

**Interreg  
Danube Region**



Co-funded by  
the European Union



**Tethys**

# Model Development

**Zsolt Jolánkai**

[Jolankai.zsolt@emk.bme.hu](mailto:Jolankai.zsolt@emk.bme.hu)

**Budapest University of Technology and Economic**

**Tethys Final Conference**

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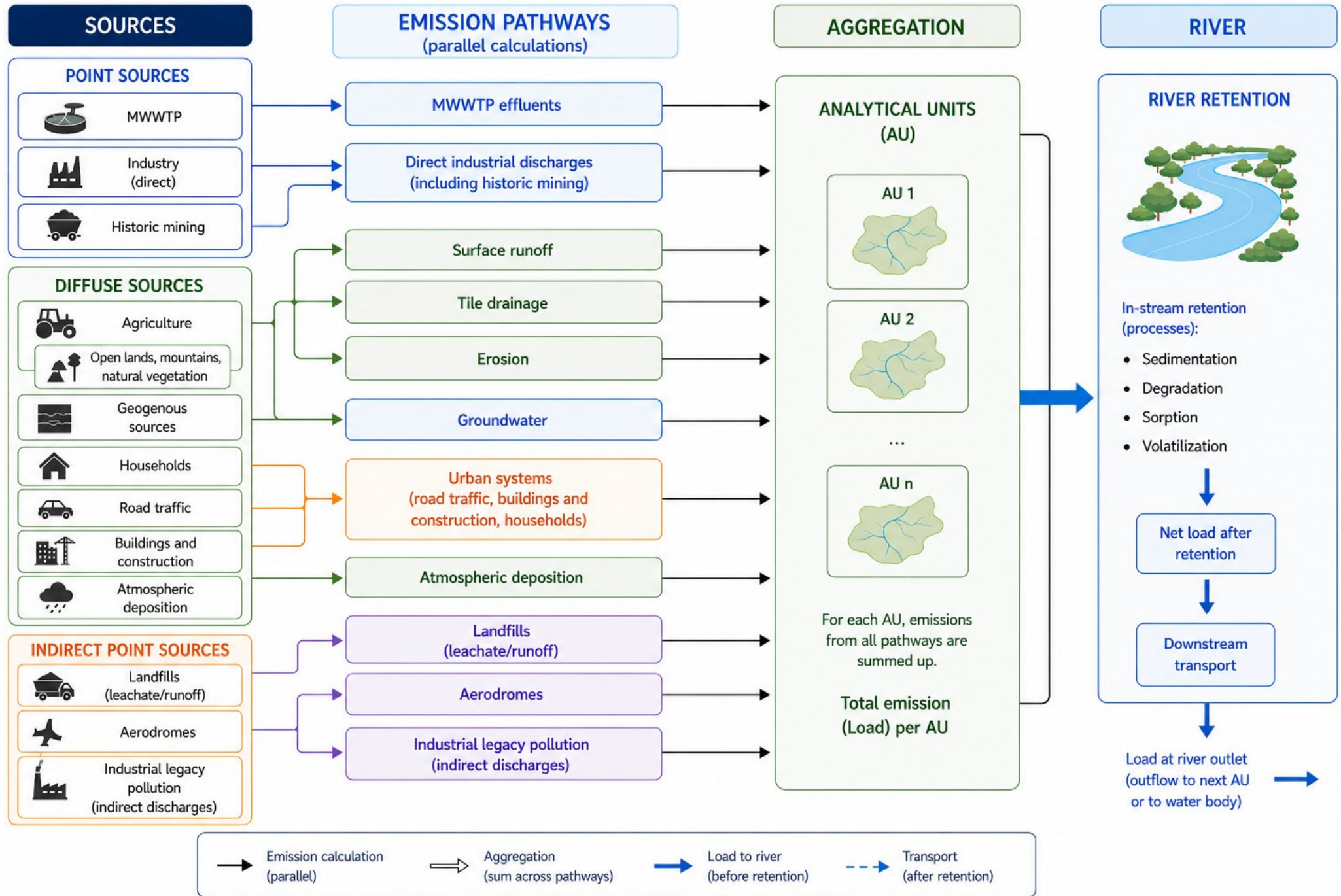


# Objective of the emission modelling

- **Understand emission patterns of priority substances in the Danube River Basin**
- **Understand the significance of specific emission hot spots/pathways**
- **Create an inventory of specific priority pollutants in the DRB to support river basin management planning**
- **Highlight information/data gaps**
- **Identify research needs**
- **Support risk assessment and mitigation evaluation**

# Method – emission modelling with MoRE modell

- **Pathway-oriented, conceptual model (Modelling of Regionalized Emissions) (Fuchs et al, Karlsruhe Institute of Technology)**
- **Algorithms based on MONERIS 2.01**
- **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**
- **Newly developed retention estimate is used for heavy metals**



# Overview of the modelled substance groups/ substances

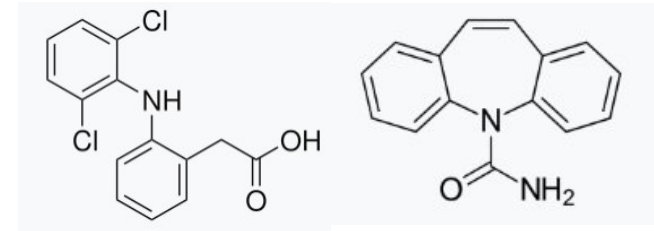
- **Heavy metals and metalloids:**

**As, Cd, Cr, Cu, Ni, Pb and Zn**



- **Pharmaceuticals:**

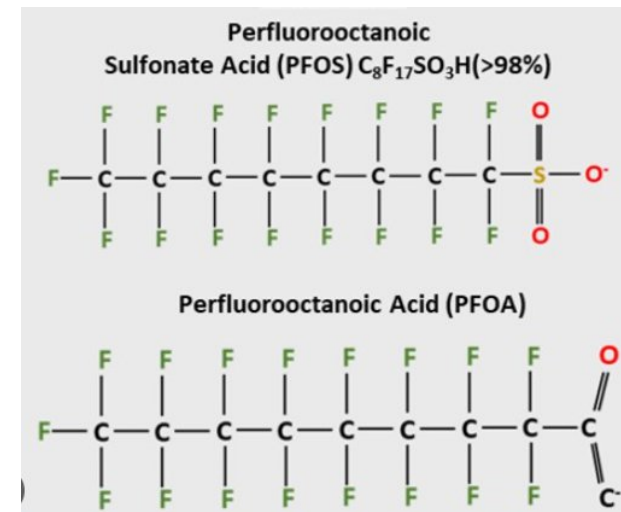
**Diclophenac (DCF) and Carbamazepine**







































**(CBZ)**

- **Per- and polyfluoroalkyl substances (PFAS):**

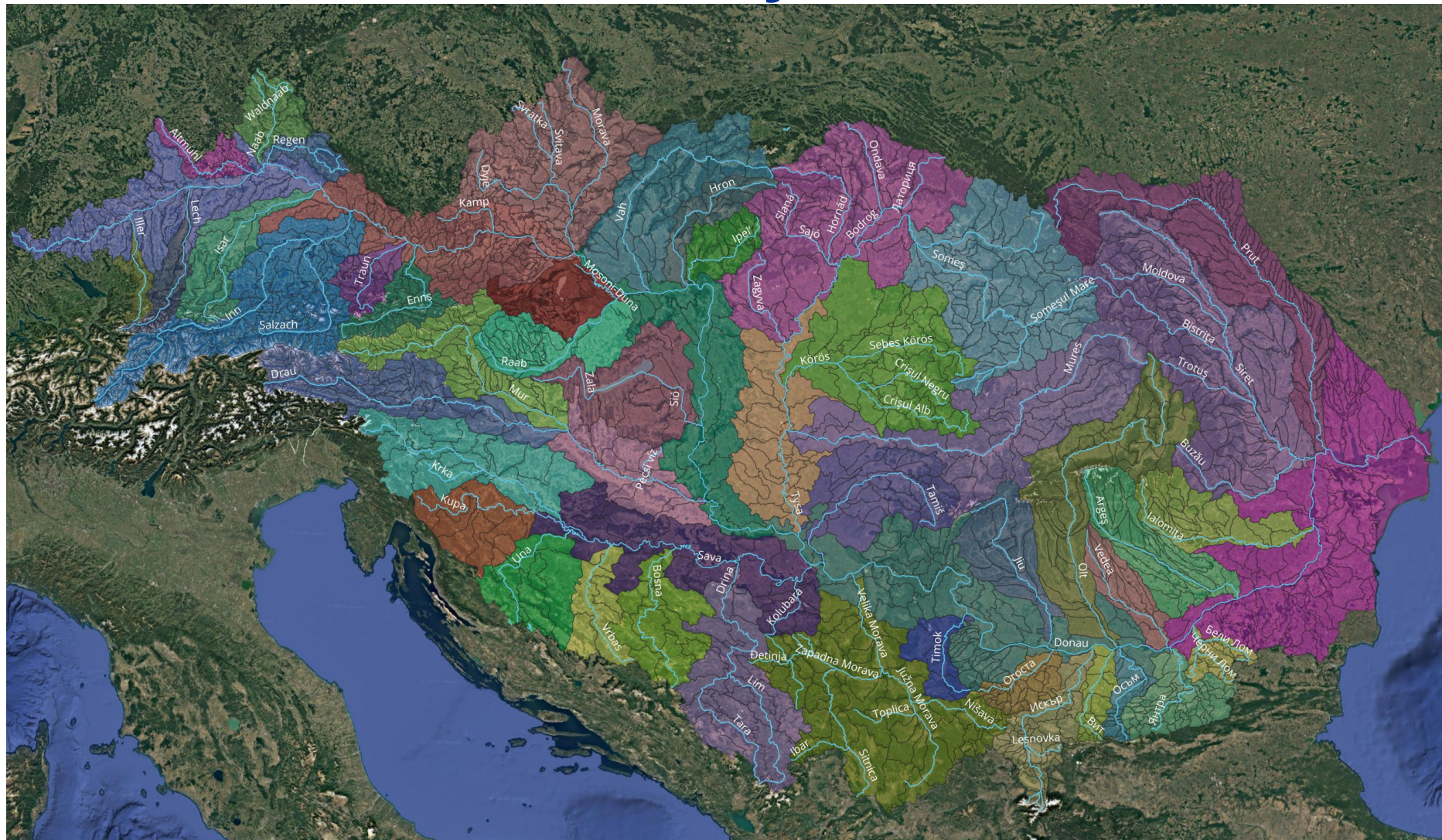
**- PFOS and PFOA**



■ Literature data (outside DRB)  
 ■ Pilot measurements within DRB  
 ■ Regional dataset  
 ■ Country dataset  
 ■ Modelled data

Process	Heavy metals	Pharmaceuticals	PFAS
Erosion	<span style="color: yellow;">■</span> 		<span style="color: orange;">■</span> 
Surface Runoff	<span style="color: red;">■</span> 		<span style="color: red;">■</span> 
Tile drainage	<span style="color: red;">■</span> 		<span style="color: red;">■</span> 
Urban emission	<span style="color: red;">■</span> 	<span style="color: red;">■</span> 	<span style="color: red;">■</span> 
Groundwater	<span style="color: yellow;">■</span> <span style="color: green;">■</span> 		<span style="color: green;">■</span> <span style="color: red;">■</span> 
Atmospheric dep.	<span style="color: purple;">■</span> <span style="color: orange;">■</span> 		<span style="color: orange;">■</span> 
Atmospheric dep. - hot spot	<span style="color: red;">■</span> <span style="color: yellow;">■</span> 		<span style="color: red;">■</span> <span style="color: yellow;">■</span> 
Point source - communal	<span style="color: orange;">■</span> <span style="color: green;">■</span> 	<span style="color: orange;">■</span> 	<span style="color: orange;">■</span> <span style="color: green;">■</span> 
Point source - industrial	<span style="color: red;">■</span> <span style="color: yellow;">■</span> <span style="color: green;">■</span> 	<span style="color: red;">■</span> 	<span style="color: red;">■</span> <span style="color: yellow;">■</span> 
Industrial diffuse hot-spots	<span style="color: red;">■</span> 		<span style="color: red;">■</span> 
Landfills	<span style="color: red;">■</span> 	<span style="color: red;">■</span> 	<span style="color: red;">■</span> 
Aerodomes and other fire fighting centres			<span style="color: red;">■</span> 

