

Project Danube Hazard m³c: *Transnational trainings on hazardous substances emission modelling and scenario evaluation*



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

October 2022

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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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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.



Agenda of event

Danube Hazard m³c

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 hazard- ous substances management (<i>Matthias Zessner, TU Wien</i>) 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 (<i>UBA</i>) Technical introduction: scope, temporal and spatial scales; data re- quirements; calculation approaches; technical requirements, condi- tions 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 (<i>Deltares</i>) Interactive and practical exercise session		



Project Danube Hazard m³c: *Transnational trainings on hazardous substances emission modelling and scenario evaluation*

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 <i>(UBA)</i>		
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, UBAExamples 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 complemen- 		
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		





Danube Hazard m³c 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

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

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- Monitoring versus Modelling
- Exposure Models
- Emission Modeling and Emission Inventories
- Predictions and Scenarios



Monitoring versus Modelling for Exposure Assessment

Monitoring versus Modelling for Exposure Assessment



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



Foresight

Calculated ("predicted") environmental concentrations (PEC)

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





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



Exposure models

Exposure models



- 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





"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

"realistic" image of the environment

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

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





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 $logK_{oc}$

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



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





EU-Guidance Document on Inventories



TIER	BUILDING BLOCKS	EXPECTED OUTPUT	RESULTS FOR THE INVENTORY		
STEP 1: ASSESSMEN	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 1	
STEP 2: APPROACHE	S FOR RELEVANT SUB	STANCES			
1. Point source information	Data on point sourcesEmissions factors	Availability of dataQuality of dataIdentification of gaps	Point source emissionsListing 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 	– Step 2	
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 		

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



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 1
STEP 2: APPROACHE	S FOR RELEVANT SUBS	STANCES		
1. Point source information	Data on point sourcesEmissions factors	Availability of dataQuality of dataIdentification of gaps	Point source emissionsListing of identified data gaps	
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3. Pathway orientated approach				– Step 2
4. Source orientated approach	Need for emission models			

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*



Danube Transnational Programme Danube Hazard m³c



Tier 1: Point source information



- 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



- 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





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







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

DHSM use of chemicals



Chemicals in the anthroposphere / technosphere

Production Industrial processes Instantaneous use In service Waste disposal

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

DOI: 10.1289/EHP9372

DHSM stock of chemicals



- 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


Model outputs (Tier 3 and 4)



- River loads and concentrations calculated based on emission loads (and storage/degradation) ⇒ 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)





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

MoRE model Vienna, 04.10.2022

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

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Scope

- Temporal and spatial scales
- Data requirements
- Calculation approaches
- Technical requirements
- Conditions and documentation for its use

Scope – MoRE Emission model



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-Excelmodel into a more stable technical framework
- Application for PAHs

Scientific publication of MoRE:

- Karlsruhe Institute of Technology
- Fuchs et al. 2017

 \bigcirc

Scope – MoRE Emission model



- Pathway-oriented, conceptual model (Modelling of Regionalized Emissions)
- 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







Scope – pathways



Scope – in the DHm3c project



Goals

Q

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

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

Benefits

providing a validated, actual Model adapted to the specific conditions (e.g. status of wastewater treatment and data availability) and a detailed system analysis Visualizing crucial system interactions, dominant pathways, sources and gaps; a precondition of a proper management



Identification of mitigation measures and assessment of their efficiency based on scenario analyses Give guidance and build capacity to master large parts of the management cycle





Pilot regions

			A						
		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	4
	Arable land [%]	60,6	10,5	0,2	42,8	50,9	11,8	30,5	9
2	Arable land > 4% slope [%]	38,9	6,7	0,2	28,9	21,2	8,2	15,4	
Legend	Pasture [%]	3,5	17,2	20,0	5,4	1,9	24,9	11,0	
test ca	Forrest [%]	24,9	48,6	64,8	45,4	38,3	58,7	45,8	
Land use:	Urban area [%]	2,8	5,6	3,2	2,3	3,3	0,4	5,4	
no dat urban arable	Runoff [mm]	60	246	959	197	66	811	40	meters

Temporal scale



- 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



- More operates on catchment scale
- > The model is related to the meso scale (catchments with $\sim 50 >100 \text{ km}^2$)
- 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



Delineation of Subcatchments



- The delineation of Analytical Units (AU) (~50->100 km²) 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



DHm3c Pilot regions















Runoff tree



- 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



 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

1	id point source 💌	year 💌	variable 💌	value 💌	variant 💌 💦	ame of input data set	💌 date	
2	201	2016 V	WWTP_ps_Q	2387050	1 National Wate	er Directorate data for 2019	30.03.20	22
3	202	2016 V	WWTP_ps_Q	493060	1 National Wate	er Directorate data for 2019	30.03.20	22
4	203	2016 V	WWTP_ps_Q	41234	1 National Wate	er Directorate data for 2019	30.03.20	22
5	204	2016 V	WWTP_ps_Q	2340	1 National Wate	er Directorate data for 2019	30.03.20	22
6	205	2016 V	WWTP_ps_Q	102076	1 National Wate	er Directorate data for 2019	30.03.20	22
7	206	2016 V	WWTP_ps_Q	72210	1 National Wate	er Directorate data for 2019	30.03.20	22
8	207	2016 V	WWTP_ps_Q	77865	1 National Wate	er Directorate data for 2019	30.03.20	22
9	208	2016 V	WWTP_ps_Q	83210	1 National Wate	er Directorate data for 2019	30.03.20	22
10	209	2016 V	WWTP_ps_Q	2400	1 National Wate	er Directorate data for 2019	30.03.20	22
11	210	2016 V	WWTP_ps_Q	4130	1 National Wate	er Directorate data for 2019	30.03.20	22
12	211	2016 V	WWTP_ps_Q	3084	1 National Wate	er Directorate data for 2019	30.03.20	22
13	212	2016 V	WWTP_ps_Q	10600	1 National Wate	er Directorate data for 2019	30.03.20	22
14	213	2016 V	WWTP_ps_Q	5000	1 National Wate	er Directorate data for 2019	30.03.20	22
15	214	2016 V	WWTP_ps_Q	77500	1 National Wate	er Directorate data for 2019	30.03.20	22
16	215	2016 V	WWTP_ps_Q	11200	1 National Wate	er Directorate data for 2019	30.03.20	22
17	216	2016 V	WWTP_ps_Q	4100	1 National Wate	er Directorate data for 2019	30.03.20	22
18	217	2016 V	WWTP_ps_Q	301178	1 National Wate	er Directorate data for 2019	30.03.20	22
19	218	2016 V	WWTP_ps_Q	123810	1 National Wate	er Directorate data for 2019	30.03.20	22
20	219	2016 V	WWTP_ps_Q	1375811	1 National Wate	er Directorate data for 2019	30.03.20	22
21	220	2016 V	WWTP_ps_Q	81310	1 National Wate	er Directorate data for 2019	30.03.20	22
•	point sources	constants	analytical u	units variables	periodical AU variables	PS dependent variables	periodical PS varia	ables river segm (+) : (

