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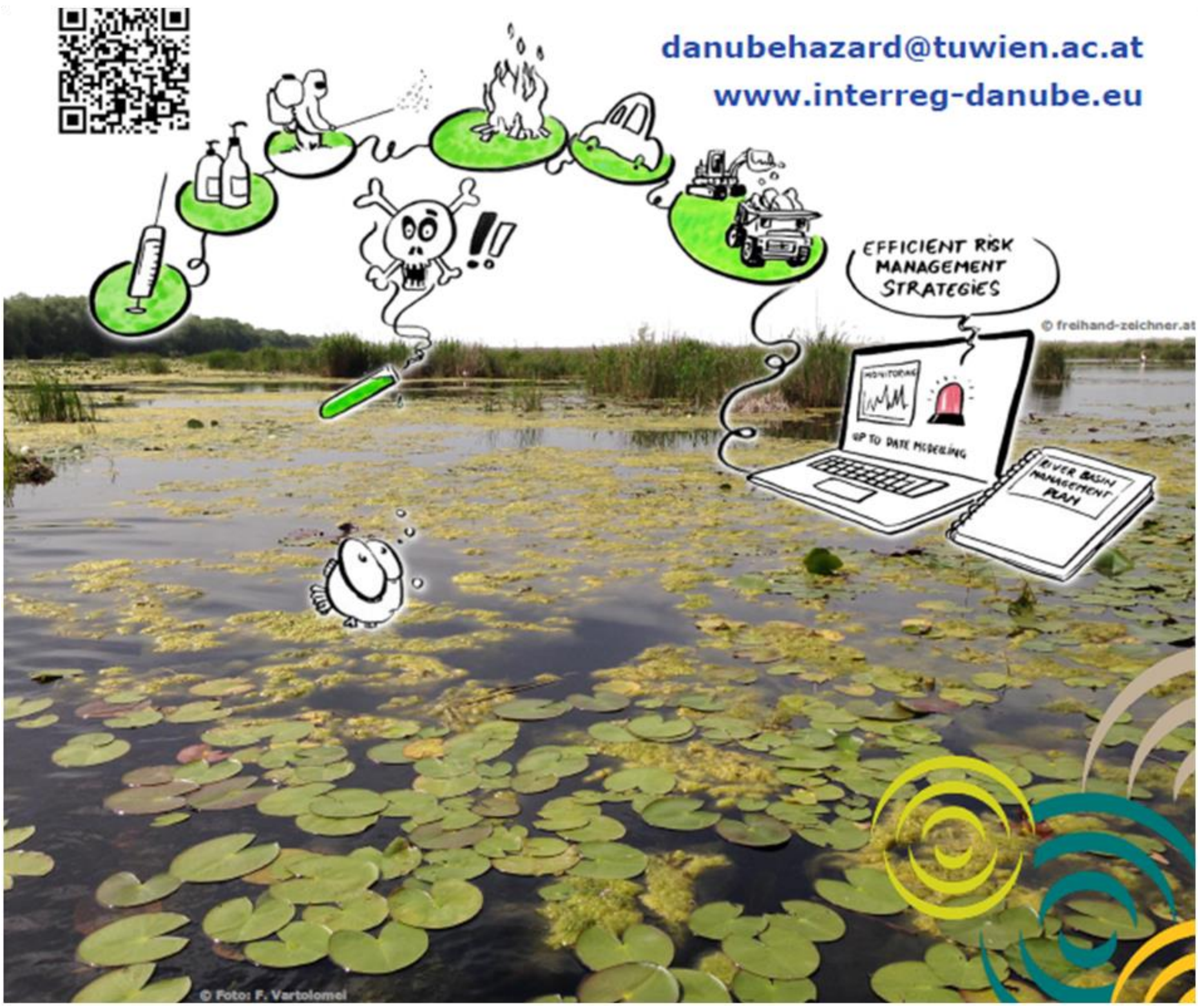
EUROPEAN UNION

Danube Transnational Programme

Danube Hazard m^{3}c



Output T2.1
Harmonized MoRE model adapted to specific territorial characteristics within the DRB
Date: 31/ March / 2023

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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1. Summary

1.1 Introduction

The MoRE model (Fuchs et al., 2017) is a semi-empirical emission model, which operates on the mesoscale (tenth to hundreds of square kilometers) and on annual time steps (in this model application period 2016-2021). It is a further development derived from the MONERIS emissions model (Behrendt et al., 2002) mainly developed for nutrients and differs in particular by a modified technical model realization.
The MoRE model, was available only in a German version for an extended number of organic and inorganic micro pollutants before this project. Additionally, a very basic application for nutrients was available in English. The latter was taken and built up into a fully functional English version for a wide range of substances and with a wide range of calculation approaches in the Danube Hazard m^{3}c project.

