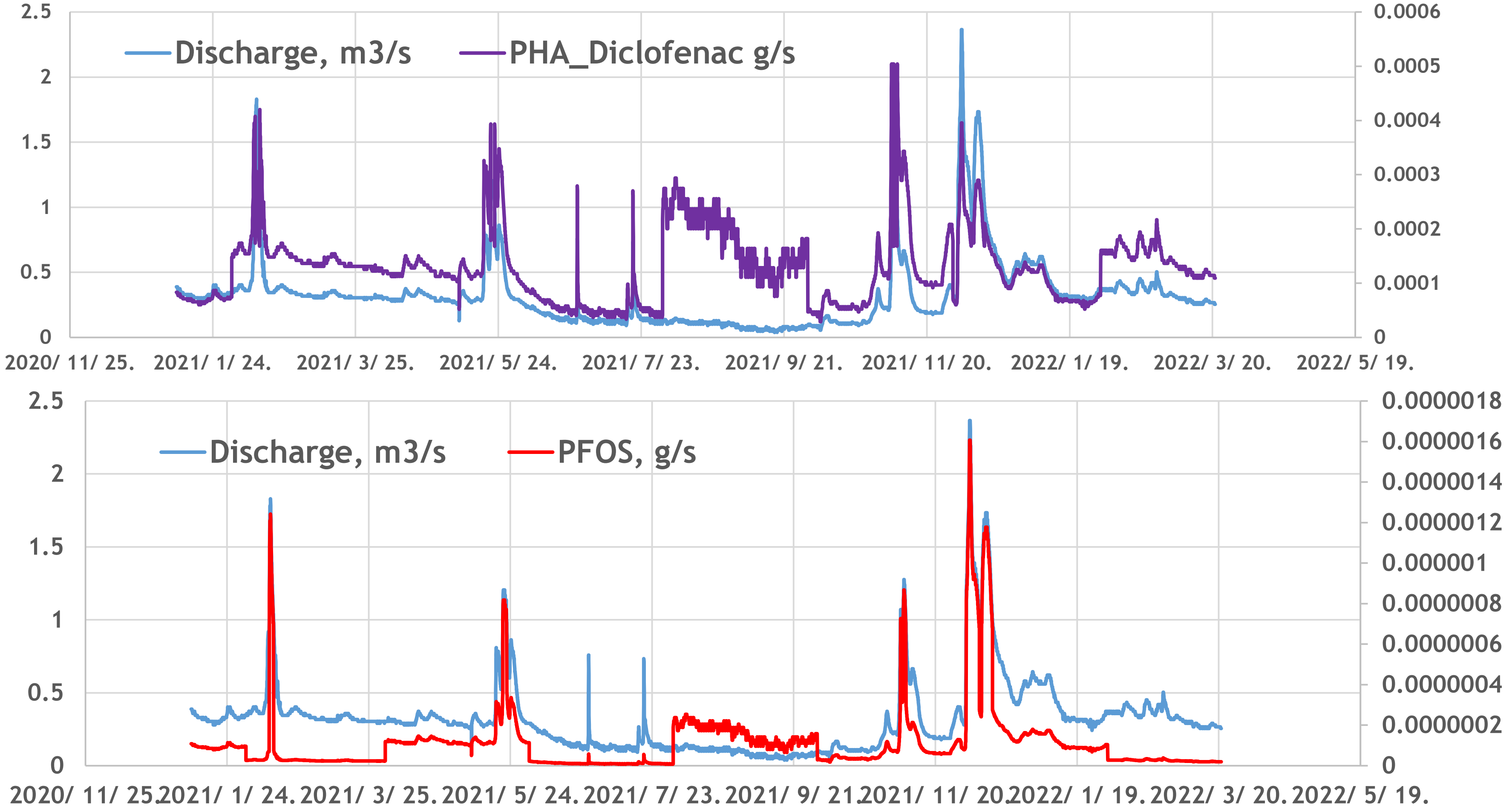




Data evaluation: calculation of SS and pollutant loads based on the applied river sampling

If $Q < Q_{10\%}$ $L_{lowflow} = \Sigma$ (Qi * C_composite)

If $Q > Q_{10\%}$ $L_{highflow} = \Sigma$ (Qi * C_flow event's average)



Danube Hazard m³c

Training on hazardous substances emission modelling and scenario evaluation

Development and implementation of programmes of measures for scenario analysis

Vienna, 05.10.2022

Project co-funded by European Union funds (ERDF, IPA, ENI) and National Funds of the participating countries

Content

- The use of the MoRE model to support assessments in the WFD management cycle and the emission inventory.
- Results from a former project are presented to address and visualize this opportunities.
- The workflow within the model application is expressed.
- The calculation of scenarios in the MoRE model is addressed.

Emission inventory-legal requirements

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According to the Article 5 of the Directive 2008/105/EC (EQS Directive), Member States shall establish an inventory, including maps, if available, of emissions, discharges and losses of all priority substances for each river basin district or part of a river basin district lying within their territory including their concentrations in sediment and biota, as appropriate.

Main objectives of the inventorying:

- Inform on the relevance of priority substances at spatial scale in the RBD
- Enable compliance check with WFD regarding the reduction of discharges, emissions and losses

Guidance document on Emission inventories

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TIER	BUILDING BLOCKS	EXPECTED OUTPUT	RESULTS FOR THE INVENTORY
STEP 1: ASSESSMENT OF RELEVANCE			
	Information sources identified in Art. 5 of EQS directive, see section I.1	Decision of relevance	List of relevant and less relevant substances
STEP 2: APPROACHES FOR RELEVANT SUBSTANCES			
1. Point source information	• Data on point sources • Emissions factors	• Availability of data • Quality of data • Identification of gaps	• Point source emissions • Listing of identified data gaps
2. Riverine load approach	add: • River concentration • Data on discharge • In stream processes	• Riverine load • Trend information • Proportion of diffuse and point sources • Identification of gaps	• Rough estimation of total lumped diffuse emissions • Verification data for pathway and source orientated approaches • Listing of identified data gaps
3. Pathway orientated approach	Need for emission models		
4. Source orientated approach			

Step 1

Step 2

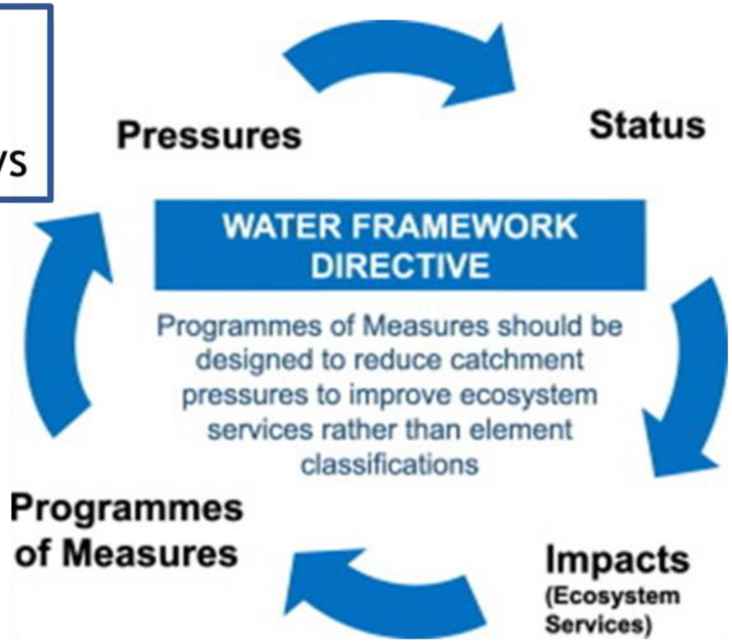
Tier approaches in Step 2

Technical Report - 2012 – 058 Common Implementation Strategy for the Water Framework Directive (2000/60/EC) *Guidance Document No. 28 Technical Guidance on the Preparation of an Inventory of Emissions, Discharges and Losses of Priority and Priority Hazardous Substances*

Use of MoRE in the management cycle

Quantification of significant pressures from different pathways

Completion of more fragmented picture of monitorig



(T. Giakoumis and N. Voulvoulis, 2019)

Gain knowledge:
relevance of pathways
relevance of sources
potential reduction of Measures (by scenarios)

Possible risk analyses on scale of modeled Analytical Units

Use of MoRE in the management cycle

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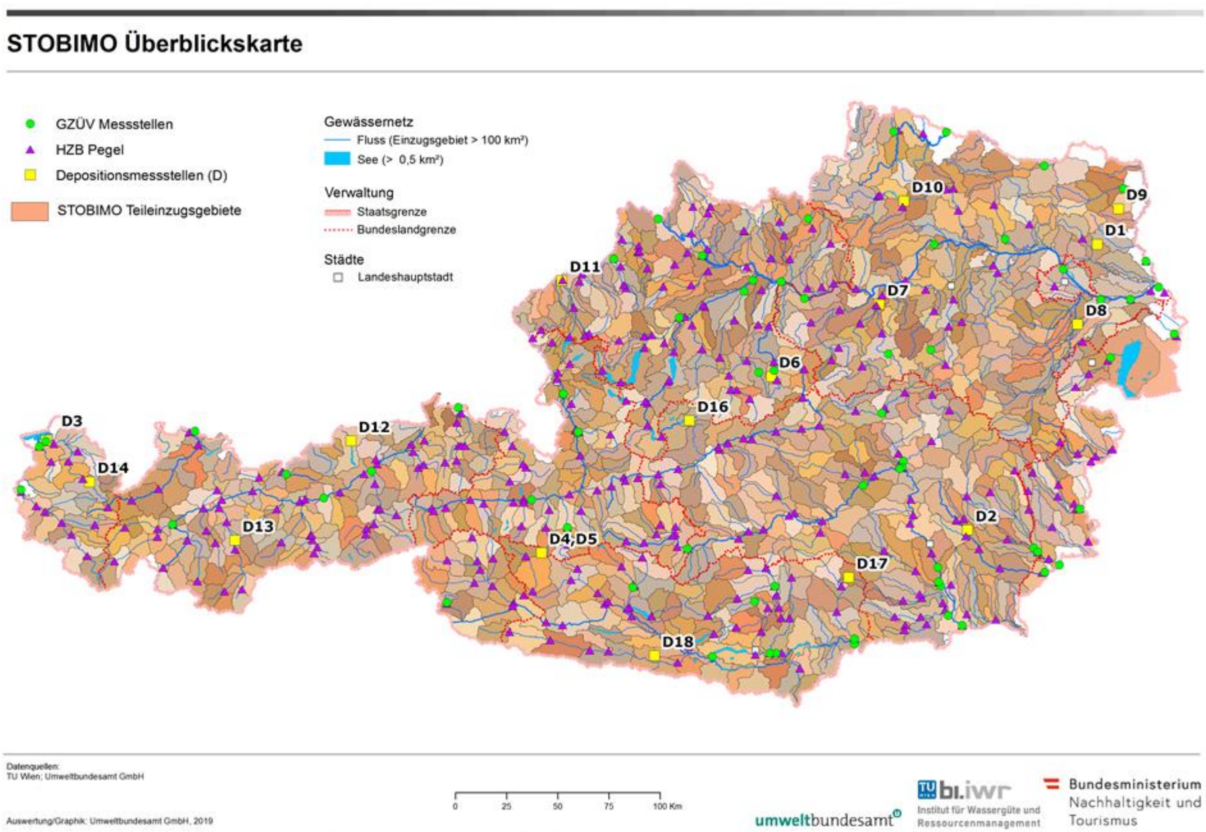
- In a project “STOBIMO SPURENSTOFFE” (2016-2019) in Austria emission modelling was applied in 754 sub-catchments



Use of MoRE in the management cycle

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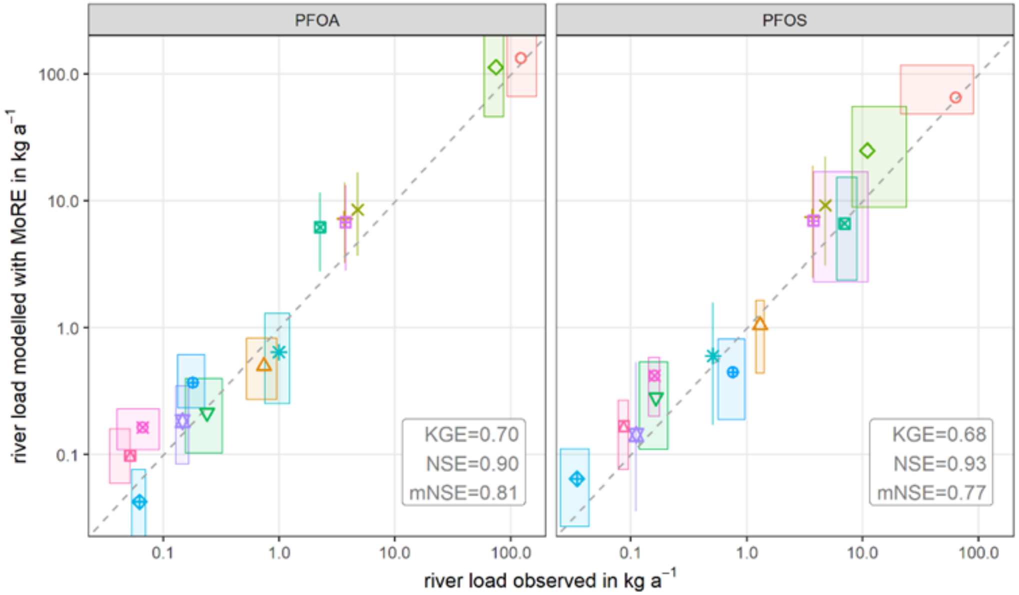
- After improving database by an intense monitoring of different technical and physical compartments MoRE was setup and validated
- A mean, maximum and minimum variant was calculated to address uncertainties
- For several substances validation was successful
- For some substances input data quality and quantification approaches were not sufficient and validation results did not justify performing a further assessment



Quantification of in stream-concentrations

Transport, degradation and retention

- No consideration of degradation processes in the river as all modelled substances are considered more or less persistent
- For PFAS no retention considered, as transport is mainly dissolved
- For strongly particle binding substances (heavy metals, PAHs) retention processes considered as in MONERIS for Phosphorus:
  - For tributaries mean retention factor calculated as mean from specific discharge approach (discharge/surface water area) and hydraulic load approach (discharge/catchment area)
  - For main rivers only the hydraulic load approach is used
- MoRE does not consider travel times

Quantification of in stream-concentrations

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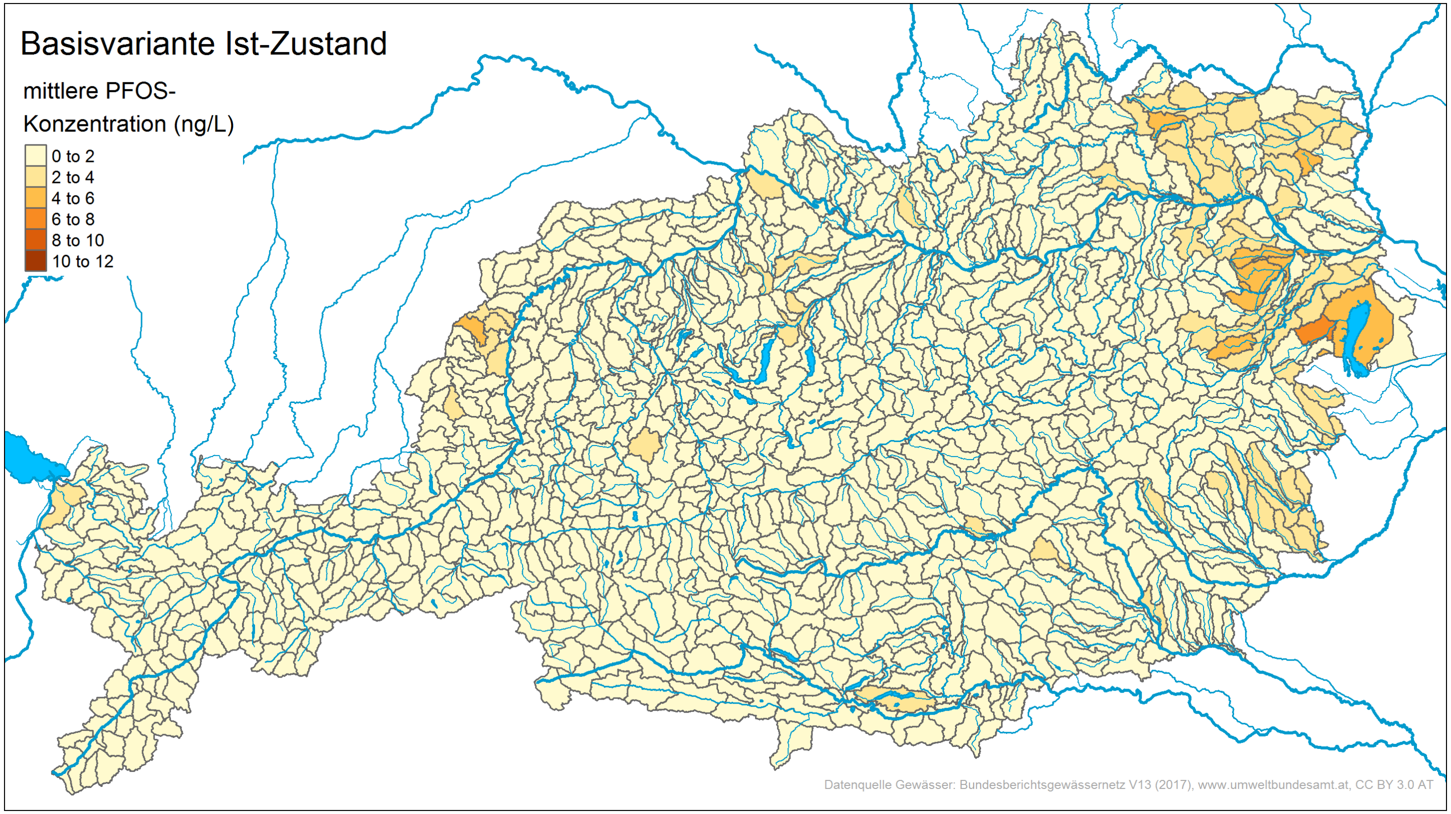
Mean modelling variant



Quantification of in stream-concentrations

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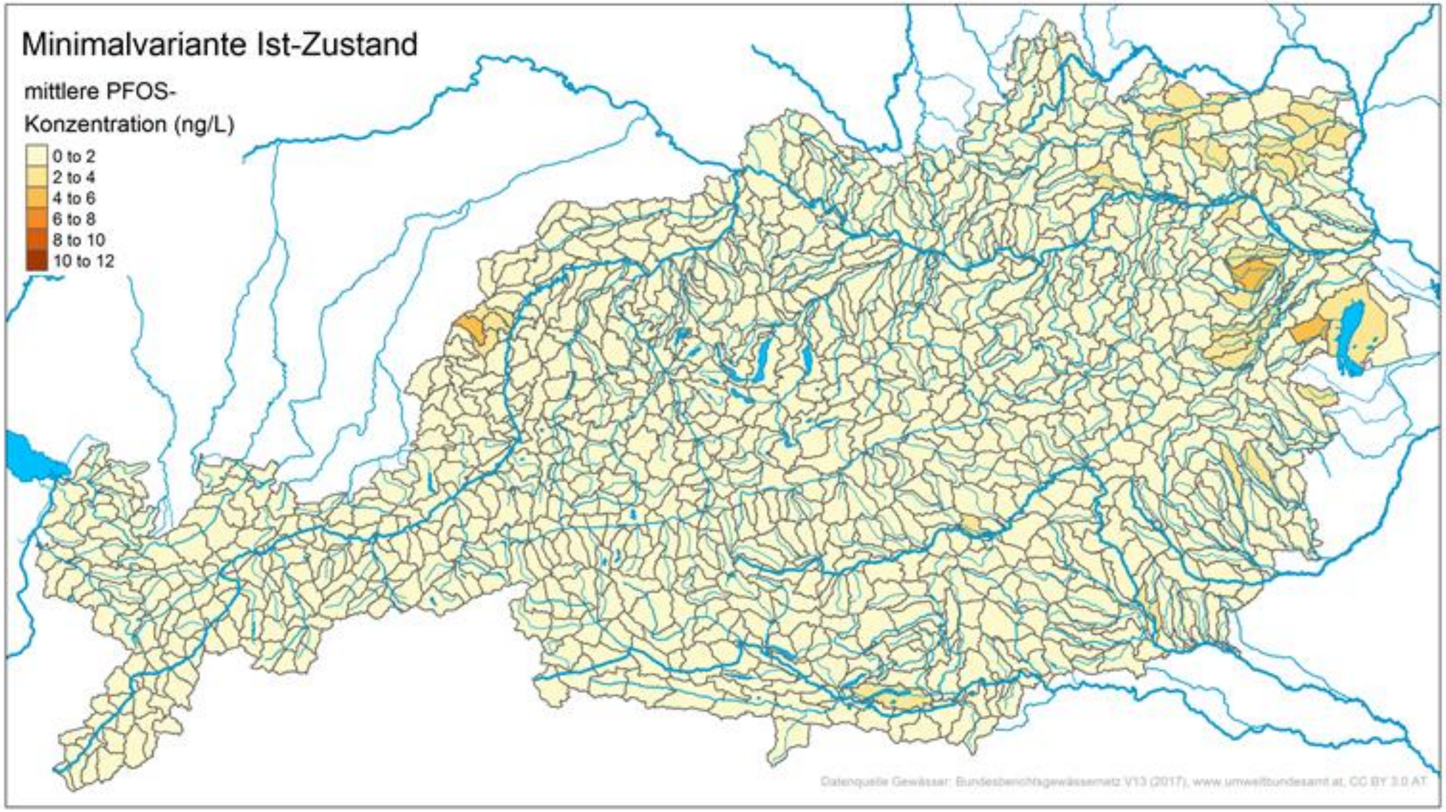
Minimum modelling variant



Quantification of in stream-concentrations

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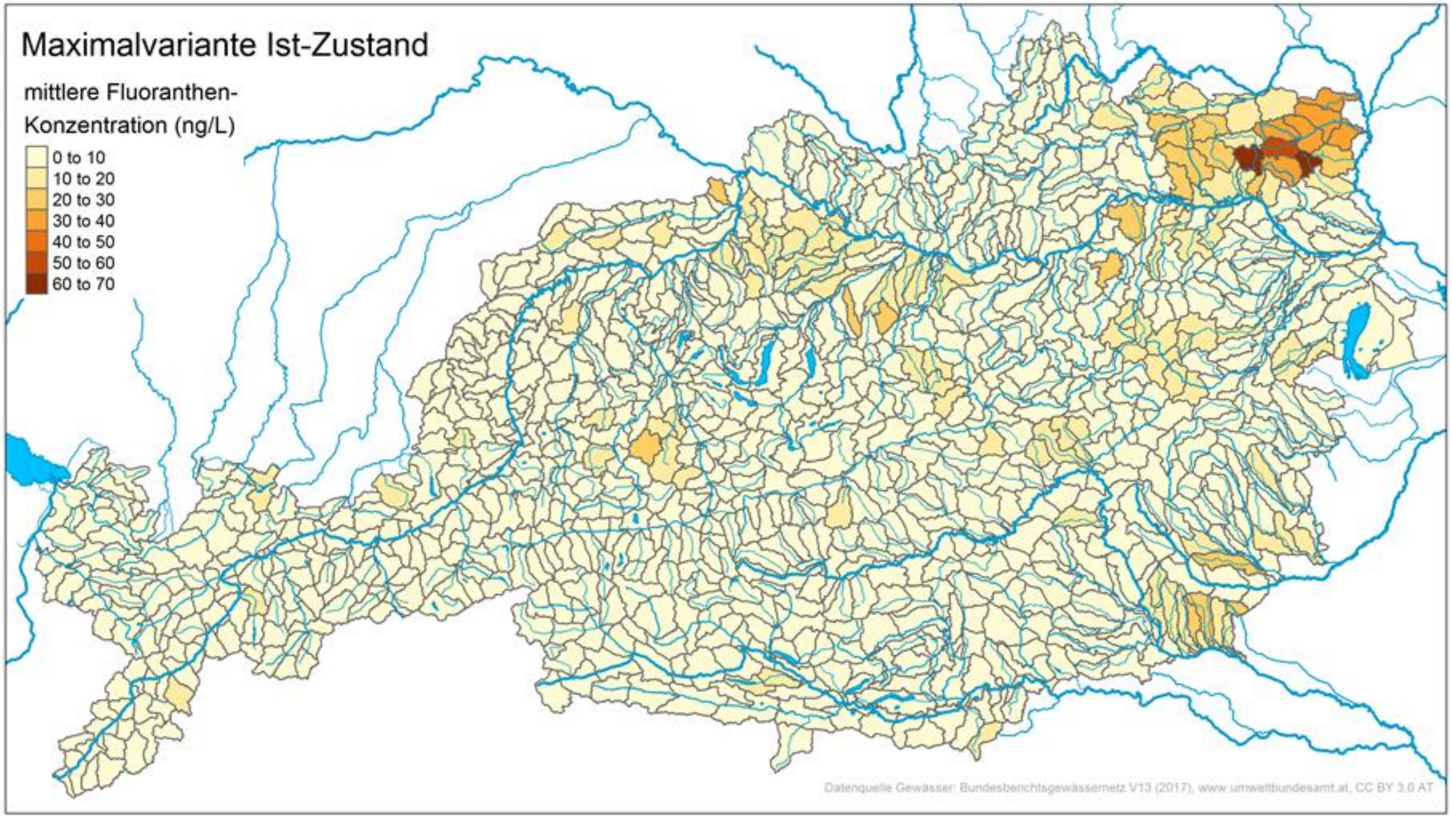
Maximum modelling variant



Risk Analyses

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- Calculation of a risk quotient ($RQ = c_{River,calculated} / EQS$) for 754 outlets from sub-catchments
- Calculation from Minimum-, Base (Mean) and Maximum variant.