Data implementation



Note		modeling > input data > constants					7 6 7	<u>Y 6 8 1</u>	1.2 II.4 X II	constant: BI ELEVA crit RAT	E dep
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Image: Second	a modeling									variable	BI_ELEVA_ort_RATE_dep
Production Product	- analytical units	SILmit_PCT_snowmet	1		0.54563728901	-				variant number	1
Products	- point sources	SKUMPCHARL MAX			800	mm/a			in the different of	value	500
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Data requirements



- 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



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

input uata type	Actual Input data code	Indille	description	- unite	v v u na	1005	Roppany	zayy va	VIL	viseu ,	Somesul Mic
Analytical Unit	BI_A	Area of analytical unit	Area of analytical units	km²	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]	km²	Available	Available	Available	Available	Available	Available	Available
Landuse	BI_A_PST	pastures		km²	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	km²	Available	Available	Available	Available	Available	Available	Available
Landuse	BI_A_FOR	naturally covered areas	woods; scrubland	km²	Available	Available	Available	Available	Available	Available	Available
Landuse	BI_A_O	open areas	alpine-mountainous area without vegetation; beaches; dunes	km²	Available	Available	Available	Available	Available	Available	Available
Landuse	BI_A_OPM	surface mining areas		km²	Corine (1.3.1)	Corine (1.3.1)	Available	Available	Available	Available	Available
Landuse	BI_A_URB	settlements	total urban areas	km²	Available	Available	Available	Available	Available	Available	Available
Landuse	BI_A_IMP	impervious urban area	paved areas inside urban areas: settlements; industrial estates; car parks	km²	Available	Available	Available	Available	Available	Available	Available
Landuse	BI_A_WL	wetlands		km²	Available	Available	Available	Available	Available	Available	Available
Landuse	BI_A_OR	country roads	paved road area; not included in settlements	km²	Available	Available	Available	Available	Available	Available	Available
Landuse	BI_A_REM	other remaining areas	if not very small, please indicate landuse as comment	km²	Available	Available	Available	Available	Available	Available	Available
Drainages	TD_SHR_a_td_agrl	Tile drained areas	from arable land and pastures	km²	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 run off from	modelling period; annual data on subcatchment level	m³/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	m³	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	m³	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	m³/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_sep	ot	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)	m³/a	Available	Available	Available	Available	Available	Available	Available
Industrial wastewater	ID_ps_Q	disch arge	runoff via industrial direct dischargers	m³/a	Available	Available	Available	Available	Available	Available	Available





Data requirements-Examples of alternative data sources Danube Hazard m³c

Source: EUROPEAN SOIL DATA CENTRE (ESDAC)JRC



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

Data requirementsgeneral



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



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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



Technical implementation



- 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

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Technical requirements



- ➢ 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:



- 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 <u>https://more.iwg.kit.edu/wiki/index.php?title=MoRE_Developer</u>
- 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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Danube Hazard m³c 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

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





Scope, temporal and spatial scales



- 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



- "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)



- 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



- 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			
Copper	x	x	x	x	X	X			
Arsenic	x		X		X	X			
Nickel	х	х	х		х	Х			
Mercury	х	х			х	х			
Zinc	х	х	х	Х	х	Х		x	
Benzo[a]pyrene	х		х		х			х	
PFOS					х				
PFOA					х				
Bisphenol A					х				
Nonylphenol			х		х	х			
4-tert-									
octylphenol					Х	Х			
Metolachlor		х			Х				
Tebuconazole		х			Х				
Carbamezepine					Х				
Diclofenac					Х				
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





- Atmospheric deposition
 - European
 Monitoring &
 Evaluation
 Programme





- 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)



- 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 we	ar (mg/vkm)	100		300	600		50	
	Brake w	/ear (mg/vkm)	10		30	40		5	
	Road su	rface wear (mg/vkm)	150		⁷⁰⁰	700		60	
Substa	ance	Tire wear (light traffic	c) Tire wear (heavy	/ traffic)	Brake wear	Tar-based asphalt	Bitum	en-based asphalt	Motor oils
Cd (g/	'g)	1.00E-06	1.00E-06		0	0		0	5.00E-07
BaP (g	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	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

Austria Per capita traffic volume Per capita traffic Per capita traffic Per capit	- +
(Mvkm/cap/y) volume (Mvkm/cap/y) volume (Mvkm/cap/y) volume (Mv	km/cap/y)

* <u>https://www.emissieregistratie.nl/</u>



- Built Environment
 - Activity rate: population
 - **Emission factor**: per capita emission (mass/cap/time)
- Provisional EFs in kg/cap/d are:
 - 1.15531^{E-05} for Zn
 - 3.90642^{E-06} for Pb
 - 1.65044^{E-06} for Cu



- 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
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Substance	Fuchs et al. (2010) ⁽¹⁾	NL-PRTR (2)	WWTP data	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		



- 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



- 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 ind	ividual PAHs in emissions	from coatings and bilge	water (Deltares and TNO, 2016).
		0 0	

РАН	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[<u>a,h</u> ,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

+



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



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



Calculation approaches: Methodology Danube Transnational Programme Danube Hazard m³c

- The SOLUTIONS project Solutions
 - 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





DHSM: Source oriented approach

Tier approaches

in Step 2



TIER	BUILDING BLOCKS	EXPECTED OUTPUT	RESULTS FOR THE INVENTORY
STEP 1: ASSESSMEN	IT 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: APPROACHE	S FOR RELEVANT SUB	STANCES	
1. Point source information	Data on point sourcesEmissions factors	 Availability of data Quality of data Identification of gaps 	Point source emissionsListing 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			
арргоаст			
4. Source orientated approach		Need for emission	models

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



• sources as defined in WFD-CIS Guidance

(Common Implementation Strategy; European Comm., 2012).