In seven pilot regions, the model approach was adapted and setup, due to specific conditions in the Danube Basin.

The original model approaches calculated for each sub-catchment includes the following pathways:

- Municipal Wastewater Treatment Plants > 2.000 PE,
- Industrial Wastewater Treatment Plants,
- Combined storm water overflows (combined system),
- Storm water overflow (storm sewer),
- Country roads and highways,
- Atmospheric deposition (direct on water surfaces),
- Surface runoff,
- Erosion (agricultural areas, natural areas (forests), open areas (mountainous)),
- Drainage (Tile drainages),
- Groundwater.

Emission from groundwater and from drainages refer to the underground flux, which enters surface waters after passing the soils. Both pathways were subsumed, describing emission from drainages and from groundwater (which integrates base flow and intermediate flow) in a single pathway, because a lack of specific data on drainage concentrations makes further differentiation impossible.

In Danube Hazard m^{3}c two specific pathways were also processed and added to the model structure, due to their high relevance in the pilot regions:

- Sewer systems not connected to Wastewater Treatment Plants and
- Untreated Wastewater from abandoned mining sites.

Potential micro pollutants of interest were already selected during project development and include the following substances:

- Per- and polyfluorinated alkyl substances (PFAS),
- 16 EPA Polycyclic aromatic hydrocarbons (PAHs),

- Mercury (Hg), Cadmium (Cd), Copper (Cu), Chrome (Cr), Nickel (Ni), Lead (Pb), Zinc (Zn), and Arsenic (As),
- Diclofenac and Carbamazepine,
- 4-tert-Octylphenol,
- Nonylphenol,
- Bisphenol A,
- Metolachlor including Metolachlor-ESA and Metolachlor-OA (metabolites),
- Tebuconazole.

1.2 Status of substances in the model

A large number of these substances were created for further use in an executable model version. According to relevance and occurrence in the pilot areas, which became apparent from the monitoring results, an additional differentiation was made:

- Substances implemented, completely parametrized and validated based on datasets from the Danube Hazard m³c database,
- Substances implemented and parametrized with a first input data set,
- Substances completely implemented but not parametrized,
- Substances not implemented.

Table 1 gives an overview on substances implemented in the model and their different processing status.

Table 1: Substance - specific model status.

Substance group	Substance	Implemented	Parametrized	Validated
PFAS*	PFOS	x	x	x
PFAS*	PFOA	x	x	x
PFAS*	Perfluorohexanoic acid	x		
PFAS*	Perfluoropentanoic acid	x		
PFAS*	Perfluorobutane sulfonic acid	x		
PAHs	EPA16-PAHs	x		
PAHs	Benzo[a]pyrene	x	x	
PAHs	Fluoranthene	x	x	
PAHs	Naphthalene	x	x	
PAHs	Phenanthrene	x	x	
Heavy metals	Mercury (Hg)	x	x	x
Heavy metals	Cadmium (Cd)	x	x	x
Heavy metals	Copper (Cu)	x	x	x
Heavy metals	Chrome (Cr)	x	x	x
Heavy metals	Nickel (Ni)	x	x	x
Heavy metals	Lead (Pb)	x	x	x
Heavy metals	Zinc (Zn)	x	x	x

Heavy metals	Arsenic (As)	x	x	x
Pharmaceuticals	Diclofenac	x	x	x
Pharmaceuticals	Carbamazepine	x	x	x
Phenols	4-tert-Octylphenol	x	x	
Phenols	Nonylphenol	x	x	
Phenols	Bisphenol A	x	x	
Pesticides	Tebuconazole	x	x	x
Pesticides	Metolachlor	x	x	x
Pesticides	Metolachlor ESA	x	x	x
Pesticides	Metolachlor OA	x	x	x

Substances not listed in the table (e.g. other PAHs or PFAS) were not implemented in the model.

For pesticides, two different model approaches were investigated. The first one is based on input data from the Danube Hazard m^{3}c database and reflects the calculation approaches used for most other modelled substances to calculate the input pathways. The second approach was established due to crop specific application rates from national pesticides statistics in Austria and Hungary. Using an Austrian datasets from a special pesticide measurement program, with 30 surface water catchments and crops from agricultural statistics (Invekos data), potential application rates were calculated and transfer functions established to estimate in - stream concentrations. However, for the application of this approach only for Hungarian and Austrian catchments crop-specific area statistics were available in a sufficient resolution.

Abandoned mining, which is a topic in one pilot region, was addresses by a first literature research on substance specific concentration in different technical (point sources) and environmental compartments (e.g. soils, groundwater, untreated abandoned mining effluent). Based on this dataset model results could reproduce the magnitude of loads and concentrations but could not map them exactly.

