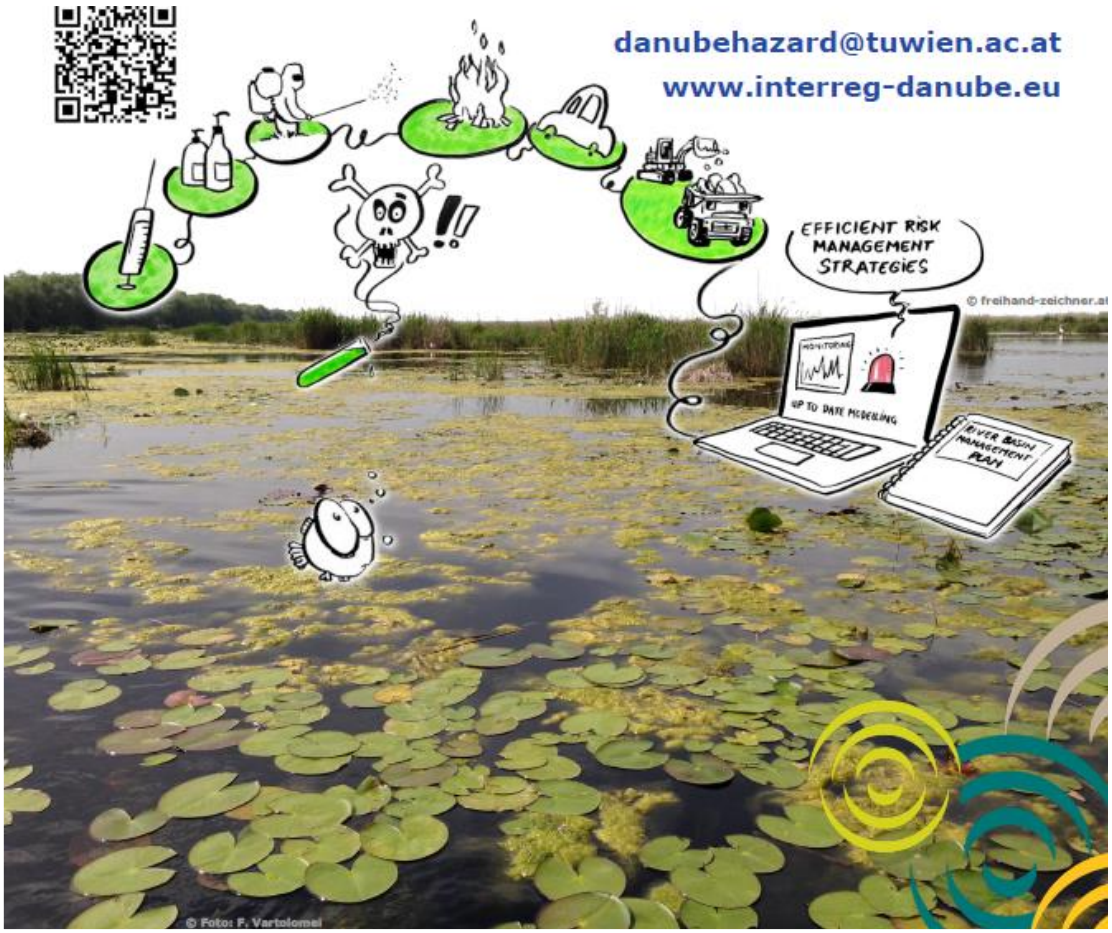

Output O.T3.2

Upgraded version of the Solutions model adapted to territorial needs for transnational modelling of HS emissions in the DRB

(Danube Hazardous Substances Model)

Interreg
EUROPEAN UNION
Danube Transnational Programme

March 2023

PROJECT TITLE: Tackling Hazardous Substances Pollution in the Danube River Basin by Measuring, Modelling-based Management and Capacity building

ACRONYM: Danube Hazard m^{3}c

PROJECT CODE: DTP3-299-2.1

DATE OF PREPARATION: 31. March.2023

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Responsible of the Output: International Commission for the Protection of the Danube River

Summary

This output constitutes the upgraded version of the Solutions model adapted to territorial needs for transnational modelling of Hazardous Substances emissions in the Danube River Basin. The model was implemented within the Danube Hazard m3c project and is denoted as Danube Hazardous Substances Model (DHSM).