• Losses of polutants distributed in space



Pathways ... from source to river



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



Pathways ... zooming in



• From Impermeable Surfaces to Surface Waters:





Model Scheme



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?



• PFOS, PFOA:



- "missing relevant sources or processes"

• Pesticides & pharma's:

longitudinal profiles plot

- lack of regionalized use data
 - "Met" & carbamazepine underestimated, "Teb" & diclofenac overestimated

Calculation approaches: results



4tO

Urban runoff

• Section 6.1 of the report:

Direct inputs

- 100% 80% 60% 40% 20% 0% Pb Cd BaP PFOS PFOA BPA Teb NP Cu As Ni Hg Zn Met Car Dic
- 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-tertoctylphenol, NP: nonylphenol, BPA: bisphenol-A, PFOS: perfluorooctanesulfonic acid, PFOA: perfluorooctanoic acid, Teb: tebuconazole, Met: metolachlor.

Soils

Mixed sewers

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

Runoff

Calculation approaches: results



Zooming in: detailed balances for compartments •



– Balance terms: In, Out, Storage, Decay

Calculation approaches: results







- 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





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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%).





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





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 - Carbamazepine: WWTPs dominant (high population and high connection rate to sewers)



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





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







- 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





- 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





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



Support/investigate source controls & precautionary measures



- 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



- 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 (<u>https://oss.deltares.nl/web/delft3d</u>)

Documentation

- general user guide (<u>https://oss.deltares.nl/web/delft3d</u>)
- 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)



Technical Reference Manual
Questions?











Danube Hazard m³c 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



*This map represents preliminary modeling results produced by the Danube Hazard m3c project based on incomplete database and an initial modeling approach. The database, the model and the results will be updated in 2022. Emission estimates were based on basin-wide data on substance use. www.icpdr.org

This EXPR product to based on national information provided by the Contracting Pagina to the EXPR (AT BA BD, CZ, Der, RF, HU, MD, ME, FO, DS, SL, SF, UJ) and C/H. EuroSbathler, data from the European exa used for all national bodynes except for AL, BA. (RE where the data from the European examination and the system and the DB and AL, TL, The and PL.

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





Riverine load

Points to remember





Riverine load

Points to remember





Riverine load

The model system lay-out





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 / advectiondiffusion 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

The software we use

Documentation:

- general user guide (<u>https://oss.deltares.nl/web/delft3d</u>)
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D-Water Quality Input File Description



Technical Reference Manual

Files and folders



(anna)	AR_Maps
1 ac	DHSM_Carbamazepine
	GIS_Maps
	H_Danube
	Programs
(unu)	WW_Man

"activity rate" maps

files for modelling a substance

some maps for GIS presentations

stored schematization, hydrology and sediment data

DELWAQ programme and supporting tools

maps related to wastewater and stormwater management

Files and folders (2)



(Junit)	input_subs	substance-specific input
B	output	final output
F.	present	presentations of results
Samuel	run	(folder where actual calculations take place)
1	system	(definition of workflows)
100 m	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

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





D-Water Quality Input File Description



Technical Reference Manual

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)



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] —							_	×					
<u>F</u> ile <u>E</u> dit	<u>O</u> ptions	En <u>c</u> oding	<u>H</u> elp										0 <u>%</u>
;	FSew 0.60 1.00 0.60 1.00 1.00 0.13 1.00 0.79 0.88 0.95 0.99 0.00 0.74	FSep 0.00	FDCTP 0.40 0.00 0.40 0.00 0.87 0.00 0.21 0.21 0.12 0.05 0.00 1.00 0.26	FTr0 0.00 0.00 0.00 0.00 0.00 0.00 1.00 0.00 0.00 0.00 1.00 0.00 1.00	FTr1 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.	FTr2 1.00 1.00 1.00 1.00 0.17 1.00 0.00 1.00 1	F\$1dInc 0.20 0.65 0.65 0.65 0.65 0.20 0.56 0.20 0.18 0.18 0.18 0.56 0.10 0.11	fComSew 0.50 0.70 0.70 0.70 0.50 0.28 0.60 0.50 0.50 0.28 0.50 0.28 0.10 0.85	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	Danube 1 2 3 4 5 6 7 8 9 10 11 11 12 13	SUBID 9000145 9000229 9000233 9000235 9000236 9000236 9000385 9000385 9000400 9000665 9000665 9000674 9000678 9000678	Country Ukraine Germany Germany Germany Ukraine Austria Moldova Hungary Hungary Austria Slovakia Czech Rep.	
<	A 00	0 00	0 40	0 00	0 00	4 00	0 00	0 7 0	-	a 1.	0000/00	en	>

Input processing



- 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)





substance-specific input

final output

presentations of results

(folder where actual calculations take place)

(definition of workflows)

run step 1: emission model (< 1 minute)

run step 2: water quality model (20-30 minutes)

run postprocessing steps

Substance specific input data



- activity rate source industry
- activity rate source navigation
- dry deposition rate
- emission factor agriculture
- emission factor built environment
- emission factor households
- emission factor road traffic
- fate and transport model parameters
- initial concentrations in top soils
- 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



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*



AR_Maps
DHSM_Carbamazepine
DHSM_Carbamazepine_ScenTest
H_Danube
Presentation
Programs
WW_Man

Deltares



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)



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	For each plant or	Annual
		effluent concentration	lumped over AU	average
Point	Industrial WWTP effluent or	Effluent loads OR water amount and	For each plant or	Annual
	direct industrial discharge	effluent concentration	lumped over AU	average
Point	Abandoned mining site	Effluent loads OR water amount and	For each site or	Annual
		effluent concentration	lumped over AU	average





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

Type of pathway	Pathway	Input data	Spatial scale	Temporal
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
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
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, ...





Danube Hazard m³c



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)
<u>E-OBS</u>	Europe	0.1°/0.25°	1950 - present	Day	NetCDF-4
ERA5 - Land	Global	0.1°	1950 - present	Month, Day, Hour	GRIB (binary grid)
<u>CarpatClim</u>	44-50°N 17-27°E	0.1°	1961 - 2010	Day	Gridded data
<u>Climate Forecast</u> System Rean. CFSR	Global	0.5°	1979 - 2017	Day, Month	GRIB
European Climate Assessment and Dataset	Global		1755 - 2020	Day, Month	Point data (CSV)
<u>GPCP</u>	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: <u>E-hype</u>, <u>CWATM</u>, <u>LISFLOOD</u>, ...