# Model domain – 1727 analytical units



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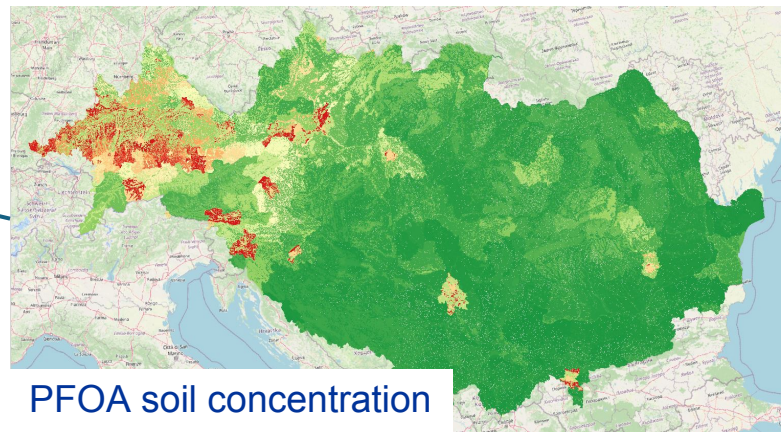
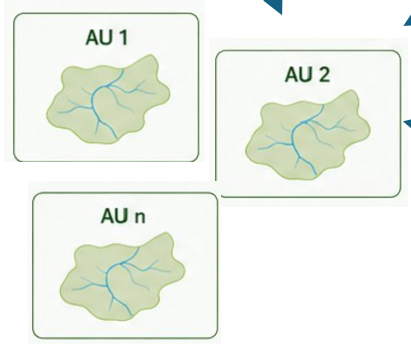
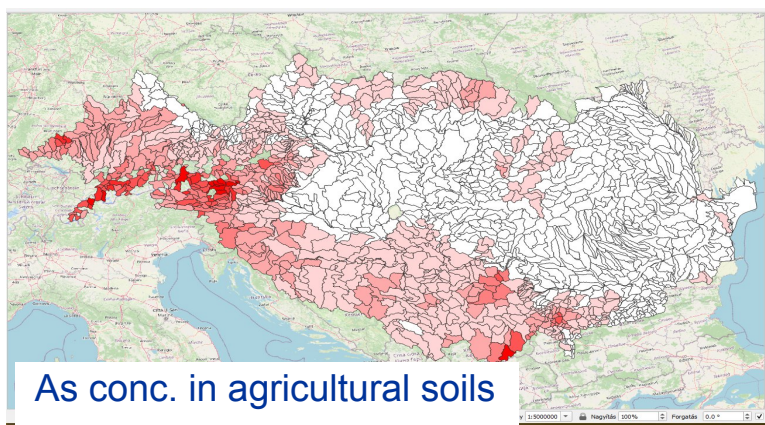
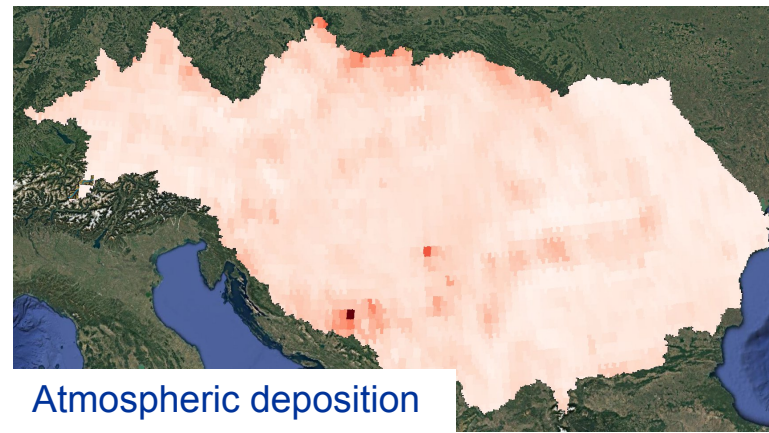
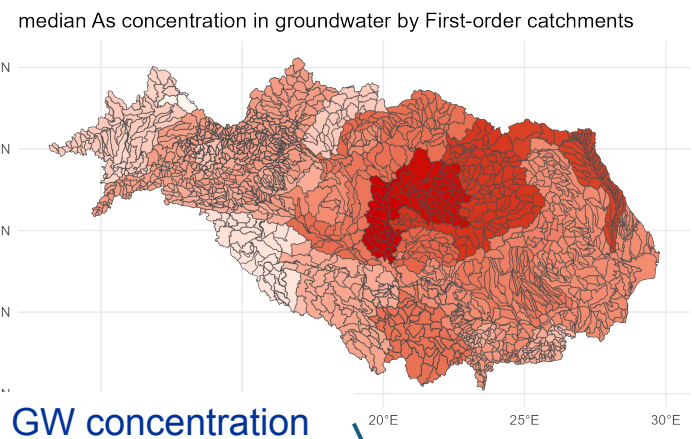
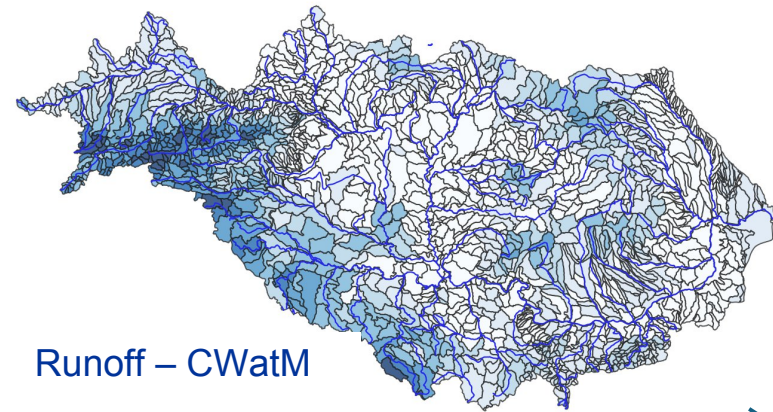
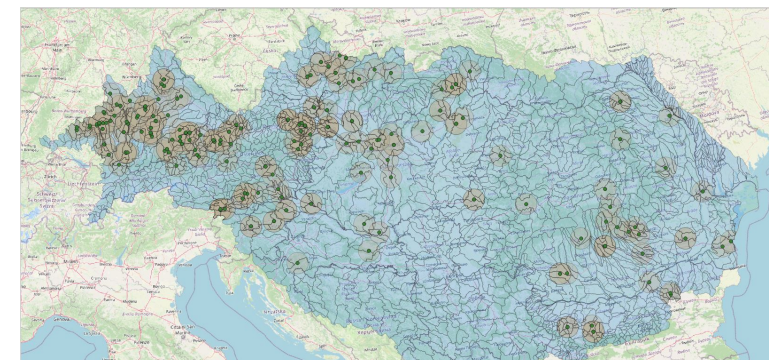
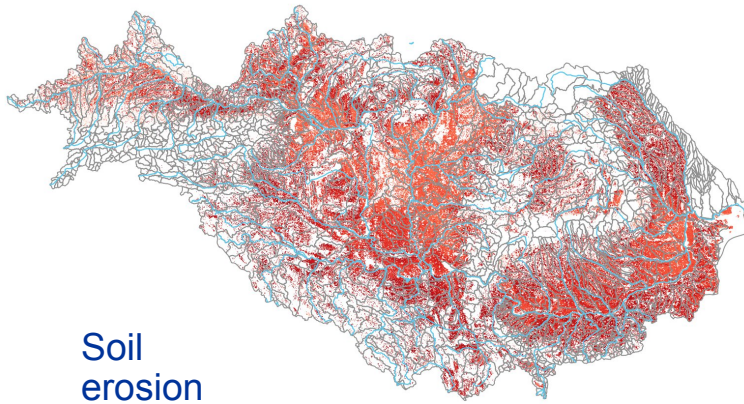
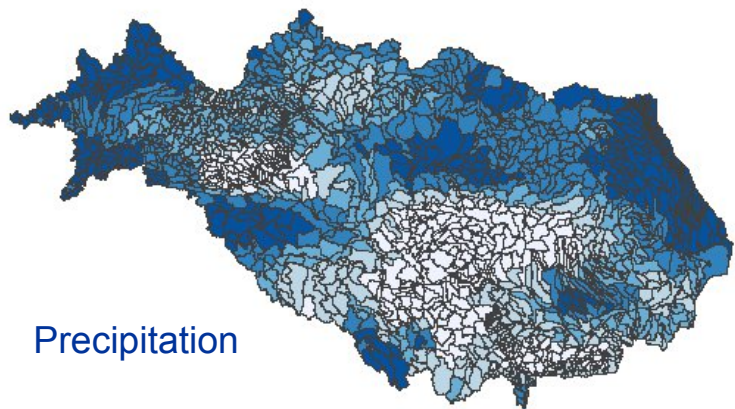
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Temporal coverage

2015-2020

# Diffuse source data



# Point source data

## Industrial emissions

I-EPR database (2007-2023)

-10.445 facilities

## Municipal sewage emissions

ICPDR – WWTP database

-5636 agglomeration

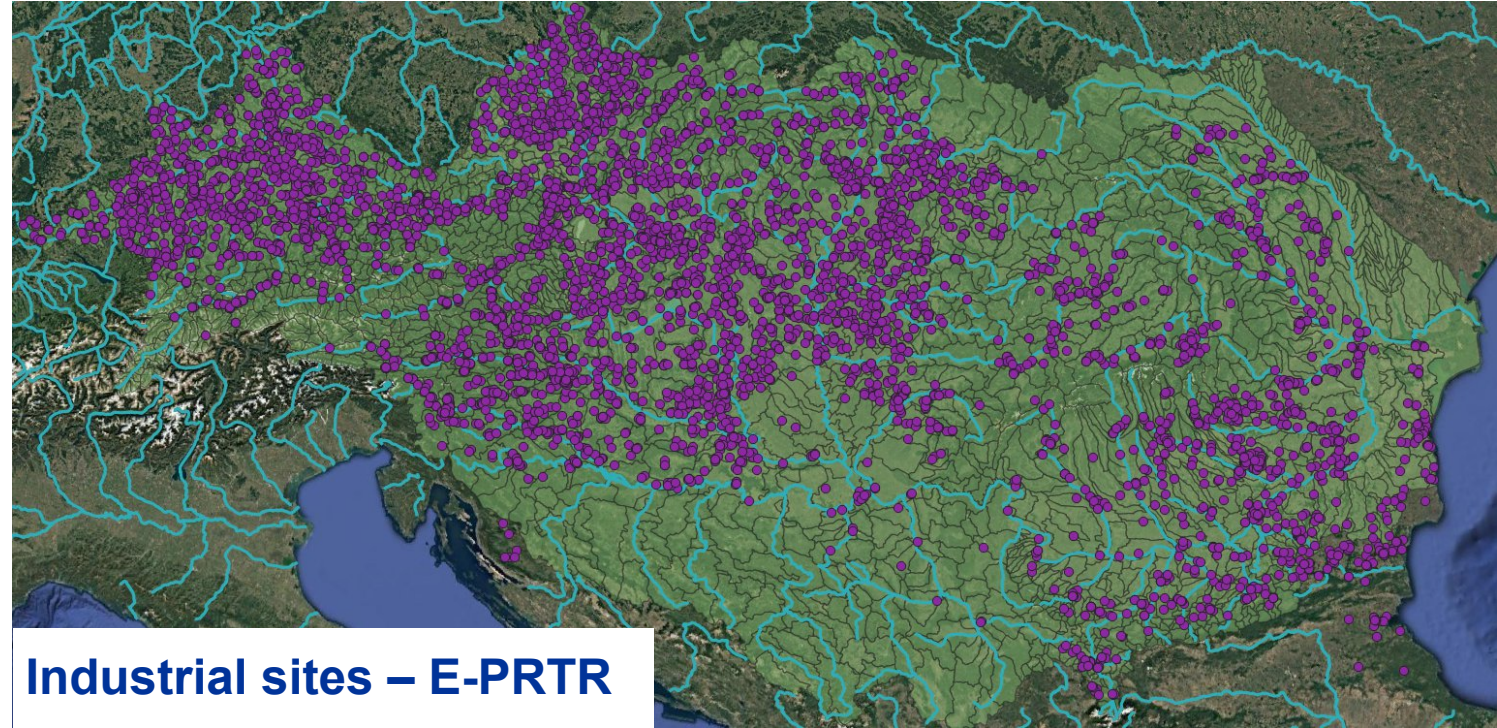
-3867 discharge point

-Total capacity: 85 million PE

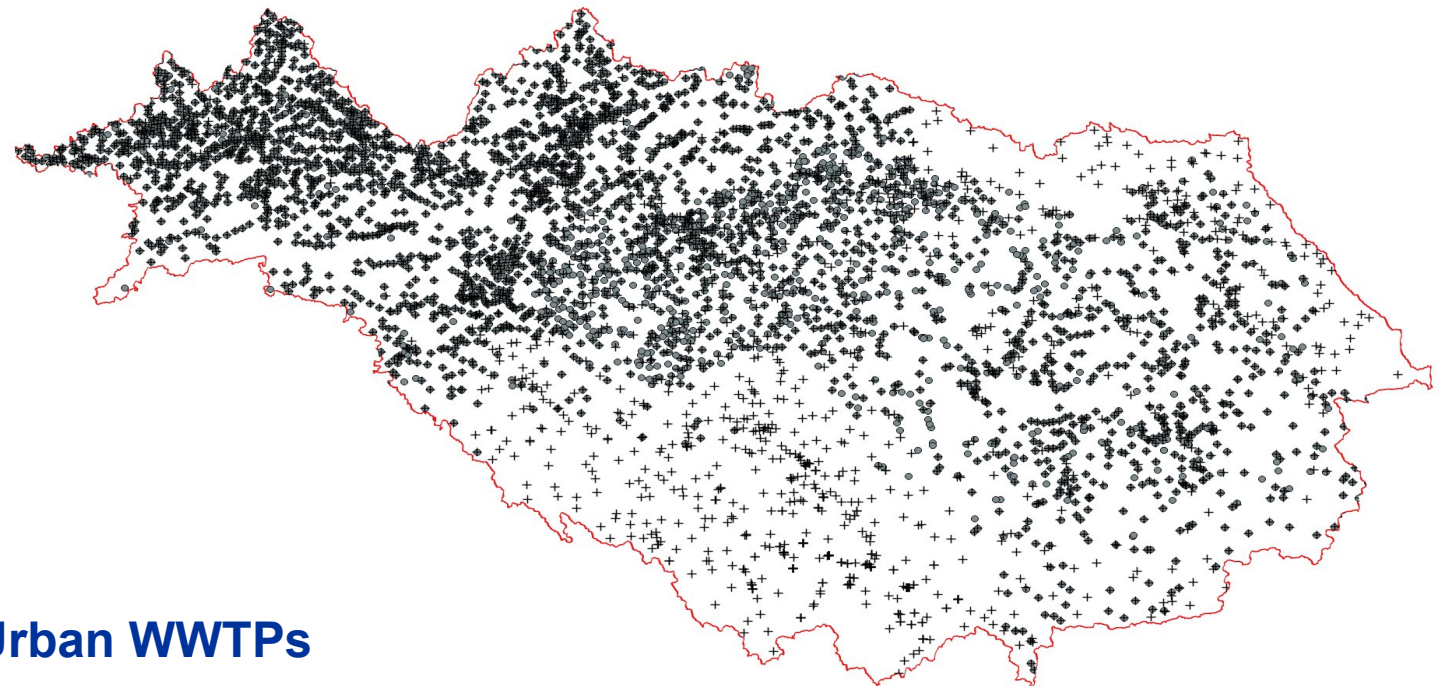
-Total discharge:

- 4.96E+09 m<sup>3</sup>/year

- 157 m<sup>3</sup>/s



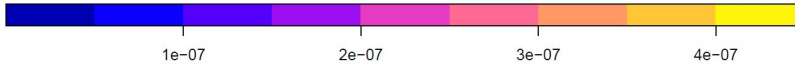
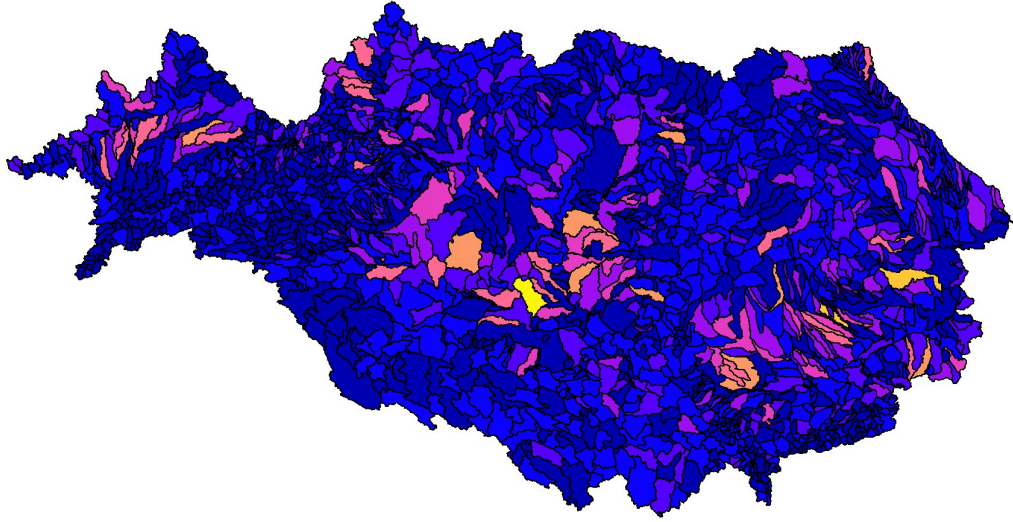
Industrial sites – E-PRTR