Parameters	Number (absolut / relativ) of EQS overshootings (RQ>1)		
	Minimum	Base	Maximum
Lead	0 / 0%	0 / 0%	0 / 0%
Dibutyltin compounds	0 / 0%	0 / 0%	0 / 0%
Naphthaline	0 / 0%	0 / 0%	0 / 0%
Cadmium	1 / 0,13%	2 / 0,27%	2 / 0,27%
Nickel	0 / 0%	0 / 0%	58 / 7,7%
Zinc	1 / 0,13%	1 / 0,13%	117 / 16%
Trybutyltin compounds	1 / 0,13%	25 / 3,3%	190 / 25%
Copper	104 / 14%	215 / 29%	301 / 40%
Fluoranthene	133 / 18%	200 / 27%	375 / 50%
PFOS	168 / 22%	754 / 100%	754 100%
Benzo(a)pyren	741 / 98%	754 / 100%	754 / 100%
PBDE	754 / 100%	754 / 100%	754 / 100%
Mercury	754 / 100%	754 / 100%	754 / 100%

Risk Analyses

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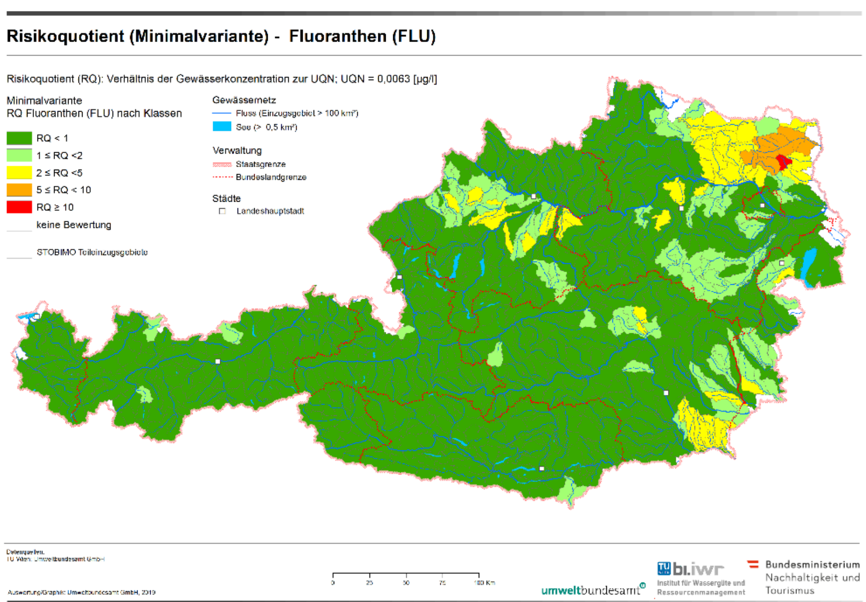

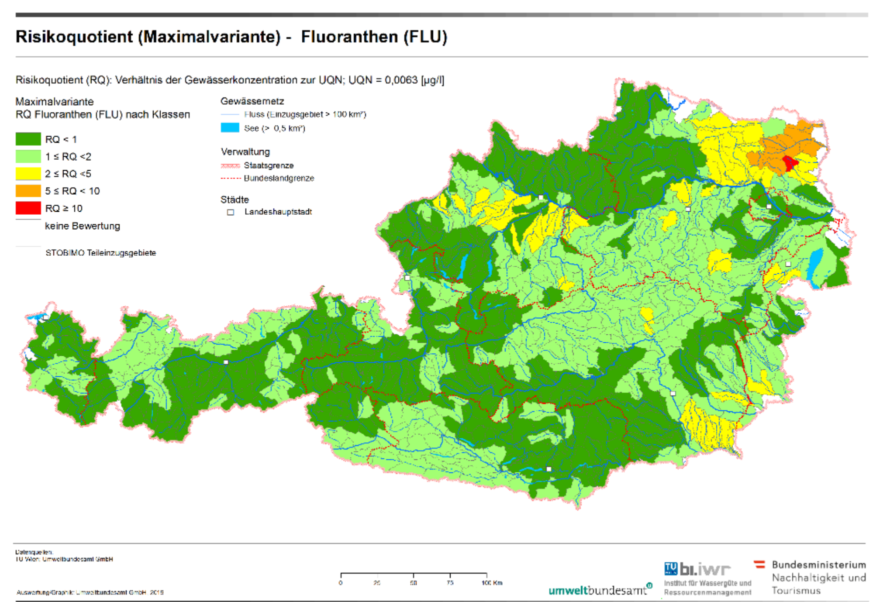

Quantification of significant pressures

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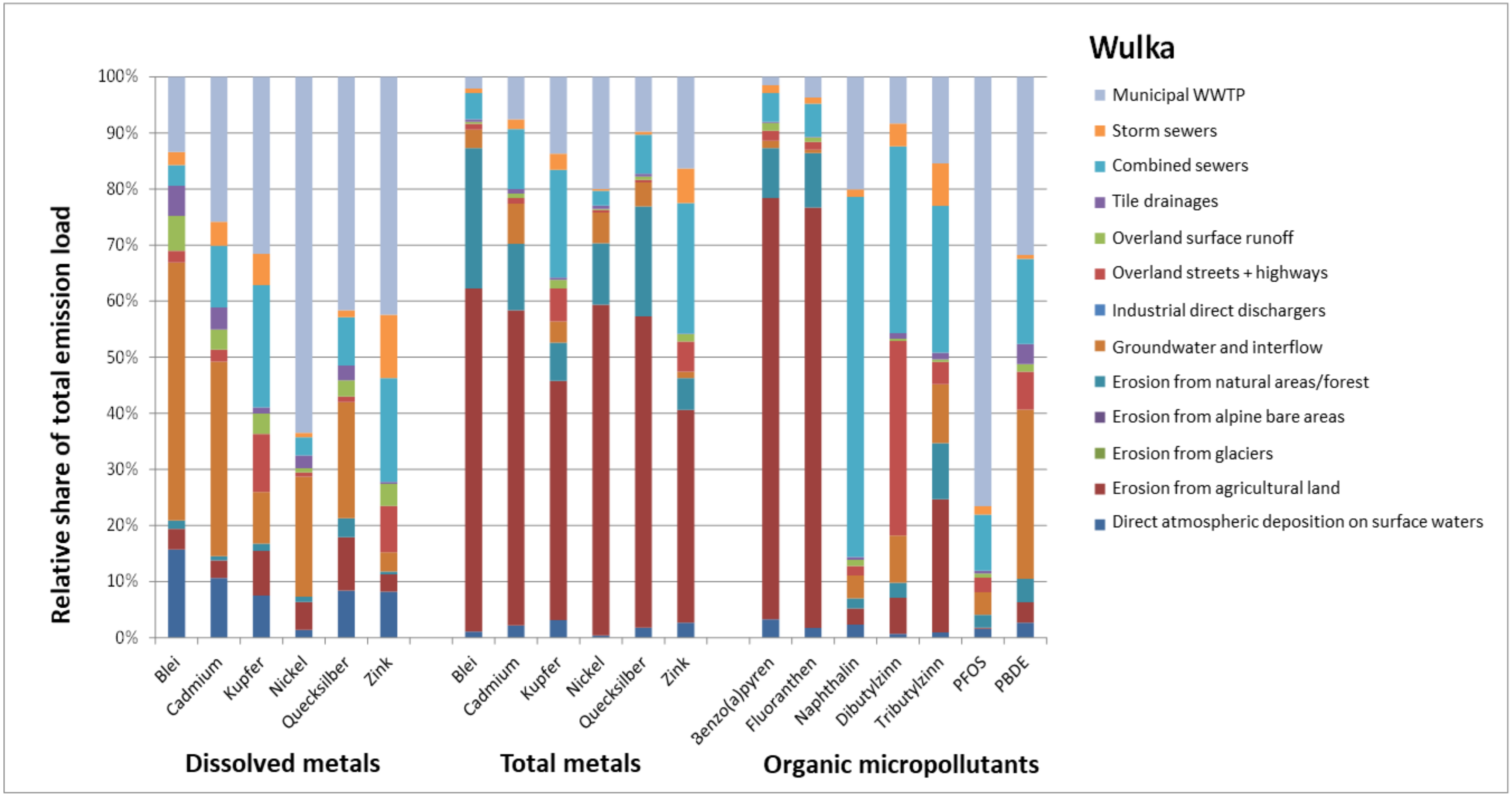
- A detailed catchments related evaluation and quantification of pathways can be used as fundament for a sound pressure analyses in catchments at risk to fail the EQS for a given substance



Quantification of significant pressures

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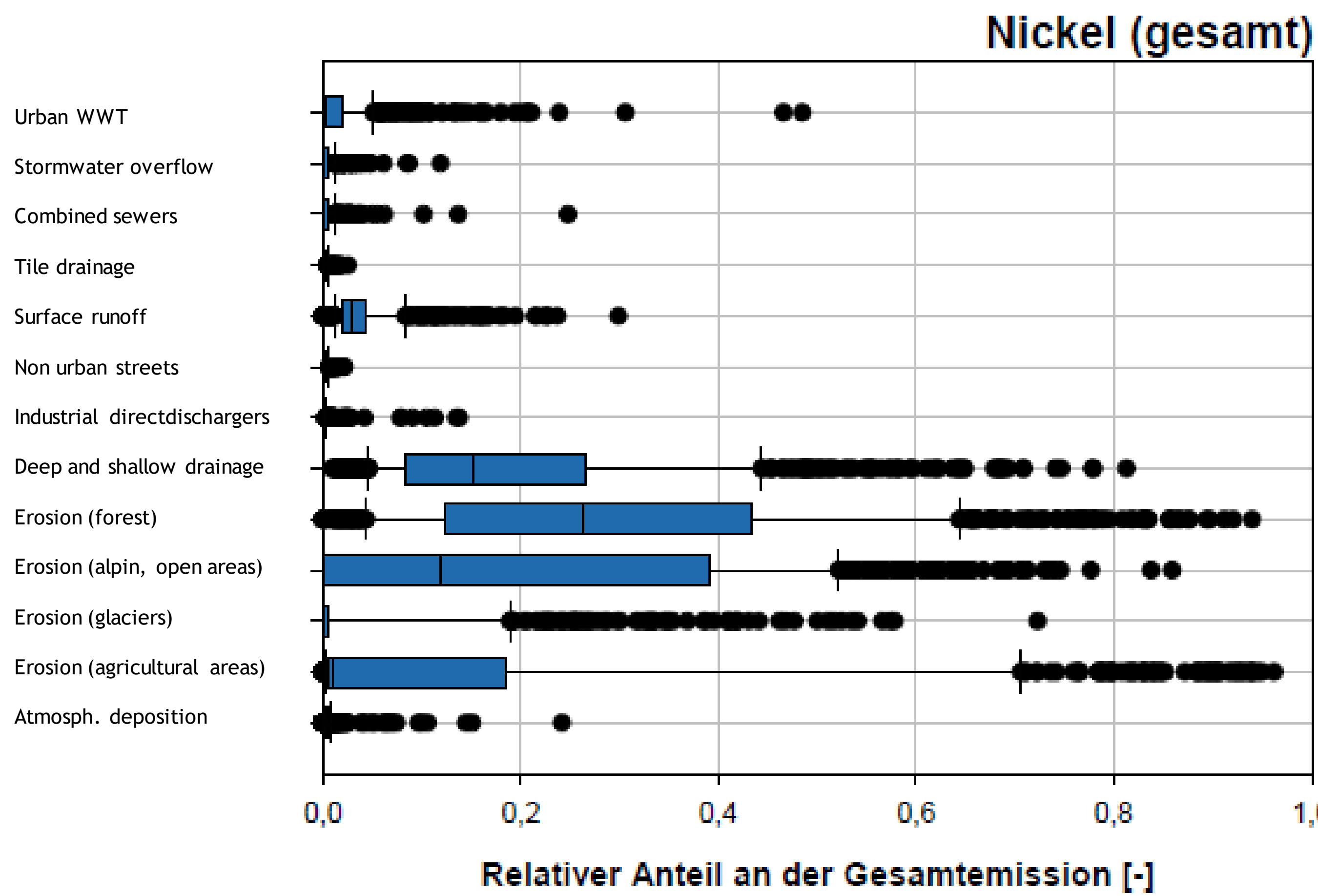
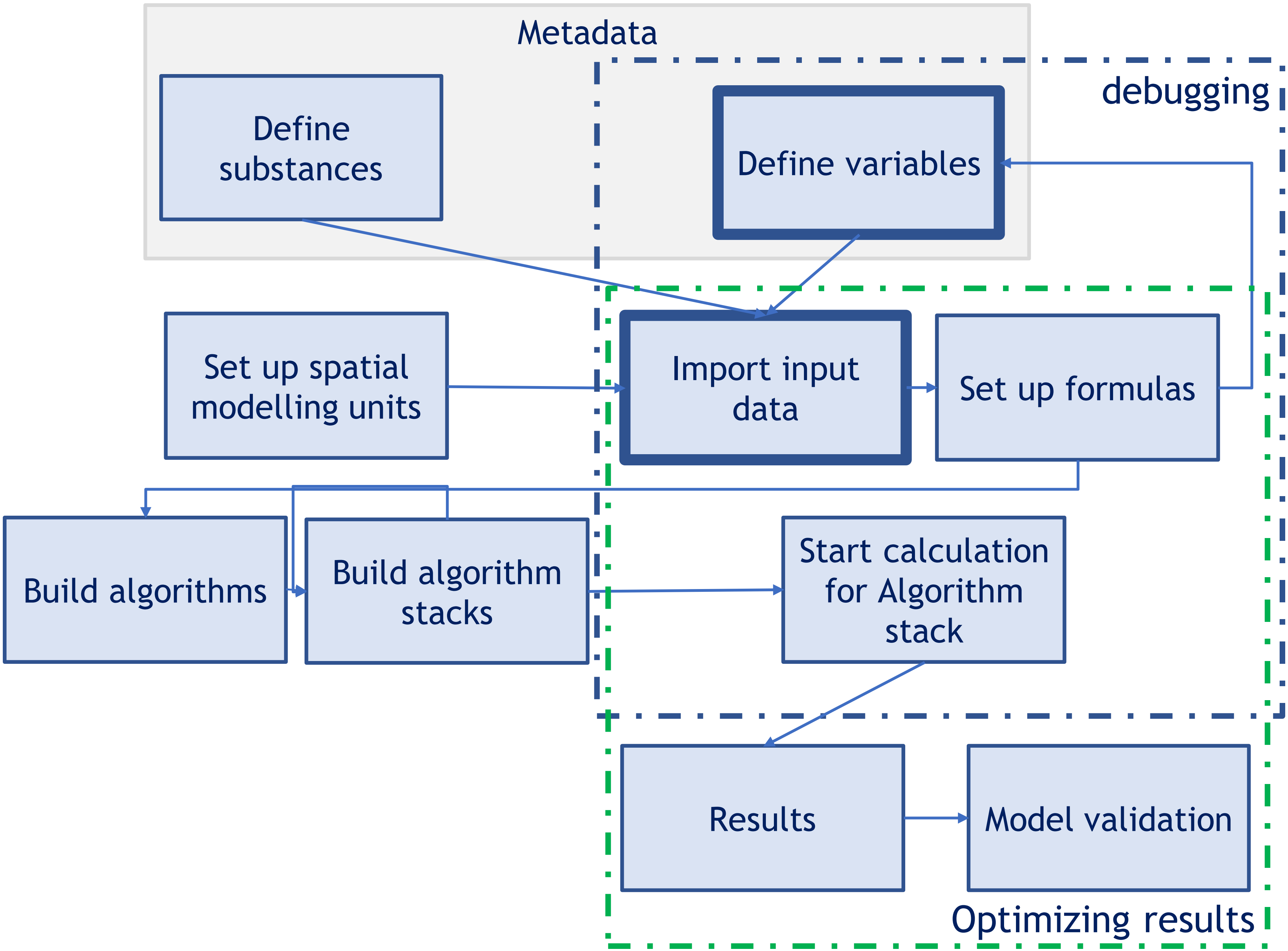
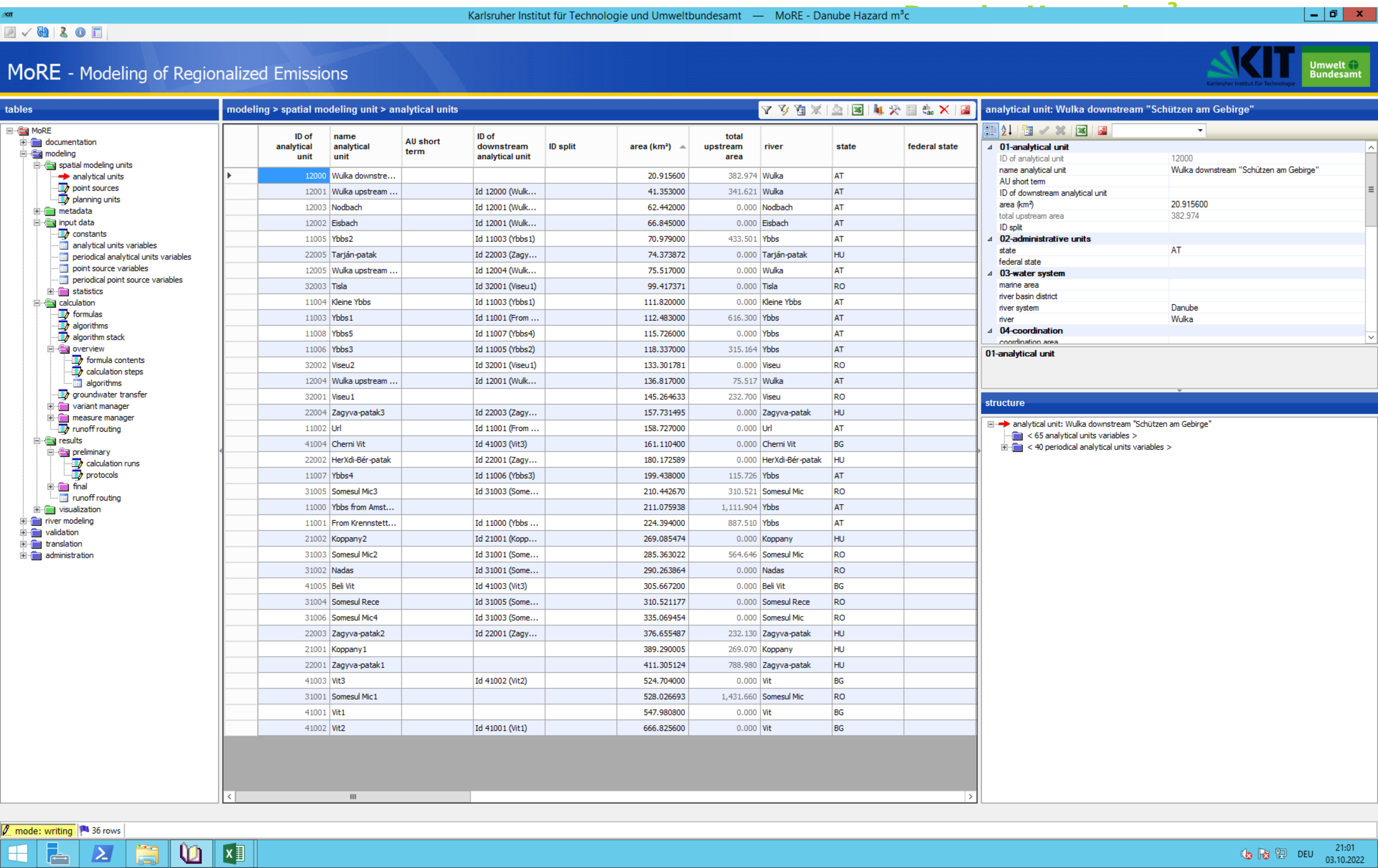


Quelle: Umweltbundesamt/TU Wien

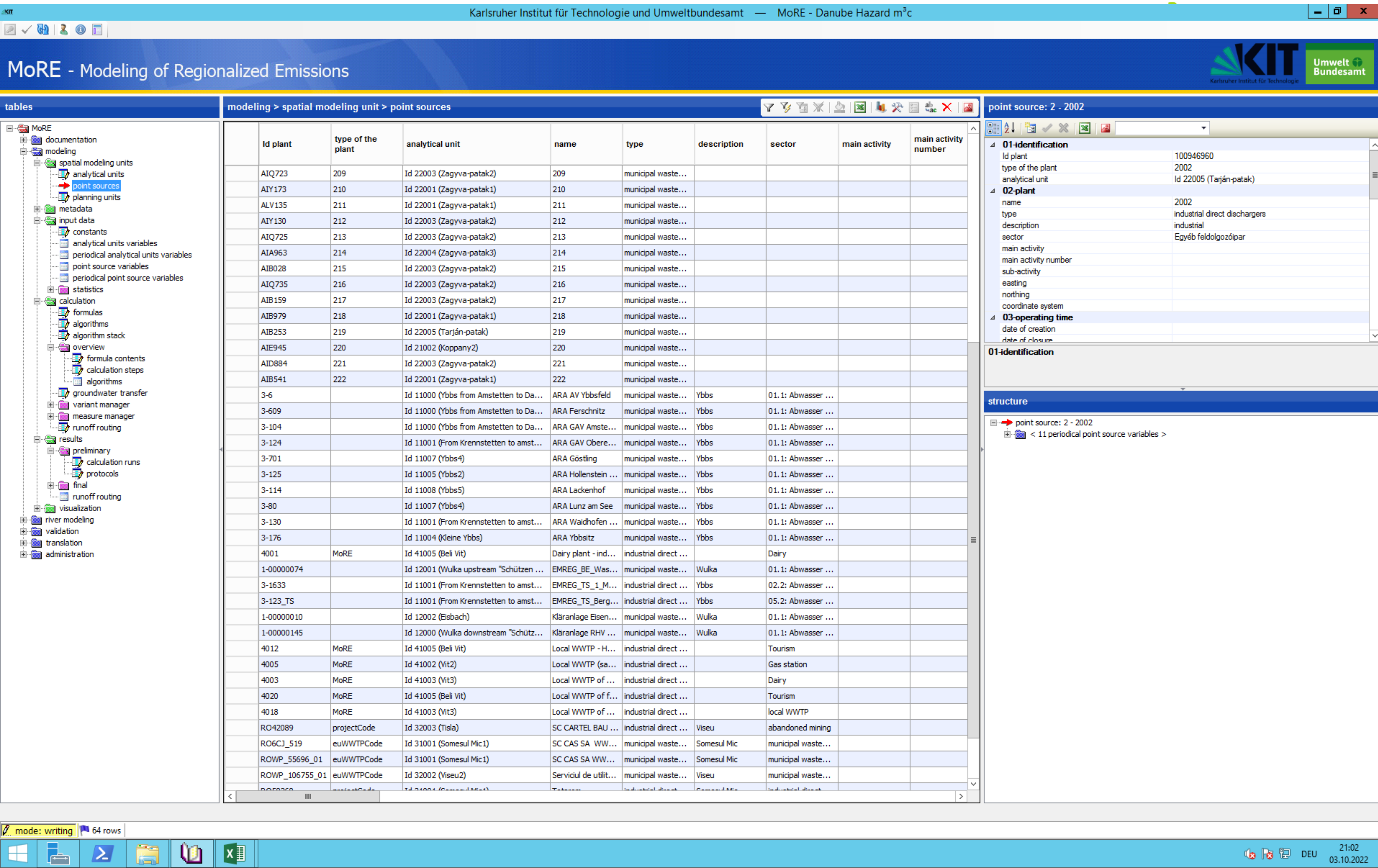
MoRE workflow


Metadata
debugging
Define substances
Define variables
Set up spatial modelling units
Import input data
Set up formulas
Build algorithms
Build algorithm stacks
Start calculation for Algorithm stack
Results
Model validation
Optimizing results

Danube Transnational Programme

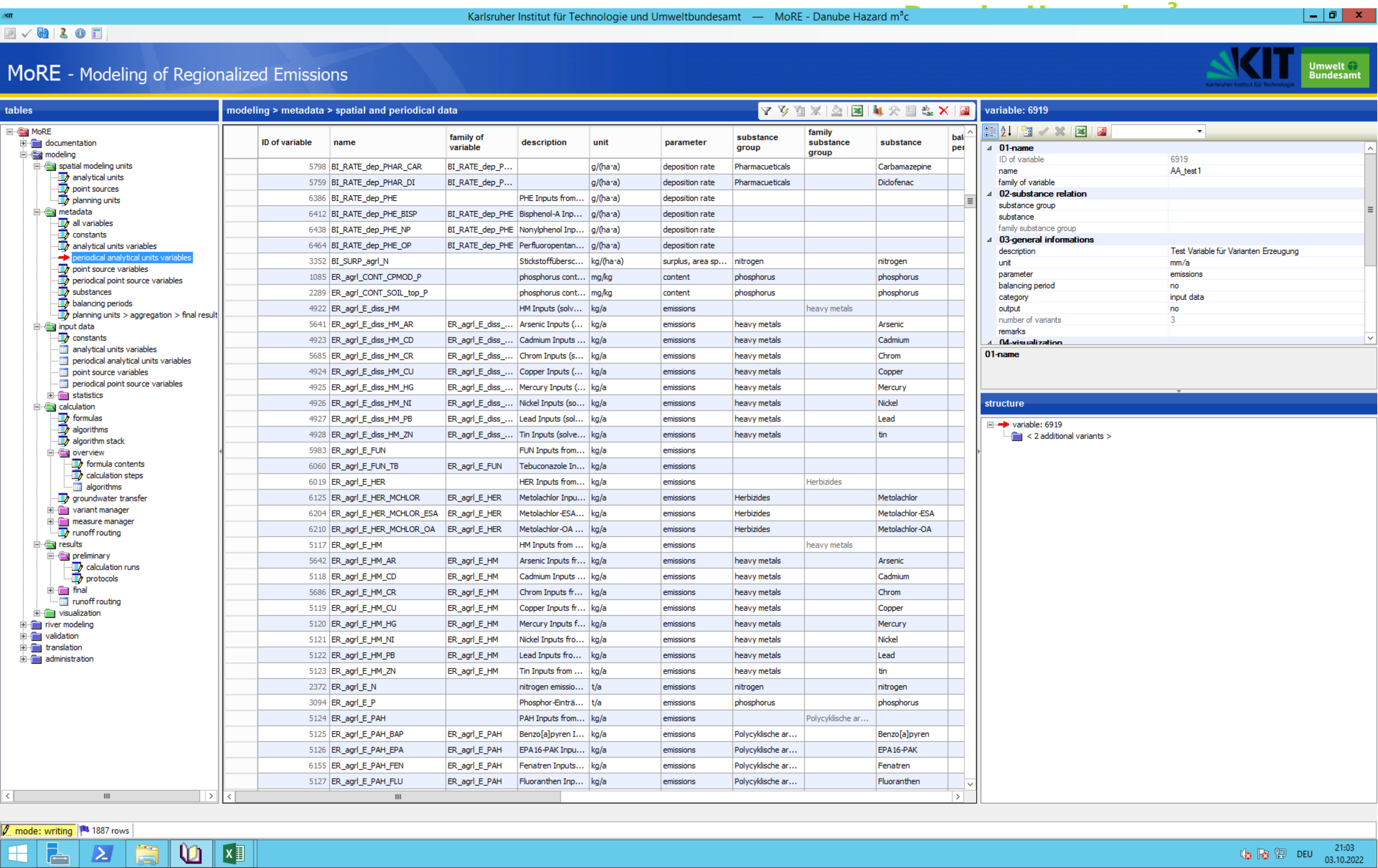


ID of analytical unit	name analytical unit	AU short term	ID of downstream analytical unit	ID split	area (km²)	total upstream area	river	state	federal state
12000	Wulka downstre…				20.915600	382.974	Wulka	AT	
12001	Wulka upstream …		Id 12000 (Wulk…		41.353000	341.621	Wulka	AT	
12003	Nodbach		Id 12001 (Wulk…		62.442000	0.000	Nodbach	AT	
12002	Eisbach		Id 12001 (Wulk…		66.845000	0.000	Eisbach	AT	
11005	Ybbs2		Id 11003 (Ybbs1)		70.979000	433.501	Ybbs	AT	
22005	Tarján-patak		Id 22003 (Zagy…		74.373872	0.000	Tarján-patak	HU	
12005	Wulka upstream …		Id 12004 (Wulk…		75.517000	0.000	Wulka	AT	
32003	Tisla		Id 32001 (Viseu1)		99.417371	0.000	Tisla	RO	
11004	Kleine Ybbs		Id 11003 (Ybbs1)		111.820000	0.000	Kleine Ybbs	AT	
11003	Ybbs1		Id 11001 (From …		112.483000	616.300	Ybbs	AT	
11008	Ybbs5		Id 11007 (Ybbs4)		115.726000	0.000	Ybbs	AT	
11006	Ybbs3		Id 11005 (Ybbs2)		118.337000	315.164	Ybbs	AT	
32002	Viseu2		Id 32001 (Viseu1)		133.301781	0.000	Viseu	RO	
12004	Wulka upstream …		Id 12001 (Wulk…		136.817000	75.517	Wulka	AT	
32001	Viseu1				145.264633	232.700	Viseu	RO	
22004	Zagyva-patak3		Id 22003 (Zagy…		157.731495	0.000	Zagyva-patak	HU	
11002	Url		Id 11001 (From …		158.727000	0.000	Url	AT	
41004	Cherni Vit		Id 41003 (Vit3)		161.110400	0.000	Cherni Vit	BG	
22002	HerXdi-Bér-patak		Id 22001 (Zagy…		180.172589	0.000	HerXdi-Bér-patak	HU	
11007	Ybbs4		Id 11006 (Ybbs3)		199.438000	115.726	Ybbs	AT	
31005	Somesul Mic3		Id 31003 (Some…		210.442670	310.521	Somesul Mic	RO	
11000	Ybbs from Amst…				211.075938	1,111.904	Ybbs	AT	
11001	From Krennstett…		Id 11000 (Ybbs …		224.394000	887.510	Ybbs	AT	
21002	Koppany2		Id 21001 (Kopp…		269.085474	0.000	Koppany	HU	
31003	Somesul Mic2		Id 31001 (Some…		285.363022	564.646	Somesul Mic	RO	
31002	Nadas		Id 31001 (Some…		290.263864	0.000	Nadas	RO	
41005	Beli Vit		Id 41003 (Vit3)		305.667200	0.000	Beli Vit	BG	
31004	Somesul Rece		Id 31005 (Some…		310.521177	0.000	Somesul Rece	RO	
31006	Somesul Mic4		Id 31003 (Some…		335.069454	0.000	Somesul Mic	RO	
22003	Zagyva-patak2		Id 22001 (Zagy…		376.655487	232.130	Zagyva-patak	HU	
21001	Koppany1				389.290005	269.070	Koppany	HU	
22001	Zagyva-patak1				411.305124	788.980	Zagyva-patak	HU	
41003	Vit3		Id 41002 (Vit2)		524.704000	0.000	Vit	BG	
31001	Somesul Mic1				528.026693	1,431.660	Somesul Mic	RO	
41001	Vit1				547.980800	0.000	Vit	BG	
41002	Vit2		Id 41001 (Vit1)		666.825600	0.000	Vit	BG	