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!





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

- + continuous online measurement of indicator parameters:
- turbidity
- conductivity



←→ High flow events:

flow proportional sampling with autosamplers







Point sources outlets

Inflow or outflow? ^(c) **Outflow** from plant, inflow into the river

Urban systems (w or w/o industrial)



WW treatment:	Not present	Present
Channel system:		
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 m³) 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 reuse. 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! 47









Concentration from single measurements over time



Danube Hazard m³c

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

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





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

Methods:

- Averaging ~ interpolation $L \approx \overline{q} \cdot \overline{c}$
- Proportion estimation
- Regression









Load calculation: stratification

Stratificaiton

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

Applicable to every method



$$L \approx \frac{365}{12} \sum_{m=1}^{12} \frac{\sum_{i} Q_{im}}{N_m} \cdot \frac{\sum_{i} c_{im}}{n_m}$$
$$L \approx \frac{365}{4} \sum_{h=1}^{4} \frac{\sum_{i} Q_{ih}}{N_h} \cdot \frac{\sum_{i} c_{ih}}{n_h}$$







Load calculation

- 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	% of SS	% of	% of SS	% of	% of SS
		runoff	load	runoff	load	runoff	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%



Danube Hazard m³c



Censored data (<LOD, <LOQ)

- LOQ \gtrless 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

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







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





Clay content

Depth (cm)

15-30

30-60

60-100

100-200



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





0 - 0.5 0.5 - 1 1 - 2 2 - 5 5 - 10 10 - 20

20 - 50 >50

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Danube Transnational Programme Modelled spatial data – Soil loss

Source: e.g. European scale map from JRC







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
 - Ftc





Danube Transnational Programme 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

	Da	Input
Example:nutrient budgets		Farm Land
	Animal products	

Input	Output	Surplus
Farm Land Soil	Farm Land S	oil Farm Land Soil

٦.

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

Source: OECD manual, 2013

Input data nitrogen surplus

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scales and resolution







Spatial data source type: application rates

Peszticide use data

- \rightarrow direct use to create map
- \rightarrow Link information to plant
- Production data
- \rightarrow 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	evapotranspiration
Precipitation	monthly values	mm	precipitation





Input data – population, canalization & point sources

name	description	unit	parameter
Statistical Data about inhabitants a	nd 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	m³	storage volume
US_cso_VOL_SOT	storage volume of stormwater overflow tanks in combined sewer systems	m³	storage volume
US_cso_VOL_spec_SOT	storage volume of stormwater overflow tanks in combined sewer systems, area-specific	m³/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 consumption
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)	m³/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	evapotranspiration
Precipitation	monthly values	mm	precipitation
Hydrology			
Net runoff from catchments	if available, otherwhise 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







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)









and pollutant loads based on the applied river sampling



2020/ 11/ 25.2021/ 1/ 24.2021/ 3/ 25.2021/ 5/ 24.2021/ 7/ 23.2021/ 9/ 21.2021/ 11/ 20.2022/ 1/ 19.2022/ 3/ 20.2022/ 5/ 19.





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 inventorylegal requirements



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



TIER	BUILDING BLOCKS	EXPECTED OUTPUT	RESULTS FOR THE INVENTORY	
STEP 1: ASSESSMEN	T 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 1
STEP 2: APPROACHE	S FOR RELEVANT SUBS	STANCES		
1. Point source information	Data on point sourcesEmissions factors	Availability of dataQuality of dataIdentification of gaps	Point source emissionsListing of identified data gaps	
2. Riverine load approach	add:River concentrationData on dischargeIn 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 approach4. Source orientated approach		Need for emission r	nodels	– 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





Use of MoRE in the management cycle



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



Use of MoRE in the management cycle



- 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





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



Mean modelling variant





Minimum modelling variant





Maximum modelling variant



Risk Analyses



- Calculation of a risk quotient (RQ = c_{River,calculated}/EQS) for 754 outlets from subcatchments
- 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



Risikoguotient (Minimalvariante) - Fluoranthen (FLU) Risikoquotient (RQ): Verhältnis der Gewässerkonzentration zur UQN; UQN = 0,0063 [µg/I] Minimalvariante Gewässemetz RQ Fluoranthen (FLU) nach Klassen Fluss (Einzugsgebiel > 100 km²) See (> 0,5 km²) RQ < 1 Verwaltung 1 ≤ RQ <2 Staatsgrenze 2 ≤ RQ <5 - Bundeslandgrenze 5 ≤ RQ < 10 Städte RQ ≥ 10 Landeshauptstadt keine Bewertung STOBIMO Teileinzugsgebiete Datenquelen. 10 Wen. Umbeitbundesamt 6mb-

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	5	25	 75	100 Km		Institut für Wasserplite und	Nachhaltigkeit und
Auswartung/Graphic Unwoltounocsamt GmbH, 2010					umweltbundesamt [®]	Ressourcenmanagement	Tourismus

Risikoquotient (Maximalvariante) - Fluoranthen (FLU)



Datempelen. 10 Wen: Umweltvandesamt GmbH							Whitiwe 1	Bundesministerium
Auswartung Graan Kr. Umwaltundasanti Gineki. 2010	ò	21	ca .	75	SOC Km	umweltbundesamt [®]	Institut für Wessergüte und Ressourcenmanagement	Nachhaltigkeit und Tourismus
	_							

Quantification of significant pressures



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





Nickel (gesamt)

Relativer Anteil an der Gesamtemission [-]

Quelle: Umweltbundesamt/TU Wien

MoRE workflow







MoRE - Modeling of Regionalized Emissions

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Umwelt 🎧 Bundesamt



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MoRE - Modeling of Regionalized Emissions

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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



MoRE - Modeling of Regionalized Emissions

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constants		6438	BI_RATE_dep_PHE_NP	BI_RATE_dep_PHE	Nonylphenol Inp	g/(ha·a)	deposition rate					family substance group		
		6464	BI_RATE_dep_PHE_OP	BI_RATE_dep_PHE	Perfluoropentan	g/(ha·a)	deposition rate					4 03-general informations	Test Variable für Varianten Erzeugung	
		3352	BI_SURP_agrl_N		Stickstoffübersc	kg/(ha·a)	surplus, area sp	nitrogen		nitrogen		unit	mm/a	
point source variables		1085	ER_agrl_CONT_CPMOD_P		phosphorus cont	mg/kg	content	phosphorus		phosphorus		parameter	emissions	
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protocols		5118	ER_agri_E_HM_CD	ER_agri_E_HM	Cadmium Inputs	kg/a	emissions	neavy metals		Cadmium				
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Translation		5121	ER_agrl_E_HM_NI	ER_agrl_E_HM	Nickel Inputs fro	kg/a	emissions	heavy metals		Nickel				
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Set up Formulas