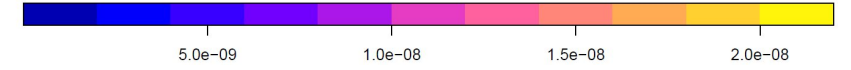
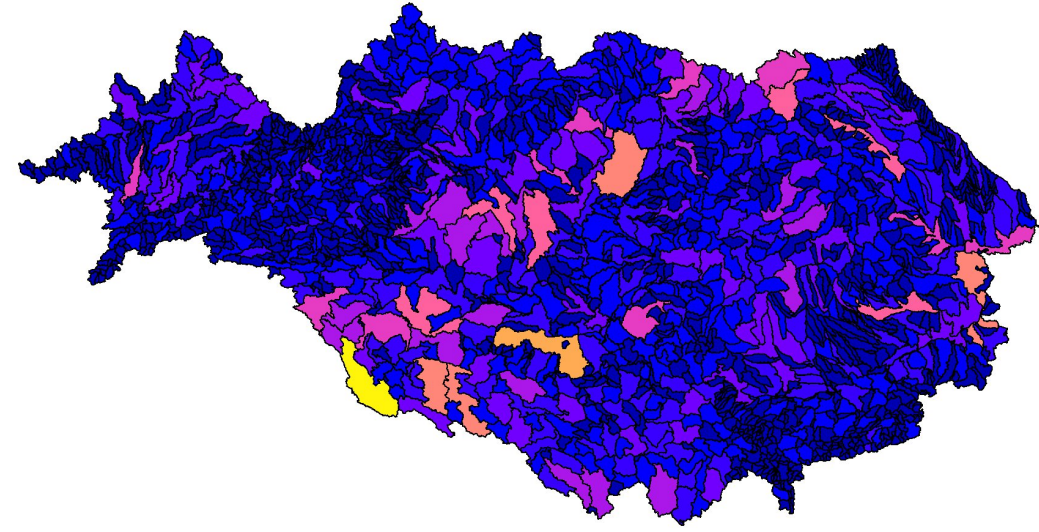
Urban WWTPs

# Retention of HM in the model - examples

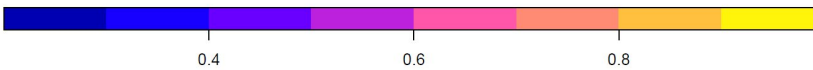
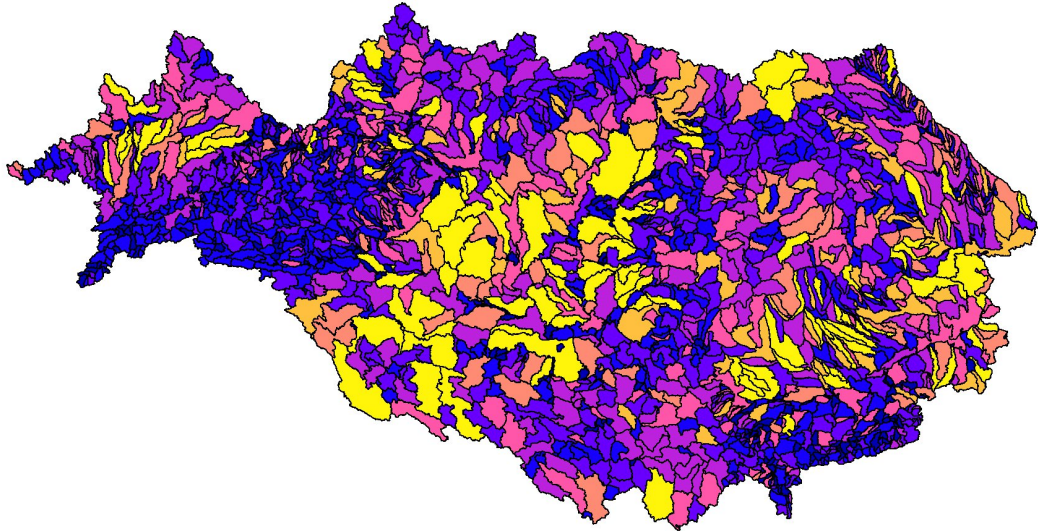
ret\_local\_As



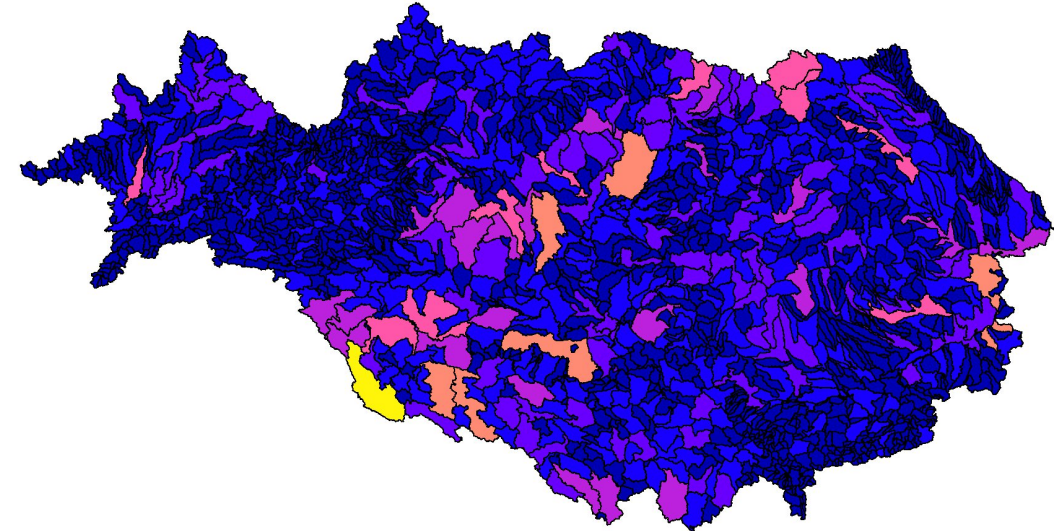
ret\_transfer\_As



ret\_local\_Pb

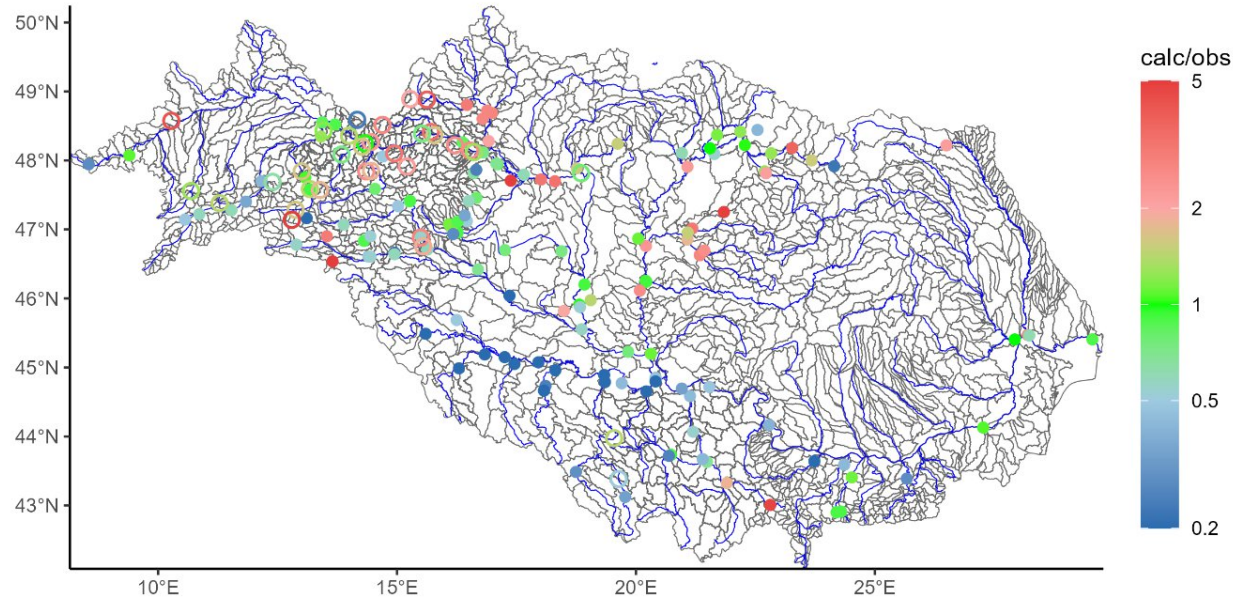


ret\_transfer\_Pb

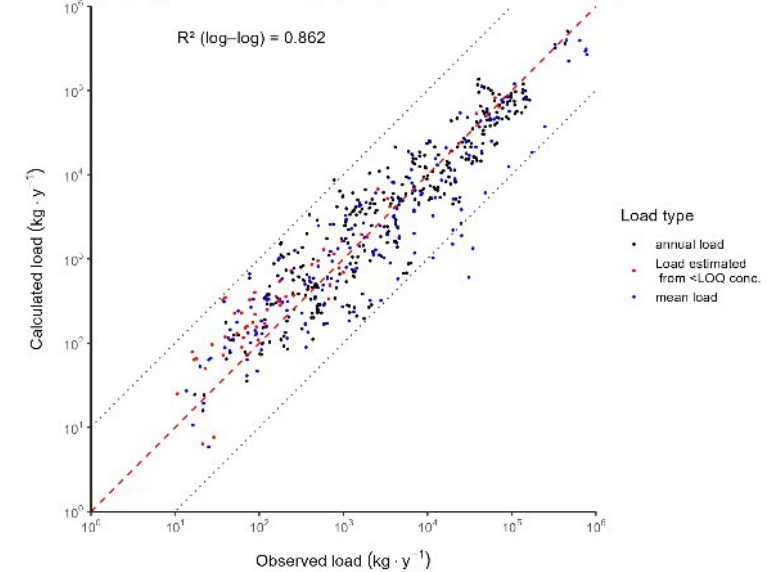


# Validation map for metalloids – arsenic, a „well” validated example

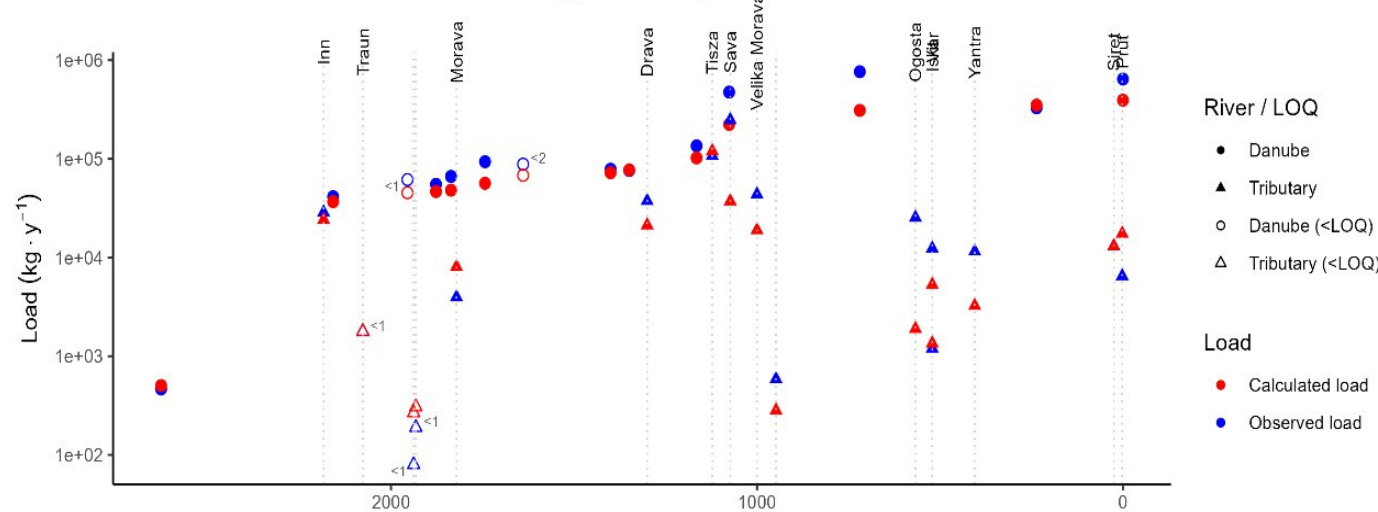
As load validation with retention and measured Q-ratio  
Calculated vs observed average loads



As load validation with retention  
(log-log) - realQ - average yearly loads 2015-2020 and avg load



As load long profile along the Danube

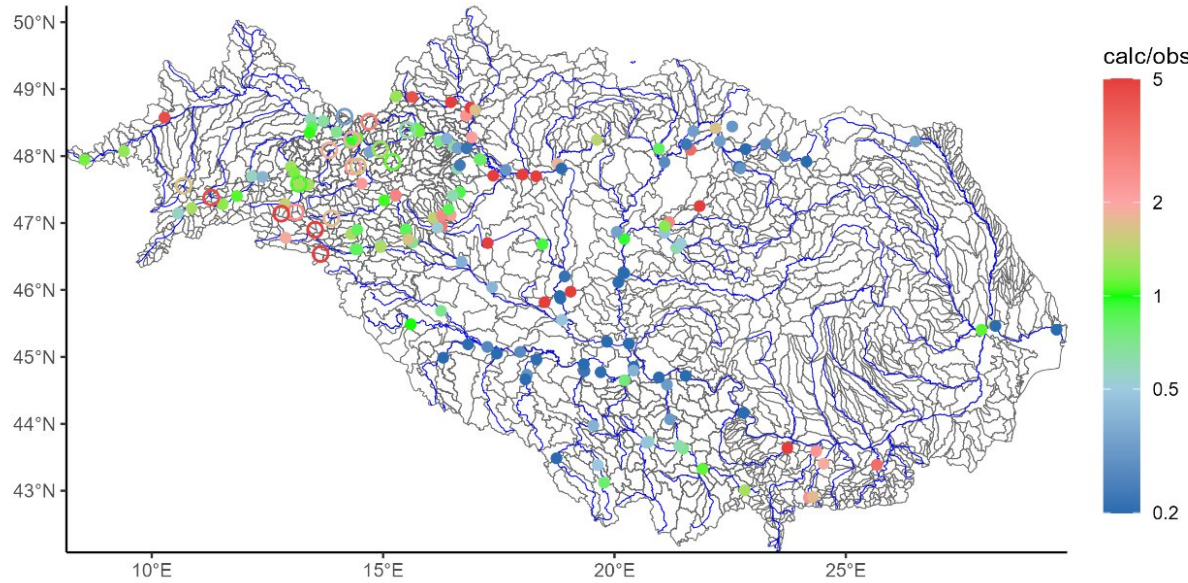


## Main observations

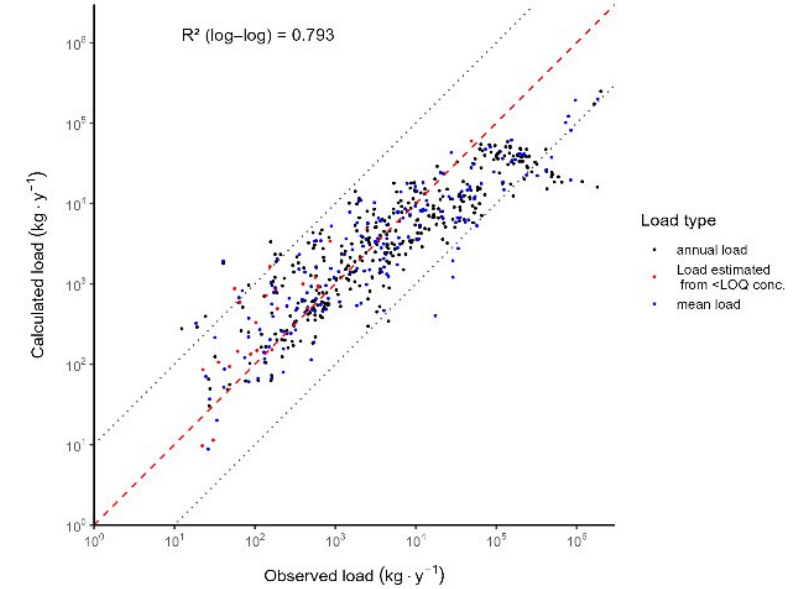
- Clear underestimation of loads in the Sava basin
- Generally good agreement of Danube loads
- Low number of groundwater wells behind derived gw. concentrations are main suspect for the underestimation of loads at Sava and lower Danube tributaries
- Lack of industry data