Karlsruher Institut für Technologie und Umweltbundesamt — MoRE - Danube Hazard m³c
MoRE - Modeling of Regionalized Emissions
KIT
Karlsruher Institut für Technologie
Umwelt Bundesamt
tables
MoRE
documentation
modeling
spatial modeling units
analytical units
point sources
planning units
metadata
input data
constants
analytical units variables
periodical analytical units variables
point source variables
periodical point source variables
statistics
calculation
formulas
algorithms
algorithm stack
overview
formula contents
calculation steps
algorithms
groundwater transfer
variant manager
measure manager
runoff routing
results
preliminary
calculation runs
protocols
final
runoff routing
visualization
river modeling
validation
translation
administration
modeling > spatial modeling unit > point sources
Id plant | type of the plant | analytical unit | name | type | description | sector | main activity | main activity number
AIQ723 | 209 | Id 22003 (Zagyva-patak2) | 209 | municipal waste...
AIY173 | 210 | Id 22001 (Zagyva-patak1) | 210 | municipal waste...
ALV135 | 211 | Id 22001 (Zagyva-patak1) | 211 | municipal waste...
AIY130 | 212 | Id 22003 (Zagyva-patak2) | 212 | municipal waste...
AIQ725 | 213 | Id 22003 (Zagyva-patak2) | 213 | municipal waste...
AIA963 | 214 | Id 22004 (Zagyva-patak3) | 214 | municipal waste...
AIB028 | 215 | Id 22003 (Zagyva-patak2) | 215 | municipal waste...
AIQ735 | 216 | Id 22003 (Zagyva-patak2) | 216 | municipal waste...
AIB159 | 217 | Id 22003 (Zagyva-patak2) | 217 | municipal waste...
AIB979 | 218 | Id 22001 (Zagyva-patak1) | 218 | municipal waste...
AIB253 | 219 | Id 22005 (Tarján-patak) | 219 | municipal waste...
AIE945 | 220 | Id 21002 (Koppany2) | 220 | municipal waste...
AID884 | 221 | Id 22003 (Zagyva-patak2) | 221 | municipal waste...
AIB541 | 222 | Id 22001 (Zagyva-patak1) | 222 | municipal waste...
3-6 | Id 11000 (Ybbs from Amstetten to Da... | ARA AV Ybbsfeld | municipal waste... | Ybbs | 01.1: Abwasser ...
3-609 | Id 11000 (Ybbs from Amstetten to Da... | ARA Ferschnitz | municipal waste... | Ybbs | 01.1: Abwasser ...
3-104 | Id 11000 (Ybbs from Amstetten to Da... | ARA GAV Amste... | municipal waste... | Ybbs | 01.1: Abwasser ...
3-124 | Id 11001 (From Krennstetten to amst... | ARA GAV Obere... | municipal waste... | Ybbs | 01.1: Abwasser ...
3-701 | Id 11007 (Ybbs4) | ARA Gösting | municipal waste... | Ybbs | 01.1: Abwasser ...
3-125 | Id 11005 (Ybbs2) | ARA Hollenstein ... | municipal waste... | Ybbs | 01.1: Abwasser ...
3-114 | Id 11008 (Ybbs5) | ARA Lackenhof | municipal waste... | Ybbs | 01.1: Abwasser ...
3-80 | Id 11007 (Ybbs4) | ARA Lunz am See | municipal waste... | Ybbs | 01.1: Abwasser ...
3-130 | Id 11001 (From Krennstetten to amst... | ARA Waidhofen ... | municipal waste... | Ybbs | 01.1: Abwasser ...
3-176 | Id 11004 (Kleine Ybbs) | ARA Ybbsitz | municipal waste... | Ybbs | 01.1: Abwasser ...
4001 | MoRE | Id 41005 (Beli Vit) | Dairy plant - ind... | industrial direct ... | Dairy
1-00000074 | Id 12001 (Wulka upstream "Schützen ... | EMREG_BE_Was... | municipal waste... | Wulka | 01.1: Abwasser ...
3-1633 | Id 11001 (From Krennstetten to amst... | EMREG_TS_1_M... | industrial direct ... | Ybbs | 02.2: Abwasser ...
3-123_TS | Id 11001 (From Krennstetten to amst... | EMREG_TS_Berg... | industrial direct ... | Ybbs | 05.2: Abwasser ...
1-00000010 | Id 12002 (Eisbach) | Kläranlage Eisen... | municipal waste... | Wulka | 01.1: Abwasser ...
1-00000145 | Id 12000 (Wulka downstream "Schütz... | Kläranlage RHV ... | municipal waste... | Wulka | 01.1: Abwasser ...
4012 | MoRE | Id 41005 (Beli Vit) | Local WWTP - H... | industrial direct ... | Tourism
4005 | MoRE | Id 41002 (Vit2) | Local WWTP (sa... | industrial direct ... | Gas station
4003 | MoRE | Id 41003 (Vit3) | Local WWTP of ... | industrial direct ... | Dairy
4020 | MoRE | Id 41005 (Beli Vit) | Local WWTP of f... | industrial direct ... | Tourism
4018 | MoRE | Id 41003 (Vit3) | Local WWTP of ... | industrial direct ... | local WWTP
RO42089 | projectCode | Id 32003 (Tisla) | SC CARTEL BAU ... | industrial direct ... | Viseu | abandoned mining
RO6CJ_519 | euWWTPCode | Id 31001 (Somesul Mic1) | SC CAS SA WW... | municipal waste... | Somesul Mic | municipal waste...
ROWP_55696_01 | euWWTPCode | Id 31001 (Somesul Mic1) | SC CAS SA WW... | municipal waste... | Somesul Mic | municipal waste...
ROWP_106755_01 | euWWTPCode | Id 32002 (Viseu2) | Serviciul de utilit... | municipal waste... | Viseu | municipal waste...
point source: 2 - 2002
01-identification
Id plant | 100946960
type of the plant | 2002
analytical unit | Id 22005 (Tarján-patak)
02-plant
name | 2002
type | industrial direct dischargers
description | industrial
sector | Egyéb feldolgozóipar
main activity
main activity number
sub-activity
easting
northing
coordinate system
03-operating time
date of creation
date of closure
01-identification
structure
point source: 2 - 2002
< 11 periodical point source variables >
mode: writing
64 rows
DEU
21:02
03.10.2022

Define variables

- All input data
- Intermediate results
- Model output
- Each part of every formula needs to be defined as a variable!
- If calculating variants (best case,worst case) each variable needs a variant
- Substance specific variables are assigned to a substance group



ID of variable	name	family of variable	description	unit	parameter	substance group	family substance group	substance
5798	BI_RATE_dep_PHAR_CAR	BI_RATE_dep_P...		g/(ha·a)	deposition rate	Pharmaceuticals		Carbamazepine
5759	BI_RATE_dep_PHAR_DI	BI_RATE_dep_P...		g/(ha·a)	deposition rate	Pharmaceuticals		Diclofenac
6386	BI_RATE_dep_PHE		PHE Inputs from...	g/(ha·a)	deposition rate			
6412	BI_RATE_dep_PHE_BISP	BI_RATE_dep_PHE	Bisphenol-A Inp...	g/(ha·a)	deposition rate			
6438	BI_RATE_dep_PHE_NP	BI_RATE_dep_PHE	Nonylphenol Inp...	g/(ha·a)	deposition rate			
6464	BI_RATE_dep_PHE_OP	BI_RATE_dep_PHE	Perfluoropentan...	g/(ha·a)	deposition rate			
3352	BI_SURP_agrl_N		Stickstoffübersc...	kg/(ha·a)	surplus, area sp...	nitrogen		nitrogen
1085	ER_agrl_CONT_CPMOD_P		phosphorus cont...	mg/kg	content	phosphorus		phosphorus
2289	ER_agrl_CONT_SOIL_top_P		phosphorus cont...	mg/kg	content	phosphorus		phosphorus
4922	ER_agrl_E_diss_HM		HM Inputs (solv...	kg/a	emissions		heavy metals	
5641	ER_agrl_E_diss_HM_AR	ER_agrl_E_diss_...	Arsenic Inputs (...	kg/a	emissions	heavy metals		Arsenic
4923	ER_agrl_E_diss_HM_CD	ER_agrl_E_diss_...	Cadmium Inputs ...	kg/a	emissions	heavy metals		Cadmium
5685	ER_agrl_E_diss_HM_CR	ER_agrl_E_diss_...	Chrom Inputs (s...	kg/a	emissions	heavy metals		Chrom
4924	ER_agrl_E_diss_HM_CU	ER_agrl_E_diss_...	Copper Inputs (...	kg/a	emissions	heavy metals		Copper
4925	ER_agrl_E_diss_HM_HG	ER_agrl_E_diss_...	Mercury Inputs (...	kg/a	emissions	heavy metals		Mercury
4926	ER_agrl_E_diss_HM_NI	ER_agrl_E_diss_...	Nickel Inputs (so...	kg/a	emissions	heavy metals		Nickel
4927	ER_agrl_E_diss_HM_PB	ER_agrl_E_diss_...	Lead Inputs (sol...	kg/a	emissions	heavy metals		Lead
4928	ER_agrl_E_diss_HM_ZN	ER_agrl_E_diss_...	Tin Inputs (solve...	kg/a	emissions	heavy metals		tin
5983	ER_agrl_E_FUN		FUN Inputs from...	kg/a	emissions			
6060	ER_agrl_E_FUN_TB	ER_agrl_E_FUN	Tebuconazole In...	kg/a	emissions			
6019	ER_agrl_E_HER		HER Inputs from...	kg/a	emissions		Herbizides	
6125	ER_agrl_E_HER_MCHLOR	ER_agrl_E_HER	Metolachlor Inpu...	kg/a	emissions	Herbizides		Metolachlor
6204	ER_agrl_E_HER_MCHLOR_ESA	ER_agrl_E_HER	Metolachlor-ESA...	kg/a	emissions	Herbizides		Metolachlor-ESA
6210	ER_agrl_E_HER_MCHLOR_OA	ER_agrl_E_HER	Metolachlor-OA ...	kg/a	emissions	Herbizides		Metolachlor-OA
5117	ER_agrl_E_HM		HM Inputs from ...	kg/a	emissions		heavy metals	
5642	ER_agrl_E_HM_AR	ER_agrl_E_HM	Arsenic Inputs fr...	kg/a	emissions	heavy metals		Arsenic
5118	ER_agrl_E_HM_CD	ER_agrl_E_HM	Cadmium Inputs ...	kg/a	emissions	heavy metals		Cadmium
5686	ER_agrl_E_HM_CR	ER_agrl_E_HM	Chrom Inputs fr...	kg/a	emissions	heavy metals		Chrom
5119	ER_agrl_E_HM_CU	ER_agrl_E_HM	Copper Inputs fr...	kg/a	emissions	heavy metals		Copper
5120	ER_agrl_E_HM_HG	ER_agrl_E_HM	Mercury Inputs f...	kg/a	emissions	heavy metals		Mercury
5121	ER_agrl_E_HM_NI	ER_agrl_E_HM	Nickel Inputs fro...	kg/a	emissions	heavy metals		Nickel
5122	ER_agrl_E_HM_PB	ER_agrl_E_HM	Lead Inputs fro...	kg/a	emissions	heavy metals		Lead
5123	ER_agrl_E_HM_ZN	ER_agrl_E_HM	Tin Inputs from ...	kg/a	emissions	heavy metals		tin
2372	ER_agrl_E_N		nitrogen emissio...	t/a	emissions	nitrogen		nitrogen
3094	ER_agrl_E_P		Phosphor-Einträ...	t/a	emissions	phosphorus		phosphorus
5124	ER_agrl_E_PAH		PAH Inputs from...	kg/a	emissions		Polycyklische ar...	
5125	ER_agrl_E_PAH_BAP	ER_agrl_E_PAH	Benzo[a]pyren I...	kg/a	emissions	Polycyklische ar...		Benzo[a]pyren
5126	ER_agrl_E_PAH_EPA	ER_agrl_E_PAH	EPA16-PAK Inpu...	kg/a	emissions	Polycyklische ar...		EPA16-PAK
6155	ER_agrl_E_PAH_FEN	ER_agrl_E_PAH	Fenatren Inputs...	kg/a	emissions	Polycyklische ar...		Fenatren
5127	ER_agrl_E_PAH_FLU	ER_agrl_E_PAH	Fluoranthen Inp...	kg/a	emissions	Polycyklische ar...		Fluoranthen

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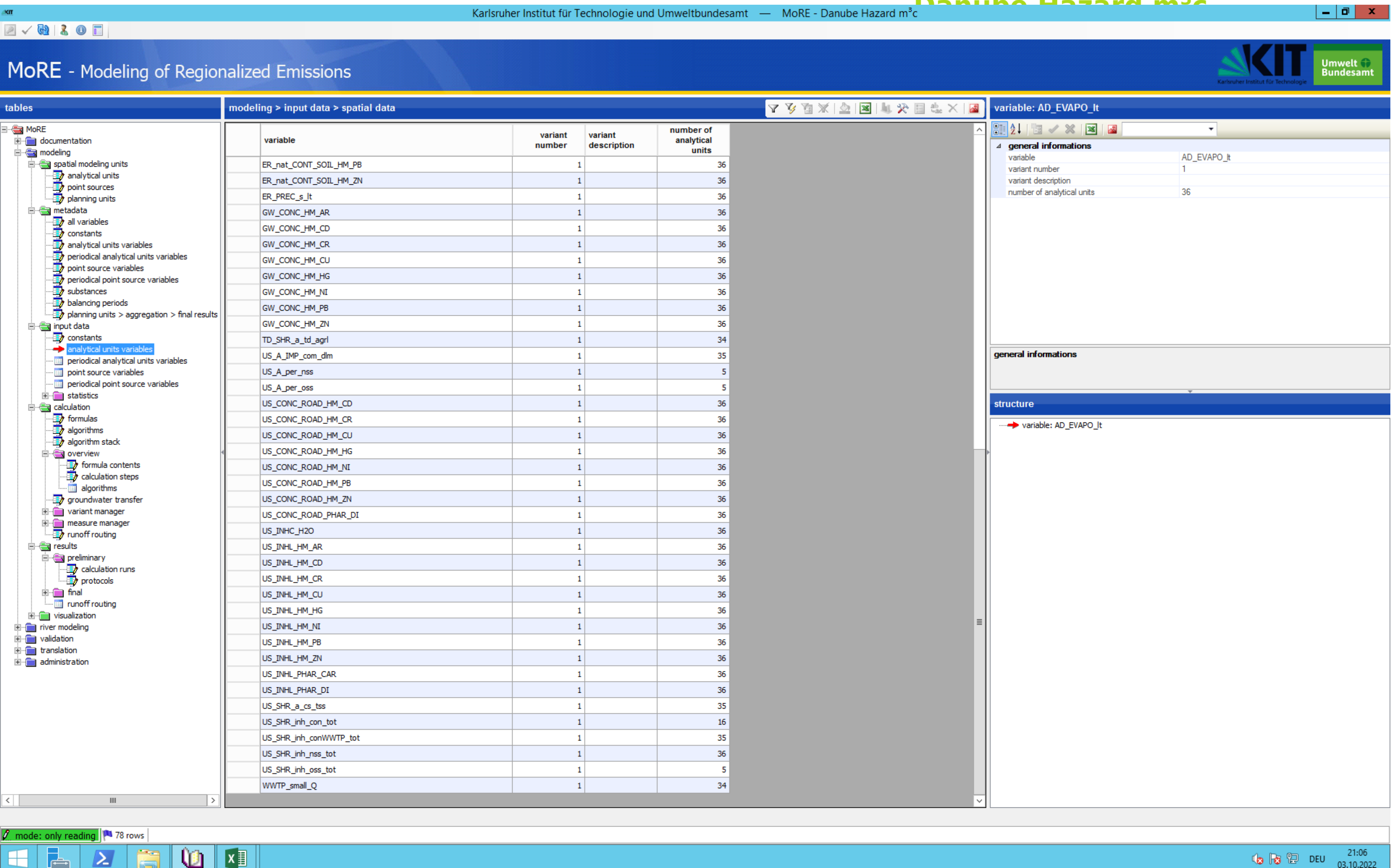

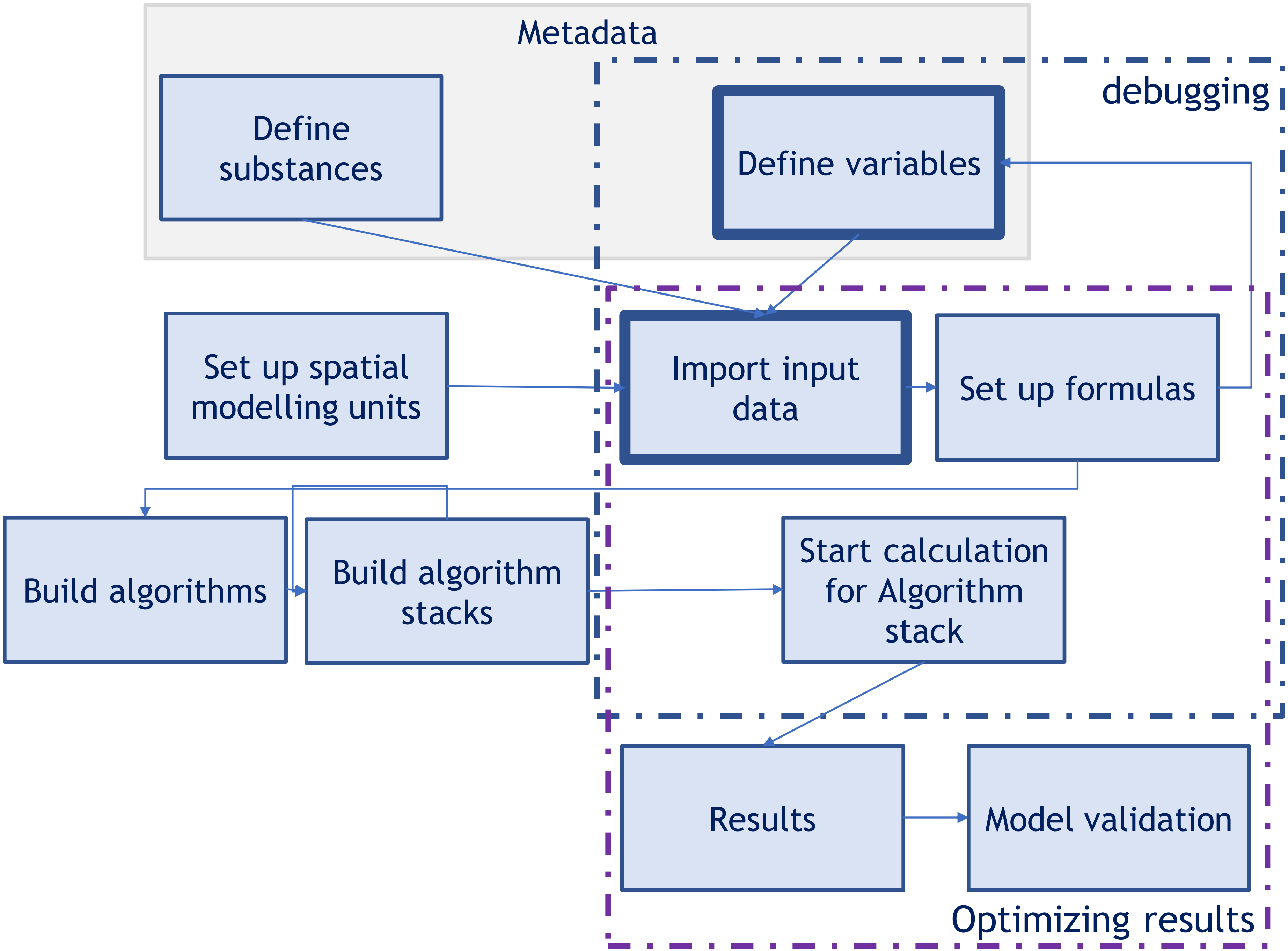
Metadata
debugging
Define substances
Define variables
Set up spatial modelling units
Import input data
Set up formulas
Build algorithms
Build algorithm stacks
Start calculation for Algorithm stack
Results
Model validation
Optimizing results

Set up Formulas

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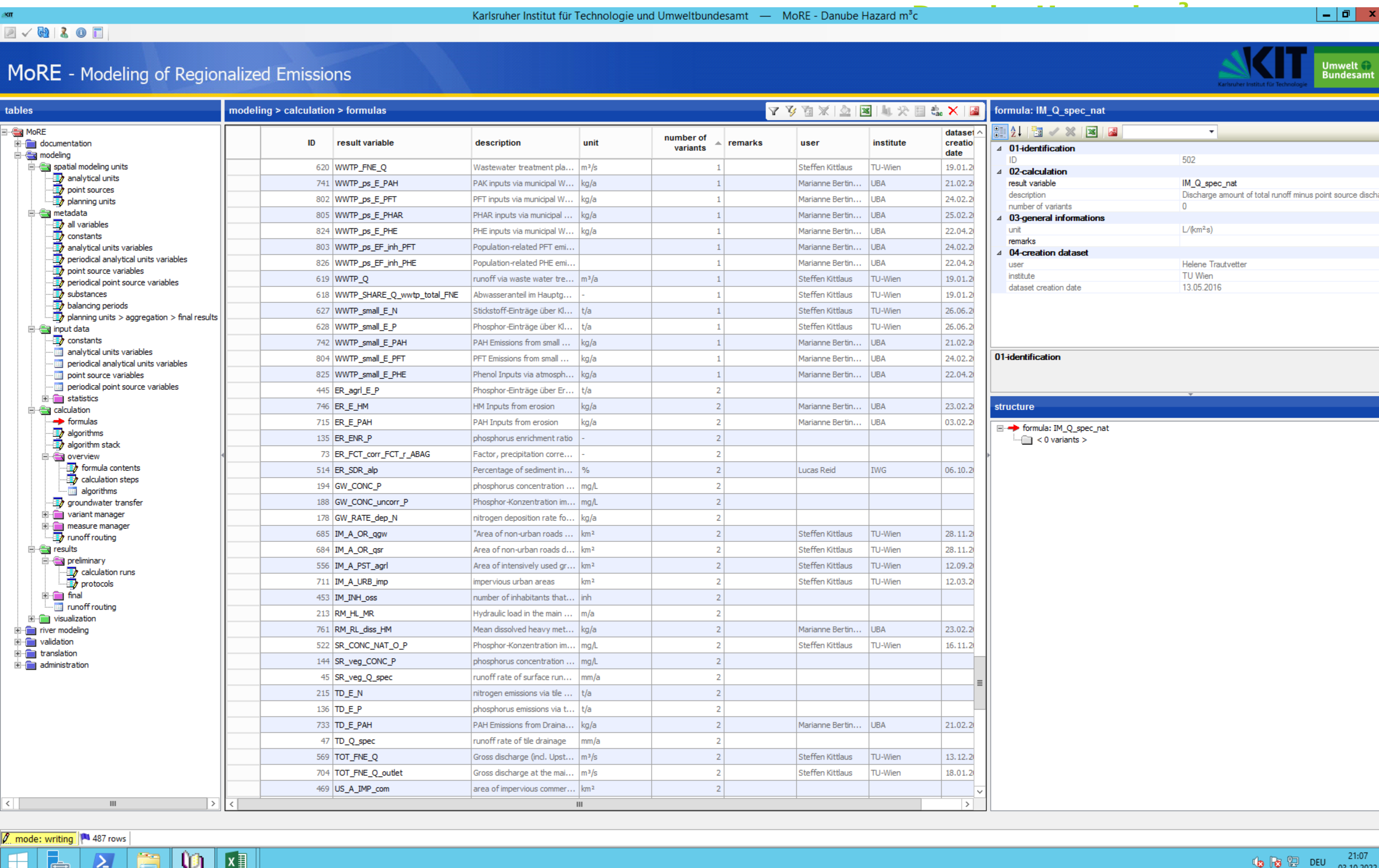
Danube Hazard m^3c