- 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



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MoRE - Modeling of Regionalized Emissions

tables		modeling > calcula	tion > formulas				Y	愛南茶 Δ 5	a lu 🛠 🗐	ab. 🗙 🛛 🜌	formula: IM Q spec nat	
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	spatial modeling units		520 WWTP_FNE_Q	Wastewater treatment pla	m³/s	1		Steffen Kittlaus	TU-Wien	19.01.2	↓ 02-calculation	502
	analytical units		741 WWTP_ps_E_PAH	PAK inputs via municipal W	kg/a	1		Marianne Bertin	UBA	21.02.2	result variable	IM_Q_spec_nat
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	periodical point source variables		519 WWTP_Q	runoff via waste water tre	m³/a	1		Steffen Kittlaus	TU-Wien	19.01.2	dataset creation date	13.05.2016
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	input data		528 WWTP_small_E_P	Phosphor-Einträge über Kl	t/a	1		Steffen Kittlaus	TU-Wien	26.06.2		
	🕎 constants		742 WWTP_small_E_PAH	PAH Emissions from small	kg/a	1		Marianne Bertin	UBA	21.02.2		
	analytical units variables		804 WWTP_small_E_PFT	PFT Emissions from small	kg/a	1		Marianne Bertin	UBA	24.02.2	01-identification	
	periodical analytical units variables		325 WWTP small E PHE	Phenol Inputs via atmosph	kg/a	1		Marianne Bertin	UBA	22.04.2		
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	formula contents		514 ER_SDR_alp	Percentage of sediment in	%	2	:	Lucas Reid	IWG	06.10.2		
	algorithms		194 GW_CONC_P	phosphorus concentration	. mg/L	2						
	🖅 groundwater transfer		188 GW_CONC_uncorr_P	Phosphor-Konzentration im	. mg/L	2	:					
۲	🚞 variant manager		178 GW_RATE_dep_N	nitrogen deposition rate fo	. kg/a	2						
±.	measure manager		585 IM_A_OR_qgw	"Area of non-urban roads	km²	2		Steffen Kittlaus	TU-Wien	28.11.2		
	results		584 IM A OR gsr	Area of non-urban roads d	km²	2		Steffen Kittlaus	TU-Wien	28.11.2		
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			136 TD_E_P	phosphorus emissions via t	. t/a	2						
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			47 TD Q spec	runoff rate of tile drainage	mm/a	2						
			569 TOT ENE O	Gross discharge (incl. Upst	m ³ /s			Steffen Kittlaus	TU-Wien	13, 12, 2		
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MoRE - Modeling of Regionalized Emissions

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MoRE - Modeling of Regionalized Emissions

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visualization		emissions > nitrogen emissions via surrace runoff	-		nitrogen			_	
i river modeling i ···· · · · · · · · · · · · · · · · ·		emissions > nitrogen emissions via die drainage			hitrogen			_	
Translation		hiver module > heavy metal river loads and concentrations, dissolved	-		heavy metals			_	
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		Areas > Areas contributing to groundwater recharge > Areas contributing to groundwater recharge	-			1			
		Emissions > Nitrogen emissions via erosion		<u> </u>	nitrogen	1			
		Gewassermodul > Phosphor Gewässerfracht > Retention im Nebenlauf		<u> </u>	phosphorus	1			
		river module > phosphorus river load > retention in main river			phosphorus	1	L	~	

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MoRE - Modeling of Regionalized Emissions

tables modeling > calculation > algorithms > calculation steps Y 🏹 🗑 💥 🖄 📓 💺 🛠 📓 calculation step 🔠 狂 🛅 🥒 💥 💌 🎴 MoRE formula 🗄 🍘 documentation step active formula formula content remarks reference ⊿ 01-identification 🖻 🍓 modeling 01 step 🖶 🍓 spatial modeling units 01 ✓ WWTP_ps_E_PHAR (variant 1) WWTP_ps_Q*WWTP_CONC_PHAR/(1000*1000) ID a space inocening and analytical units point sources planning units 02 ~ WWTP_small_E_PHAR (variant 1) WWTP_s_CONC_PHAR * WWTP_small_Q / 1000 / 1000 ⊿ 02-formula WWTP_ps_E_PHAR (variant 1) formula 03 ~ WWTP_E_PHAR (variant 1) more_psaggrau(WWTP_ps_E_PHAR) + WWTP_small_E_PHAR formula content WWTP_ps_Q*WWTP_CONC_PHAR/(1000*1000) 🛛 🍓 metadata formula reference all variables ⊿ 03-general informations active ves 📑 analytical units variables remarks periodical analytical units variables point source variables ⊿ 04-creation datase Marianne Bertine Broei periodical point source variables periodical point source variables balancing periods user UBA institute 25.02.2022 dataset creation date planning units > aggregation > final results 🖓 📺 input data 🔙 constants analytical units variables 01-identification periodical analytical units variables point source variables minimizer in periodical point source variables 🔅 🚞 statistics structure alculation algorithms algorithm stack 🖃 🦏 algorithms: Emissions > PHAR emissions via waste water treatment plants - variant 1 < 3 calculation steps :</p> 🛯 🎃 overview formula contents algorithms groundwater transfer 🗄 🛗 variant manager measure manager 🕘 results 📄 🏐 preliminary calculation runs 🗄 🚞 final - 🔟 runoff routing i visualization visicalization
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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