1.3 Basic input data

Together with all pilot region responsible project partners the high amount of necessary input data could be managed. Almost all data sets could be provided from national data sets.

Table 2: Basic input data used in MoRE. (x,t) = function of space and time; (x) = function of space; (c) = function of space using homogeneous values per country.

Actual input data code	Name	Description	Unit	Source
Analitical Unit (AU)	**Topography/Area**	**Delineation of Analytical Units**		
BI_A	Area	Area of analytical units	km²	(x)
BI_ELEVA	Digital Elevation Model	Mean hights of subcatchments	m	(x)
Landuse	**Landuse data set**	**Landuse categories in actual version**	**km²**	

Actual input data code	Name	Description	Unit	Source
BI_A_AL_slope_0-1	Arable land	5 slope classes: 0-1; 1-2; 2-4; 4-8; >8 % (if available)	km²	(x)/(x,t)
BI_A_PST	Pastures	Greenland, meadows	km²	(x)/(x,t)
BI_A_WS_mr	Water surface	Main river (also lakes; reservoirs)	km²	(x)/(x,t)
BI_A_WS_trib	Water surface	Tributaries (also lakes; reservoirs)	km²	(x)/(x,t)
BI_A_FOR	Naturally covered areas	Woods; scrubland	km²	(x)/(x,t)
BI_A_O	Open areas	Mountainous area without vegetation; beaches; dunes	km²	(x)/(x,t)
BI_A_OPM	Surface mining	Mining areas	km²	(x)/(x,t)
BI_A_URB	Settlements	Total urban areas	km²	(x)/(x,t)
BI_A_IMP	Impervious urban area	Paved areas inside urban areas: settlements; industrial estates; car parks….	km²	(x)/(x,t)
BI_A_WL	Wetlands	Area of Bog; swamp; floodplains	km²	(x)/(x,t)
BI_A_OR	Country roads	Paved road area; not included in settlements	km²	(x)/(x,t)
BI_A_REM	Other remaining areas	Other areas not listed above	km²	(x)/(x,t)
Drainages	**Melioration cadastre**			
TD_SHR_a_td_agrl	Tile drained areas	From arable land and pastures	km²	(x)
Meteorological Data	**Climatic data**			
AD_EVAPO_lt	Evapotranspiration	Longterm mean annual evapotranspiration	mm	(x)/(x,t)
BI_PREC_apr	Precipitation	Monthly values	mm	(x)
Hydrological data	**River Discharges**			
BI_Q_net	Net runoff	Modelling period; annual data	m3/s	(x)
Erosion	**Soil loss**			
ER_agrl_SL_spec_lt_AL	Soil loss	Soil loss from arable land (optional from 5 slope classes)	t/(ha·a)	(x)/(x,t)
ER_agrl_SL_spect_lt_PST	Soil loss	Soil loss from pastures	t/(ha·a)	(x)/(x,t)
Sewer sytem	**Statistical Data about inhabitants and waste water system (partly from UWWTD)**			
BI_INH	Number of inhabitants	Population	inh	(x,t)
US_cso_VOL_spec_SOT	Stormwater overflow	Storage volume of stormwater overflow tanks in combined sewer systems, area-specific	m³/ha	(x)/(x/t)
US_L_CS	Combined sewers	Length of combined sewers	km	(x)/(x/t)
US_L_SS	Stormwater sewers	Length of stormwater sewers	km	(x)/(x/t)
US_SHR_inh_con_tot	Connection rate	Percentage of inhabitants that are connected to sewer systems	%	(x)/(x/t)
US_SHR_inh_conWWTP_tot	Connection rate	Percentage of inhabitants that are connected to sewer systems and waste water treatment plants	%	(x)/(x/t)

Actual input data code	Name	Description	Unit	Source
US_SHR_inh_nss_tot	Connection rate	Percentage of inhabitants that are not connected to sewer systems	%	(x)/(x/t)
US_INHC_H2O	Water consumption	Inhabitant specific water consumption	l/(inh·d)	
US_nss_SHR_inhl_towwtp_sept		Percentage of inhabitant load that is transported from septic tanks to waste water treatment plants	%	(x)/(x/t)
US_Q_spec_COM		Runoff rate for commercial waste water	l/(ha·s)	
Point source data (one value for each treatment plant)	**Urban wastewater (partly from UWWTD)**			
WWTP_ps_INH_conWWTP	Connection rate	Number of inhabitants that are connected to sewer systems and waste water treatment plants (point sources)	Inh	(x)/(x/t)
WWTP_ps_CP	Capacity	Capacity of the waste water treatment plant (point sources)	PE	(x)
WWTP_ps_PE	Load	Nominal load of waste water treatment plant (point sources)	PE	(x,t)
WWTP_ps_TS	Treatment type	Current treatment type of waste water treatment plant (point sources)	-	(x)/(x/t)
WWTP_ps_Q	Discharge	Runoff via waste water treatment plant (point sources)	m^3/a	(x/t)
Industrial wastewater				
ID_ps_Q	Discharge	Runoff via industrial direct dischargers	m^3/a	(x/t)