The DHSM has been set up on the basis of the generic Delft3D open-source modelling framework, the central version of which is maintained by Deltares. The use of this framework is supported by a dedicated portal to download source code and manuals, to exchange experiences and to ask questions (https://oss.deltares.nl/web/delft3d).

This output consists of a file package and an annex, which can be downloaded from here: https://doi.org/10.48436/1yam1-e0y86.

Table of Contents

1 File package

The file package contains four folders:

- DHSM: the generic software plus all input files that together form the implementation of DHSM to the DRB.
- Scenarios: alternative sets of input data for the P25, best estimate (P50) and P75 emission estimates, and for the scenarios S01-S07.
- Supportive: some supportive files for presentation of the results.
- Documentation:
  - The general principles and operation of the DELWAQ framework used for the DHSM are documented in a User Manual (https://content.oss.deltares.nl/delft3d4/D-Water_Quality_User_Manual.pdf)
  - The input file format is documented in a separate manual: (https://content.oss.deltares.nl/delft3d4/D-Water_Quality_Input_File_Description.pdf)
  - The mass balances output is documented in a separate manual, included in the package[1].

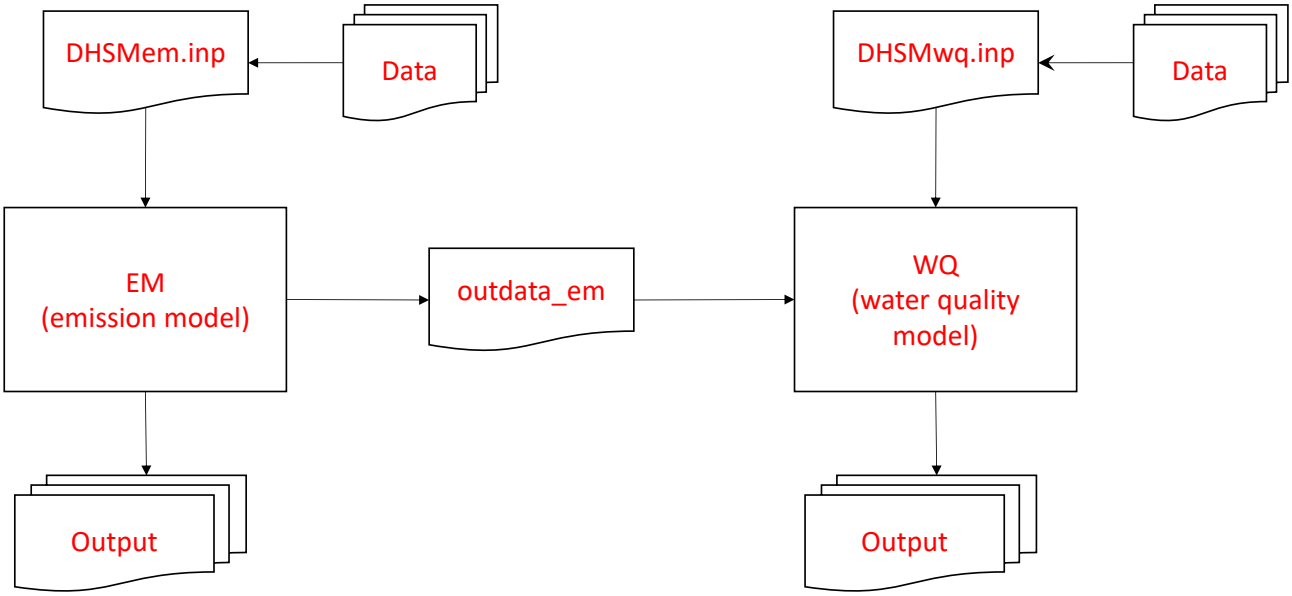
The accompanying annex "Danube River Basin Scale Assessment Report" provides a full account of the model approach and implementation.