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MoRE - Modeling of Regionalized Emissions

tables	modeling > calculation > algorithm stack					7 🏹 🗃 💥 🖄	. 🛛 🕹 🛠 1	🛯 🖞 🛦 🗙	algorithm stack: Area balance (CORIN	E)			
🥁 MoRE I 📺 documentation	name	balancing	component	substance	temporal	creation	remarks	user	2 V V V V	•			
🖻 🍓 modeling		penieu		group		uuto			name	Area balance (CORINE)			
analytical units	Area balance (CORINE)		area		2016-2021	13.05.2016 10:48			ID	246			
point sources	area calculation		area		2016-2021	16.05.2013 12:18			4 02-properties	20			
planning units	fine solids emissions via erosion		emission	Fine solids	2009-2014	16.03.2017 15:08		Lucas Reid	component	area			
🖃 👹 metadata	fine solids emissions via sewer systems		emission	Fine solids	2009-2014	15.05.2013 11:50	based on "water		substance group				
	fine solids emissions via tile drainage		emission	Fine solids	2009-2014	17.05.2013 10:03	based on "water		temporal reference	2016-2021			
analytical units variables	fine solids emissions via wastewater treatment plants		emission	Fine solids	2009-2014	14.05.2013 13:53	for AU (analytic		4 03-creation	13 05 2016			
periodical analytical units variables	heavy Metal emmisions		emission	heavy metals	2016-2022	16.09.2022 14:10		Marianne Bertin	⊿ 04-creation dataset	13.03.2010			
point source variables	Heavy metal river loads and concentrations		load, modelled	heavy metals	2016-2022	27.09.2022 13:24		Marianne Bertin	user				
substances	nitrogen emissions		emission	nitrogen	2009-2014	17.07.2012 14:57			institute	12.05.2010			
balancing periods	nitrogen river loads		load, modelled	nitrogen	2009-2014	07.12.2016 17:36		Snezhina Tosho	dataset creation date 13.05.2016				
planning units > aggregation > final results	Pharmacueticals emissions		emission	Pharmacueticals	2016-2022	30.09.2022.14:22		Marianne Bertin	remarks				
constants	Pharmacueticals river loads and concentrations		load modelled	Pharmacueticals	2016-2022	30.09.2022 14:25		Marianne Bertin					
analytical units variables	Pharmacdeddais i Verifodds and concerta adons		ioau, modelleu		2010-2022	12 10 2017 11:27		Chaffee Kittlesse	01-identification				
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point source variables	phosphorus emissions via atmospheric deposition		emission	pnospnorus	2009-2014	23.02.2012 11:21							
statistics	phosphorus emissions via erosion		emission	phosphorus	2009-2014	07.10.2016 15:59		Snezhina Tosho		¥			
acalculation	phosphorus emissions via groundwater		emission	phosphorus	2009-2014	05.12.2014 17:35			structure				
······································	phosphorus emissions via industrial direct dischargers		emission	phosphorus	2009-2014	04.11.2014 17:28			□ → algorithm stack: Area balance (CORINE)				
algorithm stack	phosphorus emissions via sewer systems		emission	phosphorus	2009-2014	05.12.2014 17:31			└ (main algorithms >				
e 🔄 overview	phosphorus emissions via surface runoff		emission	phosphorus	2009-2014	05.12.2014 17:18							
···· 🔤 formula contents	phosphorus emissions via tile drainage		emission	phosphorus	2009-2014	06.11.2014 15:46							
algorithms	phosphorus emissions via waste water treatment plants		emission	phosphorus	2009-2014	23.02.2012 13:51							
groundwater transfer	phosphorus emissions, total		emission	phosphorus	2009-2014	03.04.2012 17:56							
🗉 👜 variant manager	phosphorus river loads and concentrations		load, modelled	phosphorus	2009-2014	10.08.2018 11:46		Steffen Kittlaus					
measure manager runoff routing	Retention particulate		load, modelled	Fine solids	2009-2014	18.12.2018 15:04		Steffen Kittlaus					
results	Solids inputs, total (solids balance)		emission	Fine solids	2009-2014	27.05.2013 14:43	based on "water						
🖶 🍓 preliminary	Wastewater share of area runoff		runoff		2016-2021	19.01.2018 16:51		Steffen Kittlaus					
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MoRE - Modeling of Regionalized Emissions

tables		mode	ling > calculatio	n > algorithm stack > algorithms	7 7 1 1	△ ■ ■ ↓ ※	· 🗄 🗄 🗙 🔛	algorithm	
	ocumentation odeling B control modeling units		step	algorithm	algorithm stack as calculation step	substance group	active	21 3 2 8 8 3 21 3 2 8 1 3 2 8 1 3 2 1 3 1 3	284
	a spatial modeling units	•	01		Water balance		Image: A state of the state	ID	1292
	point sources		02	Emissions > fine solids emissions via erosion (variant 1)			Image: A state of the state	algorithm	
			03	Emissions > Heavy metal emissions via roads ouside of settlements (variant 1)		heavy metals	 Image: A start of the start of	algorithm stack as calculation step	Water balance
	all variables		04	Emissions > Heavy metal emissions via waste water treatment plants (variant 1)		heavy metals	Image: A state of the state	step	01
	constants		05	Emissions > Heavy metal emissions via industrial direct dischargers (variant 1)		heavy metals	~	substance group	
	analytical units variables		06	Emissions > Heavy metal emissions via atmospheric deposition onto water surfaces (variant 1)		heavy metals	Image: A state of the state	active	yes
	point source variables		07	Emissions > Heavy metal emissions via surface runoff (variant 1)		heavy metals	 Image: A start of the start of	remarks	
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	balancing periods		09	Emissions > Heavy metal emissions via groundwater (variant 1)		heavy metals	~	institute	UBA
	planning units > aggregation > final results		10	Emissions > Heavy metal emissions via sewer systems (variant 1)		heavy metals	Image: A state of the state	dataset creation date	16.09.2022
8-4	input data		11	Emissions > Heavy metal emissions via tile drainage (variant 1)		heavy metals	~		
	analytical units variables		12	Emissions > Heavy metal emissions, total (variant 1)		heavy metals	Image: A state of the state	01:	
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Calculate a algorithm stack



- 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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SKIT