Not all input data are available in all pilot regions in the same quality. Consequently, in some pilot regions alternative data sets must be used. For example, soil loss data, available in Hungary and Austria from nation-wide, long-term soil loss investigations are not available for Romanian and Bulgarian pilot regions. Here the soil loss information from the European JRC soil loss calculation approach were used.

A detailed description of basic input data used in each pilot catchment is presented in Deliverable "D.T2.1.1 Datasets containing basic input data for pilot regions", which is available as Appendix I. A detailed description of used substance specific input data is given in Output "O.T2.2 Report on improved system understanding".

1.4 Model approaches

All model approaches to calculate emission from the different pathways listed above are described in Deliverable "D.T2.1.2 Technical description of the model setup in the pilot regions" made available as Appendix II.

A condensed, technical description is presented in flowcharts, available for all relevant model approaches (Appendix III).

Figure 1 gives an example of a flowchart describing the variables and the formulas used for calculating the emission of PAH from industrial point sources.

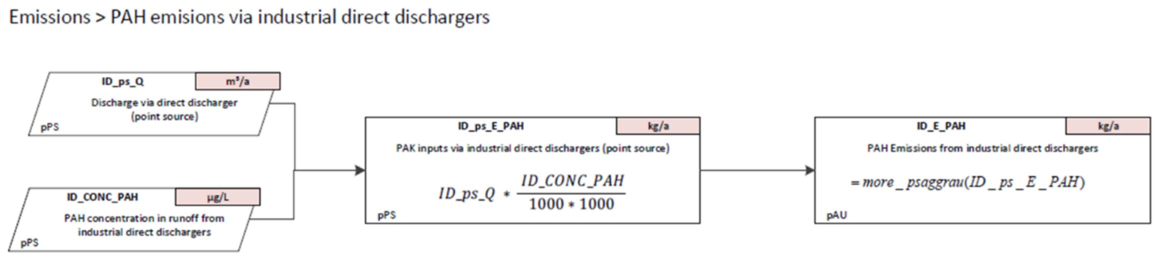

Figure 1: Example of a flowchart – PAH emission from industrial point sources.

1.5 Technical workflow

The standardized technical workflow to setup and run the MoRE model can be summarized in four main steps:

- Evaluation and pre-processing of input data,
- The creation of variables (constants, time and catchment-related variables, time-related point source variables) and import of data,
- Creation and definition of calculation approaches (formulas, calculation paths, calculation stacks),
- Calculation of catchment-related emission and concentration by use of the model quantification kernel for all pathways.

Based on the modelling results further steps are necessary:

- Comparison of model results with data from monitoring (run-off, loads and concentration),
- Check and interpretation of the pathway-related results,
- Visualization of model results.

Detailed results from this evaluation can be found in Output "O.T2.2 Report on improved system understanding".

A slimmed-down model (stand-alone version) is provided, which only contains the model approaches used in the pilot regions. This reduced SQLite version is available as DHm^{3}c project output T2.1 *Harmonized MoRE model adapted to specific territorial characteristics within the DRB* in Appendix III together with the technical flowcharts.

1.6 Short introduction to the SQLite application

The stand alone SQLite application is provided as a .exe application which can be stored locally or on a USB-stick or hard drive. To use the application simply open the application, no installation is needed. The MoRE application will start and can be used with all functionalities of the MoRE model.
When the application starts, the graphical user interface (GUI) shows the references used in the model.