[1] Deltares (2018). Water Quality Modelling. Using the mass balances facilities. User Manual. Jos van Gils, Jan van Beek, Erwin Meijers, Version: 5.01. SVN Revision: 57623. August 30, 2018.

2 Guidance on the use of DHSM

2.1 General

The procedure to run DHSM is shown in the below figure:



This figure shows two modelling steps:

1. The emission model, starting from the input file DHSMem.inp
2. The water quality model, starting from the input file DHSMwq.inp

Both steps make use of the same software.

For both steps, the input file contains references to other files, indicated in the scheme as “Data”. The organisation of these files is completely free. This is further explained in the Input File Description Manual. The way this is organized in the current output is just one way to do it and was chosen by the modelling team that developed the DHSM.

The running of both EM and WQ again requires two separate steps. The first step entails the reading of the input file and included data files. The second step is the true simulation. This is explained in the User Manual of the DELWAQ framework.

These two steps are conducted from the command line:

```
delwaq1.exe DHSMem.inp -p<proc_def_em>
delwaq2.exe DHSMem.inp -openpb<em.dll>

delwaq1.exe DHSMwq.inp -p<proc_def_wq>
delwaq2.exe DHSMwq.inp -openpb<wq.dll>
```

where items enclosed in < > are references to system files. The above is a simplified representation. The true commands need to reflect the file locations of the executables, input files and system files.

The output is provided in different text and binary files, as described in the User Manual of the DELWAQ framework. Some supportive tools are available to convert this output to various tabulated text files.

2.2 Organization of the run process

As mentioned above, the organisation of the input file and the references to additional data files is completely free. The DHSM development team has chosen an approach that completely avoids duplication of input for different hazardous substances. Therefore, the primary input files DHSMem and DHSMwq are independent of the modelled substance. Different substances are modelled by copying different versions of the substance dependent data files from the data folder (\DHSM\Data\) to the run folder (\DHSM\Q_Danube\).

The output files inherit their name from the input files. As the same input files are used for all substances, the output files initially have a generic name. They are given a substance specific name and copied to a separate folder (\DHSM\Q_Danube\output\).

This whole process is arranged by a sequence of bat-fles, that starts from:

\DHSM\Q_Danube\runall-em.bat

\DHSM\Q_Danube\runall-wq.bat

We repeat that this is just one way of organizing the simulation process. This organization can be modified as desired, evidently satisfying constraints formulated in the manuals.

2.3 Input

Input files are stored in different folders:

- \DHSM\H_Danube\: data on the schematization and the hydrology;
- \DHSM\S_Danube\: data on the sediment delivery to streams and the in-stream concentrations of SPM;
- \DHSM\Data\: all input for the hazardous substances modelling, including general data and substance-specific data.

The \DHSM\Data\ folder is organized as follows:

Name	description
raintot.inc	File containing space dependent total rainfall
agrlu_km2.inc	File containing space dependent area with agricuoture land use
population.inc	File containing space dependent population
flows.inp	File containing flow data to extract output for pilot regions for high flows and low flows in the correct year
FrRainSew.inc	File containing space dependent connection rate to central stormwater collection
wwman_final.inc	File containing space dependent wastewater management data
AR_traffic.inc	File containing space dependent traffic activity rates
CSO_thres.inc	File containing space dependent rainfall threshold for CSOs
pcww.inc	File containing per capita generated waste water

Name	description
Built	Folder with files providing source data for built environment
Drydep	Folder with files providing source data for atmospheric deposition
dummy	Folder with files providing dummy data for undefined sources
farms	Folder with files providing source data for agriculture
Households	Folder with files providing source data for households
Industry	Folder with files providing source data for industry
Navigation	Folder with files providing source data for navigation
S1	Folder with files providing data for initial concentrations in soils and soil fate and transport parameters
SubsProps	Folder with files providing data for surface water fate and transport parameters
traffic	Folder with files providing source data for traffic
Treatment	Folder with files providing data for treatment

All input in the \DHSM\Data\ is in text format and contains in most cases either a constant value or a series of 3477 values for all schematization elements in the correct order. Constant values are specified as

```
CONSTANTS name DATA number
```

Space dependent input is specified as:

```
PARAMETERS name ALL DATA 3477 numbers
```

It is noted that a specific format to repeat a certain value is sometimes used (note the absence of spaces in this sequence):

```
3477*1.0
```

Input is recognized by prescribed names, which are listed in section 3.