# Validation map for metalloids – copper, the worst validated example

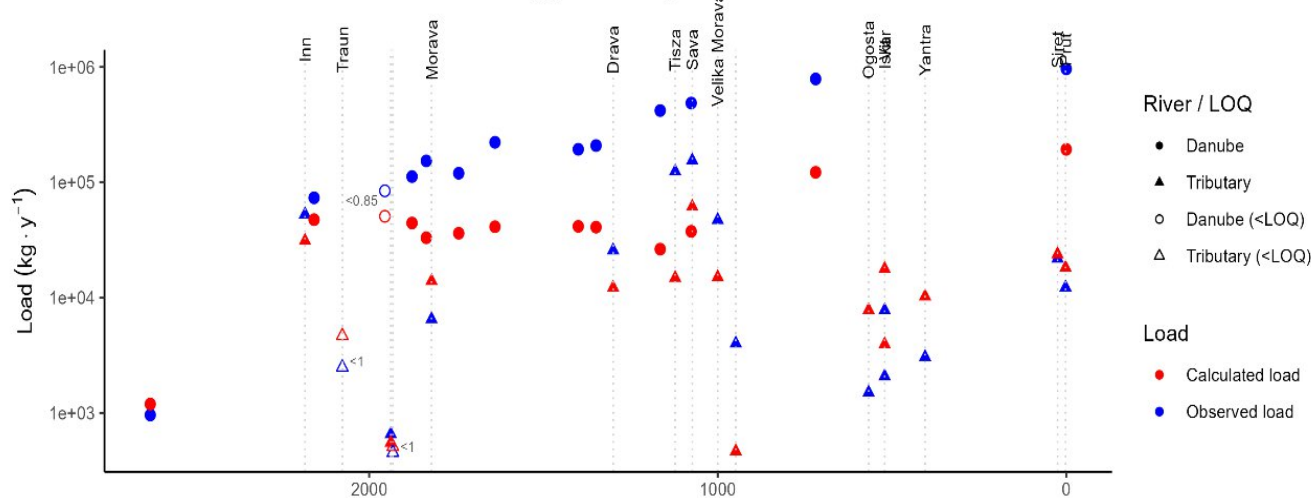
Cu load validation with retention and measured Q-ratio  
Calculated vs observed average loads



Cu load validation with retention  
(log-log) - realQ - average yearly loads 2015-2020 and avg load



Cu load long profile along the Danube

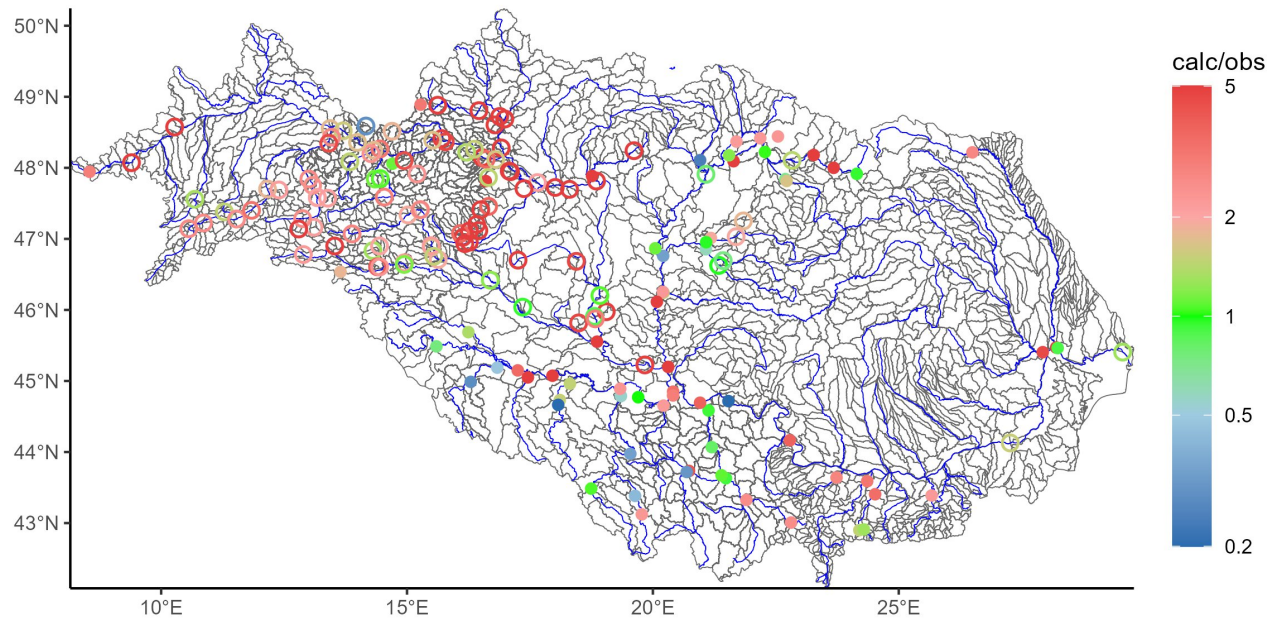


## Main observations

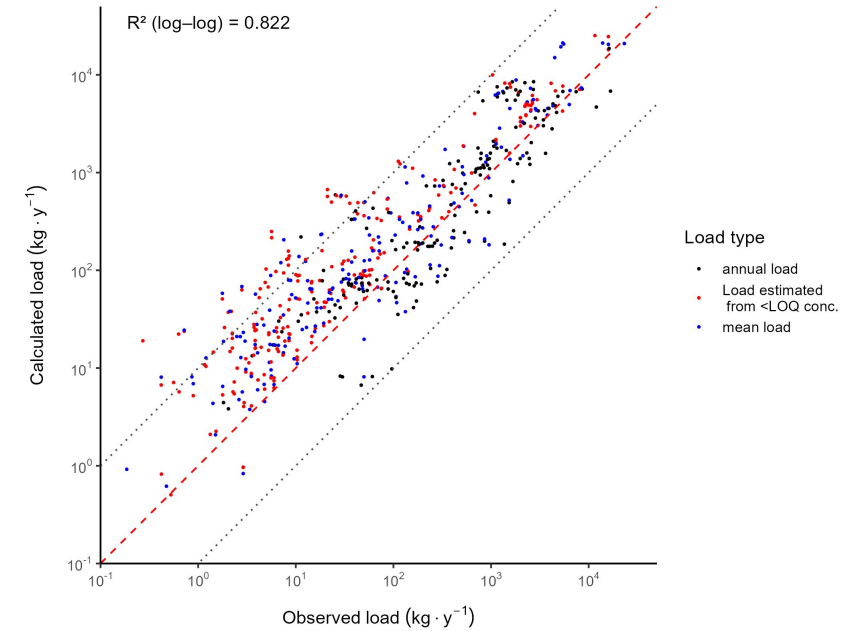
- Clear underestimation of loads in the Sava and Tisza basins
- Strong underestimation of Danube loads
- Loads at Tisza and Sava are comparable to the upper Danube loads
- Lack of industry data/industrial underestimation?
- Orchards/Vinyard soils as hot-spots?

# Validation map for metalloids – cadm

Cd load validation with retention and measured Q-ratio  
Calculated vs observed average loads



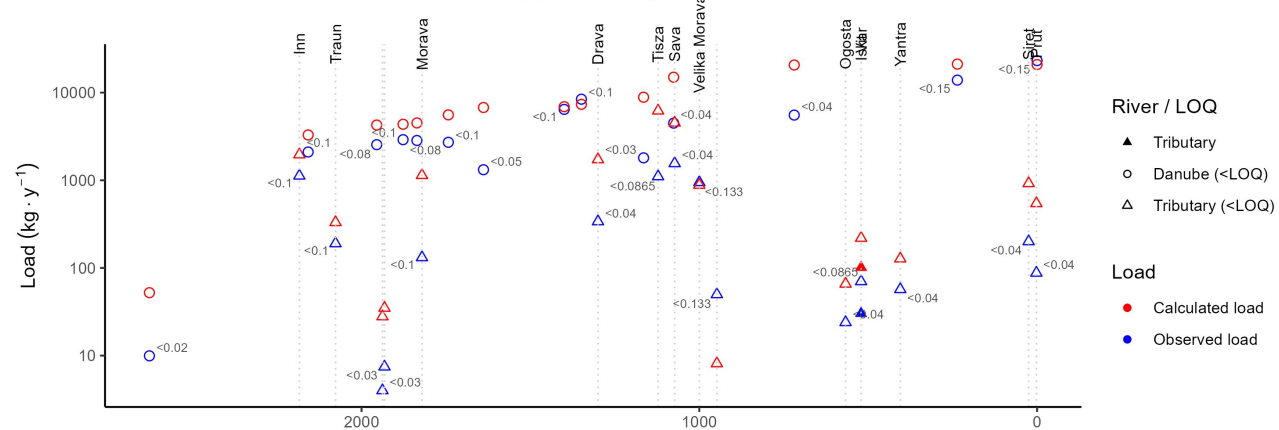
Cd load validation with retention  
(log-log) - realQ - average yearly loads 2015-2020 and avg load



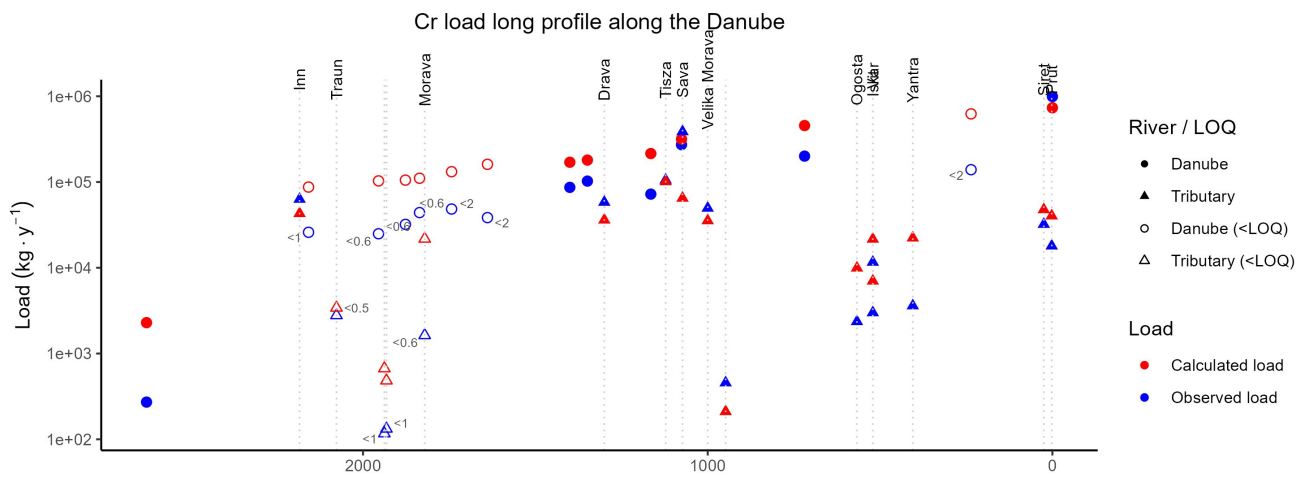
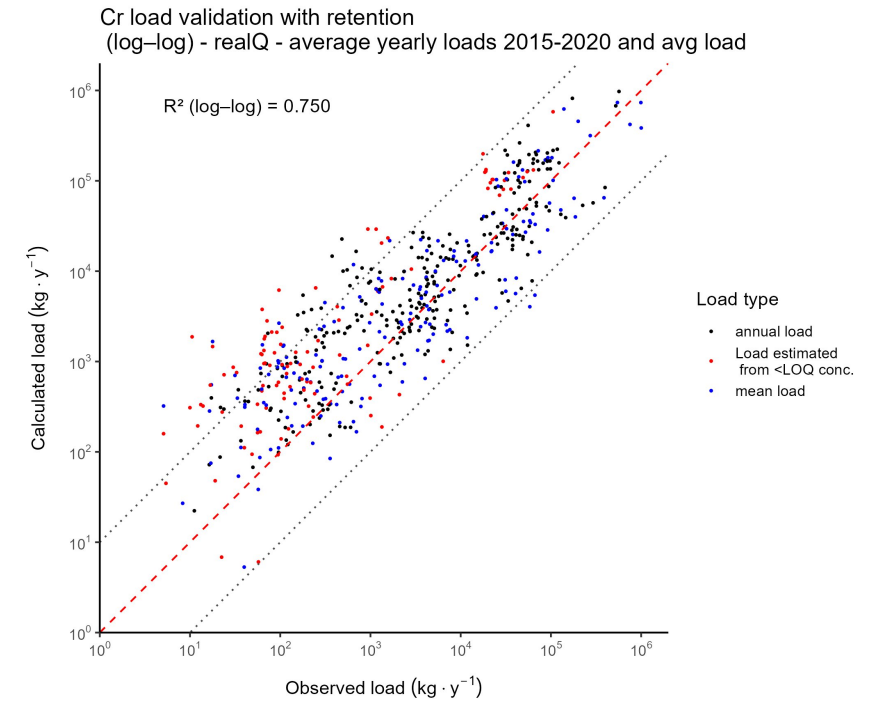
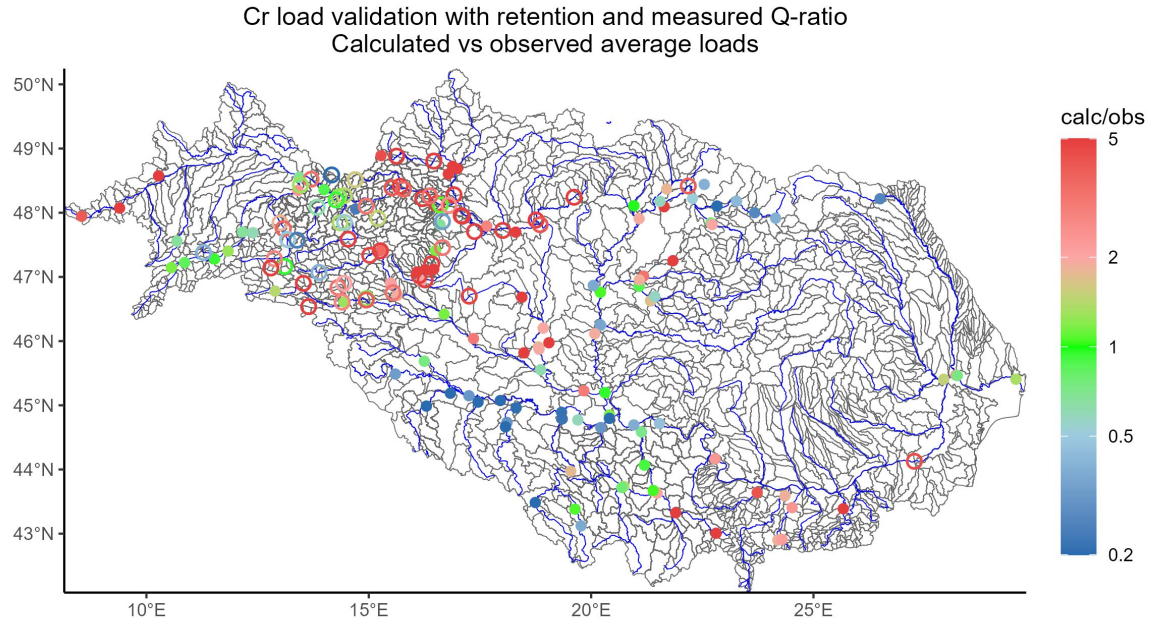
## Main observations