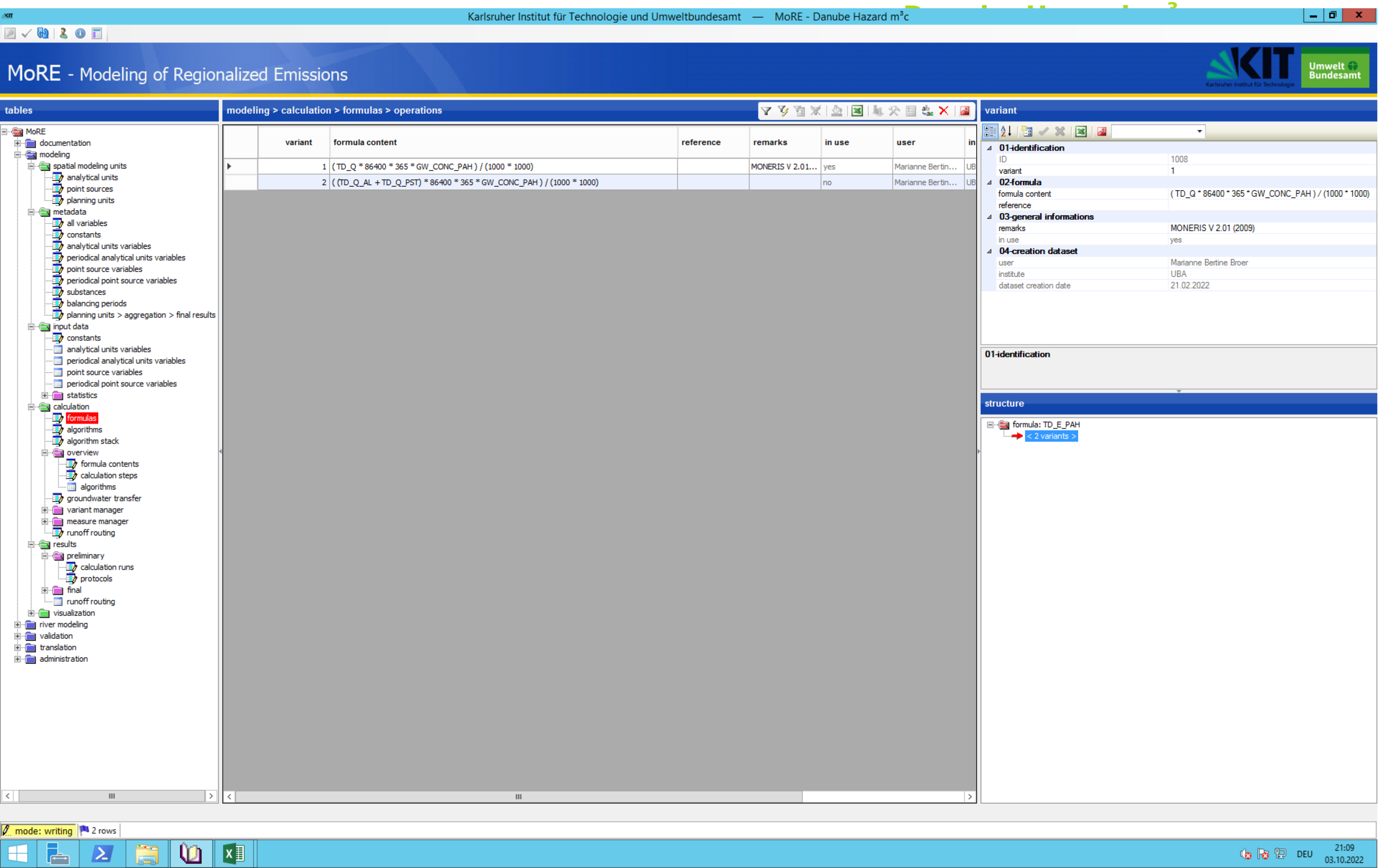
- Defined by result variable
- One results variable can have more then one formula (switch on and of)
- Defined for a substance group

Build Algorithms

- Reflects one pathway for one substance group (also land use or parts of the water balance)
- Consist of one or more formulas



ID	result variable	description	unit	number of variants	remarks	user	institute	dataset creation date
620	WWTP_FNE_Q	Wastewater treatment pla…	m³/s	1		Steffen Kittlaus	TU-Wien	19.01.2
741	WWTP_ps_E_PAH	PAK inputs via municipal W…	kg/a	1		Marianne Bertin…	UBA	21.02.2
802	WWTP_ps_E_PFT	PFT inputs via municipal W…	kg/a	1		Marianne Bertin…	UBA	24.02.2
805	WWTP_ps_E_PHAR	PHAR inputs via municipal …	kg/a	1		Marianne Bertin…	UBA	25.02.2
824	WWTP_ps_E_PHE	PHE inputs via municipal W…	kg/a	1		Marianne Bertin…	UBA	22.04.2
803	WWTP_ps_EF_inh_PFT	Population-related PFT emi…		1		Marianne Bertin…	UBA	24.02.2
826	WWTP_ps_EF_inh_PHE	Population-related PHE emi…		1		Marianne Bertin…	UBA	22.04.2
619	WWTP_Q	runoff via waste water tre…	m³/a	1		Steffen Kittlaus	TU-Wien	19.01.2
618	WWTP_SHARE_Q_wwtp_total_FNE	Abwasseranteil im Hauptg…	-	1		Steffen Kittlaus	TU-Wien	19.01.2
627	WWTP_small_E_N	Stickstoff-Einträge über Kl…	t/a	1		Steffen Kittlaus	TU-Wien	26.06.2
628	WWTP_small_E_P	Phosphor-Einträge über Kl…	t/a	1		Steffen Kittlaus	TU-Wien	26.06.2
742	WWTP_small_E_PAH	PAH Emissions from small …	kg/a	1		Marianne Bertin…	UBA	21.02.2
804	WWTP_small_E_PFT	PFT Emissions from small …	kg/a	1		Marianne Bertin…	UBA	24.02.2
825	WWTP_small_E_PHE	Phenol Inputs via atmosph…	kg/a	1		Marianne Bertin…	UBA	22.04.2
445	ER_agrl_E_P	Phosphor-Einträge über Er…	t/a	2				
746	ER_E_HM	HM Inputs from erosion	kg/a	2		Marianne Bertin…	UBA	23.02.2
715	ER_E_PAH	PAH Inputs from erosion	kg/a	2		Marianne Bertin…	UBA	03.02.2
135	ER_ENR_P	phosphorus enrichment ratio	-	2				
73	ER_FCT_corr_FCT_r_ABAG	Factor, precipitation corre…	-	2				
514	ER_SDR_alp	Percentage of sediment in…	%	2		Lucas Reid	IWG	06.10.2
194	GW_CONC_P	phosphorus concentration …	mg/L	2				
188	GW_CONC_uncorr_P	Phosphor-Konzentration im…	mg/L	2				
178	GW_RATE_dep_N	nitrogen deposition rate fo…	kg/a	2				
685	IM_A_OR_qgw	"Area of non-urban roads …	km²	2		Steffen Kittlaus	TU-Wien	28.11.2
684	IM_A_OR_qsr	Area of non-urban roads d…	km²	2		Steffen Kittlaus	TU-Wien	28.11.2
556	IM_A_PST_agrl	Area of intensively used gr…	km²	2		Steffen Kittlaus	TU-Wien	12.09.2
711	IM_A_URB_imp	impervious urban areas	km²	2		Steffen Kittlaus	TU-Wien	12.03.2
453	IM_INH_oss	number of inhabitants that…	inh	2				
213	RM_HL_MR	Hydraulic load in the main …	m/a	2				
761	RM_RL_diss_HM	Mean dissolved heavy met…	kg/a	2		Marianne Bertin…	UBA	23.02.2
522	SR_CONC_NAT_O_P	Phosphor-Konzentration im…	mg/L	2		Steffen Kittlaus	TU-Wien	16.11.2
144	SR_veg_CONC_P	phosphorus concentration …	mg/L	2				
45	SR_veg_Q_spec	runoff rate of surface run…	mm/a	2				
215	TD_E_N	nitrogen emissions via tile …	t/a	2				
136	TD_E_P	phosphorus emissions via t…	t/a	2				
733	TD_E_PAH	PAH Emissions from Draina…	kg/a	2		Marianne Bertin…	UBA	21.02.2
47	TD_Q_spec	runoff rate of tile drainage	mm/a	2				
569	TOT_FNE_Q	Gross discharge (incl. Upst…	m³/s	2		Steffen Kittlaus	TU-Wien	13.12.2
704	TOT_FNE_Q_outlet	Gross discharge at the mai…	m³/s	2		Steffen Kittlaus	TU-Wien	18.01.2
469	US_A_IMP_com	area of impervious commer…	km²	2				


Karlsruher Institut für Technologie und Umweltbundesamt — MoRE - Danube Hazard m³c
MoRE - Modeling of Regionalized Emissions
KIT
Umwelt Bundesamt
tables
MoRE
documentation
modeling
spatial modeling units
analytical units
point sources
planning units
metadata
all variables
constants
analytical units variables
periodical analytical units variables
point source variables
periodical point source variables
substances
balancing periods
planning units > aggregation > final results
input data
constants
analytical units variables
periodical analytical units variables
point source variables
periodical point source variables
statistics
calculation
formulas
algorithms
algorithm stack
overview
formula contents
calculation steps
algorithms
groundwater transfer
variant manager
measure manager
runoff routing
results
preliminary
calculation runs
protocols
final
runoff routing
visualization
river modeling
validation
translation
administration
modeling > calculation > formulas > operations
variant | formula content | reference | remarks | in use | user | in
1 | (TD_Q * 86400 * 365 * GW_CONC_PAH) / (1000 * 1000) | | MONERIS V 2.01... | yes | Marianne Bertin... | UB
2 | ((TD_Q_AL + TD_Q_PST) * 86400 * 365 * GW_CONC_PAH) / (1000 * 1000) | | | no | Marianne Bertin... | UB
variant
01-identification
ID 1008
variant 1
02-formula
formula content (TD_Q * 86400 * 365 * GW_CONC_PAH) / (1000 * 1000)
reference
03-general informations
remarks MONERIS V 2.01 (2009)
in use yes
04-creation dataset
user Marianne Bertine Broer
institute UBA
dataset creation date 21.02.2022
01-identification
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formula: TD_E_PAH
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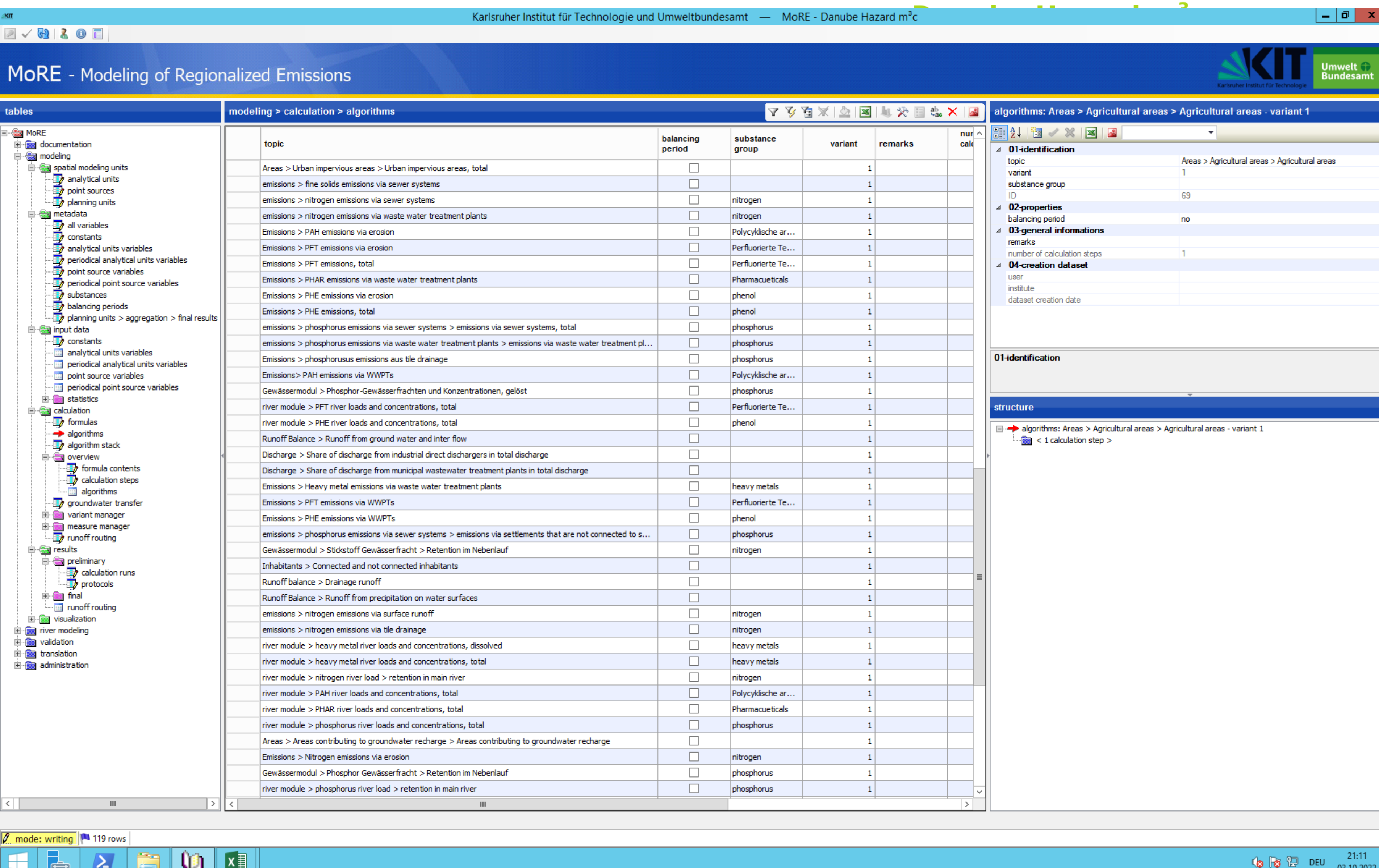
mode: writing
2 rows
DEU
21:09
03.10.2022


Karlsruher Institut für Technologie und Umweltbundesamt — MoRE - Danube Hazard m³c
MoRE - Modeling of Regionalized Emissions
Umwelt Bundesamt
tables
modeling > calculation > algorithms
algorithms: Areas > Agricultural areas > Agricultural areas - variant 1
MoRE
documentation
modeling
spatial modeling units
analytical units
point sources
planning units
metadata
all variables
constants
analytical units variables
periodical analytical units variables
point source variables
periodical point source variables
substances
balancing periods
planning units > aggregation > final results
input data
constants
analytical units variables
periodical analytical units variables
point source variables
periodical point source variables
statistics
calculation
formulas
algorithms
algorithm stack
overview
formula contents
calculation steps
algorithms
groundwater transfer
variant manager
measure manager
runoff routing
results
preliminary
calculation runs
protocols
final
runoff routing
visualization
river modeling
validation
translation
administration
topic
balancing period
substance group
variant
remarks
Areas > Urban impervious areas > Urban impervious areas, total 1
emissions > fine solids emissions via sewer systems 1
emissions > nitrogen emissions via sewer systems nitrogen 1
emissions > nitrogen emissions via waste water treatment plants nitrogen 1
Emissions > PAH emissions via erosion Polycyklische ar… 1
Emissions > PFT emissions via erosion Perfluorierte Te… 1
Emissions > PFT emissions, total Perfluorierte Te… 1
Emissions > PHAR emissions via waste water treatment plants Pharmaceuticals 1
Emissions > PHE emissions via erosion phenol 1
Emissions > PHE emissions, total phenol 1
emissions > phosphorus emissions via sewer systems > emissions via sewer systems, total phosphorus 1
emissions > phosphorus emissions via waste water treatment plants > emissions via waste water treatment pl… phosphorus 1
Emissions > phosphorusus emissions aus tile drainage phosphorus 1
Emissions> PAH emissions via WWPTs Polycyklische ar… 1
Gewässermodul > Phosphor-Gewässerfrachten und Konzentrationen, gelöst phosphorus 1
river module > PFT river loads and concentrations, total Perfluorierte Te… 1
river module > PHE river loads and concentrations, total phenol 1
Runoff Balance > Runoff from ground water and inter flow 1
Discharge > Share of discharge from industrial direct dischargers in total discharge 1
Discharge > Share of discharge from municipal wastewater treatment plants in total discharge 1
Emissions > Heavy metal emissions via waste water treatment plants heavy metals 1
Emissions > PFT emissions via WWPTs Perfluorierte Te… 1
Emissions > PHE emissions via WWPTs phenol 1
emissions > phosphorus emissions via sewer systems > emissions via settlements that are not connected to s… phosphorus 1
Gewässermodul > Stickstoff Gewässerfracht > Retention im Nebenlauf nitrogen 1
Inhabitants > Connected and not connected inhabitants 1
Runoff balance > Drainage runoff 1
Runoff Balance > Runoff from precipitation on water surfaces 1
emissions > nitrogen emissions via surface runoff nitrogen 1
emissions > nitrogen emissions via tile drainage nitrogen 1
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river module > heavy metal river loads and concentrations, total heavy metals 1
river module > nitrogen river load > retention in main river nitrogen 1
river module > PAH river loads and concentrations, total Polycyklische ar… 1
river module > PHAR river loads and concentrations, total Pharmaceuticals 1
river module > phosphorus river loads and concentrations, total phosphorus 1
Areas > Areas contributing to groundwater recharge > Areas contributing to groundwater recharge 1
Emissions > Nitrogen emissions via erosion nitrogen 1
Gewässermodul > Phosphor Gewässerfracht > Retention im Nebenlauf phosphorus 1
river module > phosphorus river load > retention in main river phosphorus 1
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topic Areas > Agricultural areas > Agricultural areas
variant 1
substance group
ID 69
02-properties
balancing period no
03-general informations
remarks
number of calculation steps 1
04-creation dataset
user
institute
dataset creation date
01-identification
structure
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DEU
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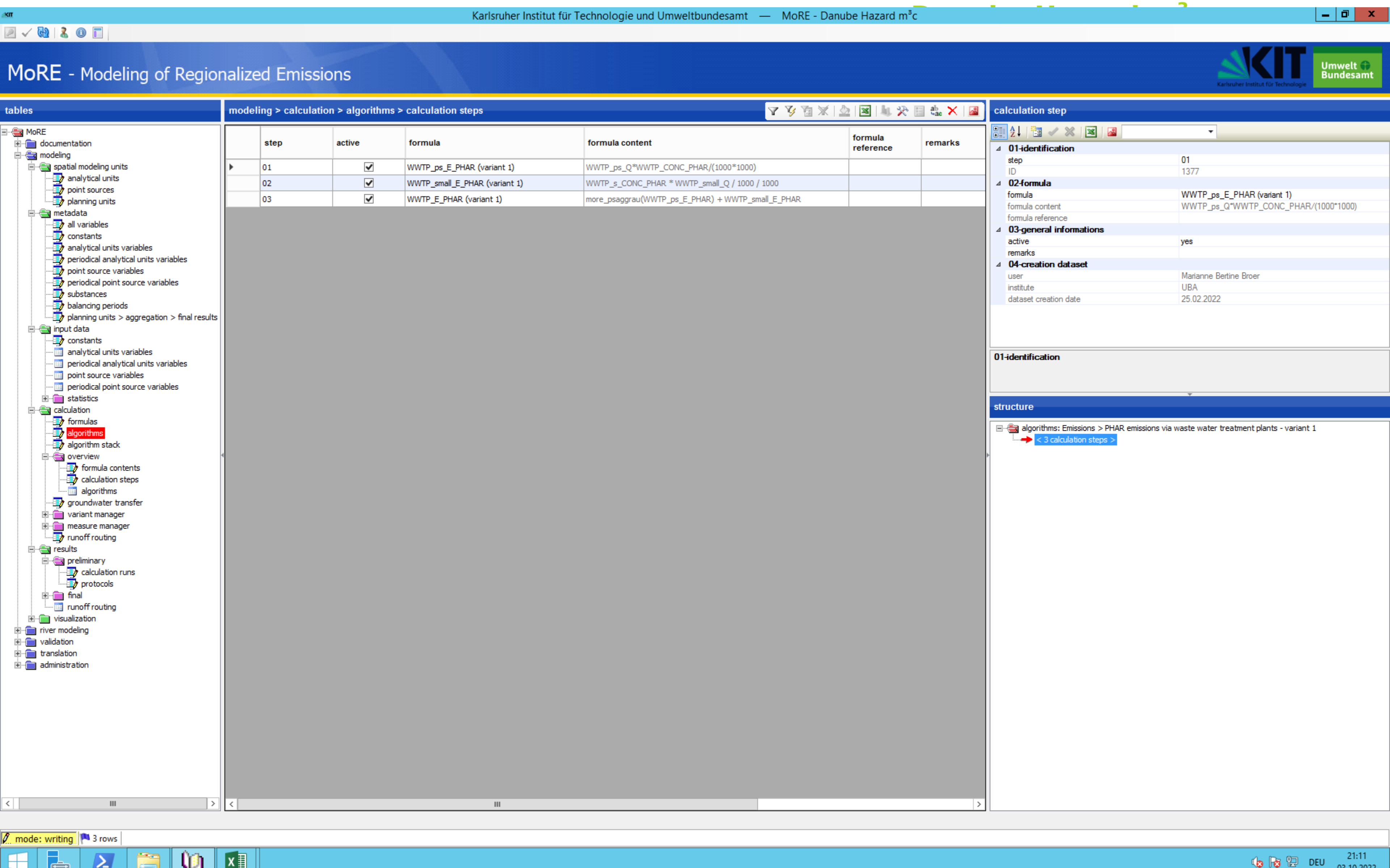
03.10.2022


Karlsruher Institut für Technologie und Umweltbundesamt — MoRE - Danube Hazard m³c
MoRE - Modeling of Regionalized Emissions
KIT
Umwelt Bundesamt
tables
MoRE
documentation
modeling
spatial modeling units
analytical units
point sources
planning units
metadata
all variables
constants
analytical units variables
periodical analytical units variables
point source variables
periodical point source variables
substances
balancing periods
planning units > aggregation > final results
input data
constants
analytical units variables
periodical analytical units variables
point source variables
periodical point source variables
statistics
calculation
formulas
algorithms
algorithm stack
overview
formula contents
calculation steps
algorithms
groundwater transfer
variant manager
measure manager
runoff routing
results
preliminary
calculation runs
protocols
final
runoff routing
visualization
river modeling
validation
translation
administration
modeling > calculation > algorithms > calculation steps
step | active | formula | formula content | formula reference | remarks
01 | ☑ | WWTP_ps_E_PHAR (variant 1) | WWTP_ps_Q*WWTP_CONC_PHAR/(1000*1000)
02 | ☑ | WWTP_small_E_PHAR (variant 1) | WWTP_s_CONC_PHAR * WWTP_small_Q / 1000 / 1000
03 | ☑ | WWTP_E_PHAR (variant 1) | more_psaggrau(WWTP_ps_E_PHAR) + WWTP_small_E_PHAR
calculation step
01-identification
step 01
ID 1377
02-formula
formula WWTP_ps_E_PHAR (variant 1)
formula content WWTP_ps_Q*WWTP_CONC_PHAR/(1000*1000)
formula reference
03-general informations
active yes
remarks
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user Marianne Bertine Broer
institute UBA
dataset creation date 25.02.2022
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structure
algorithms: Emissions > PHAR emissions via waste water treatment plants - variant 1
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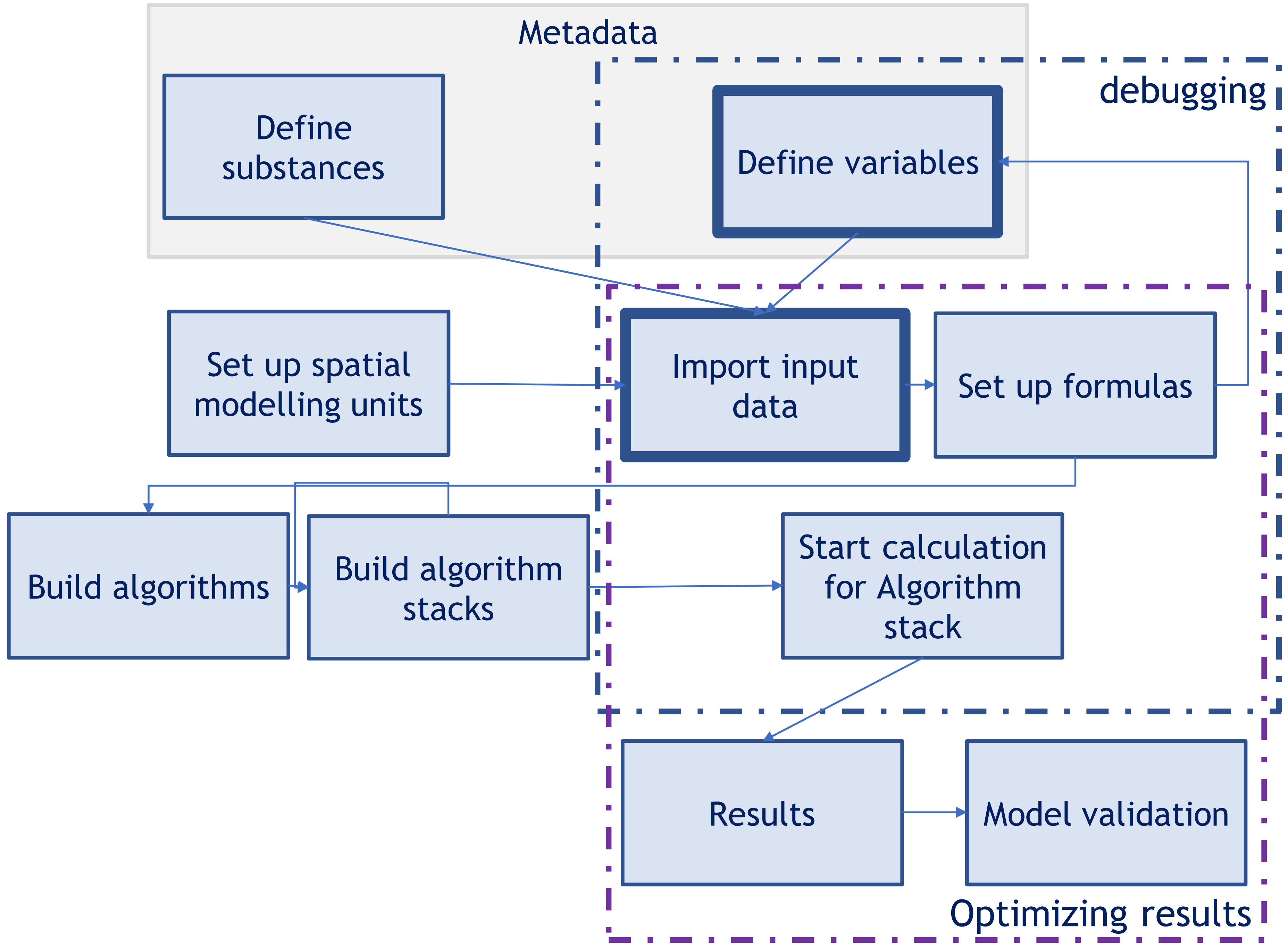
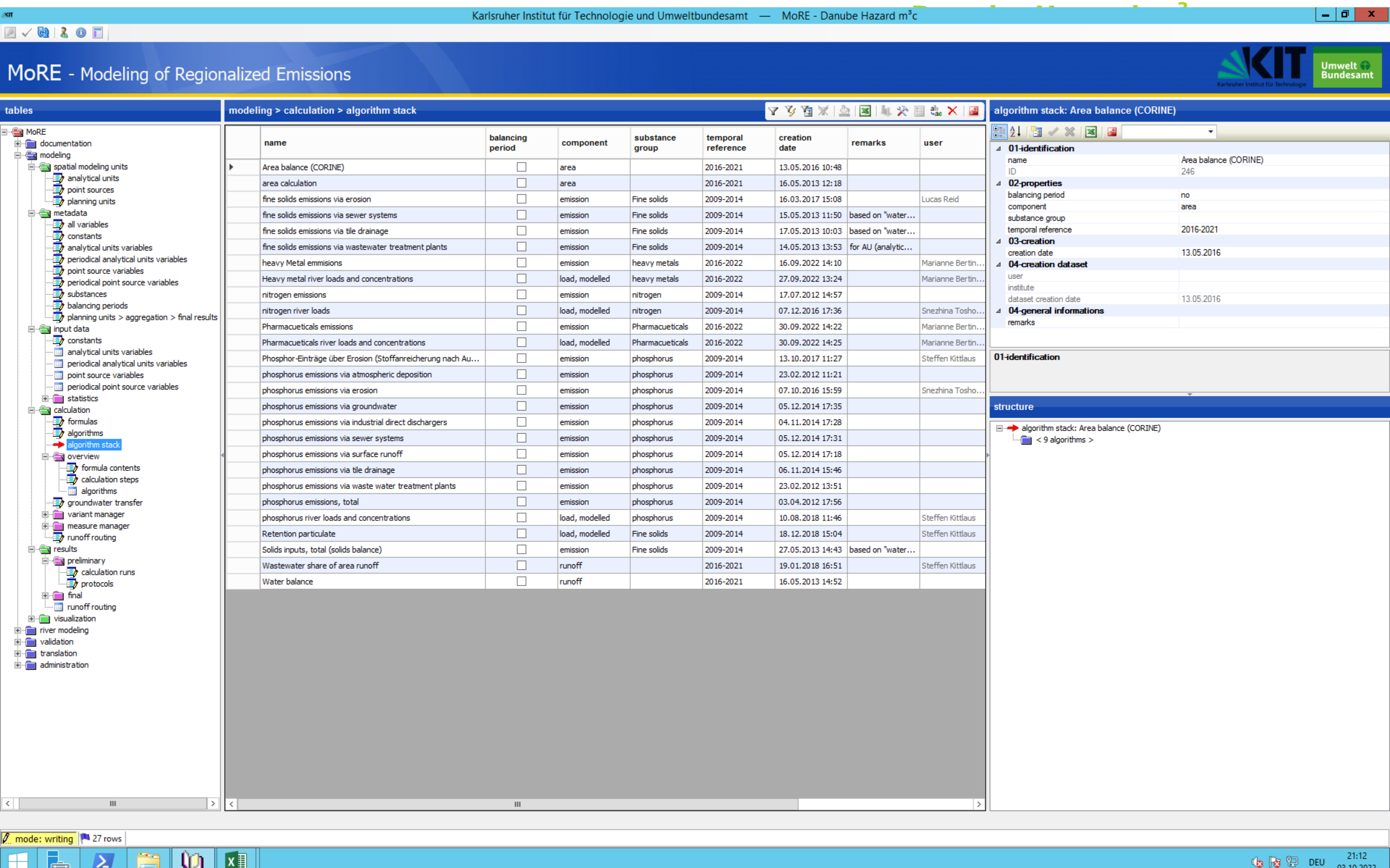
03.10.2022