2.4 Output

The procedure included in the file package collects 8 output files per substance (XX represents a substance abbreviation used in the running of DHSM):

Name	Contents
XX_DHSMem-bal.his	From EM: all mass balance terms for all simulated compartments, for “mass balance areas” for every time step
XX_DHSMem-stat.map	From EM: annual means of the emissions to water for 10 years and all schematization elements
XX_DHSMem.his	From EM: time series of masses in all simulated compartments plus additional output at request, for “mass balance areas” for every time step
XX_outdata_em.bin	From EM: emissions data for use in WQ
XX_outdata_em.txt	From EM: emissions description for use in WQ
XXwq-bal.his	From WQ: mass balances per day for the whole model domain

Name	Contents
XXwq-stat.map	From WQ: annual means of the total and dissolved concentrations for 10 years and all schematization elements
XXwq.his	From WQ: time series of concentrations at selected points for every time step

The “mass balance areas” can be defined in two ways:

1. Country-by-country (file: \DHSM\Q_Danube\zones\em-countries.inc)
2. For individual schematization elements (file: \DHSM\Q_Danube\zones\em-maps.inc)

This is arranged in two different versions of \DHSM\Q_Danube\runall-em.bat.

Each of the two versions allows different forms of output processing. The second version leads to long runtimes, big output files and long output processing times, and should only be used to produce output for maps.

As the output files are custom and binary, some tools are provided to extract information. These tools are operated by bat files in the run folder. Each one of these invokes a tool, reads a file with the extension “.def” that defines the information to extract and writes a text file in comma-separated-value format.

Bat file	Purpose	Remarks
balance-em-sources-pathways-emissions.bat	Extracts basin-wide EM mass balance terms for all compartments	For producing figures 2-3 to 2-8 of D.T3.4.1
balance-wq.bat	Extracts basin-wide WQ mass balance terms for surface waters	For producing figure 2-9 of D.T3.4.1
collect-concentrations-annual-averages-tot-dis.bat	Extracts annual concentration averages for total and dissolved concentrations respectively	For producing figures 8-1 to 8-17 of D.T3.4.1
collect-concentrations-pilots.bat	Extracts time series of concentration at pilot areas outlet points	For producing figures in section 9.4 of D.T3.4.1
collect-emissions-annual-totals.bat	Extracts annual total emissions for all segments	For producing figure 3-1 of D.T3.4.1
collect-emissions-countries.bat	Extracts total emissions per pathway for all countries	For producing lower part of figures 2-10 to 2-14 of D.T3.4.1, *will not work if EM is run with map balance areas*
collect-emissions-maps.bat	Extracts total emissions per pathway for all segments	For producing upper part of figures 2-10 to 2-14 of D.T3.4.1, *will only work if EM is run with map balance areas*
aggregate_emission_mapresults.bat	Further processes results from previous step	As above, converts to area-specific values and clusters pathways

Ìt is noted that the output files can also be read using tools like MatLab, Python and R. Reference is made to the User Manual.

Output is provided with prescribed names, which are listed in section 3.

2.5 Supportive files

The file package also provides some supportive files that are needed to prepare input or present output. This concerns:

- File DHSM_spatial_31012023.xlsx that provides spatial data including the order, ID and key properties of the schematization elements.
- File EHype-DBRD.shp that provides the shapes of the schematization elements.

- File DRBMP2021_River4000-DHSM.shp that provides the network of rivers, cut in sections with an attribute “subid-corr” that defines the equivalent schematization element. This file could be used to produce a map with river segments coloured according to their concentrations.
- File DRBMP2021_LWBody100-DHSM.shp that provides the larger lakes, with an attribute “subid” that defines the equivalent schematization element. This file could be used to produce a map with lakes coloured according to their concentrations.