MoRE - Modeling of Regionalized Emissions modeling > spatial modeling unit > analytical units Y 🏹 🌆 🗶 🖄 📓 🜬 🛠 📓 analytical unit: Ybbs5 tables 21 🔁 🗸 🗶 📓 - 🍓 MoRE ID of name ID of total documentation AU short analytical analytical downstream ID solit area (km²) upstream river state federal state ⊿ 01-analytical unit 🗄 🍓 modeling term unit unit analytical unit area 11008 ID of analytical unit -spatial modeling units name analytical unit Ybbs5 + analytical units 11000 Ybbs from Amst.. 211.075938 1,111.904 Ybbs AT AU short term point sources AT 11001 From Krennstett. Id 11000 (Ybbs . 224.394000 887.510 Ybbs ID of downstream analytical unit ld 11007 (Ybbs4) 🗒 planning units 115 726000 metadata all variables constants 11002 Url Id 11001 (From . 158.727000 0.000 Url AT area (km²) total upstream area 0.000 AT 11003 Ybbs1 Id 11001 (From . 112.483000 616.300 Ybbs ID split 111.820000 0.000 Kleine Ybbs AT analytical units variables periodical analytical units point source variables 11004 Kleine Ybbs Id 11003 (Ybbs1) 4 02-administrative units state AT Id 11003 (X 11005 Ybbs2 MoRE: calculation engine periodical analytical units variables federal state 11006 Ybbs3 Id 11005 (periodical point source variables periodical point source variables substances balancing periods ⊿ 03-water system 11007 Ybbs4 Id 11006 (marine area start calculation engine river basin district Danube river system planning units > aggregation > final results 12000 Wulka downstre... Ybbs 🗄 🕘 input data ⊿ 04-coordination 12001 Wulka upstream Id 12000 (constants algorithm stack: # 2016-2022 + Heavy metal river loads and concentrations coordination area analytical units variables 12002 Fishach Td 12001 0 01-analytical unit periodical analytical units variables 12003 Nodbach Id 12001 (substances: Cadmium, Copper, Lead, Mercury, Nickel, tin point source variables 12004 Wulka upstream . Id 12001 () ------- periodical point source variables vears 2020 v . statistics Id 12004 0 12005 Wulka upstream structure eaculation szenarios 21001 Koppany1 algorithms algorithm stack analytical unit: Ybbs5 21002 Koppany2 Id 21001 () type - < 74 analytical units variables > 22001 Zagyva-patak1 name 🛛 🔄 overview 22002 HerXdi-Bér-patal Id 22001 (formula contents 22003 Zagyva-patak2 Id 22001 (2 detailed protocol algorithms Id 22003 (2 22004 Zagyva-patak3 🔄 🚽 groundwater transfer 22005 Tarján-patak Id 22003 (2 🗄 🚞 variant manager 00:00:00 measure manager runoff routing 31001 Somesul Mic1 31002 Nadas Id 31001 (🖻 🍓 results Id 31001 (31003 Somesul Mic2 🚊 🍓 preliminary calculation runs Id 31005 (31004 Somesul Rece start calculation engine 31005 Somesul Mic3 Id 31003 (🗄 🚞 final runoff routing 31006 Somesul Mic4 Id 31003 (Se wisualization 32001 Viseu1 145.264633 232.700 Viseu RO 🗄 💼 river modeling 32002 Viseu2 Id 32001 (Viseu1) 133.301781 0.000 Viseu RO 🗄 🛅 validation 🗄 💼 translation 32003 Tisla Id 32001 (Viseu1) 99.417371 0.000 Tisla RO . administration 41001 Vit1 547.980800 0.000 Vit BG 41002 Vit2 Id 41001 (Vit1) 666.825600 0.000 Vit BG 41003 Vit3 Id 41002 (Vit2) 524.704000 0.000 Vit BG 41004 Cherni Vit Id 41003 (Vit3) 161 110400 0.000 Cherni Vit BG 41005 Beli Vit Id 41003 (Vit3) 305.667200 0.000 Beli Vit BG ш