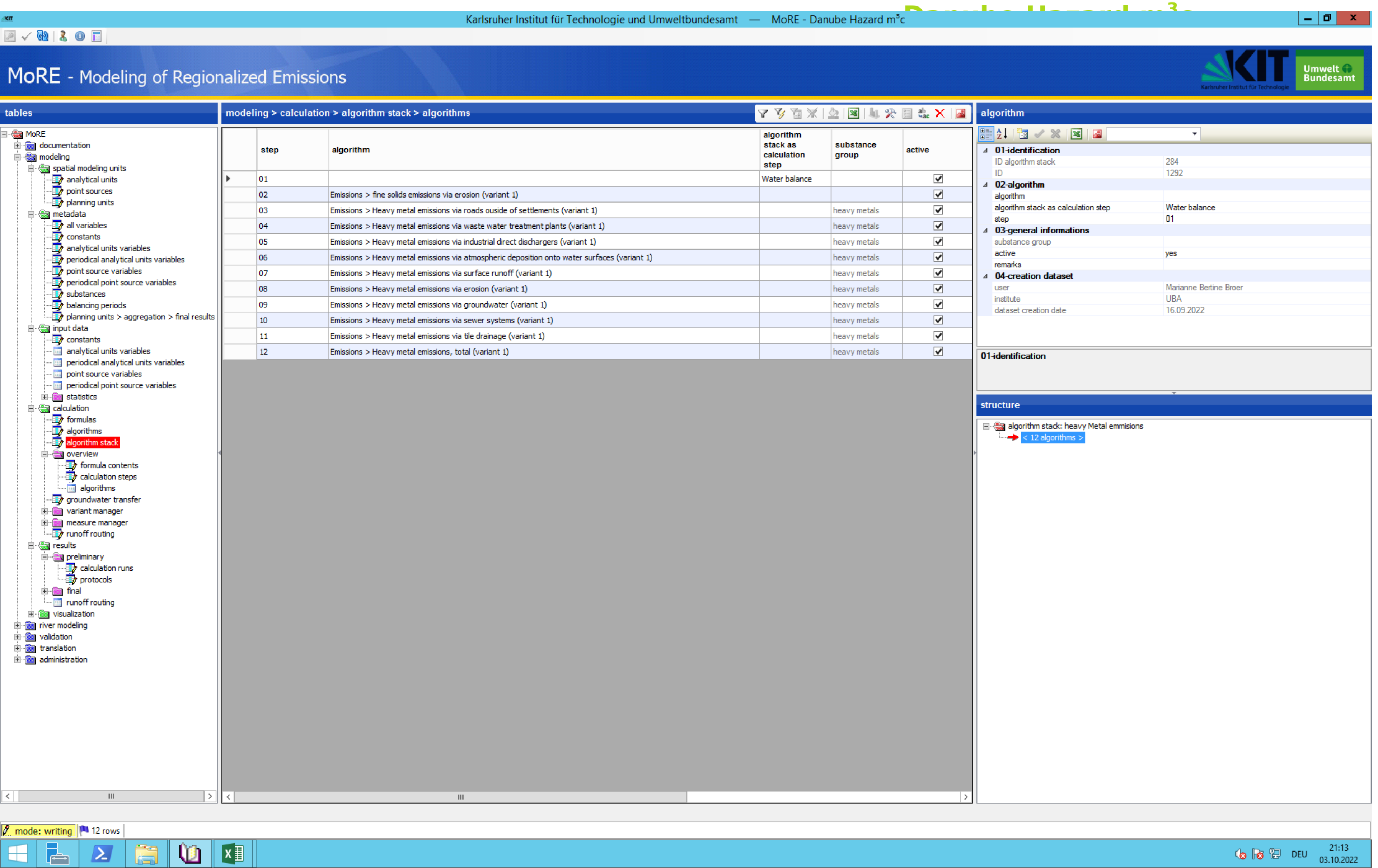

Metadata
debugging
Define substances
Define variables
Set up spatial modelling units
Import input data
Set up formulas
Build algorithms
Build algorithm stacks
Start calculation for Algorithm stack
Results
Model validation
Optimizing results

Built algorithm stacks

- Combine different algorithms into a stack
  - Total emissions
  - River concentrations & river loads
- Calculation is done per stack
- One algorithm stack can be starting point for another algorithm stack



name	balancing period	component	substance group	temporal reference	creation date	remarks	user
Area balance (CORINE)	☐	area		2016-2021	13.05.2016 10:48		
area calculation	☐	area		2016-2021	16.05.2013 12:18		
fine solids emissions via erosion	☐	emission	Fine solids	2009-2014	16.03.2017 15:08		Lucas Reid
fine solids emissions via sewer systems	☐	emission	Fine solids	2009-2014	15.05.2013 11:50	based on "water…	
fine solids emissions via tile drainage	☐	emission	Fine solids	2009-2014	17.05.2013 10:03	based on "water…	
fine solids emissions via wastewater treatment plants	☐	emission	Fine solids	2009-2014	14.05.2013 13:53	for AU (analytic…	
heavy Metal emmisions	☐	emission	heavy metals	2016-2022	16.09.2022 14:10		Marianne Bertin…
Heavy metal river loads and concentrations	☐	load, modelled	heavy metals	2016-2022	27.09.2022 13:24		Marianne Bertin…
nitrogen emissions	☐	emission	nitrogen	2009-2014	17.07.2012 14:57		
nitrogen river loads	☐	load, modelled	nitrogen	2009-2014	07.12.2016 17:36		Snezhina Tosho…
Pharmacueticals emissions	☐	emission	Pharmacueticals	2016-2022	30.09.2022 14:22		Marianne Bertin…
Pharmacueticals river loads and concentrations	☐	load, modelled	Pharmacueticals	2016-2022	30.09.2022 14:25		Marianne Bertin…
Phosphor-Einträge über Erosion (Stoffanreicherung nach Au…	☐	emission	phosphorus	2009-2014	13.10.2017 11:27		Steffen Kittlaus
phosphorus emissions via atmospheric deposition	☐	emission	phosphorus	2009-2014	23.02.2012 11:21		
phosphorus emissions via erosion	☐	emission	phosphorus	2009-2014	07.10.2016 15:59		Snezhina Tosho…
phosphorus emissions via groundwater	☐	emission	phosphorus	2009-2014	05.12.2014 17:35		
phosphorus emissions via industrial direct dischargers	☐	emission	phosphorus	2009-2014	04.11.2014 17:28		
phosphorus emissions via sewer systems	☐	emission	phosphorus	2009-2014	05.12.2014 17:31		
phosphorus emissions via surface runoff	☐	emission	phosphorus	2009-2014	05.12.2014 17:18		
phosphorus emissions via tile drainage	☐	emission	phosphorus	2009-2014	06.11.2014 15:46		
phosphorus emissions via waste water treatment plants	☐	emission	phosphorus	2009-2014	23.02.2012 13:51		
phosphorus emissions, total	☐	emission	phosphorus	2009-2014	03.04.2012 17:56		
phosphorus river loads and concentrations	☐	load, modelled	phosphorus	2009-2014	10.08.2018 11:46		Steffen Kittlaus
Retention particulate	☐	load, modelled	Fine solids	2009-2014	18.12.2018 15:04		Steffen Kittlaus
Solids inputs, total (solids balance)	☐	emission	Fine solids	2009-2014	27.05.2013 14:43	based on "water…	
Wastewater share of area runoff	☐	runoff		2016-2021	19.01.2018 16:51		Steffen Kittlaus
Water balance	☐	runoff		2016-2021	16.05.2013 14:52		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MoRE - Modeling of Regionalized Emissions
KIT
Umwelt Bundesamt
tables
modeling > calculation > algorithm stack > algorithms
algorithm
MoRE
documentation
modeling
spatial modeling units
analytical units
point sources
planning units
metadata
all variables
constants
analytical units variables
periodical analytical units variables
point source variables
periodical point source variables
substances
balancing periods
planning units > aggregation > final results
input data
constants
analytical units variables
periodical analytical units variables
point source variables
periodical point source variables
statistics
calculation
formulas
algorithms
algorithm stack
overview
formula contents
calculation steps
algorithms
groundwater transfer
variant manager
measure manager
runoff routing
results
preliminary
calculation runs
protocols
final
runoff routing
visualization
river modeling
validation
translation
administration
step
algorithm
algorithm stack as calculation step
substance group
active
01 Water balance
02 Emissions > fine solids emissions via erosion (variant 1)
03 Emissions > Heavy metal emissions via roads ouside of settlements (variant 1) heavy metals
04 Emissions > Heavy metal emissions via waste water treatment plants (variant 1) heavy metals
05 Emissions > Heavy metal emissions via industrial direct dischargers (variant 1) heavy metals
06 Emissions > Heavy metal emissions via atmospheric deposition onto water surfaces (variant 1) heavy metals
07 Emissions > Heavy metal emissions via surface runoff (variant 1) heavy metals
08 Emissions > Heavy metal emissions via erosion (variant 1) heavy metals
09 Emissions > Heavy metal emissions via groundwater (variant 1) heavy metals
10 Emissions > Heavy metal emissions via sewer systems (variant 1) heavy metals
11 Emissions > Heavy metal emissions via tile drainage (variant 1) heavy metals
12 Emissions > Heavy metal emissions, total (variant 1) heavy metals
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ID algorithm stack 284
ID 1292
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algorithm stack as calculation step Water balance
step 01
03-general informations
substance group
active yes
remarks
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user Marianne Bertine Broer
institute UBA
dataset creation date 16.09.2022
01-identification
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algorithm stack: heavy Metal emmisions
< 12 algorithms >
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12 rows
DEU
21:13
03.10.2022

Calculate a algorithm stack

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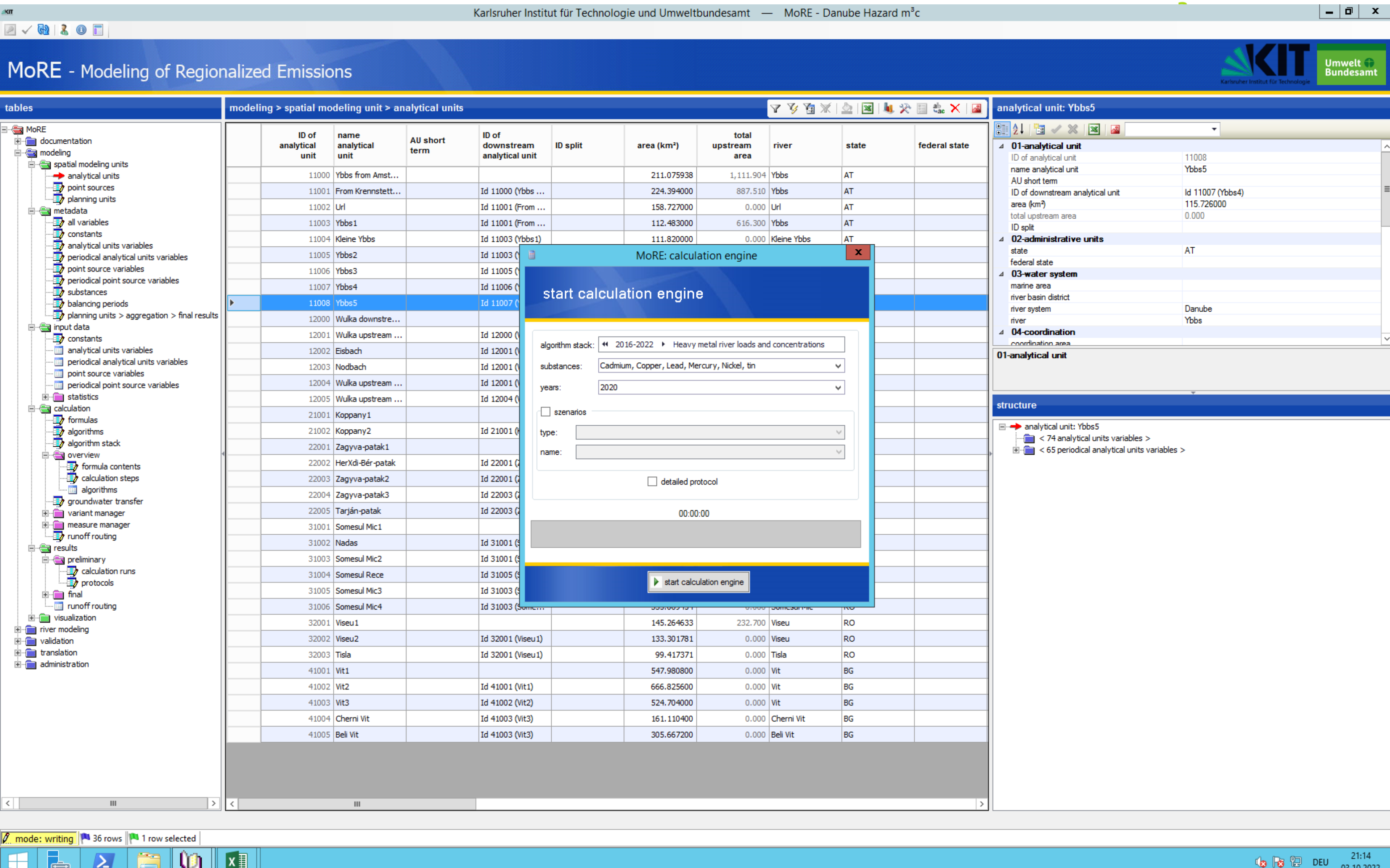
- Debug! (involving variables, input data & formulas)
- Fill in missing data
- Protocoll contains all calculation steps (very handy to debug)
- Compare results with monitored load
- Adjust input data, formulas etc.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MoRE - Modeling of Regionalized Emissions
KIT
Umwelt Bundesamt
tables
modeling > spatial modeling unit > analytical units
analytical unit: Ybbs5
ID of analytical unit
name analytical unit
AU short term
ID of downstream analytical unit
ID split
area (km²)
total upstream area
river
state
federal state
MoRE: calculation engine
start calculation engine
algorithm stack:
2016-2022
Heavy metal river loads and concentrations
substances:
Cadmium, Copper, Lead, Mercury, Nickel, tin
years:
2020
szenarios
type:
name:
detailed protocol
00:00:00
start calculation engine
01-analytical unit
02-administrative units
03-water system
04-coordination
structure
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1 row selected

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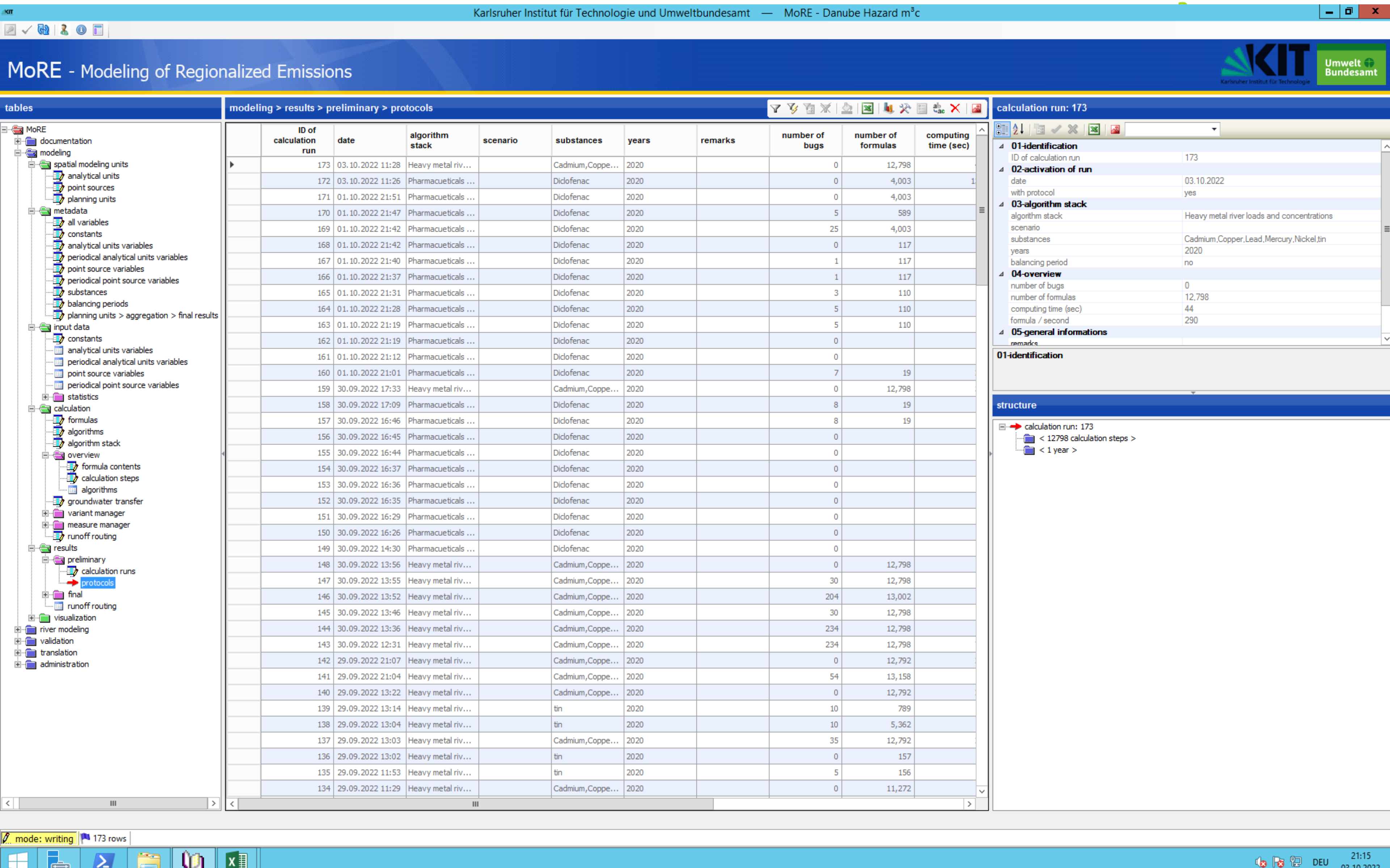