3 Names of model input and output items

3.1 Definitions in EM

The EM part of DHSM distinguishes 6 compartments:

Compartment	Description
Sew	Mixed sewers and WWTPs
Pav	Impermeable surfaces
Unp	Permeable surfaces
Stw	Separated sewers
Sfw	Surface waters (what arrives in this compartment is passed to WQ as emissions)
Soi	Top soil (thickness from the hydrology model)

The sources are numbered as follows:

Source	Description
1	Agriculture
2	Road traffic
3	Built environment
4	Households
5	Industry
6	Navigation
7	Mining (not implemented)
8	Empty

3.2 Input for EM

Item	Description	Unit
ADTot	Total deposition	(g/km2/y)
RainTot	Mean annual rainfall	(mm/y)
FrWet	Fraction allocated to wet deposition	(-)
EV_Bii	Activity rate for source ii	(X)
EF_Bii	emission factor for source ii	(kg/d/X)
BiitoWW	released fraction of source ii to wastewater (further allocated to compartments depending on local infrastructure)	(-)
BiitoSew	released fraction of source ii to receptor Sew	(-)
BiitoPav	released fraction of source ii to receptor Pav	(-)
BiitoUnp	released fraction of source ii to receptor Unp	(-)
BiitoStw	released fraction of source ii to receptor Stw	(-)
BiitoSfw	released fraction of source ii to receptor Sfw	(-)

Item	Description	Unit
BiitoSoi	released fraction of source ii to receptor Soi	(-)
Pest2Unp	Fraction to soil (pesticides)	(-)
Pest2Air	Fraction to air (pesticides), used to estimate fraction to water	(-)
TotArea	total surface area	(m2)
fPaved	fraction paved	(-)
fUnpaved	fraction unpaved	(-)
fOpenWater	fraction open water	(-)
Rainfall	actual rainfall	(m3/s)
RunoffPav	runoff from paved surfaces	(m3/s)
RunoffUnp	runoff from unpaved surfaces	(m3/s)
Infiltr	infiltration	(m3/s)
Exfiltr	exfiltration	(m3/s)
FrRainSew	fraction of stormwater to sewer systems	(-)
Population	population	(cap)
PCWastWat	per capita production of wastewater	(L/cap/d)
FrSewered	fraction of wastewater to sewer systems	(-)
FrSldgRem	fraction of sludge removed (not reused)	(-)
FrSeptic	fraction of wastewater to septic tanks	(-)
FrTreat1	fraction primary treated of collected wastewater	(-)
FrTreat2	fraction secondary treated of collected wastewater	(-)
FrTreat3	fraction tertiary treated of collected wastewater	(-)
Eff_Septic	fraction to surface water from septic tanks	(-)
Eff_Treat1	fraction to effluent for primary treatment	(-)
Eff_Treat2	fraction to effluent for secondary treatment	(-)
Eff_Treat3	fraction to effluent for tertiary treatment	(-)
Sld_Septic	fraction to soils for septic tanks	(-)
Sld_Treat1	fraction to sludge for primary treatment	(-)
Sld_Treat2	fraction to sludge for secondary treatment	(-)
Sld_Treat3	fraction to sludge for tertiary treatment	(-)
Eff_RS	Fraction to effluent of rain sewers influent	(-)
Sld_RS	Fraction to sludge of rain sewers influent	(-)
fComSew	fraction of combined sewers	(-)
SewLeakage	sewer leakage / CSO definition	(- or mm)
SoilThick	soil thickness	(m)
SoilPoros	soil porosity	(-)
RhoDM	soil dry matter density	(kg/m3)
FacErod	scale factor on erosion terms	(-)
ErodIM1	erosion flux of 1st fraction	(g/d)
kBurial	burial rate of unpaved pool	(-)
DecPav	decay rate paved	(/d)
DecUnp	decay rate unpaved	(/d)