- Most measurements are calculated from partly censored data
- Clear overestimation of Danube loads
- Generally overestimated in the upper Danube

Cd load long profile along the Danube



# Validation map for metalloids – ch

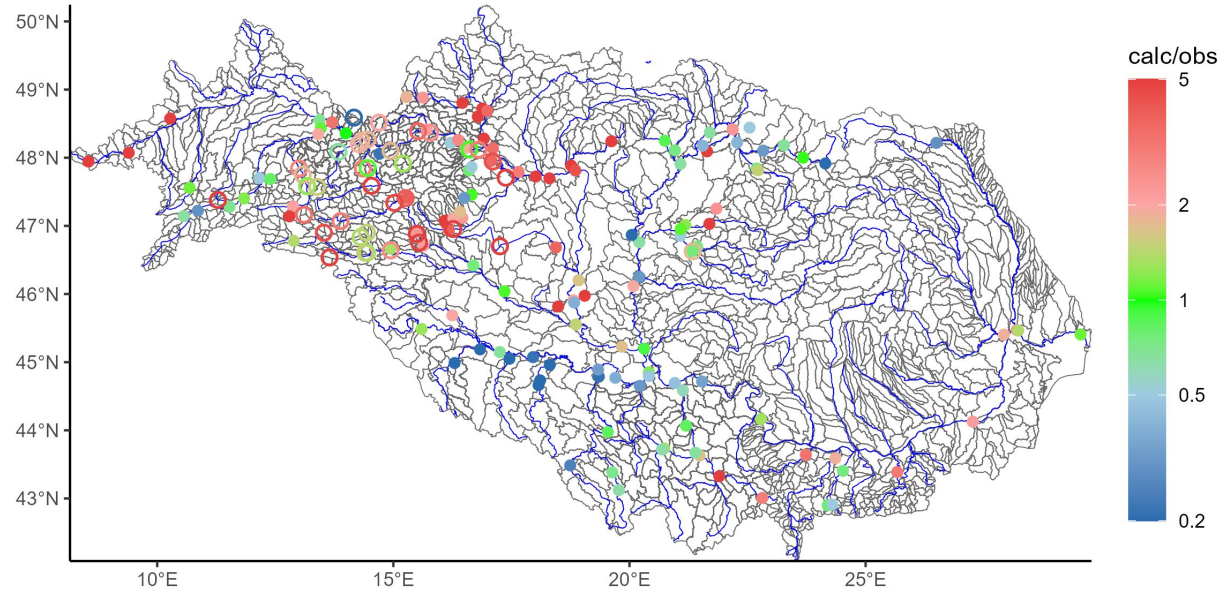


## Main observations

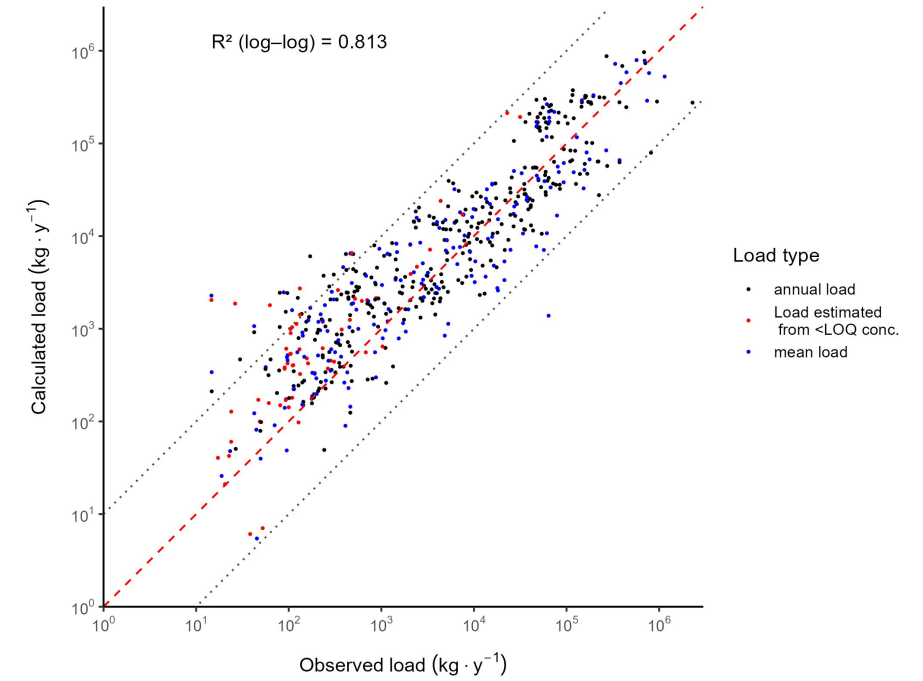
- Clear underestimation of loads in the Sava and Tisza basins
- Strong underestimation of Danube loads
- Loads at Tisza and Sava are comparable to the upper Danube loads
- Lack of industry data/industrial underestimation?
- Orchards/Vinyard soils as hot-spots?

# Validation map for metalloids – nic

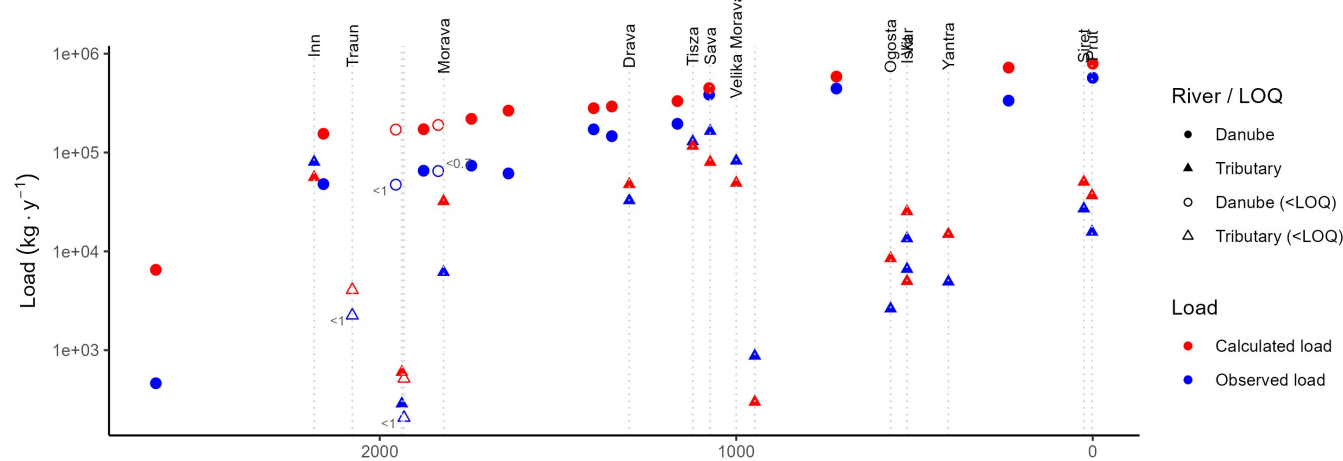
Ni load validation with retention and measured Q-ratio  
Calculated vs observed average loads



Ni load validation with retention  
(log-log) - realQ - average yearly loads 2015-2020 and avg load



Ni load long profile along the Danube

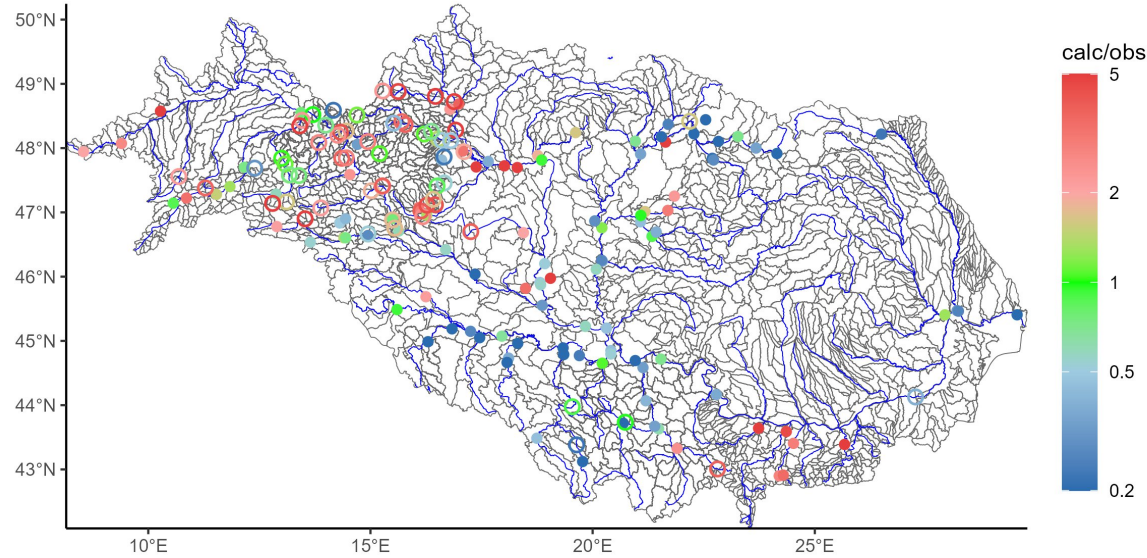


## Main observations

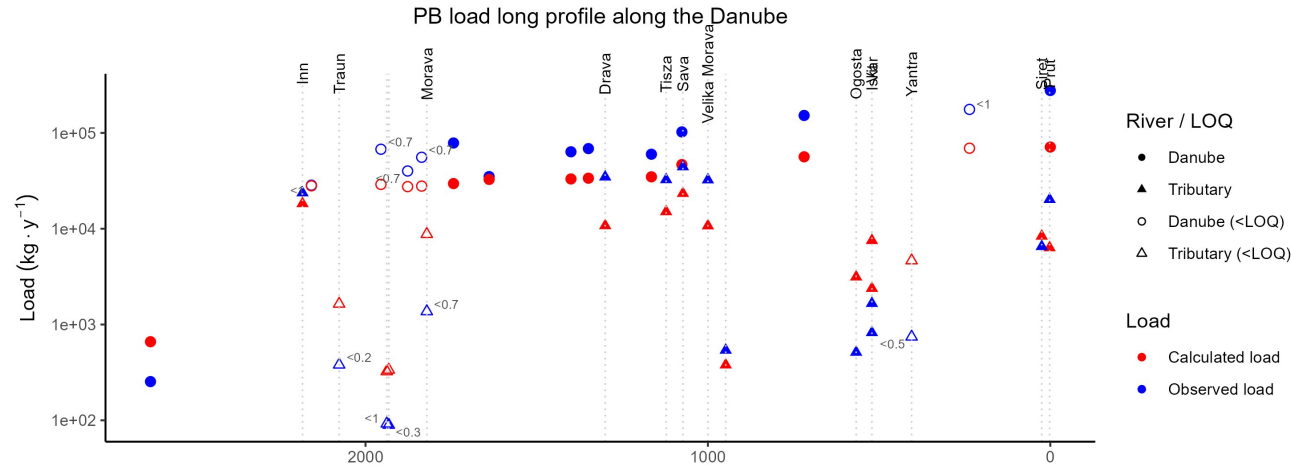
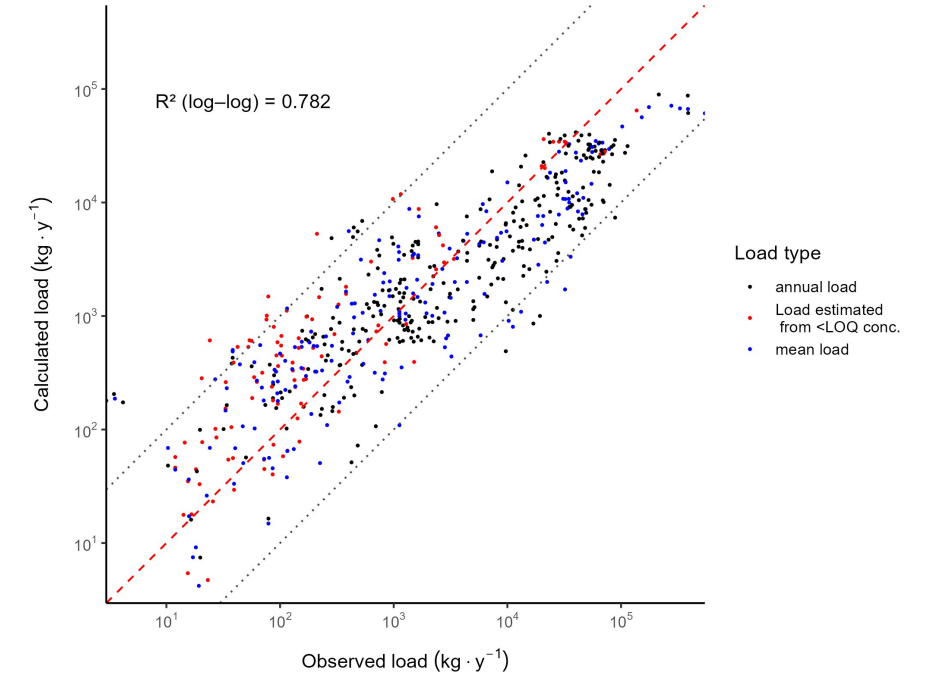
- Clear underestimation of loads in the Sava basin
- Strong overestimation of Danube loads in the upper basin

# Validation map for metalloids – Ie

PB load validation with retention and measured Q-ratio  
Calculated vs observed average loads



PB load validation with retention  
(log-log) - realQ - average yearly loads 2015-2020 and avg load