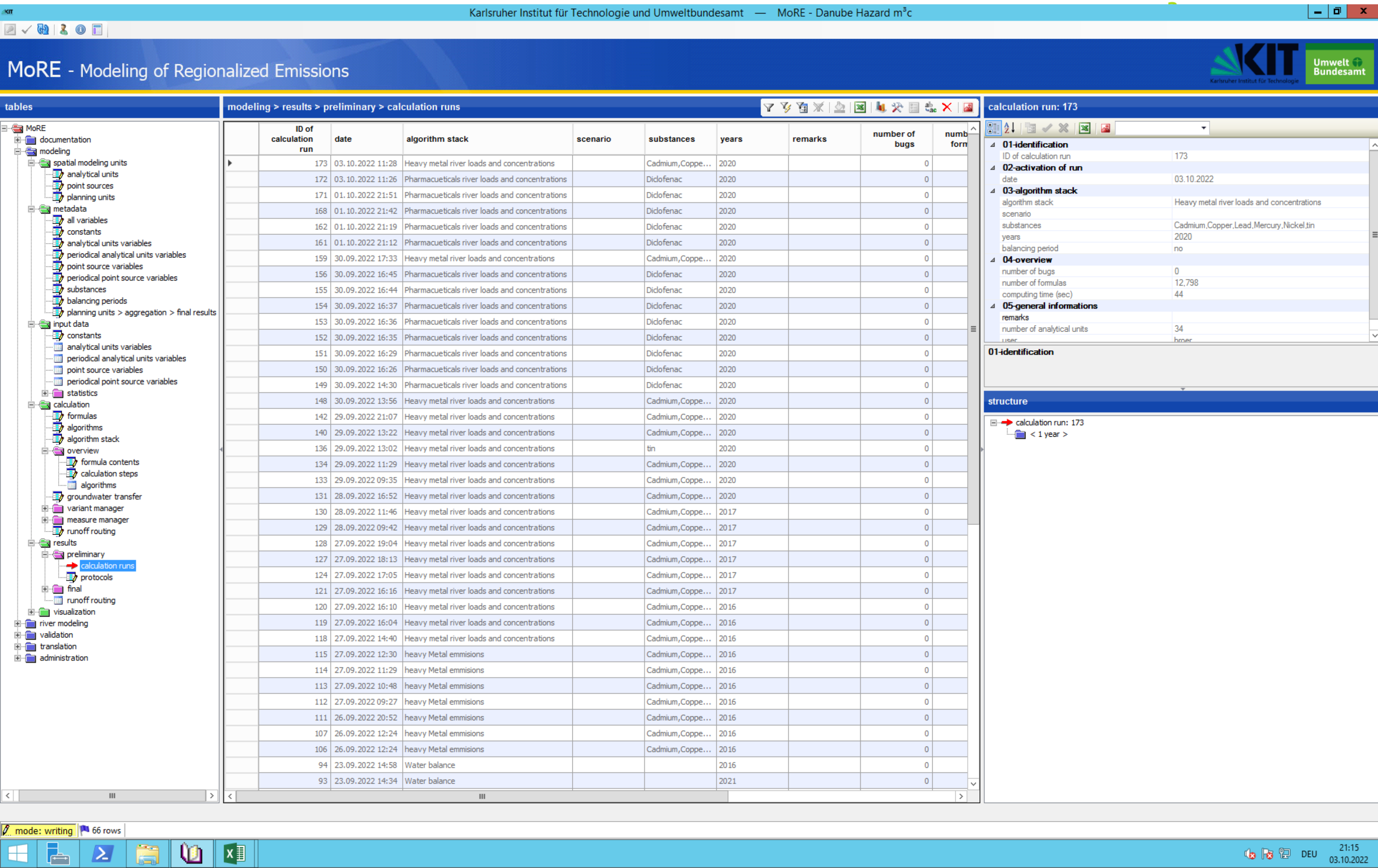

ID of calculation run	date	algorithm stack	scenario	substances	years	remarks	number of bugs	numb form
173	03.10.2022 11:28	Heavy metal river loads and concentrations		Cadmium,Coppe...	2020		0	
172	03.10.2022 11:26	Pharmaceuticals river loads and concentrations		Diclofenac	2020		0	
171	01.10.2022 21:51	Pharmaceuticals river loads and concentrations		Diclofenac	2020		0	
168	01.10.2022 21:42	Pharmaceuticals river loads and concentrations		Diclofenac	2020		0	
162	01.10.2022 21:19	Pharmaceuticals river loads and concentrations		Diclofenac	2020		0	
161	01.10.2022 21:12	Pharmaceuticals river loads and concentrations		Diclofenac	2020		0	
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153	30.09.2022 16:36	Pharmaceuticals river loads and concentrations		Diclofenac	2020		0	
152	30.09.2022 16:35	Pharmaceuticals river loads and concentrations		Diclofenac	2020		0	
151	30.09.2022 16:29	Pharmaceuticals river loads and concentrations		Diclofenac	2020		0	
150	30.09.2022 16:26	Pharmaceuticals river loads and concentrations		Diclofenac	2020		0	
149	30.09.2022 14:30	Pharmaceuticals river loads and concentrations		Diclofenac	2020		0	
148	30.09.2022 13:56	Heavy metal river loads and concentrations		Cadmium,Coppe...	2020		0	
142	29.09.2022 21:07	Heavy metal river loads and concentrations		Cadmium,Coppe...	2020		0	
140	29.09.2022 13:22	Heavy metal river loads and concentrations		Cadmium,Coppe...	2020		0	
136	29.09.2022 13:02	Heavy metal river loads and concentrations		tin	2020		0	
134	29.09.2022 11:29	Heavy metal river loads and concentrations		Cadmium,Coppe...	2020		0	
133	29.09.2022 09:35	Heavy metal river loads and concentrations		Cadmium,Coppe...	2020		0	
131	28.09.2022 16:52	Heavy metal river loads and concentrations		Cadmium,Coppe...	2020		0	
130	28.09.2022 11:46	Heavy metal river loads and concentrations		Cadmium,Coppe...	2017		0	
129	28.09.2022 09:42	Heavy metal river loads and concentrations		Cadmium,Coppe...	2017		0	
128	27.09.2022 19:04	Heavy metal river loads and concentrations		Cadmium,Coppe...	2017		0	
127	27.09.2022 18:13	Heavy metal river loads and concentrations		Cadmium,Coppe...	2017		0	
124	27.09.2022 17:05	Heavy metal river loads and concentrations		Cadmium,Coppe...	2017		0	
121	27.09.2022 16:16	Heavy metal river loads and concentrations		Cadmium,Coppe...	2017		0	
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114	27.09.2022 11:29	heavy Metal emmisions		Cadmium,Coppe...	2016		0	
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107	26.09.2022 12:24	heavy Metal emmisions		Cadmium,Coppe...	2016		0	
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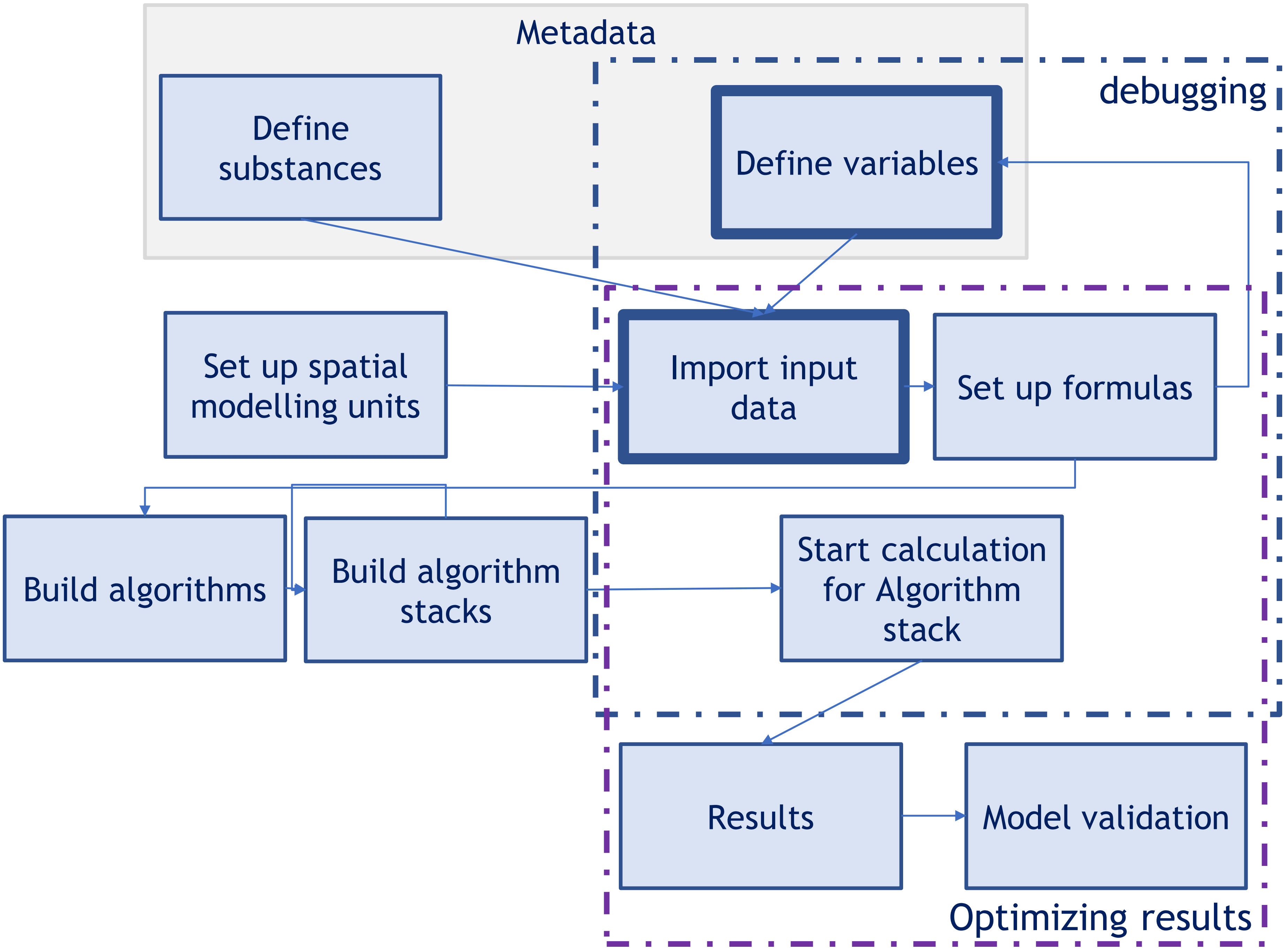
94	23.09.2022 14:58	Water balance			2016		0	
93	23.09.2022 14:34	Water balance			2021		0	


Metadata
debugging
Define substances
Define variables
Set up spatial modelling units
Import input data
Set up formulas
Build algorithms
Build algorithm stacks
Start calculation for Algorithm stack
Results
Model validation
Optimizing results

Scenario calculation

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Implementation of emission mitigation measure scenarios in MoRE

- Examples
- Way of implementation

Scenario calculation

MoRE Scenarios
• Basically restricted to interventions directly into represented pathways, • Alternatively impacts of scenarios on pathways can be calculated externally and be implemented into the model • Climate scenarios may be implemented depended on the underlying hydrological and erosion model

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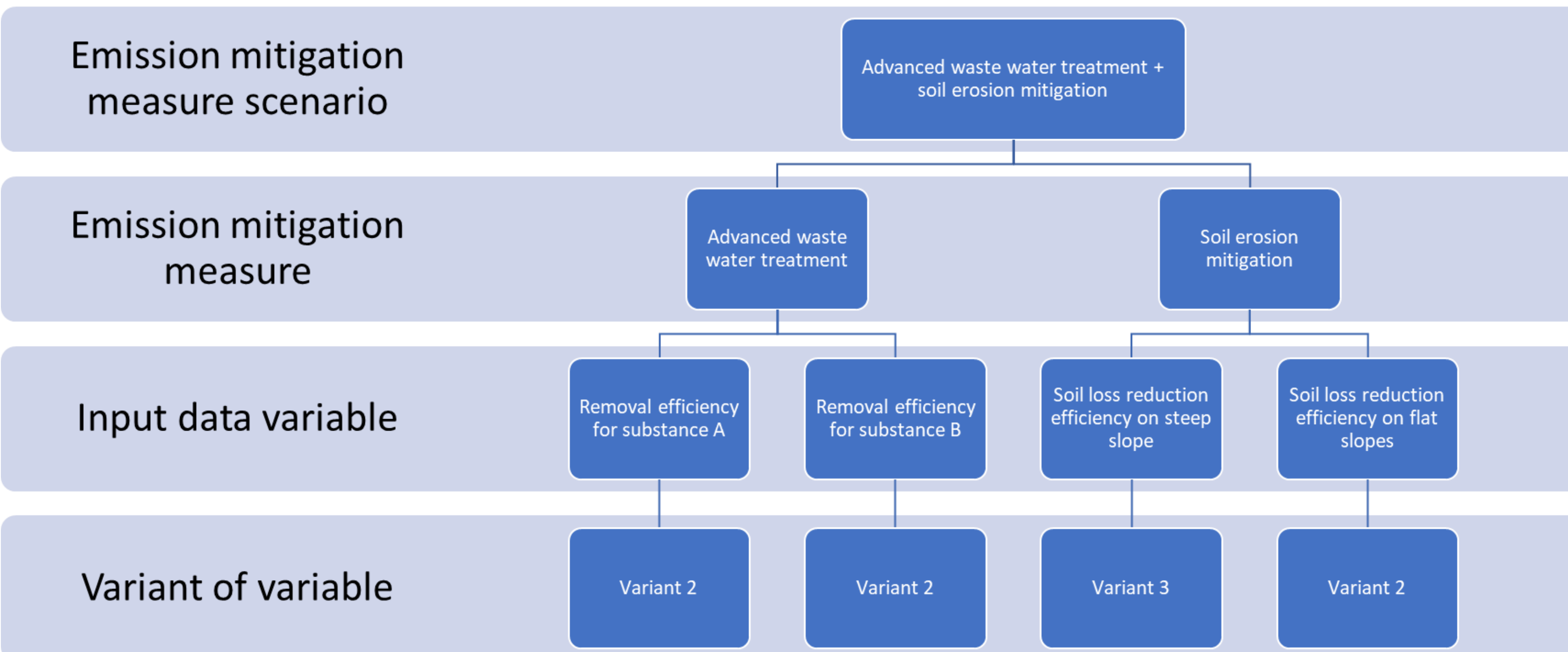
Implementation of emission mitigation measure scenarios in MoRE

Examples:

- Implementation of state of the art conventional waste water treatment for all settlements
- Implementation of advanced waste water treatment (micro pollutant removal):
  - On large municipal waste water treatment plants (>100 000 PE)
  - On large and medium size municipal waste water treatment plants (>50 000 PE)
  - With activated carbon (η_{PFOS} = 75%)
  - With ozonation (η_{PFOS} = 20%)
- Storm water treatment in combined and separate sewer systems:
  - Reduction of suspended particulate matter emissions (CSO = 30%, storm sewers = 20%)
  - Effect on micro pollutants calculated over the K_D value of the substance
- Air pollution control: reduction of atmospheric deposition for e.g. Hg by 25 %
- Soil erosion mitigation measures:
  - Reduction of soil erosion from agricultural areas by 50 %

Scenario calculation

Hierarchical approach of emission mitigation measure scenario implementation in MoRE



Picture: S. Kittlaus, TU Wien

Scenario calculation

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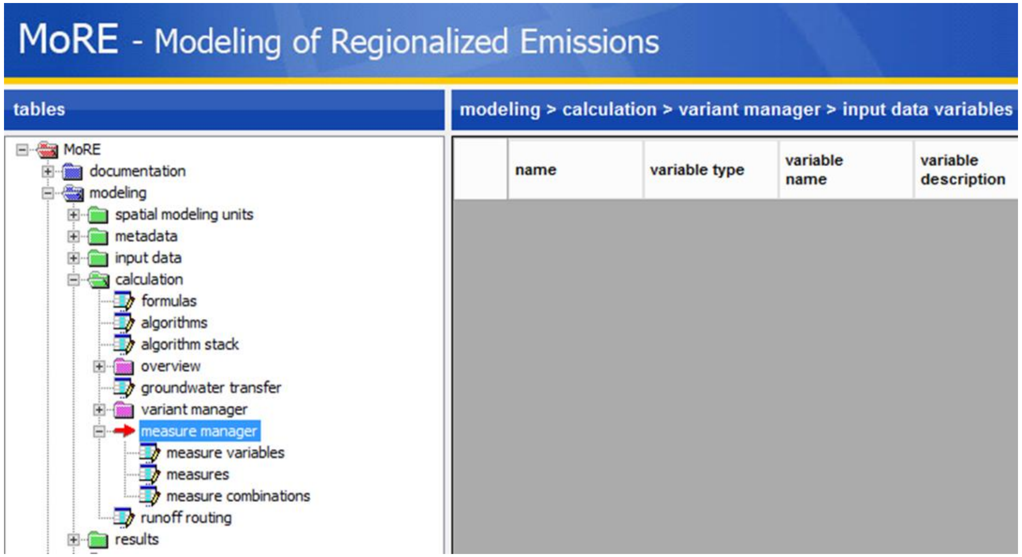
MoRE Developer GUI

- The „measure manager" can be found under „MoRE > modelling > calculation" beside the „variant manager"
- The underlying data structure is the same, therefore a combination of calculation with different variants of input data with the „variant manager" and the evaluation of mitigation measure scenario with the „measure manager can NOT be combined.



Scenario calculation

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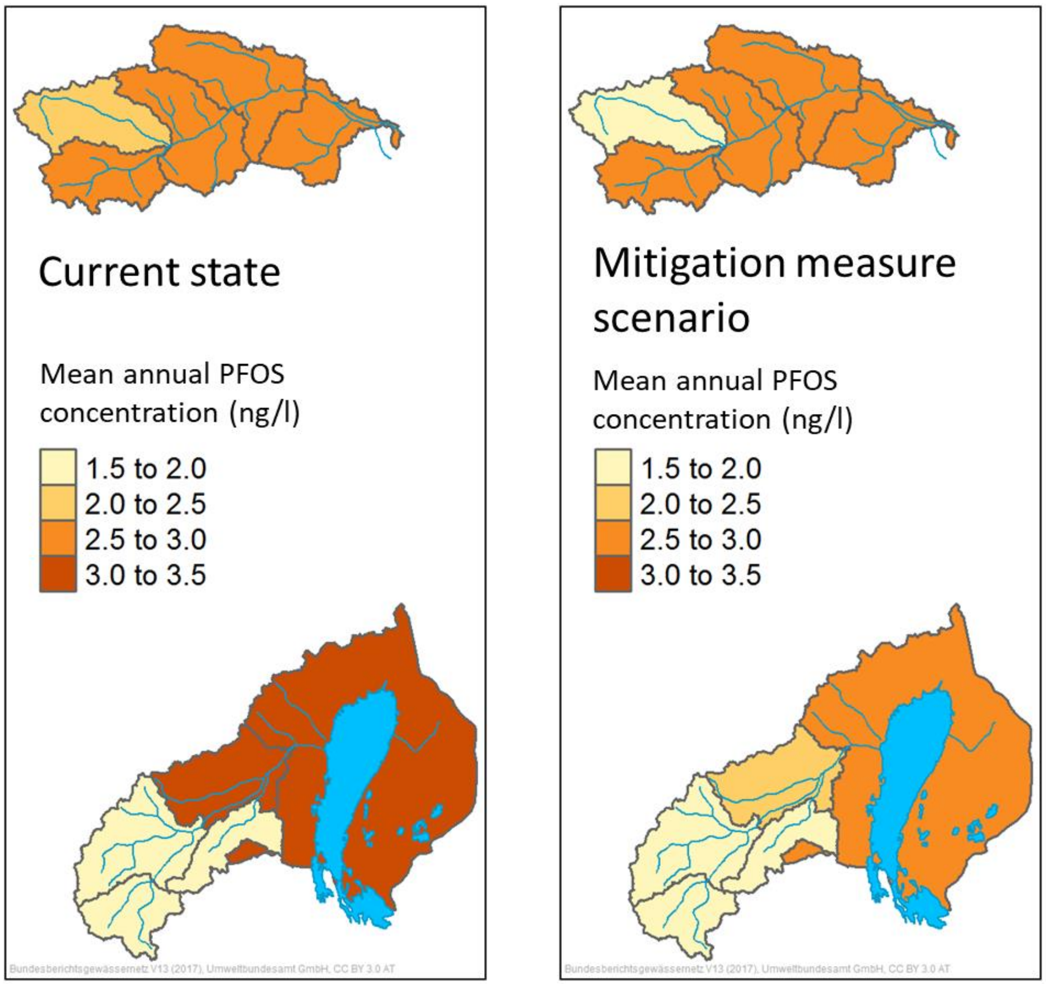
Example results



Picture: S. Kittlaus, TU Wien, Preliminary results

Scenario definition:
Combination of:

- advanced waste water treatment with activated carbon on WWTP > 50 000 PE
  $\eta_{PFOS} = 75\%$
- Storm water treatment with increased fine sediment retention. Efficiency 30 % in CSO and 20% in storm sewers

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Training on hazardous substances emission modelling and scenario evaluation

Comparison of MoRE and DHSM

Vienna, October 5th 2022

Project co-funded by European Union funds (ERDF, IPA, ENI) and National Funds of the participating countries

Content

- Critical comparison of the two models and discussion of complementary aspects.
- Lessons learned in the Danube Hazard m3c project.

Tier according to EU- Guidance Document No. 28

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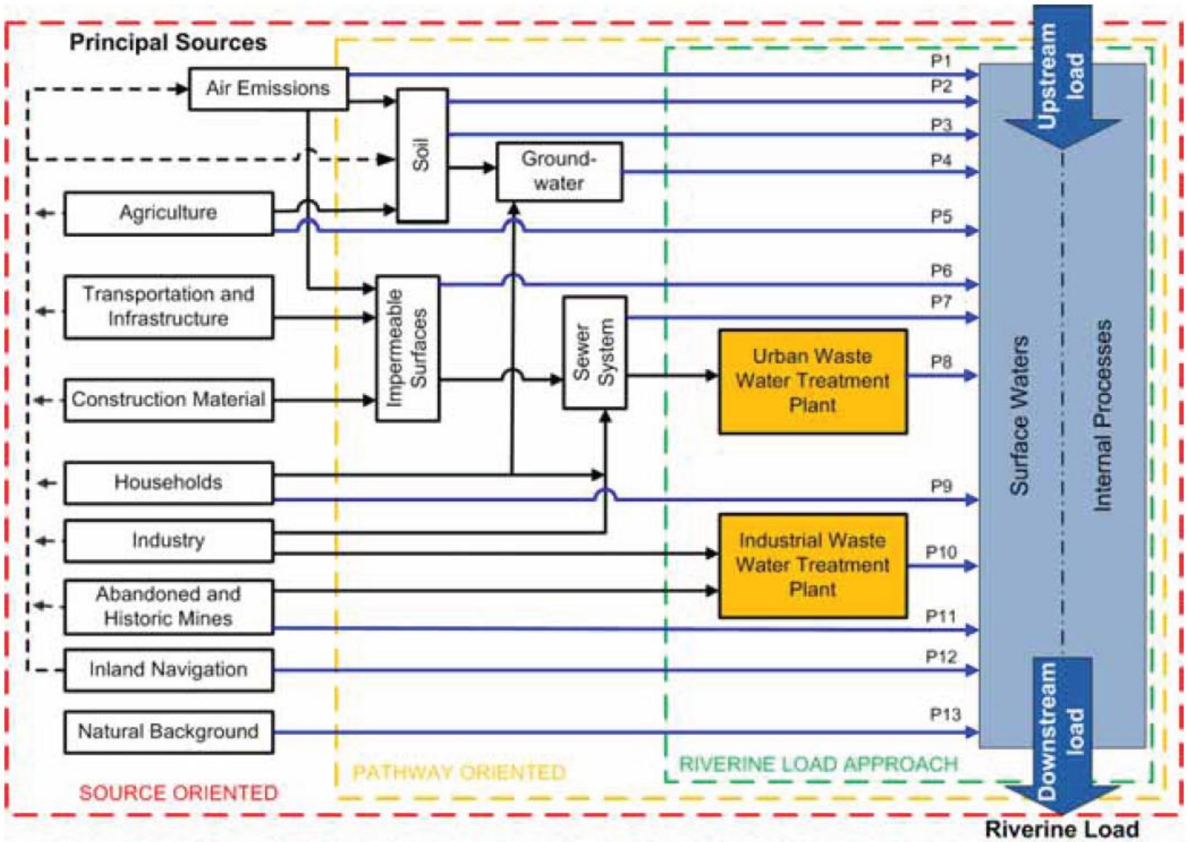
MoRE	DHSM
Tier 3	Tier 4



Tier 4 Tier 3

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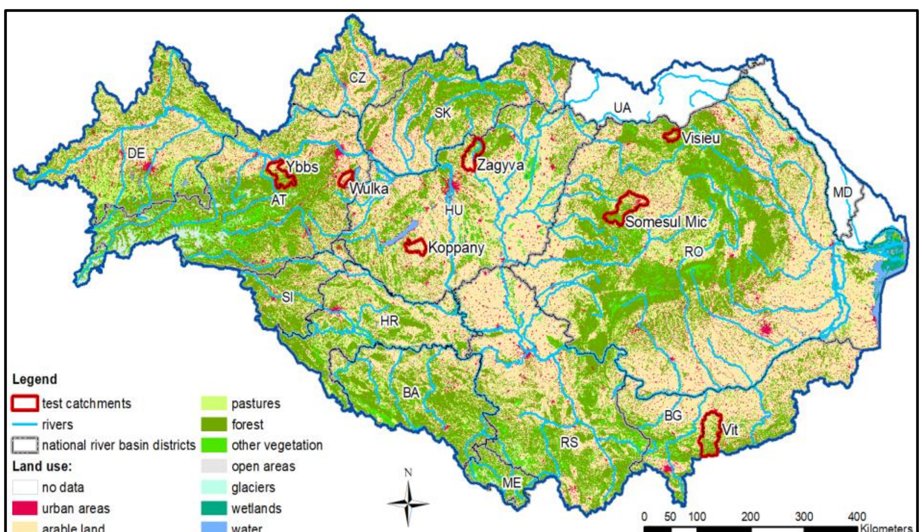
Spatial resolution

MoRE	DHSM
• medium to large scale • (sub-) catchment (> 100 km2) • Depending on data (dis-) aggregation • Currently available for pilot catchments	• large scale • (sub-) catchment(> 1000 km2) • Depending on data (dis-) aggregation • In its current form available for Danube Basin



Spatial resolution

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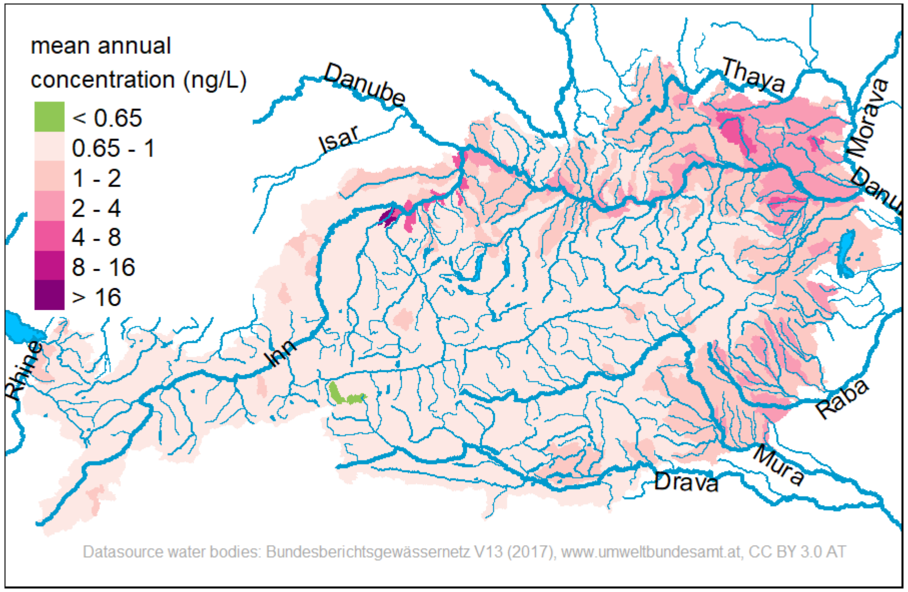
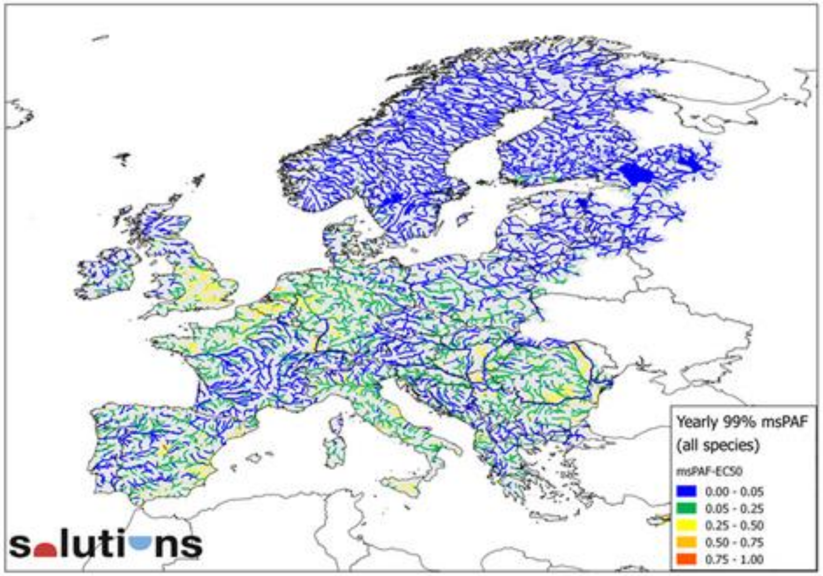
Danube Hazard m³c

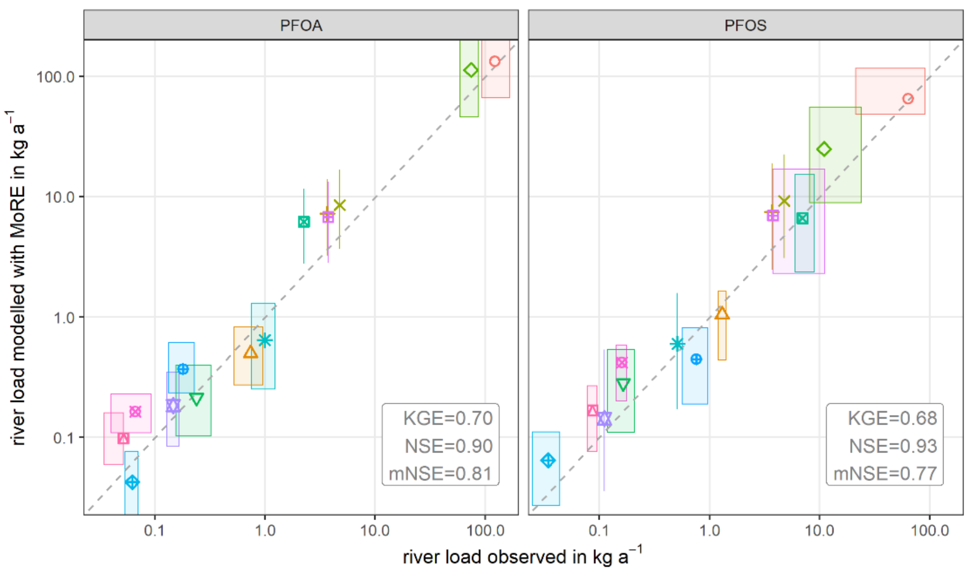
MoRE	DHSM
• medium to large scale • (sub-) catchment • Depending on data (dis-) aggregation • Currently available for pilot catchments • additional versions for national territory of Germany and Austria	• large scale • (sub-) catchment • Depending on data (dis-) aggregation • In its current form available for Danube Basin, • other applications across Europe