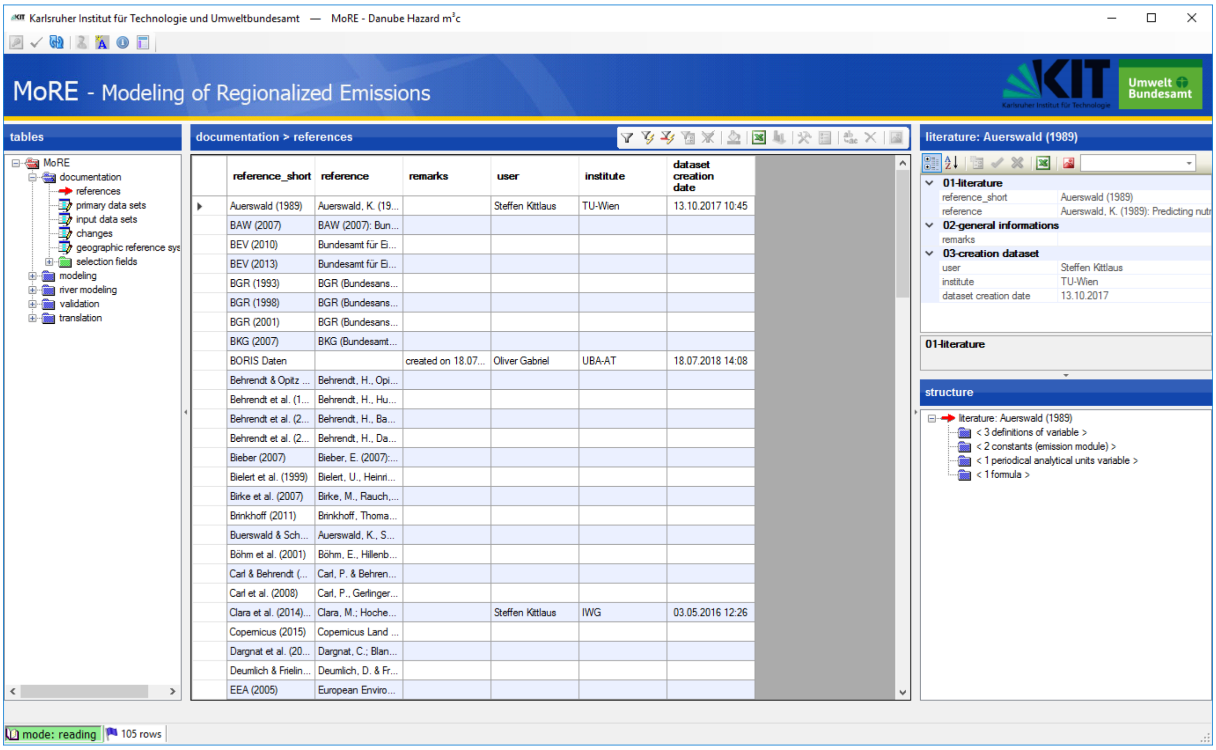

Figure 2: Screenshot of the reference menu in MoRE.

To start a model run first open the modeling menu at the left side of the GUI and then the spatial modeling units menu. Select the analytical units for which the calculation should be carried out as can be seen in Figure 3. It is also possible to select all analytical units.

