



Output O.T1.1
Inventory of concentrations of hazardous substances in the Danube River Basin
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ACRONYM: Danube Hazard m³c

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Link to data repository:

<https://doi.org/10.48436/xwve4-h7v43>

1. Introduction

1.1. Target of setting up the inventory data base

The setup of inventories of hazardous substances emissions into surface waters is a heavily data driven process. The most important part of this data is substance-specific data which are necessary to quantify the emission loads. This can be concentrations in different environmental or technical matrices (e.g. waste water or soil), surface-specific rates (e.g. atmospheric deposition rates), emissions factors for different activities (emissions per vehicle and driven kilometre) or emission loads (e.g. industrial emission reported to PRTR register). Based on such data, different types of emissions and transport models can be used to quantify the overall emissions. Such models need to be validated, which again needs measured concentration data from surface waters. To collect these data together with all necessary metadata, an inventory database of concentrations was created in the Danube Hazard m³c project (DHm³c).

The aim of this activity was to collect pre-existing data from the Danube basin which were available from different sources and in different formats and combine them together with the monitoring data generated within DHm³c to generate a data base as broad as possible for following applications:

1. Generate input data for emission models, especially the MoRE model (Fuchs, et al., 2017) which is mainly based on representative concentrations in different pathways.
2. Supply validation data for emission models as the source driven Danube Hazard Substance Model (DHSM) (van Gils, et al., 2020) and the pathway driven model MoRE.
3. Supply harmonized data for surface water status assessment.
4. Create a data base for research of drivers behind the concentration patterns, which can lead to a better system understanding which then can be transformed into better emission models.

The concept and the role of data base are illustrated in Figure 1.

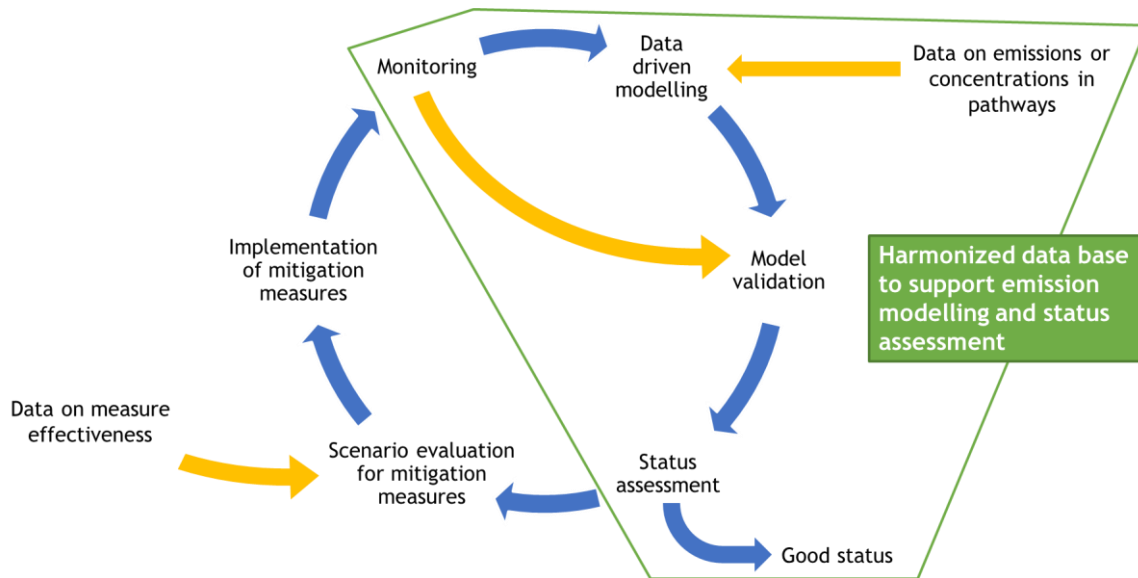


Figure 1: The cycle of hazardous substance management at the river basin scale (blue), the role of data in this cycle (yellow) and which part the data base presented here should cover (green) (Kittlaus 2023, CC-BY-SA 4.0)

1.2. Considered ideas and requirements

As this activity had a strong focus on capitalization of pre-existing knowledge, available data sources were investigated regarding their structure and the use of controlled vocabularies. These were the following data bases with data available for the Danube Basin:

- Hosted by the ICPDR data base¹:
 - Transnational Monitoring Network (TMNM)
 - Joint Danube Survey Results (JDS1, JDS2, JDS3)
- Hosted by the NORMAN EMPODAT database²:
 - Joint Danube Survey 4 Results
- Hosted by the European Environment Agency (EEA)
 - Reported monitoring data in the WISE framework
 - Reported emissions under the UWWT directive
 - Reported emissions under the E-PRTR directive

Regarding the selection of the technical framework to store the data, it was considered essential to have a system which meets the following requirements:

- Possibility of rigorous quality control of the collected data and metadata during data import.
- Easy handling of large data amounts without any restrictions.
- Data workflow to be handled with the available skills of the project team.

¹ <https://www.icpdr.org/wq-db/>

² <https://www.norman-network.com/nds/empodat/>

To make data available in the best possible way the principles of FAIR data (Findability, Accessibility, Interoperability, and Reuse) were considered as far as possible.

2. Implementation of the inventory data base

For the storage of the data, a relational database was chosen and implemented in PostgreSQL (Version 9.6, later migrated to 15.2)³, as a PostgreSQL-server was already available, known by some team members and is a powerful open-source data management system which can handle huge amount of data.

The data base consists of many tables, which are connected by columns, that refer from one table to another. There are main tables which contain the actual data and supporting tables, which contain the allowed entries for columns with controlled vocabularies. The use of controlled vocabularies is of utmost importance to harmonize the meta data from different data sources and make the data evaluable as one.

Separate tables were created for the following environmental and technical matrices:

- Water bodies:
 - surface water including suspended particulate matter samples
 - ground water
- Waste water treatment plants: municipal and industrial, influent and effluent
- Storm water: combined sewer overflows and storm water outlets in separate sewer systems
- Atmospheric deposition
- Soil

As the inventory was designed to include original monitoring data wherever possible, but also data published in an aggregated form, e.g. in scientific publications and other reports, each section contains tables for single measurements as well as tables for aggregated measurements.

Further tables contain meta data about the hazardous substances (names, identifiers) and the data sources (license, data owner) and are referenced from every data set in the main data tables (concentrations).

3. Accessibility of the inventory data base

It was not possible to develop the data base within this project into a full operational web service. Nevertheless, it was considered a useful tool, which should be made available for further use to administrations and researchers in the Danube basin. Therefore, the data base

³ <https://www.postgresql.org>

was exported into a SQL-file, zipped and published in this form in the TU Wien research data repository:

<https://doi.org/10.48436/xwve4-h7v43>

The zip file can be downloaded, unzipped and run on a PostgreSQL data base server (and with some modifications on other SQL-Servers as well) to recreate the data base structure and its content.

Along with the data base itself a PDF-file with a documentation of the different tables in the data base is available alongside in the TU Wien research data repository to support the user.

Not all data collected in the project could be included in the published data base, as some institutions preferred to keep their data undisclosed or a publication and license agreement could not be achieved within the project duration. If for further data sets a publication agreement will be achieved, new versions of the data base including more data will be published.

4. Further information and use cases

In the technical guidance document (Output O.T4.5, chapter 3) the important aspects of the workflow to develop the data base, collect, check and import data, evaluate the data and retrieve meaningful results from the data base content is explained and examples are given.

The technical guidance document can be found on the project website:

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

A rough overview of the amount of data available in the data base can be retrieved from Table 1.

Table 1: Data sources and the amount of data available in the data base

data source identifier	full citation	compartment	number of different parameters	number of measurements
AT-GZUV-GW-public	Federal Ministry for Agriculture, Regions and Tourism, Republic of Austria, National monitoring data. Supplied via the Umweltbundesamt GmbH.	ground water	275	3506129
AT-GZUV-RW-public		surface water	116	146754
AT-INN-public	Fuchs, S., Kaiser, M., Reid, L., Toshovski, S., Nickel, J. P., Gabriel, O., Clara, M., Hochedlinger, G., Trautvetter, H., Hepp, G., Kittlaus, S., Zessner, M., Kaul, U. and Forstner, S. (2019) Grenzüberschreitende Betrachtung des Inn-Salzach-Einzugsgebietes als Grundlage für ein transnationales Gewässermanagement, Umweltbundesamt (Deutschland); Umweltbundesamt GmbH	surface water	72	2484