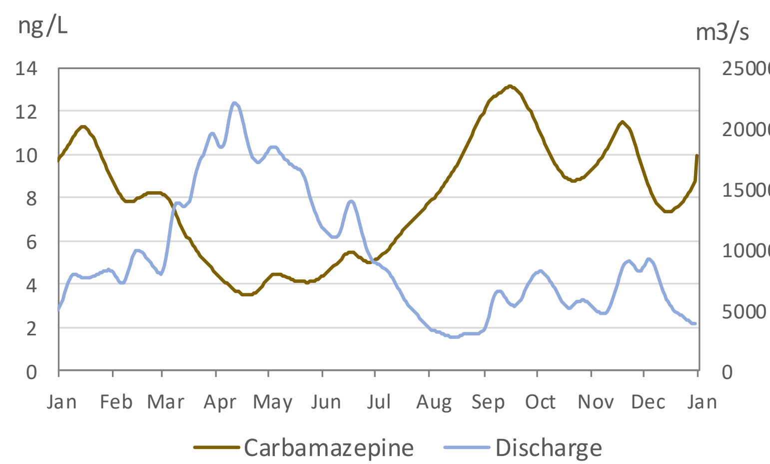




Temporal resolution

MoRE	DHSM
• Yearly average • (Monthly resolution possible with significant additional effort)	• Daily resolution





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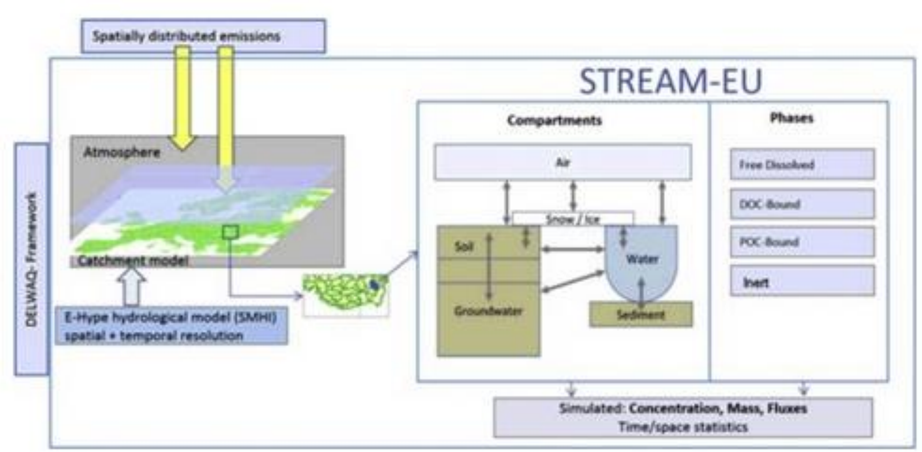
General input data

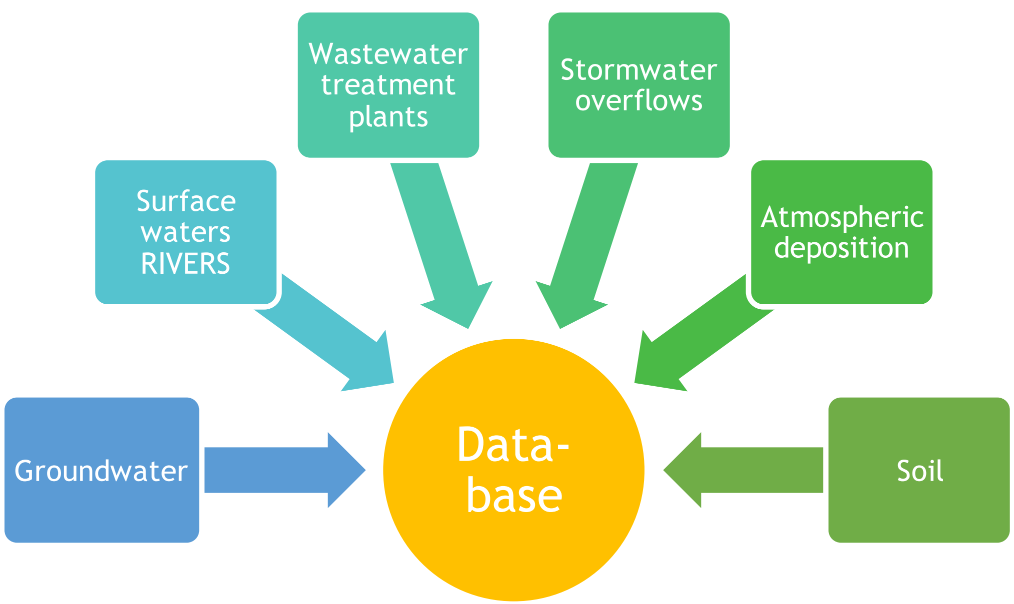
MoRE	DHSM

• Geomorphological data (slope and catchments)
• Land cover and land use
• Hydrological data:
    • Monthly precipitation
    • Potential evapotranspiration
    • Net runoff per catchment
• Urban hydrology: discharge from
    • Municipal waste water treatment plants
    • Industrial direct dischargers
    • Combined sewer overflows
    • Storm sewers
    • Sewers without treatment
• Soil loss and sediment input stratified by land cover
	• Hydrology (rainfall, run-off, water volumes and fluxes)
	• Sediment (erosion, SPM, POC, DOC, settling)
	• Socio-economic variables explaining emissions (population, land-use, …)
	• Infrastructure and management (sewage collection, treatment, stormwater, sludge)



Substance specific data requirements

MoRE	DHSM
• High, • Regionalized information on concentrations in different pathways, • Information on environmental behavior (degradation, adsorption)	• Medium to very high, • Depending on required sectoral resolution and accuracy, from release patterns and chemical/physical substance properties to regionalized information emission factors of all implemented activities including environmental stocks



Substances implementation

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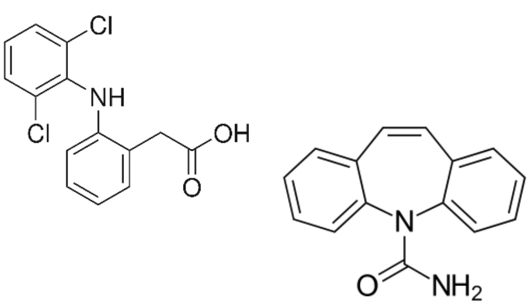
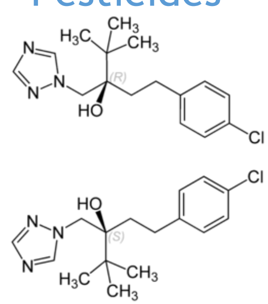
MoRE	DHSM
• Depending on available data, currently about 20 substances on national and pilot level	• > 1700 as screening tool, • Currently about 20 substances as management tool for the DRB

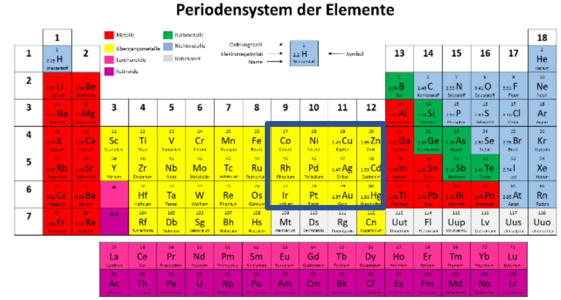
Pharmaceuticals



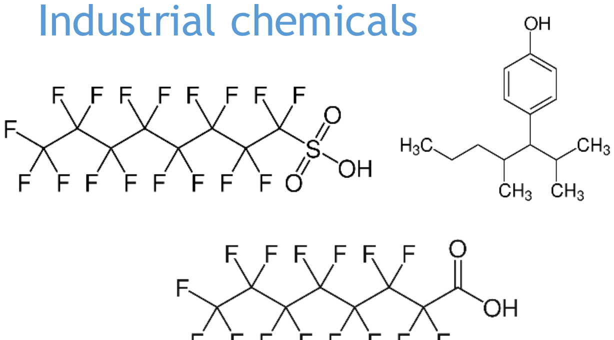
Pesticides



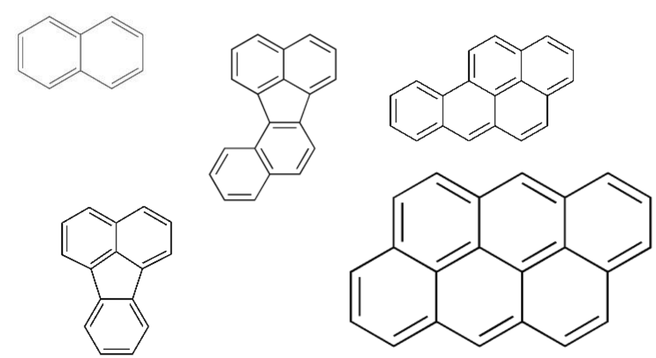
Metals

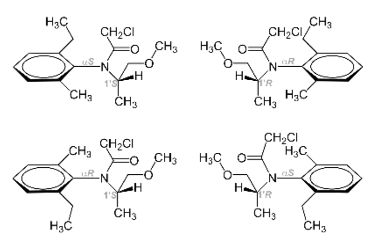


Industrial chemicals



Burning residues (PAH)





Availability, technical requirements

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MoRE	DHSM
• Licensed under GNU Affero General Public License • The server setup needs advanced technical knowledge • The technical requirements are: Windows based PC (8 GB RAM, 100 GB storage) PostgreSQL data base V 9.6, .NET-Framework >= V 4.5.1	• The technical requirements for the DHSM are a Windows based PC (OS Windows 10, 8GB RAM, 20-40 GB storage). • The availability of the model (compiled software + data) is determined by ICPDR. The source code of the software used is open (https://oss.deltares.nl/web/delft3d)

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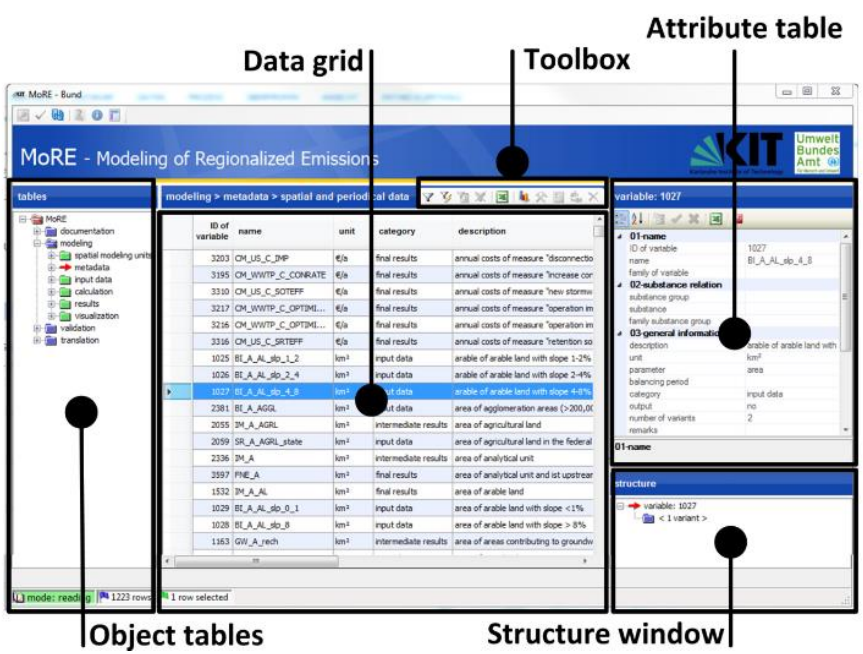
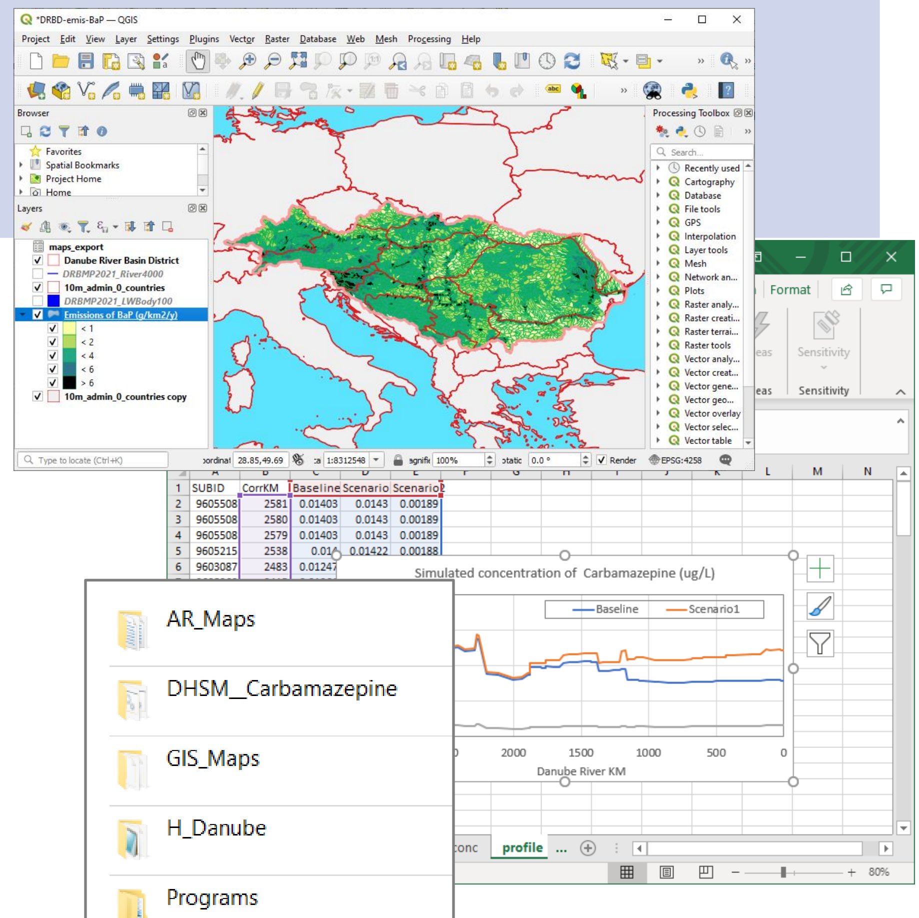
Required technical skills

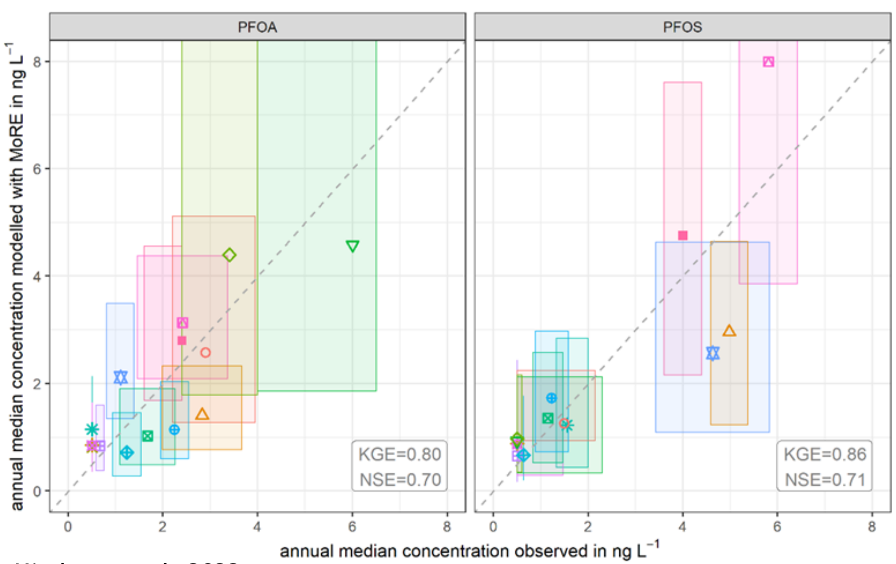
MoRE	DHSM
• Data Preparation: • Geodata management • data analysis • Model usage: • Knowledge of the underlaying quantification approaches	• Data processing & GIS tools



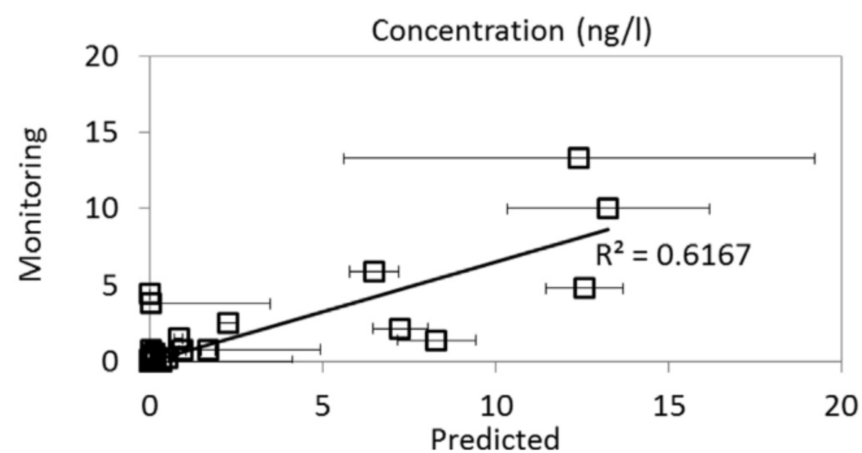


Accuracy

MoRE	DHSM
• Good accuracy has been shown an national level in e.g. Austria for some parameters – very low for other, • challenges increase with relevance of particulate transport	• Depending on substance and data availability; • Challenges increase with legacy pollution and relevance of particulate transport • Decreasing accuracy with decreasing size of catchment



Kittlaus et al. 2022



Lindim et al. 2017

Accuracy (DHm³c, preliminary DHSM)

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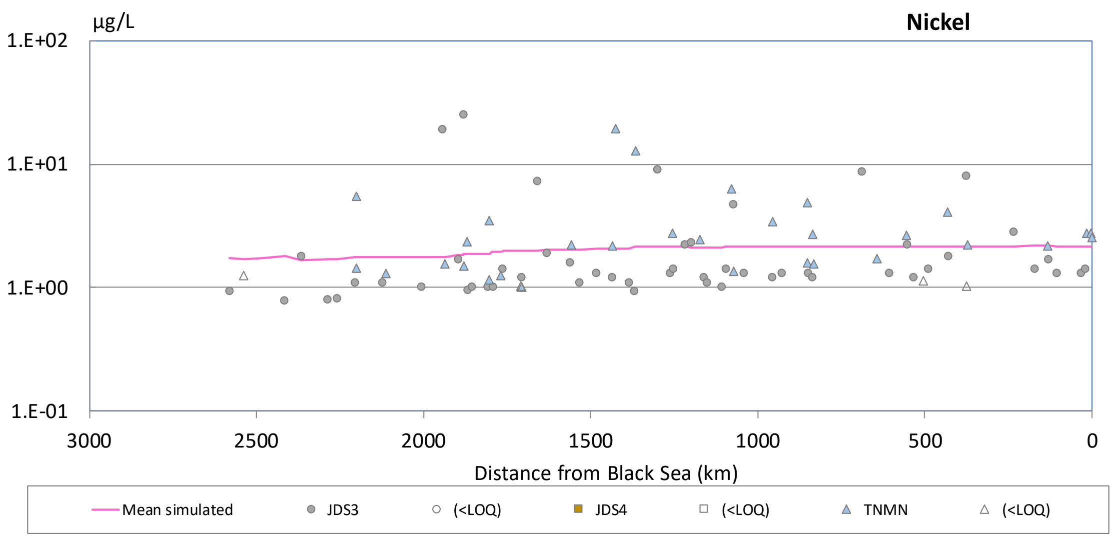

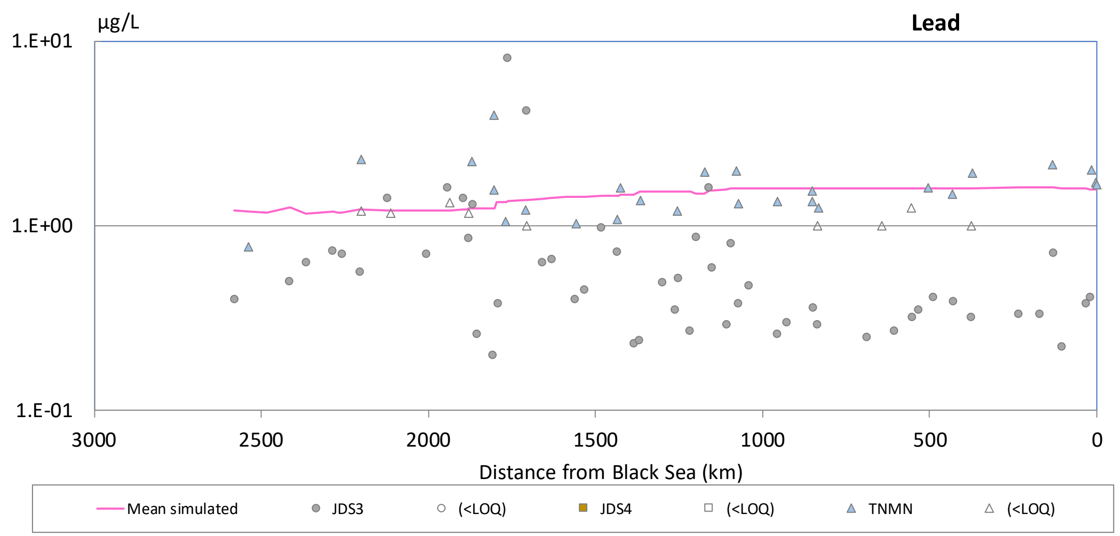

Accuracy (DHm³c, preliminary MoRE)

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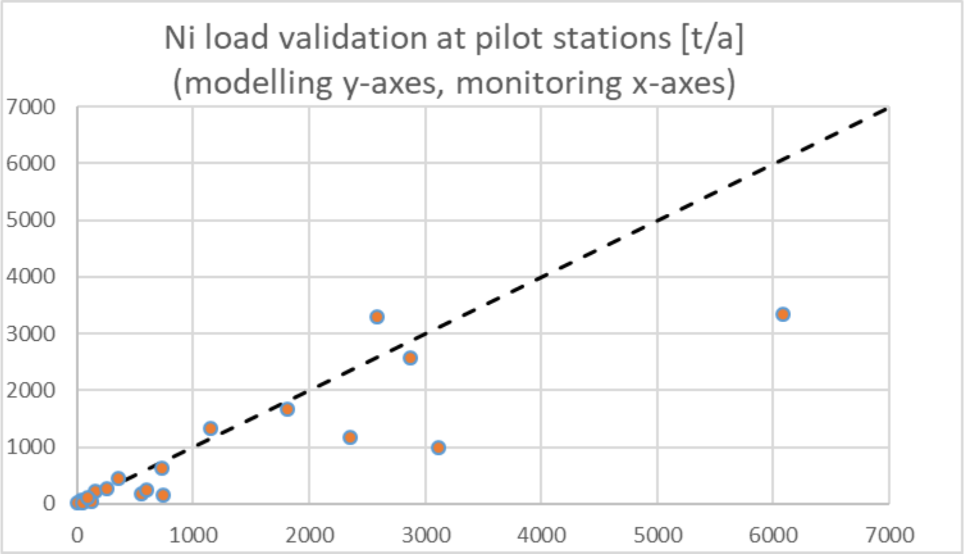

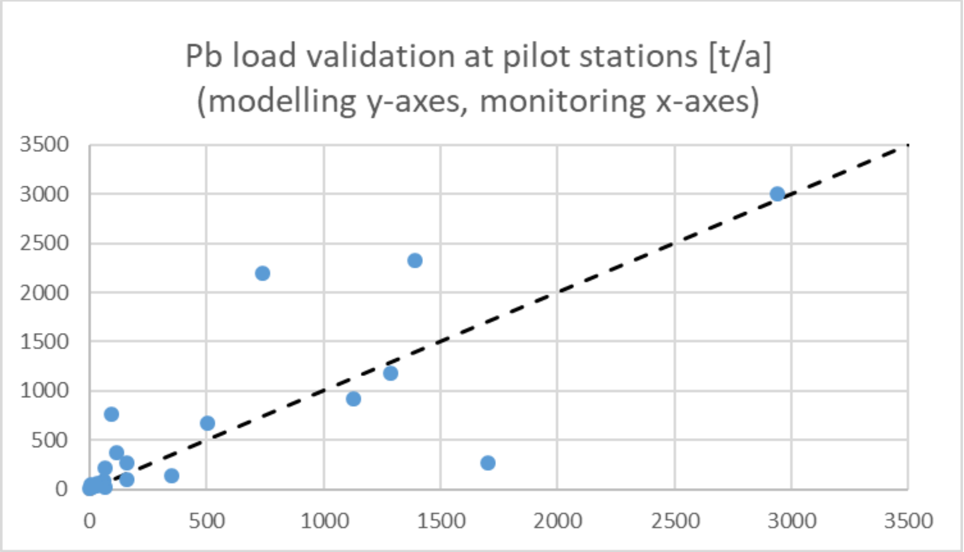

Accuracy (Pilot Regions)