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MORE - Modeling	of Regionalized	Emissions
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tables	notening - resurts - premininary - protocols					Y 9 🗄 X 🖂 🖼 📲 X 🛅 🐝 🔨 📓								
		ID of calculation	date	algorithm	scenario	substances	years	remarks	number of	number of	computing			•
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analytical units variables		168	01.10.2022 21:42	Pharmacueticals		Diclofenac	2020		0	117			substances	Cadmium,Copper,Lead,Mercury,Nickel,tin
periodical analytical units variables		167	01.10.2022 21:40	Pharmacueticals		Diclofenac	2020		1	117			balancing period	2020
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planning units > apprenation > final results		164	01.10.2022 21:28	Pharmacueticals		Diclofenac	2020		5	110			computing time (sec)	44
input data		163	01.10.2022 21:19	Pharmacueticals		Diclofenac	2020		5	110			tomula / second	290
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elculation		158	30.09.2022 17:09	Pharmacueticals		Diclofenac	2020		8	19		st	ructure	
		157	30.09.2022 16:46	Pharmacueticals		Diclofenac	2020		8	19			al calculation curs 172	
······································		156	30.09.2022 16:45	Pharmacueticals		Diclofenac	2020		0			11 -	Calculation run: 173	
algorithm stack		155	30.09.2022.16.44	Pharmacueticals		Diclofenac	2020		0				< 1 year >	
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		152	30.09.2022 16:35	Pharmacueticals		Diclofenac	2020		0					
🗄 💼 variant manager		151	30.09.2022 16:29	Pharmacueticals		Diclofenac	2020		0					
measure manager		150	30.09.2022 16:26	Pharmacueticals		Diclofenac	2020		0					
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		139	29.09.2022 13:14	Heavy metal riv		tin	2020		10	789		1		
		138	29.09.2022 13:04	Heavy metal riv		tin	2020		10	5,362				
		137	29.09.2022 13:03	Heavy metal riv		Cadmium,Coppe	2020		35	12,792		1		
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Karlsruher Institut für Technologie und Umweltbundesamt — MoRE - Danube Hazard m³c 2 🗸 🔂 🐍 🛛 🗖 MoRE - Modeling of Regionalized Emissions 🛛 🏹 🌆 💥 🖄 🖼 📕 🧩 🗐 🏭 🗙 🔛 calculation run: 173 tables modeling > results > preliminary > calculation runs 📜 🤰 🛅 🛹 💥 💌 🌌 - 🍓 MoRE ID of number of numh i documentation calculation date algorithm stack scenario substances years remarks ⊿ 01-identification buas form 🗄 🍓 modeling run ID of calculation run : B - Constant and the second analytical units 173 03.10.2022 11:28 Heavy metal river loads and concentrations Cadmium,Coppe. 0 ₄ 02-activation of run 172 03.10.2022 11:26 Pharmacueticals river loads and concentrations Diclofenac 2020 0 03 10 2022 ⊿ 03-algorithm stack 171 01.10.2022 21:51 Pharmacueticals river loads and concentrations 2020 Diclofenac 0 🗒 planning units Heavy metal river loads and concentrations algorithm stack e 🖶 metadata 168 01.10.2022 21:42 Pharmacueticals river loads and concentrations Diclofenac 0 scenario 162 01.10.2022 21:19 Pharmacueticals river loads and concentrations Diclofenac 2020 substances Cadmium,Copper,Lead,Mercury,Nickel,tin 0 률 constants 2020 vears analytical units variables 161 01.10.2022 21:12 Pharmacueticals river loads and concentrations 2020 Diclofenac 0 balancing period no periodical analytical units variables 159 30.09.2022 17:33 Heavy metal river loads and concentrations Cadmium,Coppe 2020 0 △ 04-overview point source variables 156 30.09.2022 16:45 Pharmacueticals river loads and concentrations number of bugs Diclofenac 2020 0 12,798 number of formulas 155 30.09.2022 16:44 Pharmacueticals river loads and concentrations Diclofenac 2020 0 computing time (sec) 44 balancing periods 154 30.09.2022 16:37 Pharmacueticals river loads and concentrations Diclofenac 2020 4 05-general informations 0 planning units > aggregation > final results remarks 153 30.09.2022 16:36 Pharmacueticals river loads and concentrations Diclofenac 2020 0 🗄 🕘 input data 34 number of analytical units constants 152 30.09.2022 16:35 Pharmacueticals river loads and concentrations Diclofenac 2020 0 analytical units variables 01-identification 151 30.09.2022 16:29 Pharmacueticals river loads and concentrations Diclofenac 2020 0 periodical analytical units variables point source variables 150 30.09.2022 16:26 Pharmacueticals river loads and concentrations Diclofenac 2020 0 — periodical point source variables 149 30.09 2022 14:30 Pharmacueticals river loads and concentrations 2020 0 Diclofenac . statistics 148 30.09.2022 13:56 Heavy metal river loads and concentrations 2020 0 Cadmium.Coppe. structure eaculation algorithms algorithm stack 142 29.09.2022 21:07 Heavy metal river loads and concentrations Cadmium,Coppe. 2020 0 calculation run: 173 140 29.09.2022 13:22 Heavy metal river loads and concentrations 2020 0 Cadmium.Coppe.. — (1) year > 136 29.09.2022 13:02 Heavy metal river loads and concentrations tin 2020 0 🗠 🥁 overview formula contents 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 algorithms 0 🔄 🚽 groundwater transfer 131 28.09.2022 16:52 Heavy metal river loads and concentrations Cadmium,Coppe. H i variant manager 130 28.09.2022 11:46 Heavy metal river loads and concentrations Cadmium.Coppe... . 2017 0 measure manager manager manager manager manager 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 🖻 🍓 results Cadmium,Coppe.. 2017 0 🖻 🝓 preliminary 127 27.09.2022 18:13 Heavy metal river loads and concentrations Cadmium,Coppe... 2017 0 calculation 124 27.09.2022 17:05 Heavy metal river loads and concentrations Cadmium,Coppe. 2017 0 🗄 🚞 final 121 27.09.2022 16:16 Heavy metal river loads and concentrations Cadmium.Coppe... 2017 0 runoff routing 120 27.09.2022 16:10 Heavy metal river loads and concentrations Cadmium,Coppe... 2016 0 • isualization 119 27.09.2022 16:04 Heavy metal river loads and concentrations Cadmium,Coppe... 2016 🗄 🍘 river modeling 0 🗄 🍘 validation 118 27.09.2022 14:40 Heavy metal river loads and concentrations Cadmium,Coppe... 2016 0 🗄 💼 translation 115 27.09.2022 12:30 heavy Metal emmisions Cadmium,Coppe... 2016 0 🗄 🍘 administration 114 27.09.2022 11:29 heavy Metal emmisions Cadmium Coppe 2016 0 113 27.09.2022 10:48 heavy Metal emmisions Cadmium, Coppe... 2016 0 112 27.09.2022 09:27 heavy Metal emmisions Cadmium, Coppe... 2016 0 111 26.09.2022 20:52 heavy Metal emmisions Cadmium,Coppe... 2016 0 107 26.09.2022 12:24 heavy Metal emmisions Cadmium,Coppe.. 2016 0 106 26.09.2022 12:24 heavy Metal emmisions Cadmium, Coppe... 2016 0 94 23.09.2022 14:58 Water balance 2016 0 93 23.09.2022 14:34 Water balance 2021

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Scenario calculation



Implementation of emission mitigation measure scenarios in MoRE

- Examples
- Way of implementation


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



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 ($\eta_{PFOS} = 75\%$)
 - With ozonation ($\eta_{PFOS} = 20\%$)
- 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 $\rm K_{\rm D}$ 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 %



Hierarchical approach of emission mitigation measure scenario implementation in MoRE



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.



MoRE - Modeling of Regionalized Emissions					
tables	modeling > calculation > variant manager > input data variables				
MoRE	name	variable type	variable	variable description	



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

 η_{PFOS} = 75%

 Storm water treatment with increased fine sediment retention. Efficiency 30 % in CSO and 20% in storm sewers



Danube Hazard m³c 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





- 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



Danube Transnational Programme Danube Hazard m³c

MoRE	DHSM
Tier 3	Tier 4



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





Temporal resolution



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



General input data

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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)
	Spatially distributed emissions Spatially distributed emissions STREAM-EU Compartments Hare Free Dissolved Free Dissolved DOC dourd Poc

Substance specific data requirements



MoREDHSMHigh,
Regionalized information
on concentrations in
different pathways,
Information on
environmental behavior• 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

 Wastewater
treatment
plants
 Stormwater
overflows

 Surface
waters
RIVERS
 Atmospheric
deposition

 Groundwater
 Data-
base
 Soil

(degradation, adsorption)



Substances implementation



Danube Hazard m³c



Availability, technical requirements



- Licensed under GNU Affero General Public License
- The server setup needs advanced technical knowledge

MoRE

- 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).

DHSM

 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)





Required technical skills

MoRE

DHSM

- Data Preparation:
 - Geodata management
 - data analysis
- Model usage:
 - Knowledge of the underlaying quantification approaches

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Data processing & GIS tools







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









Accuracy (DHm³c, preliminary MoRE)





Accuracy (Pilot Regions)







Accuracy (Pilot Regions)







■ DHSM ■ MoRE ■ Observed □ Observed (uncertain)

Sources and pathways





Pathways (comparison of results)



Danube Transnational Programme



Pathways (comparison of results)



Shares of pathways (copper)

Danube Transnational Programme Danube Hazard m³c



Capability for scenario implementation



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 reuse, 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





Some thoughts on model comparison and selection

Danube Transnational Programme Danube Hazard m³c

- 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