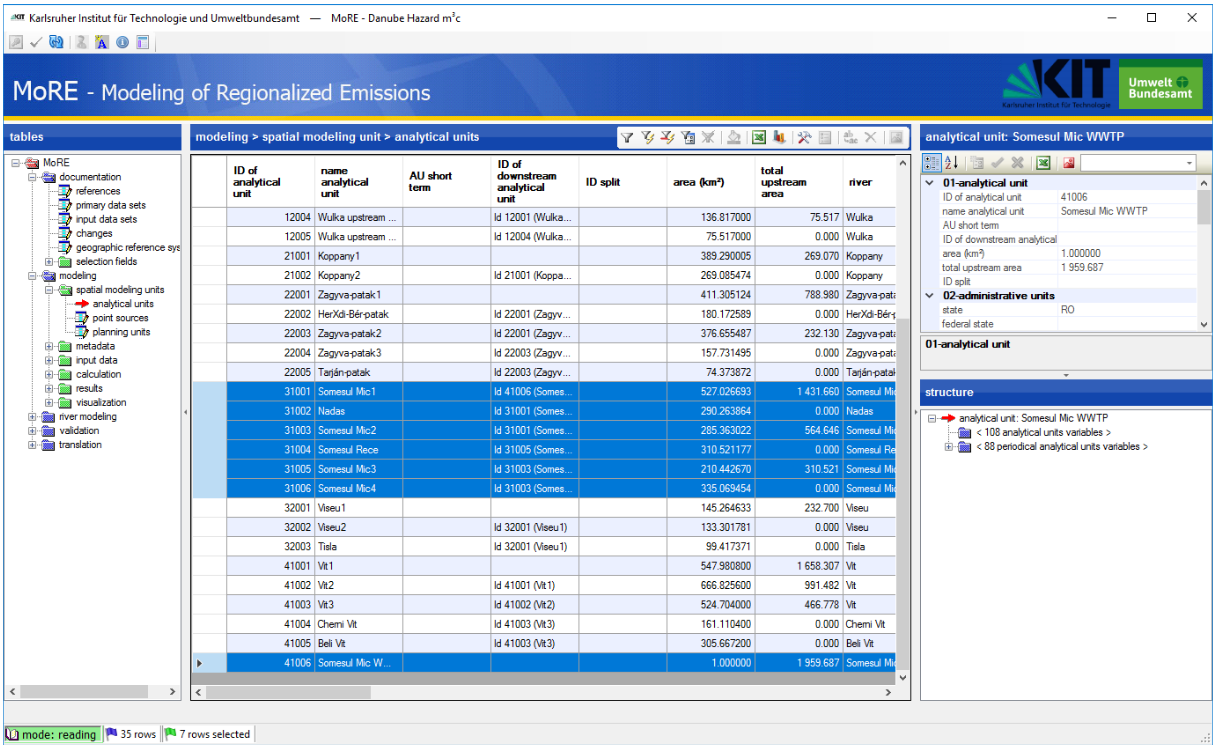

Figure 3: Screenshot of analytical units present in the provided SQLite version of MoRE.

Table 3 shows the IDs of the analytical units per pilot area. Please be aware that for the pilot area Somesul Mic the IDs 31001 through 31006 and 41006 have to be selected.

Table 3: Overview of the IDs of analytical units per pilot area.

Pilot area	Country	IDs of analytical unit
Ybbs	AT	11001 - 11008
Wulka	AT	12001 - 12005
Koppany	HU	21001, 21002
Zagyva	HU	22001 - 22005
Somesul Mic	RO	31001 - 31006 & 41006
Viseu	RO	32001 - 32003
VIT	BG	41001 - 41005

Select the toolbox icon at the right top of the GUI and then select execute calculation run → calculation for single years → OK.

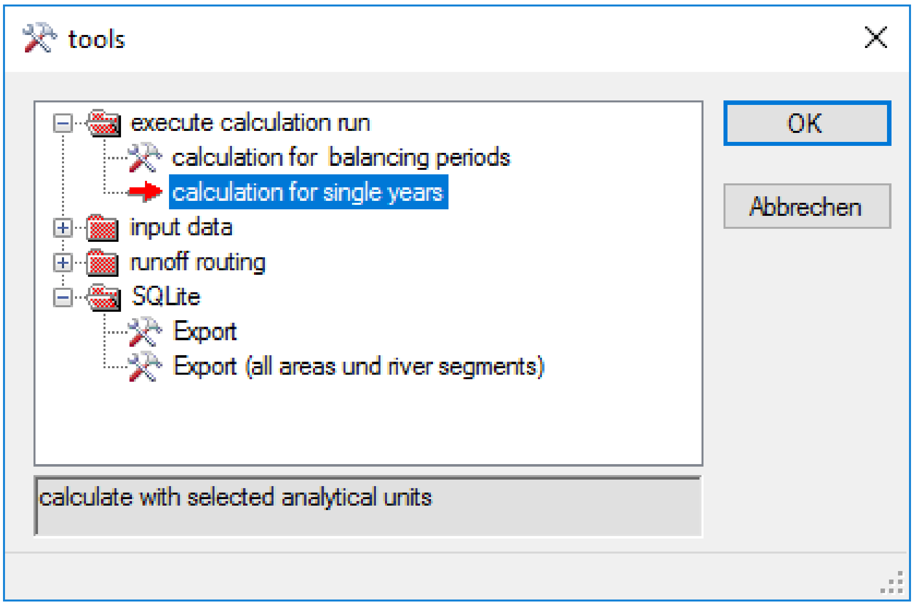

Figure 4: Screenshot of the toolbox in MoRE.

A new screen opens where the algorithm that will be calculated has to be selected, in addition the substances and the years can be selected or deselected. The algorithm stacks that calculated the modelled load contain the land use balance, the water balance and the total emissions for the selected substance group; therefore, this is good starting point to learn about the MoRE model. It is also possible to select a variant (best-case or worst-case). In order to do this the scenarios checkbox has to be checked.