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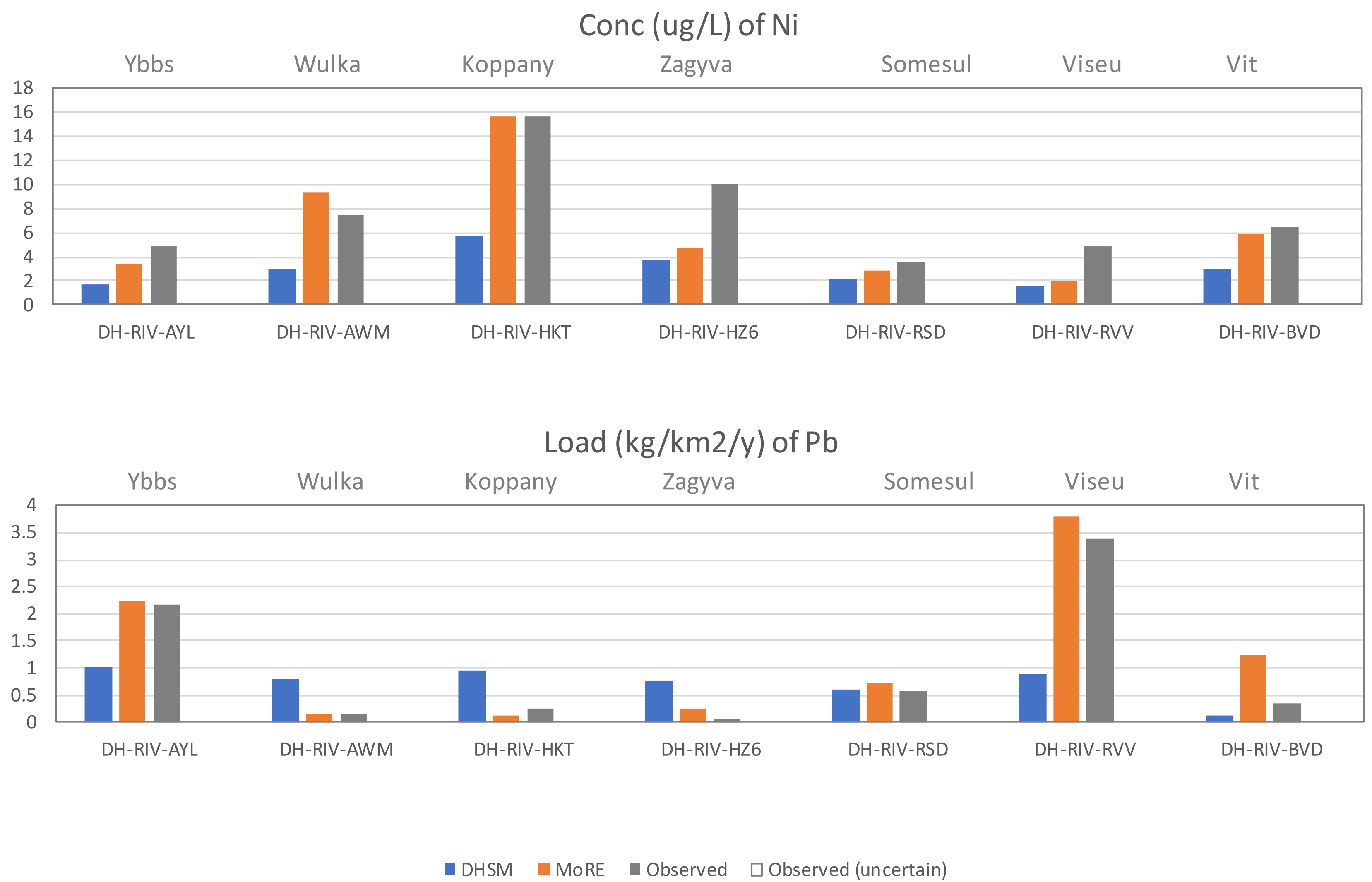

Accuracy (Pilot Regions)

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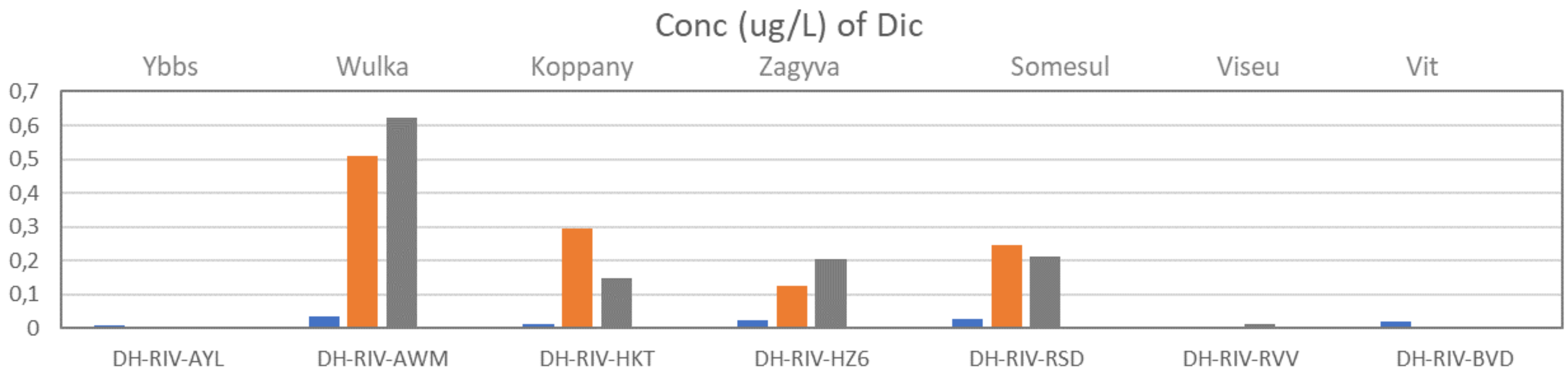

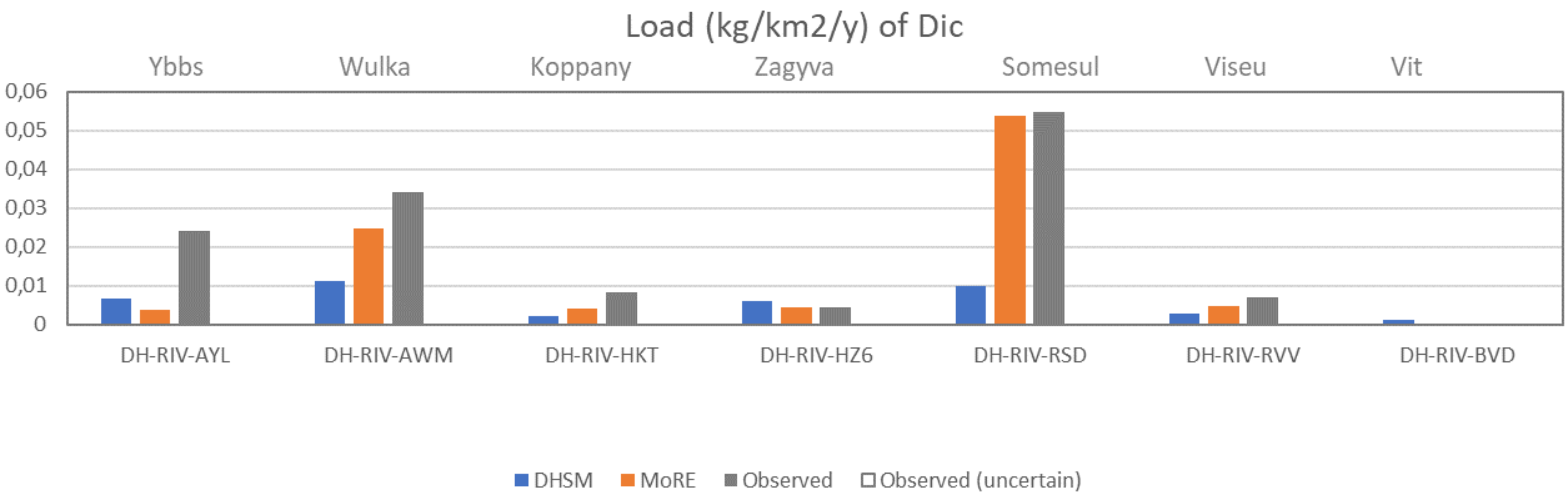

Sources and pathways

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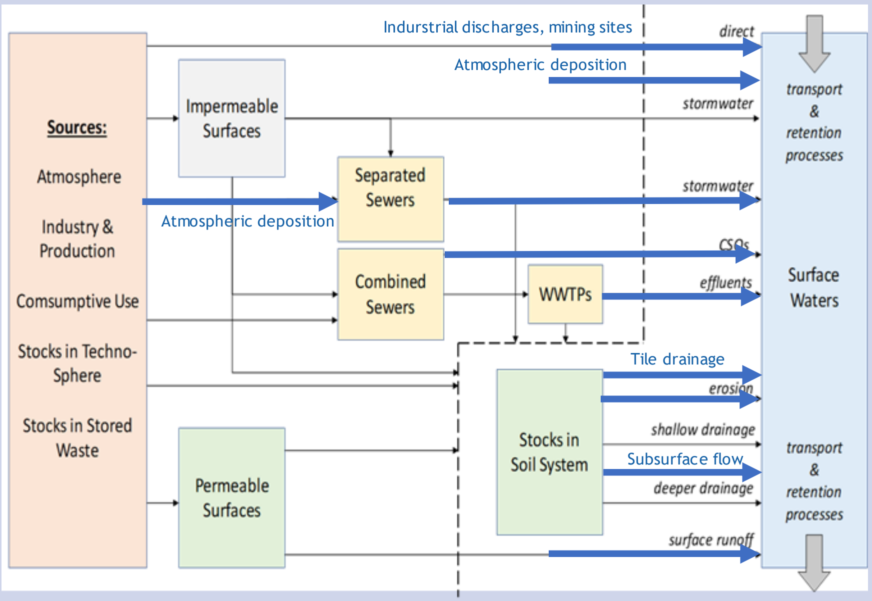
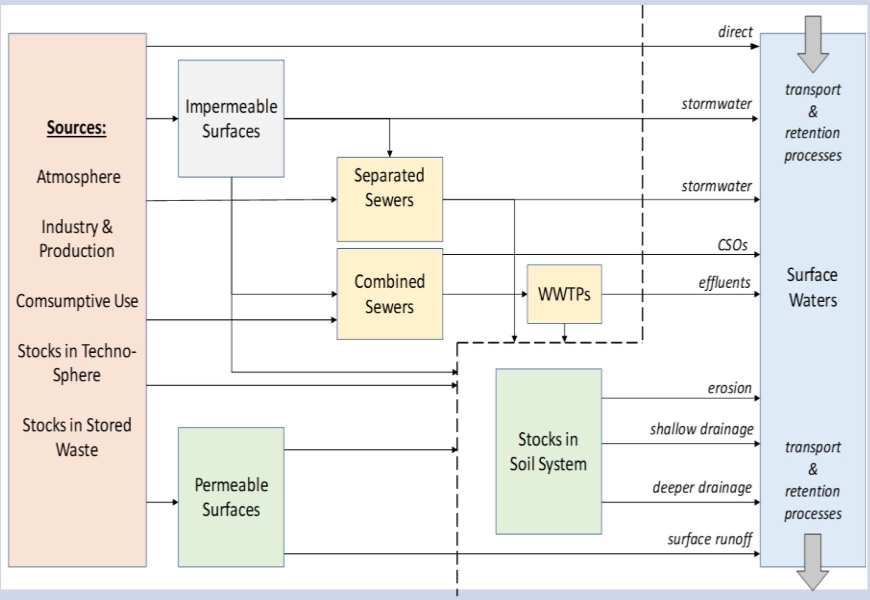
MoRE	DHSM





Pathways (comparison of results)

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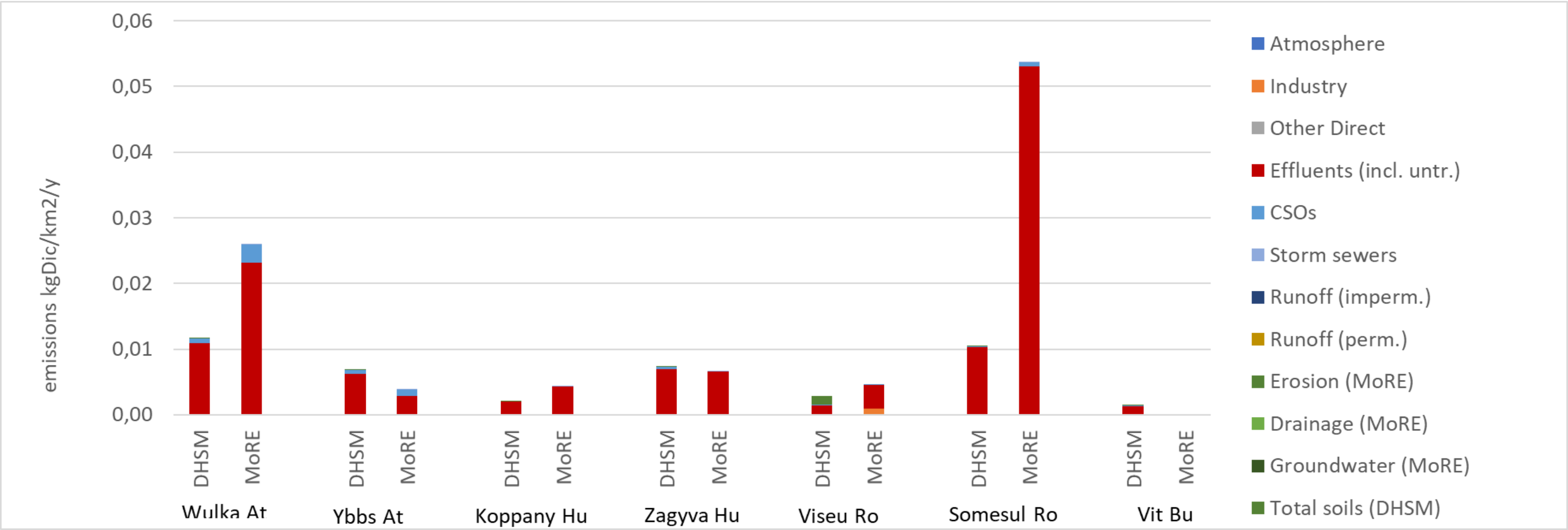
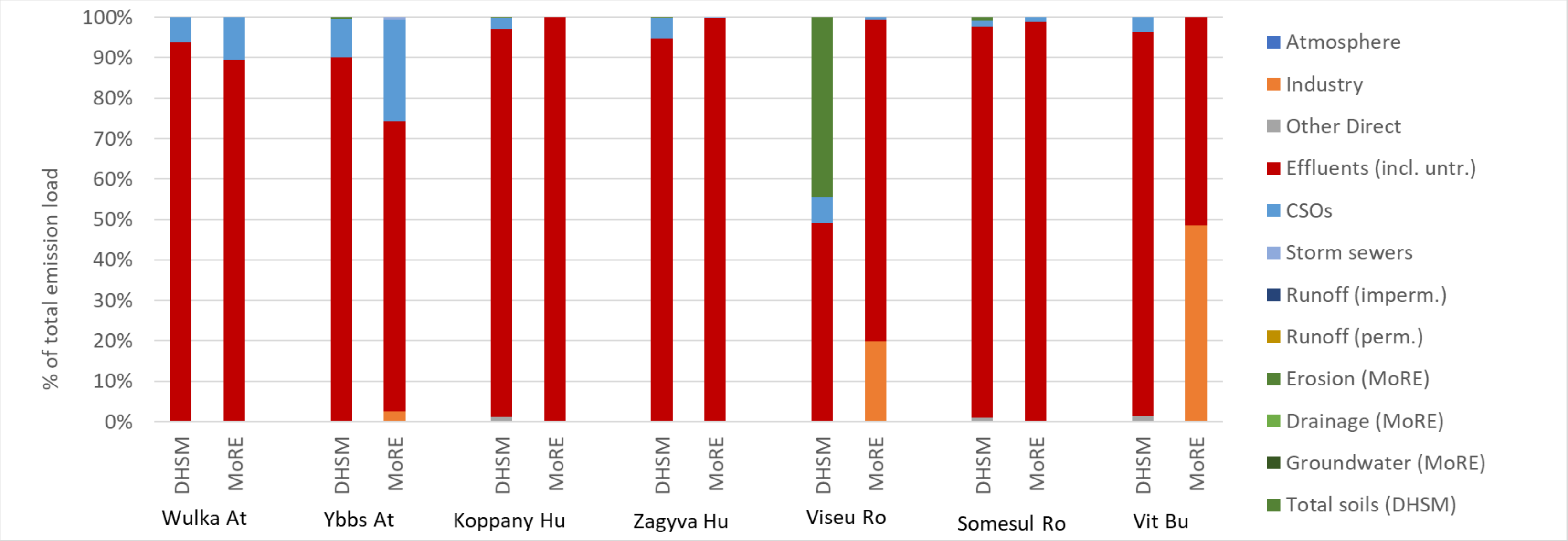
Shares of pathways (Diclofenac)





Pathways (comparison of results)

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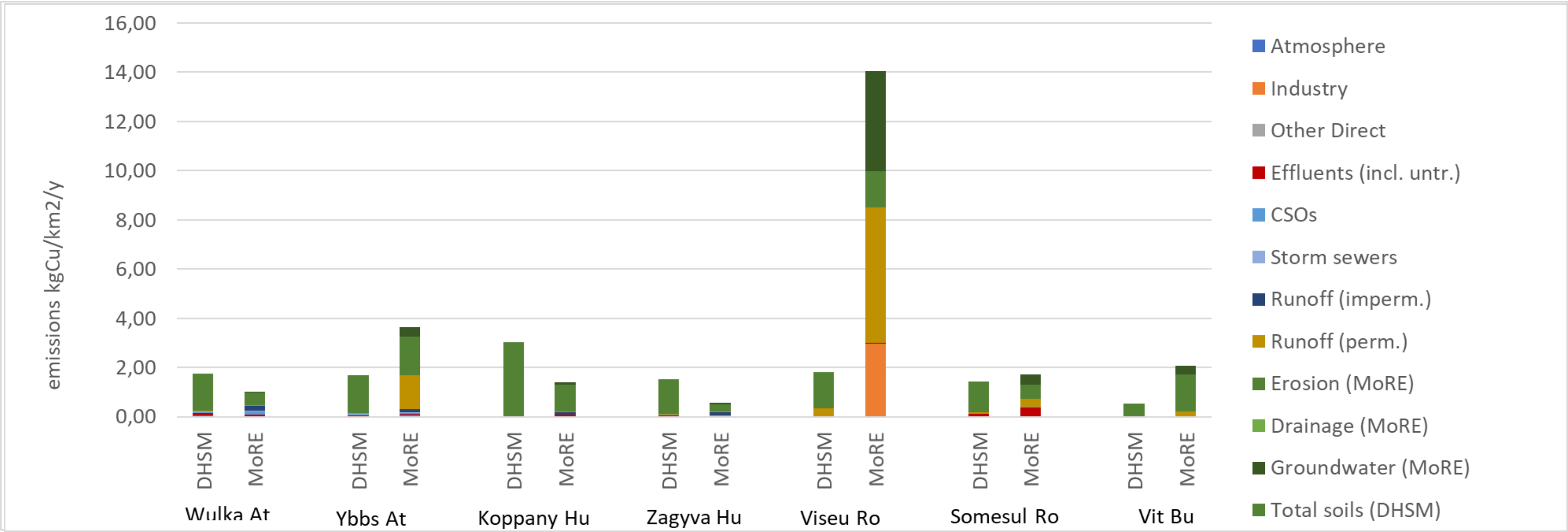
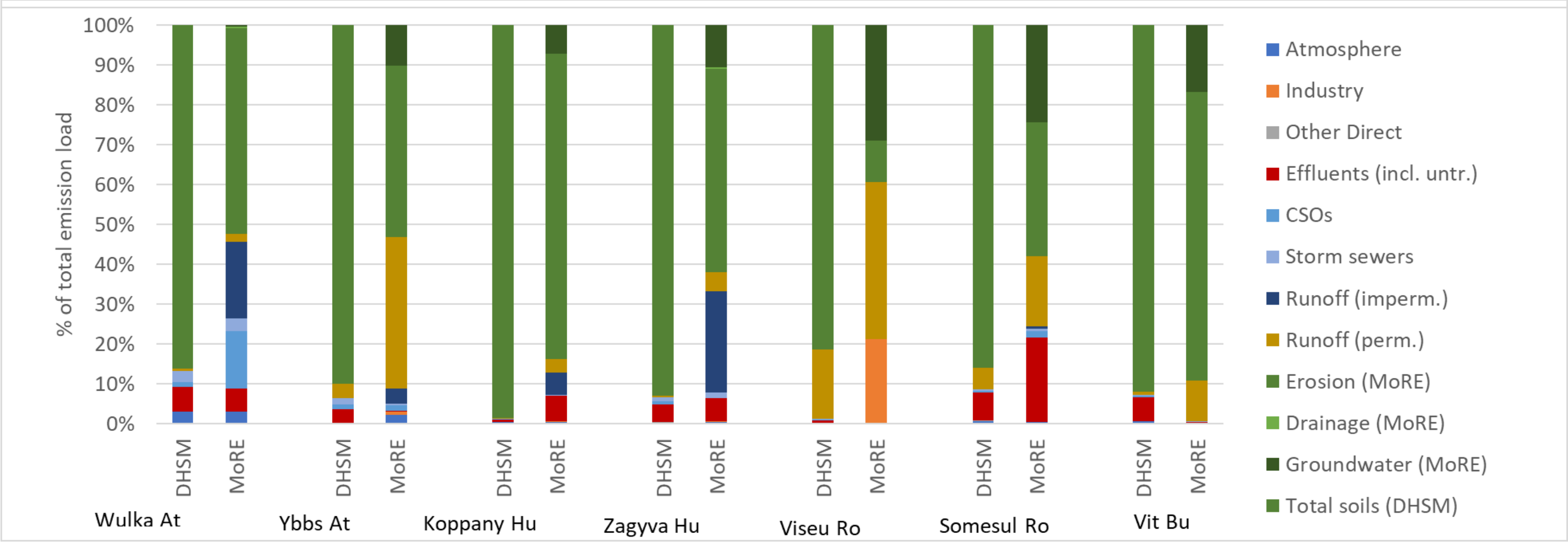
Shares of pathways (copper)





Capability for scenario implementation

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MoRE	DHSM
• Basically restricted to interventions directly into represented pathways, • Alternatively impacts of scenarios on pathways can be calculated externally and be implemented into the model • Climate scenarios may be implemented depended on the underlying hydrological and erosion model	• Changes of sources (use of chemicals, stocks of legacy chemicals) • Changes of management practices affecting pathways (e.g. wastewater collection and treatment, sludge re-use, stormwater collection and management). • The explicit handling of climate scenarios and erosion related measures relies on alternative hydrology and sediment forcing data (not part of DH m3c). • PPs and subcontractors plan to arrange this in future EU funded R&D projects.

Scenarios examples

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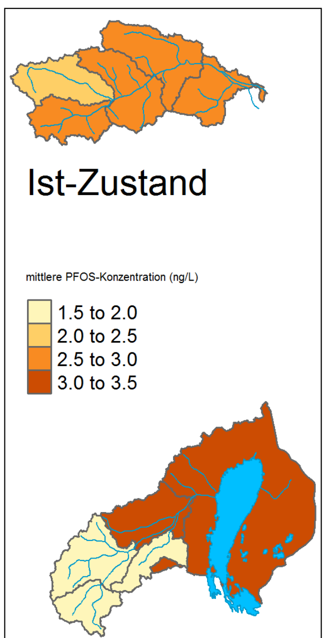
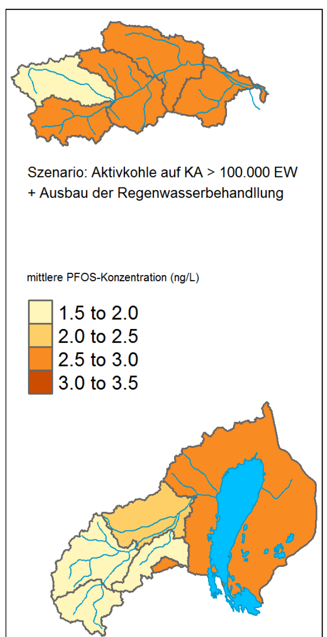
MoRE

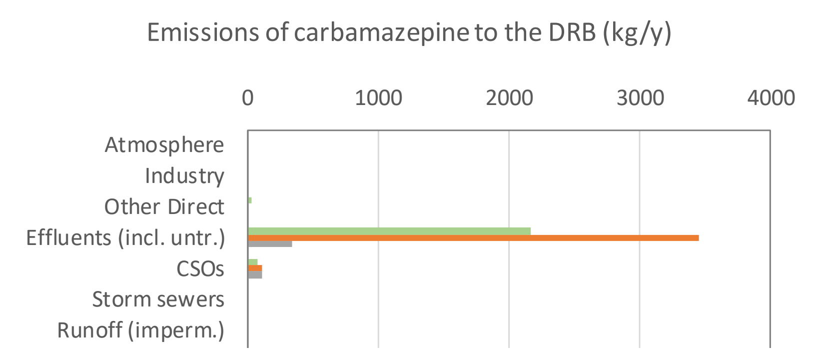
- advanced waste water treatment with activated carbon on WWTP > 50 000 PE ηPFOS = 75%
- Storm water treatment with increased fine sediment retention. Efficiency 30 % in CSO and 20% in storm sewers

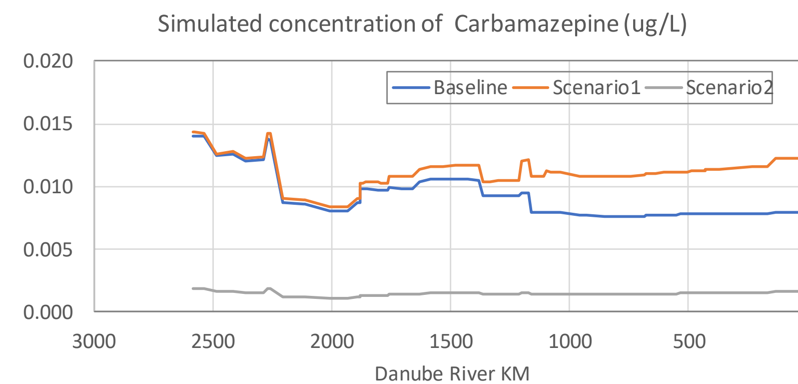




DHSM

- Hypothetical for Carbamazepine:
- Scen 1: all Danube Basin citizens connected to sewer systems
- Scen 2: all treatment advanced





Some thoughts on model comparison and selection

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- Both models have strength and weaknesses.
- Favored Model application highly depends on data availability and needs of countries/applicants.
    - Which data are available or can be collected?
    - Which regional or temporal resolution is required?
    - Which scenarios shall be implemented?
- DHMS gives higher flexibility in selection of parameters, has higher temporal resolution and includes source information – nevertheless to make use of this advantages, sufficient input data are necessary.
- In contrast MoRE is more secure in respect to data management, documentation of model variants and applications by non modelling specialists
- MoRE has the capability to better consider regional differences, more specifically address some pathways and therefore being more accurate at smaller scales – but again, only if regional information is available

Some thoughts on model comparison and selection

- **Performance of both highly depends on quality of input data - models are nothing magic (good hydrological basis is essential).**
- Data storage and data handling are major challenges (especially for longer term usage of a model -> more than just one project)
- Technical skills are required for both models -> training needed, therefore in many cases modelers stick to their "own" model and model selection is a question of tradition to some extent. Requirements to stick to predefined structure is much higher in MoRE, DHSM gives more freedom – which also requires more experiences.

Synergy within DH m3c

- MoRE: good tool for analysis of pathways contributing to emissions and in-stream loads of HS in pilot regions
- DHSM: the instrument for upscaling
- Differences observed in pilot region modelling with MoRE and DHSM to be investigated
- Knowledge and understanding gained used to improve the basin-wide application