Item	Description	Unit
KdUnpa	mobile fraction in Unp	(-)
DecSoi	decay rate soils	(/d)
KdSoi	mobile fraction in Soi	(-)
ro_lothr	run-off from hard surfaces lower threshold	(mm/d)
ro_hithr	run-off from hard surfaces upper threshold	(mm/d)
disp_hithr	dissolved transport, threshold for runoff + infilt	(mm/d)

3.3 Output from EM

Fluxes in balances:

Item	Description	Unit
dInitSoi	release to receptor Soi at initialization	(g/d)
dRelAtmxxx	release from atmospheric deposition to receptor xxx	(g/d)
dRelBiixxx	release from source ii to receptor xxx	(g/d)
dpav2sew	paved areas to mixed sewers	(g/d)
dpav2stw	paved areas to separated sewers	(g/d)
dpav2sfw	paved areas to surface waters (direct)	(g/d)
dpav2soi	paved areas to soils	(g/d)
dpav2dec	degradation on paved areas	(g/d)
dunp2sfwro	surface runoff from permeable areas	(g/d)
dunp2soiin	infiltration from permeable areas into soils	(g/d)
dunp2soibu	burial from permeable areas to soils	(g/d)
dunp2dec	degradation on permeable areas	(g/d)
dsew2sfwl	combined sewer overflows or leakages	(g/d)
dsew2rem	removal in treatment plants	(g/d)
dsew2sfwe	effluents from treatment to surface waters	(g/d)
dsew2soi	distributed sludge from treatment	(g/d)
dsew2sfwu	discharges from unconnected sewers	(g/d)
dstw2rem	removal in stormwater collection systems	(g/d)
dstw2sfw	from separated sewers to surface waters	(g/d)
dstw2soi	from separated sewers to soils	(g/d)
dsoi2rem	removal in soils	(g/d)
dsoi2sfwer	from soils to surface waters (erosion)	(g/d)
dsos2sfw	from soils to surface waters (subsurface)	(g/d)
dsfw2exp	total emissions to surface waters from EM to WQ	(g/d)

Other output:

Item	Description	Unit
Emis_Sfw	emission to water	(g/s)
RO2ComSew	runoff from paved areas to mixed sewers	(m3/s)
WW2ComSew	wastewater to mixed sewers	(m3/s)
ConcROp	concentration in runoff from paved areas	(g/m3)
ConcROu	concentration in runoff from unpaved areas	(g/m3)
ConcWW	concentration in raw WWTP influents	(g/m3)
ConcDR	concentration in drainage from soils	(g/m3)
Sew	mass in compartment Sew	(g)
Pav	mass in compartment Pav	(g)
Unp	mass in compartment Unp	(g)
Stw	mass in compartment Stw	(g)
Sfw	mass in compartment Sfw	(g)
Soi	mass in compartment Soi	(g)

3.4 Definitions in WQ

The WQ part of DHSM has a single state variable:

Item	Description	Unit
HAZ	Hazardous Substance	(g/m3)

3.5 Input for WQ

Item	Description	Unit
ErodIM1	fine sediment delivered to streams	(g/d)
IM1	inorganic matter (IM1), represents SPM	(gDW/m3)
VSedIM1	net settling velocity IM1	(m/d)
KdHAZIM1	partition coefficient to IM1	(m3/kgDM)
RcHAZ	first-order rate const. loss HAZ	(1/d)
TcHAZ	temperature coefficient loss HAZ in water	(-)

3.6 Output from WQ

Fluxes in balances:

Item	Description	Unit
dEmis	Emission flux received from EM part	(g/d)
dLossHAZ	overall loss flux HAZ in water	(g/d)
dSedHAZ	net settling flux HAZ towards sediment	(g/d)

Other output:

Item	Description	Unit
FrHAZDis	fraction free dissolved HAZ in water column	(-)
FrHAZIM1	fraction adsorbed to IM1	(-)
DisHAZ	free dissolved HAZ in water column	(g/m3)
QHAZSS	overall suspended solid quality HAZ	(mg/kgDW)
fSedHAZ	sedimentation flux HAZ towards S1	(gHAZ/m2/d)