data source identifier	full citation	compartment	number of different parameters	number of measurements
	(Österreich); Bundesministerium für Nachhaltigkeit und Tourismus (BMNT); Bayerisches Landesamt für Umwelt (LfU), Dessau, Augsburg, Wien, 145 pp.			
AT-RIVERCHARGE-GW-public	EU Project "Ri(ver)-Charge"	ground water	11	609
AT-RIVERCHARGE-RW-public		surface water	11	561
AT-STOBIMO-public	Amann, A., Clara, M., Gabriel, O., Hochedlinger, G., Humer, M., Humer, F., Kittlaus, S., Kulcsar, S., Scheffknecht, C., Trautvetter, H., Zessner, M. and Zoboli, O. 2019 STOBIMO Spurenstoffe: Stoffbilanzmodellierung für Spurenstoffe auf Einzugsgebietsebene, Bundesministerium für Nachhaltigkeit und Tourismus (BMNT), Wien.	atmospheric deposition	36	568
AT-STOBIMO-public		soil	36	648
AT-STOBIMO-public		surface water	38	2400
AT-STOBIMO-public		waste water treatment plant	36	713
DanubeHazard	Data collected in the Danube Hazard m3c project - Tackling hazardous substances pollution in the Danube River Basin by Measuring, Modelling-based Management and Capacity building. An Interreg project under the Danube Transnational Programme	atmospheric deposition	45	2397
DanubeHazard		soil	51	3570
DanubeHazard		surface water	173	25210
DanubeHazard		waste water treatment plant	102	3771
DE_IS-ESB.2020	Information System of the German Environmental Specimen Bank (IS ESB)	soil	72	1128
DE_IS-ESB.2020		surface water	85	3560
DE-KIT-MPDS-public	Nickel, Jan Philip; Sacher, Frank; Fuchs, Stephan (2021): Dataset of micropollutant concentrations and standard water quality parameters in wastewater treatment plants, combined sewer overflows, and stormwater outfalls in Germany. Karlsruhe Institute of Technology (KIT). DOI: 10.35097/449	storm water	113	12181
DE-KIT-MPDS-public		waste water treatment plant	167	79936
EU-JDS3-public	Joint Danube Survey 3 2015	surface water	193	17634
EU-JDS4-public	Joint Danube Survey 4 2019	ground water	360	4333
EU-JDS4-public		surface water	2316	118116
EU-JDS4-public		waste water treatment plant	2317	50962

data source identifier	full citation	compartment	number of different parameters	number of measurements
EU-TNMN-public	TransNational Monitoring Network (TNMN) 1996-2019	surface water	172	769365
RO-ECARO-GW-limited	Part of the RO national database (Evaluarea Calității Apelor din România - ECARO) for ground water 2015-2020	ground water	42	6468
RO-ECARO-limited	Part of the RO national database (Evaluarea Calității Apelor din România - ECARO) 2010-2020	waste water treatment plant	25	3006
RO-ECARO-SW-aggregated	Part of the RO national database (Evaluarea Calității Apelor din România - ECARO) for surface water 2010-2020	surface water	55	2780
RO-ECARO-SW-public	Part of the RO national database (Evaluarea Calității Apelor din România - ECARO) 2013-2017	surface water	17	62419
RO-EPRTR	European Pollutant Release and Trasfer Register (E-PRTR) / direct industrial releases into surface waters within the Danube River Basin District	waste water treatment plant	17	166
RS-WISE	Wise report of Republic of Serbia for years 2013-2019	ground water	97	30498
RS-WISE		surface water	109	211138
SI-SEA-GW-public	Slovenian Environmental Agency - SEA	ground water	98	41585
SI-SEA-SOIL-public		soil	15	880
SI-SEA-spat-non-public		waste water treatment plant	34	5084
SI-SEA-SW-public		surface water	188	277916
SK-National-Chem-DB		surface water	101	509255

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