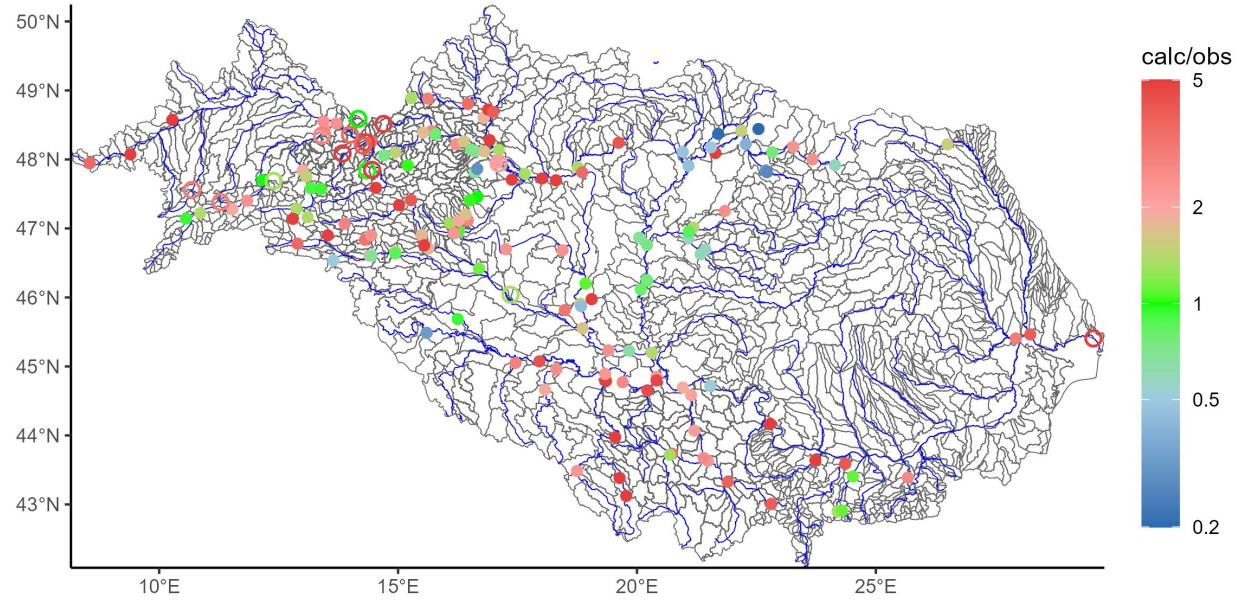


## Main observations

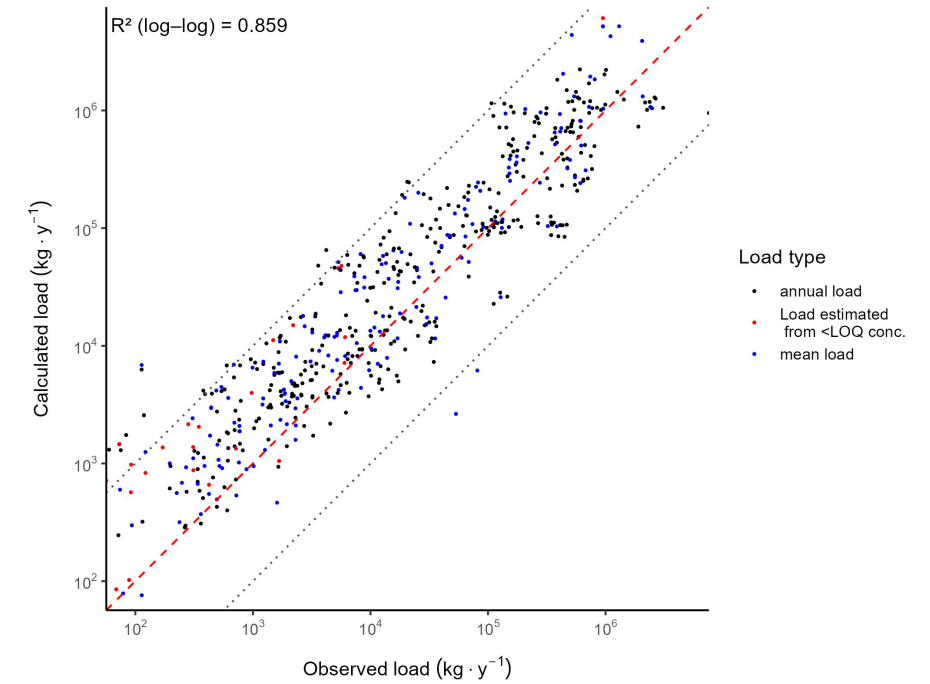
- Clear underestimation of loads in the Sava and Tisza basins
- Strong underestimation of Danube loads
- Too high loads in the south-east DRB

# Validation map for metalloids – zi

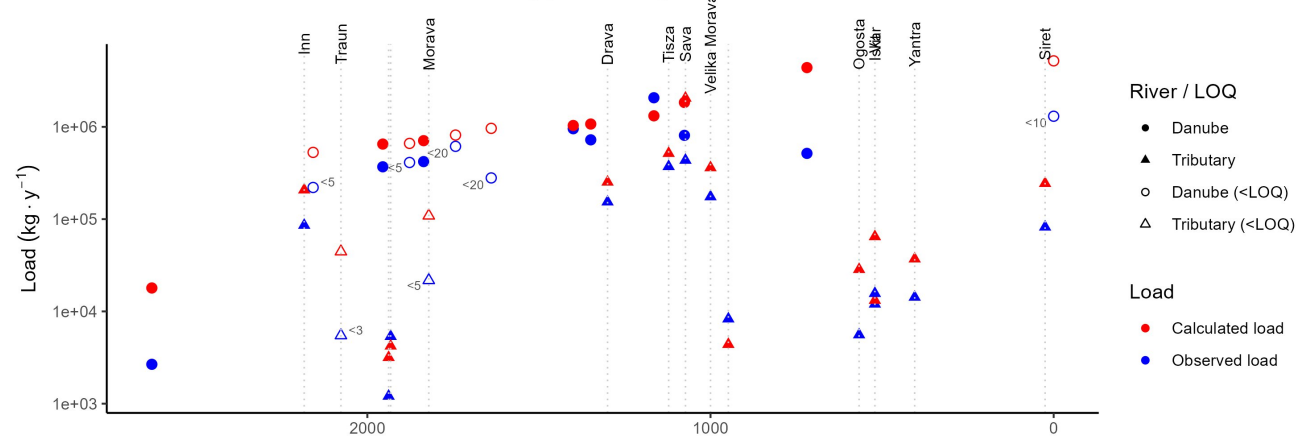
ZN load validation with retention and measured Q-ratio  
Calculated vs observed average loads



ZN load validation with retention  
(log-log) - realQ - average yearly loads 2015-2020 and avg load



ZN load long profile along the Danube

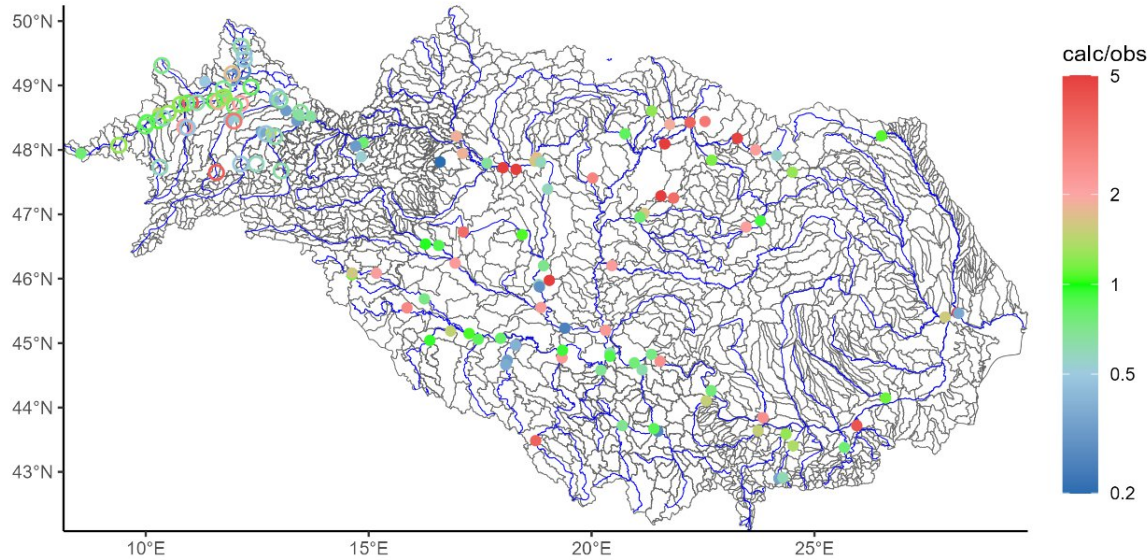


## Main observations

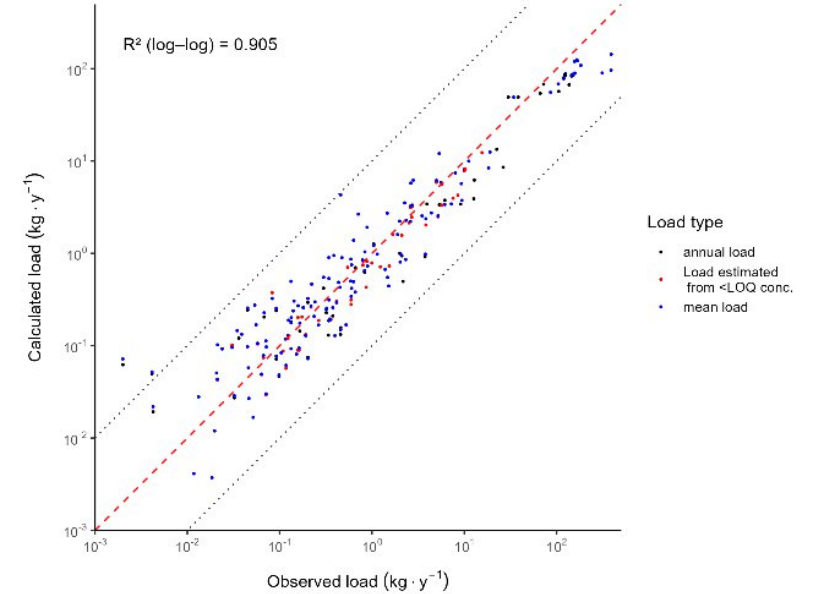
- Fairly stable model performance across the basin
- Strong drop of loads in the lower Danube section
- Highly overestimated in the Sava basin

# Validation map for PFAS – PFOA

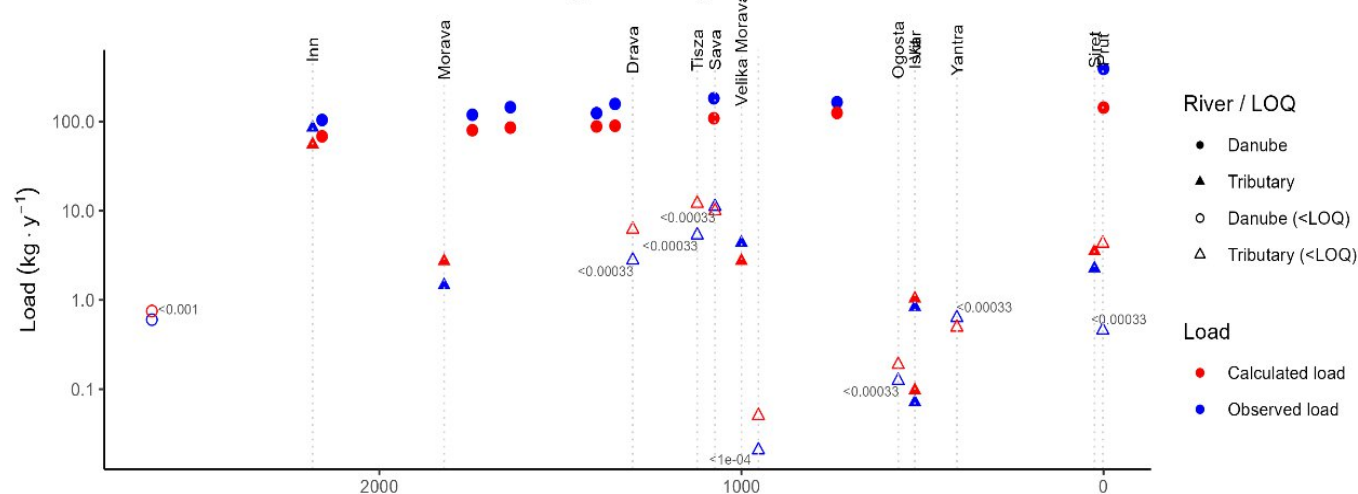
PFOA load validation without retention and measured Q-ratio  
Calculated vs observed average loads



PFOA load validation without retention  
(log-log) - realQ - average yearly loads 2015-2020 and avg load



PFOA load long profile along the Danube

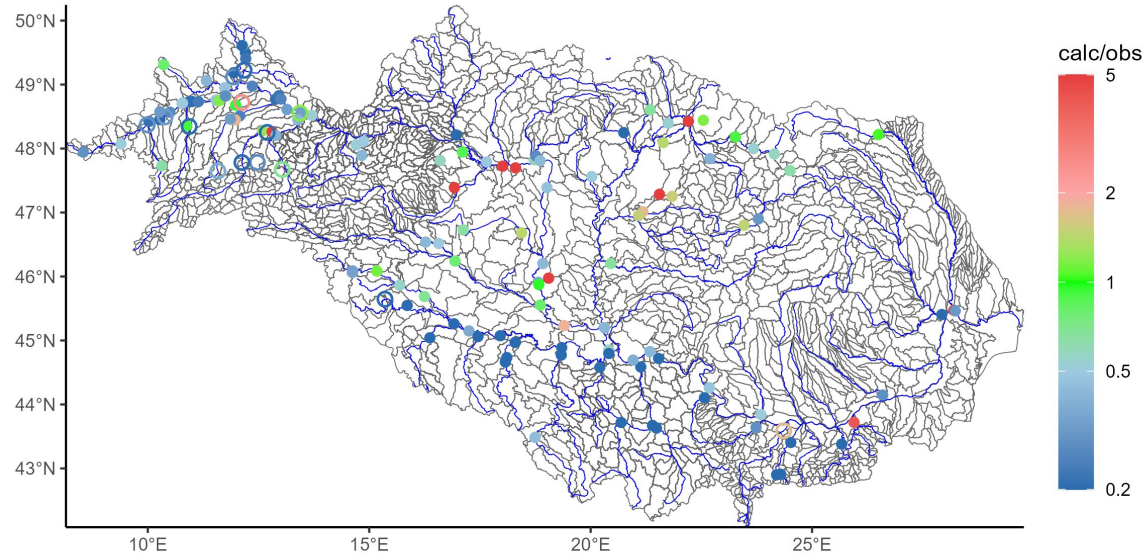


## Main observations

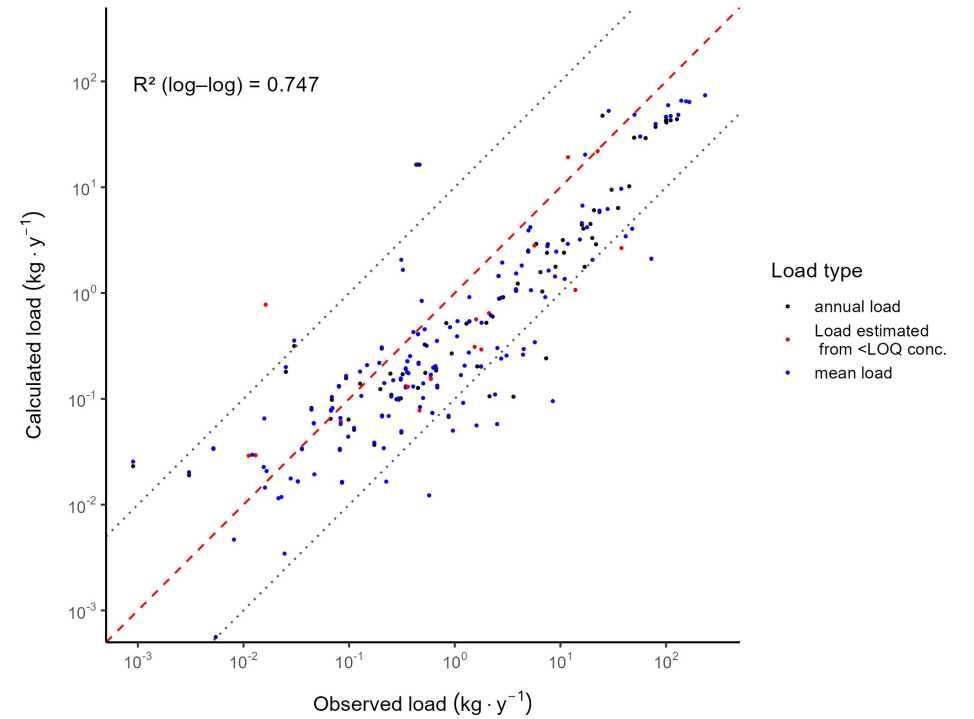
- Less reliable validation datasets (1,2 measurements per year in some cases)
- Strong overestimation at some smaller rivers
- Clear underestimation along the Danube
- Most loads come from upper Danube region
- No significant retention in rivers