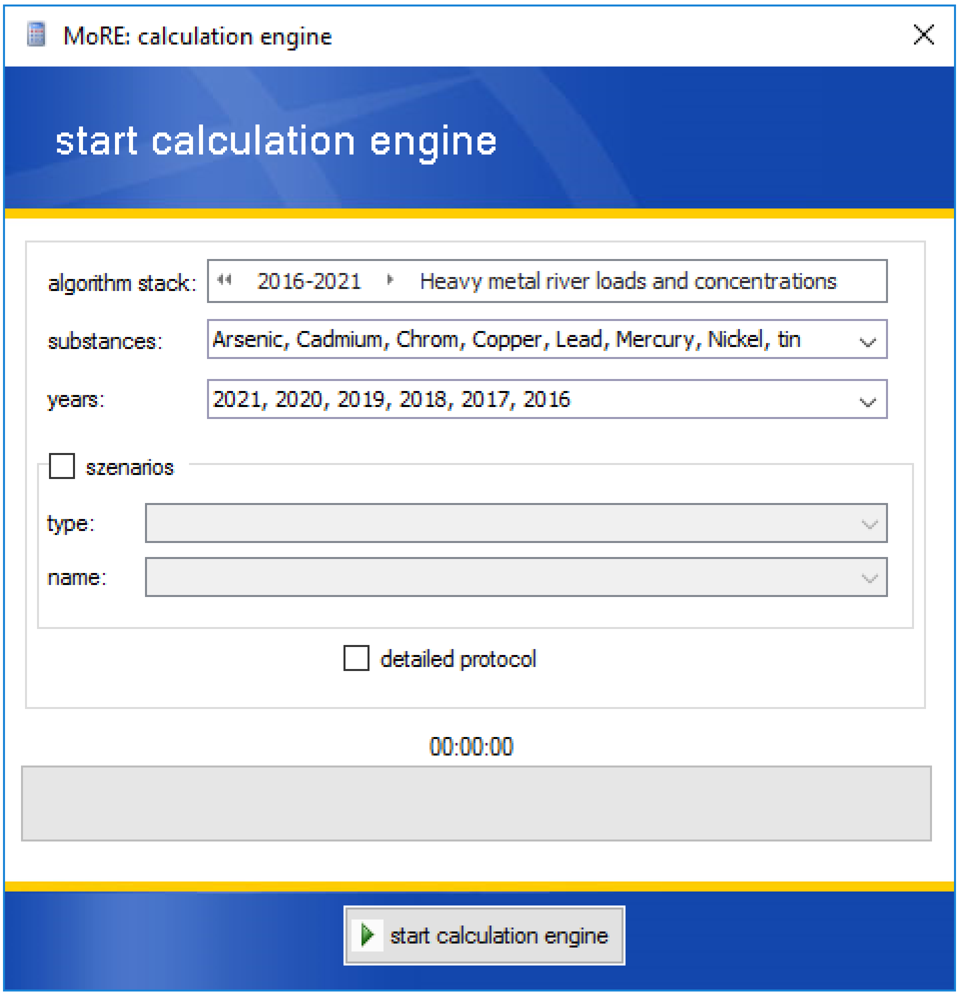

Figure 5: Screenshot of the calculation engine in MoRE

After a successful calculation run, the results can be found in the menu results → preliminary → calculation run. To export the results, select the calculation run and press the toolbox icon at the right top.

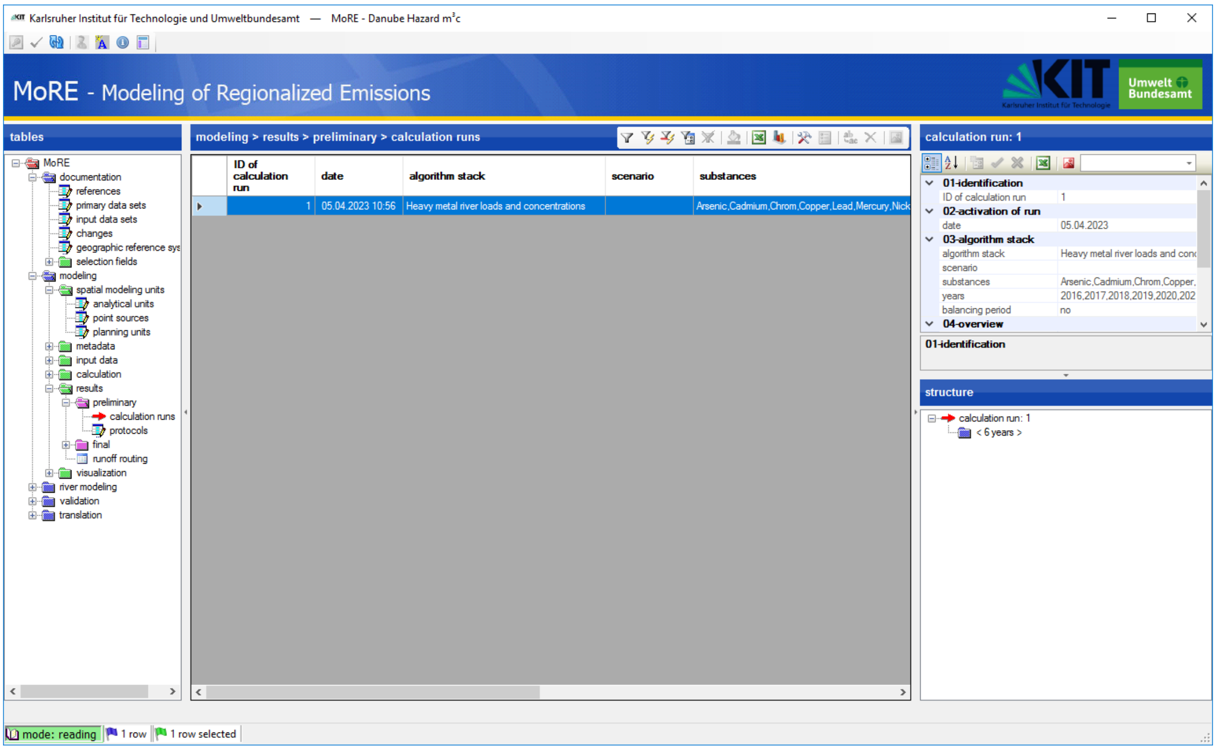

Figure 6: Screenshot of results menu in MoRE.

The results can be exported either in .csv or .xls. After choosing the format the variables that should be exported have to be selected, it is also possible to select all variables.

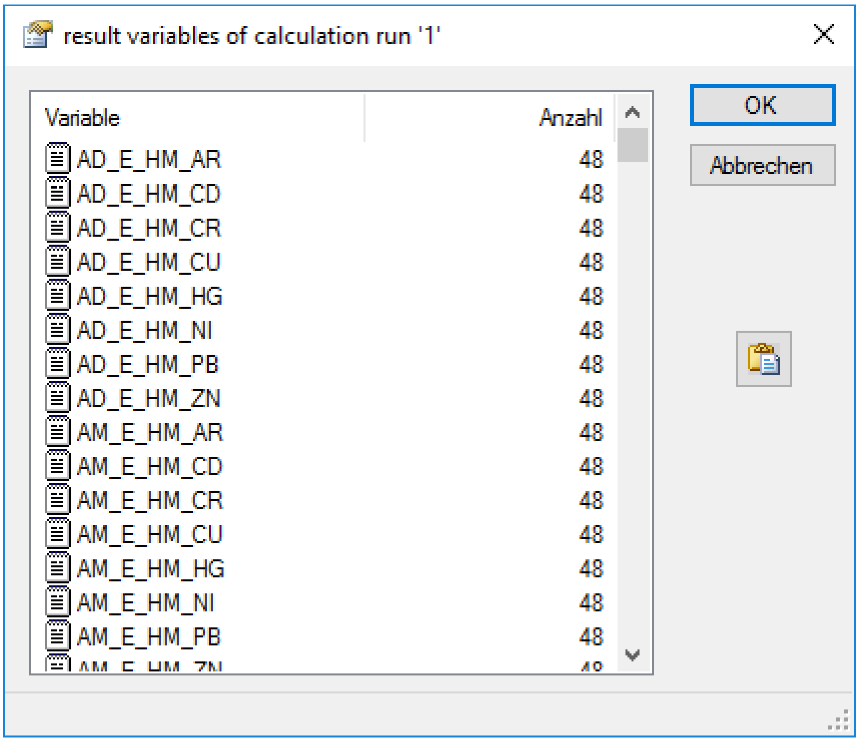

Figure 7: Screenshot of the results variables of a calculation run

Please be aware that by executing calculation runs, no changes in the model are made and therefore no errors can be generated. If the model is not functioning anymore for some reason, it is always possible to download the SQLite MoRe Model again.

For more detailed information please see the english MoRE WIKI.

Literature

Behrendt H., Huber P., Kornmilch M., Opitz D., SchmollL O., Scholz G., Uebe R., 2002. Estimation of the nutrient inputs into river basins – experiences from German rivers. Regional Environmental Changes 3: 107–117

Deliverable D.T2.1.1 (2021): Datasets containing basic input data for pilot regions.

Deliverable D.T2.1.2 (2021):

English MoRE Wiki (visited on 05.04.2023) https://more.iwg.kit.edu/wiki-en/index.php?title=MoRE_Developer

Fuchs, S., M. Kaiser, L. Kiemle, S. Kittlaus, S. Rothvoß, S. Toshovski, A. Wagner, R. Wander, T. Weber, S. Ziegler (2017). Modeling of Regionalized Emissions (MoRE) into Water Bodies: An Open-Source River Basin Management System; Water, 9, 4; pp. 239/1 - 239/13.

O.T2.2 Report on improved system understanding.

Appendix

Appendix I: Deliverable “D.T2.1.1 Datasets containing basic input data for pilot regions”.

Appendix II: Deliverable “D.T2.1.2 Technical description of the model setup in the pilot regions”.

Appendix III: Model application and flowcharts of all relevant model approaches as a Zip-File.