# Validation map for PFAS – PFC

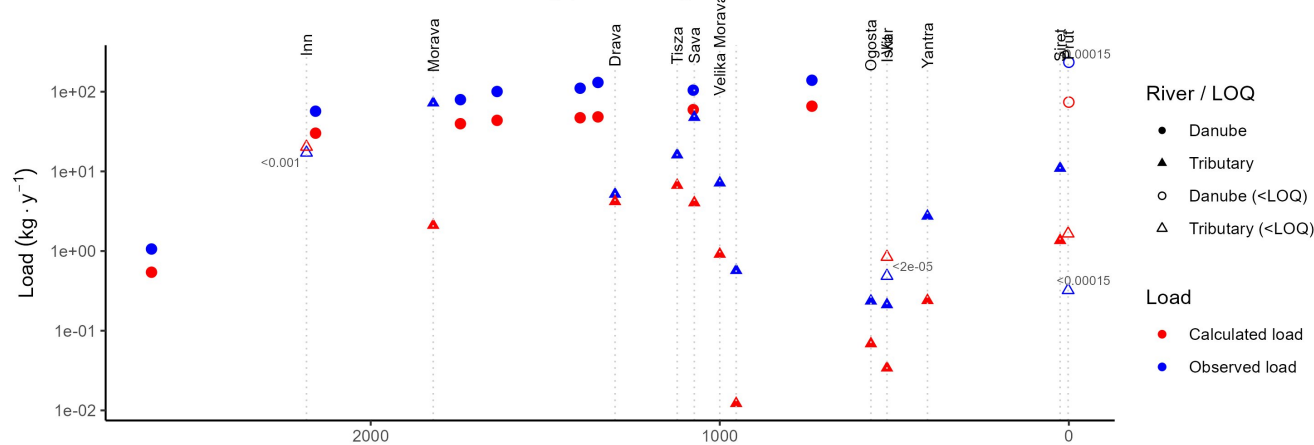
PFOS load validation without retention and measured Q-ratio  
Calculated vs observed average loads



PFOS load validation without retention  
(log-log) - realQ - average yearly loads 2015-2020 and avg load



PFOS load long profile along the Danube

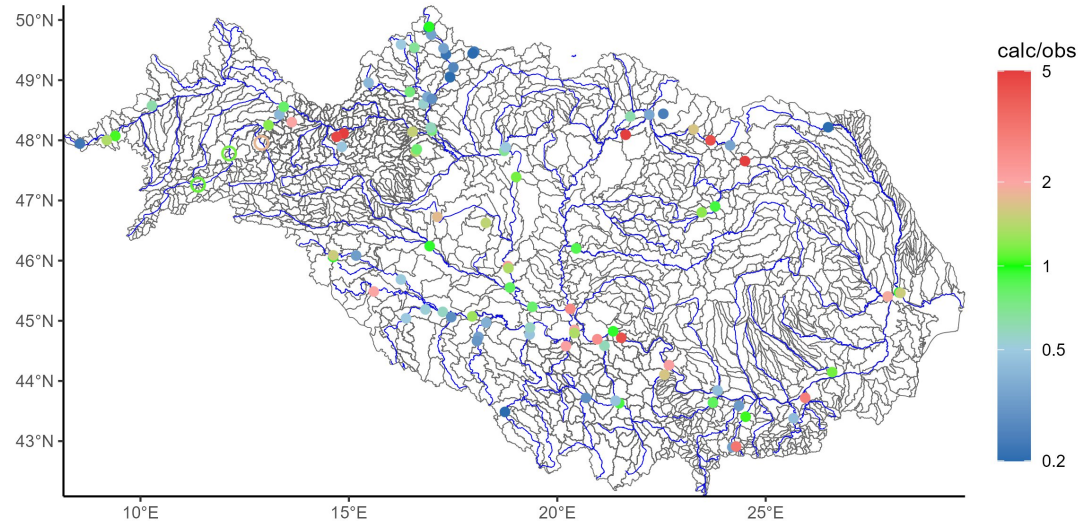


## Main observations

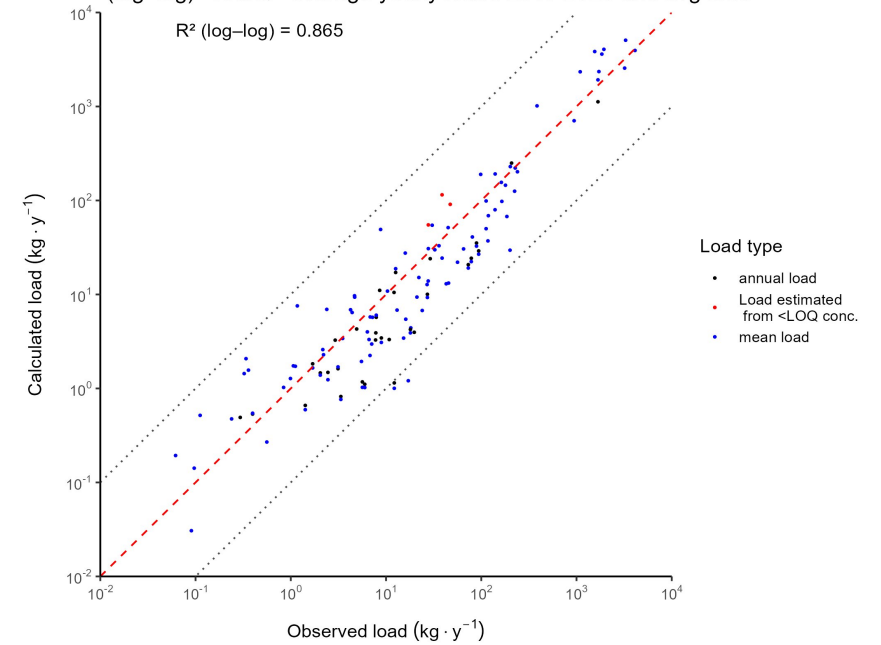
- Less reliable validation datasets (1,2 measurements per year in some cases)
- Strong regional differences in model performance
- Heavy underestimation in the Danube and in most tributaries

# Validation map for pharmaceuticals - carbamazepine

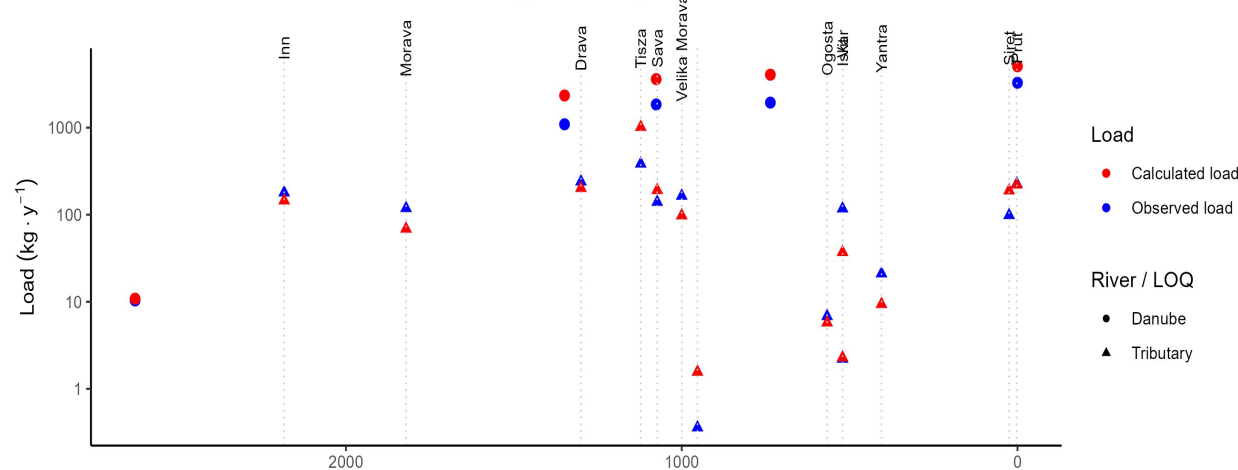
CBZ load validation without retention and measured Q-ratio  
Calculated vs observed average loads



CBZ load validation without retention  
(log-log) - real Q - average yearly loads 2015-2020 and avg load



CBZ load long profile along the Danube

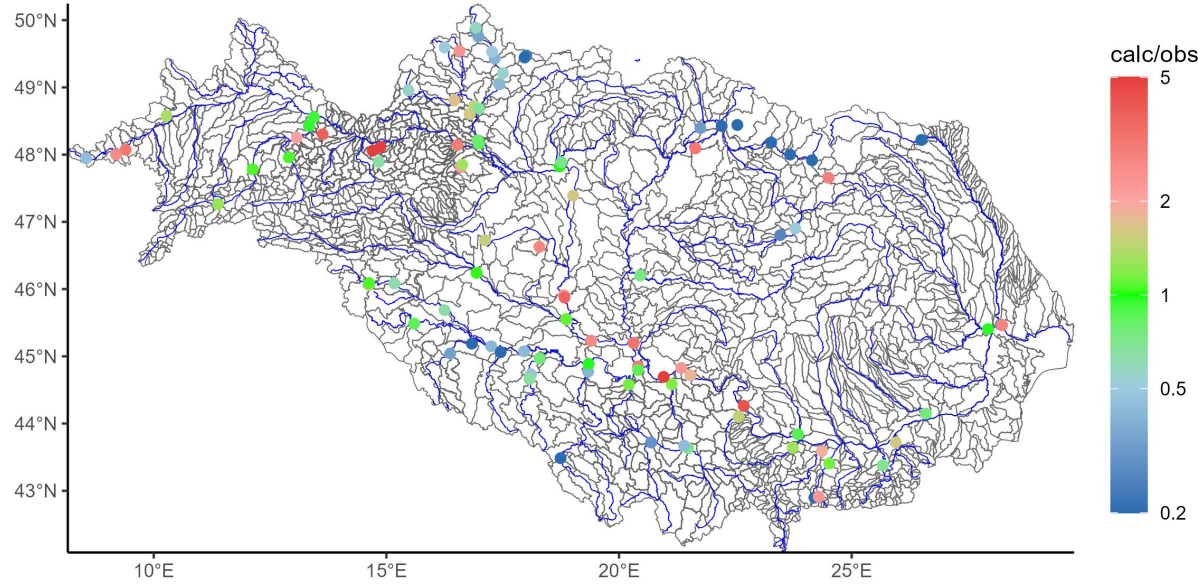


## Main observations

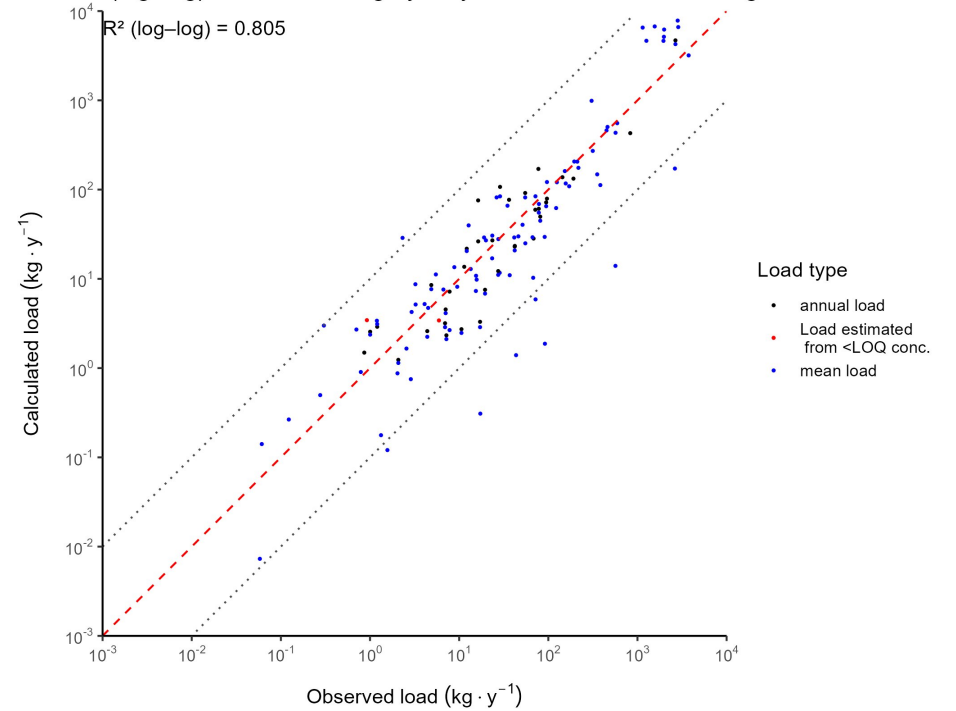
- Less reliable validation datasets (1,2 measurements per year in some cases)
- Overestimation of loads in the Danube river
- Obvious underestimation in major tributaries (Morava, Sava)
- No significant retention in rivers

# Validation map for pharmaceuticals - diclophenac

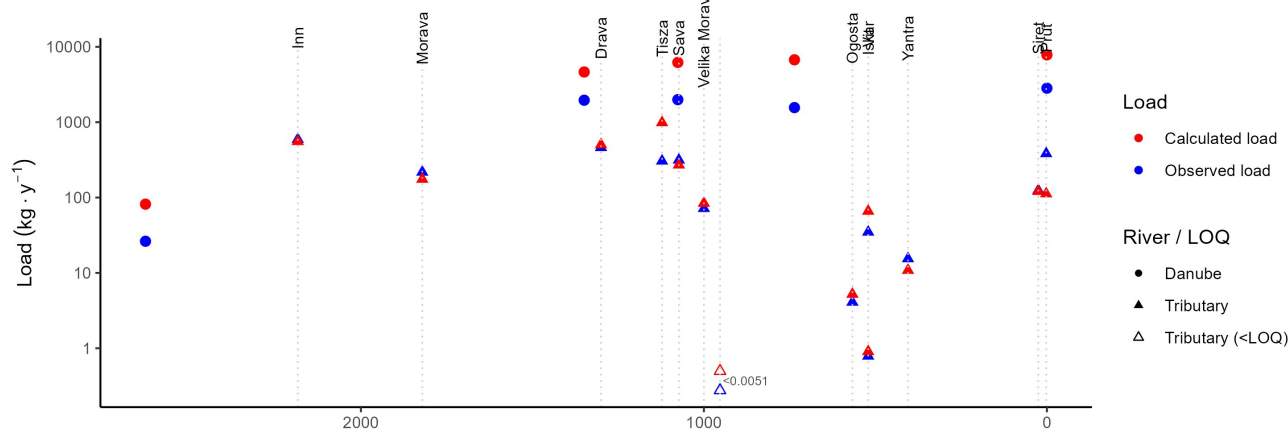
DCF load validation with Moneris retention and measured Q-ratio  
Calculated vs observed average loads



DCF load validation with Moneris retention  
(log-log) - realQ - average yearly loads 2015-2020 and avg load



DCF load long profile along the Danube

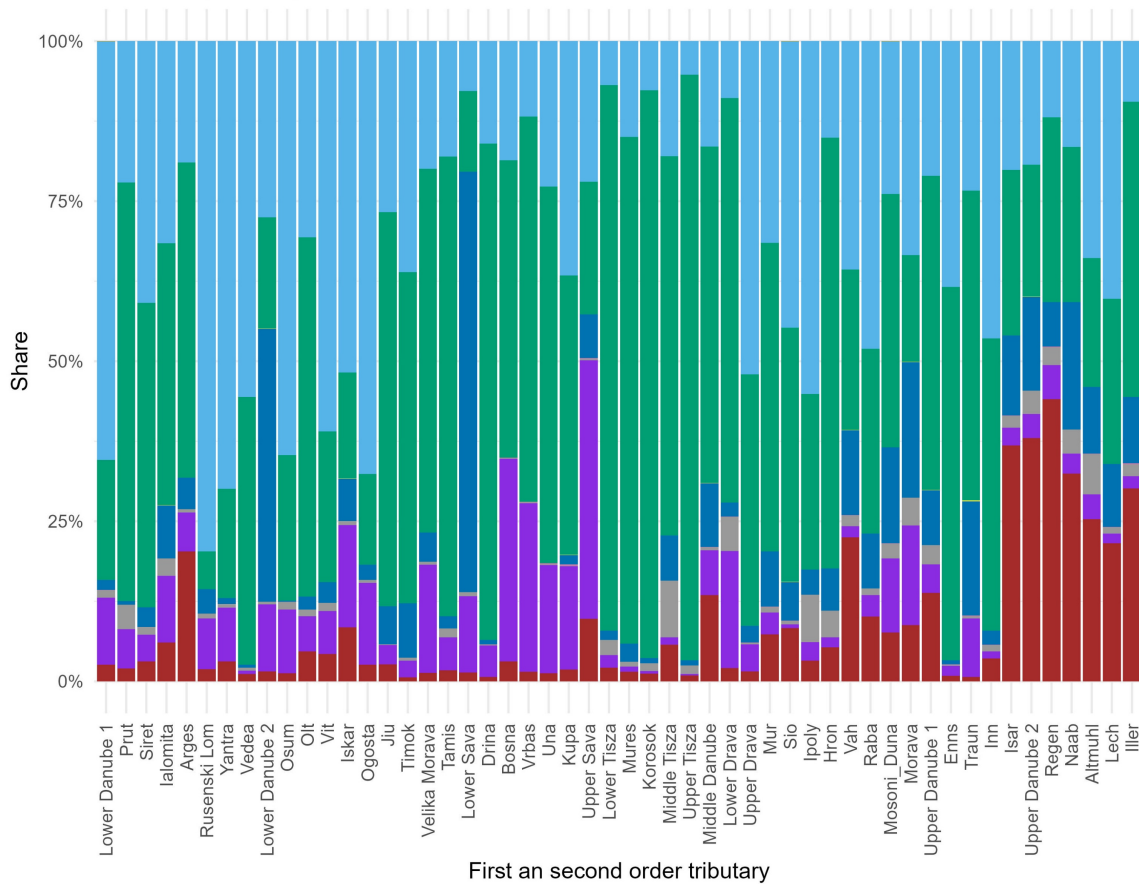


## Main observations

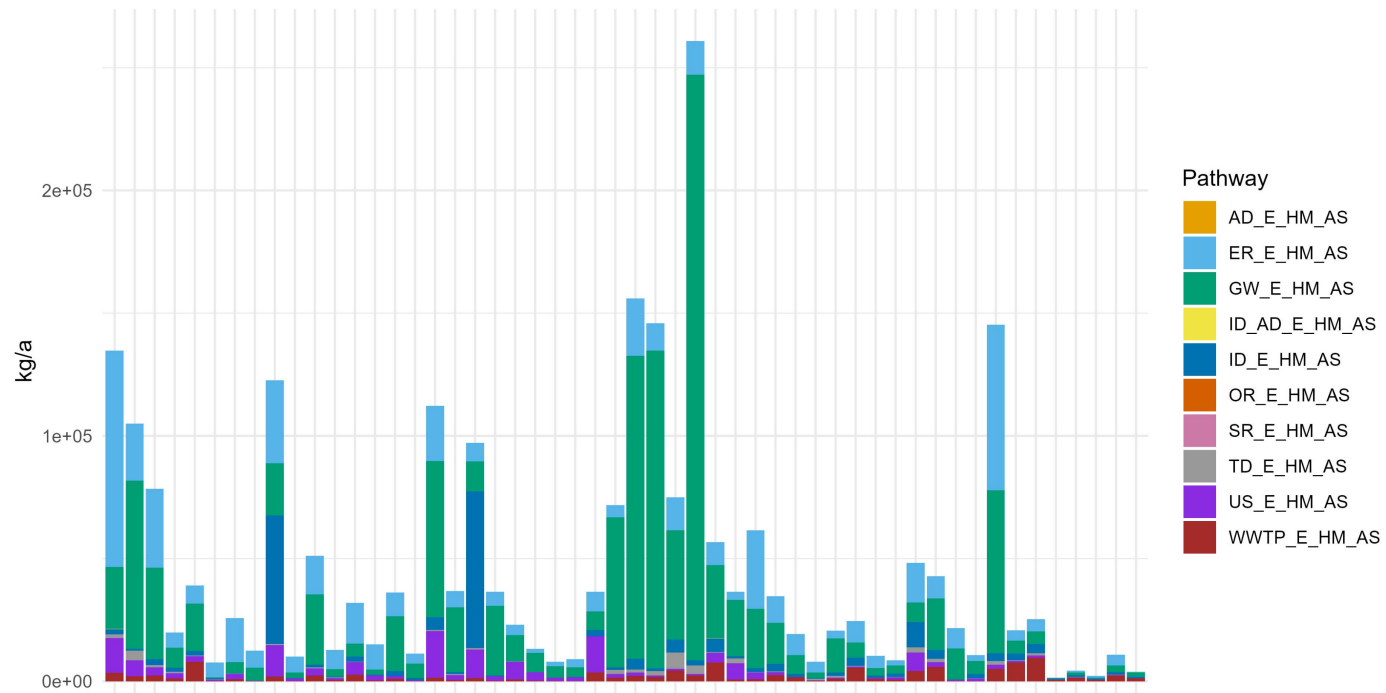
- Less reliable validation datasets (1,2 measurements per year in some cases)
- Strong overestimation of loads in the Danube river
- Riverine retention for Danube is very likely, not yet in the model!!

# As emissions in the DRB

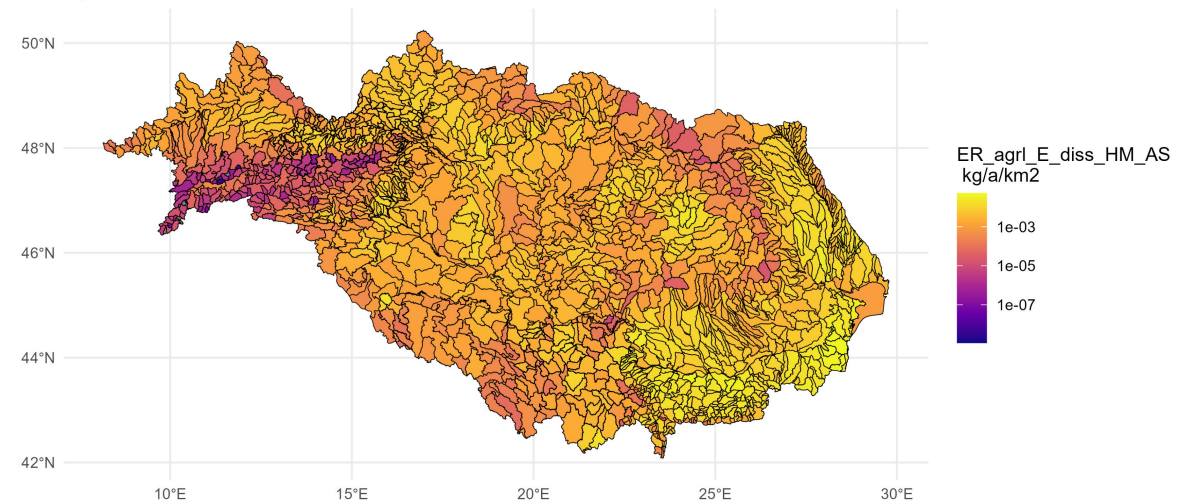
Share of pathways for HM AS



Absolute pathway loads for HM AS



Specific emission of HM AS

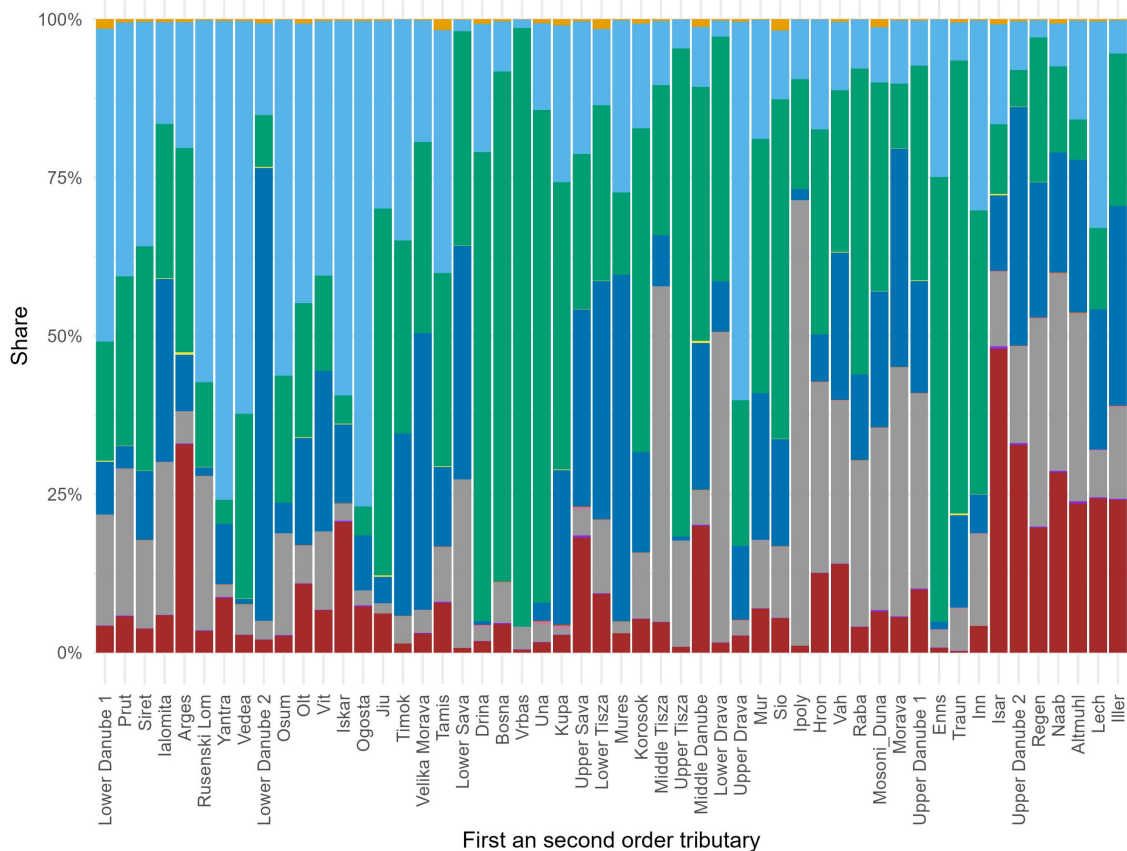


## Main observations

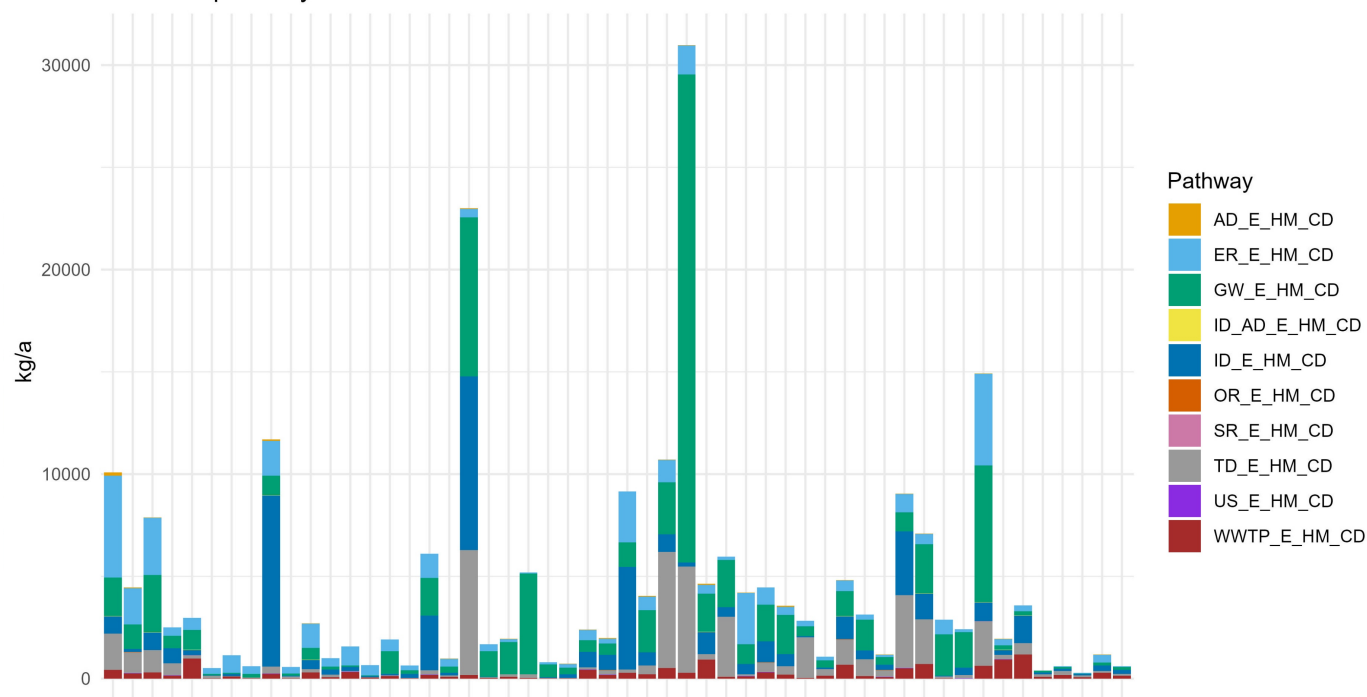
- Strong regional patterns in total loads
- Groundwater is the main overall source, especially in the middle Danube
- Erosion is significant, especially in the lower Danube
- WWTP load is a small share in total terms

# Cd emissions in the DRB

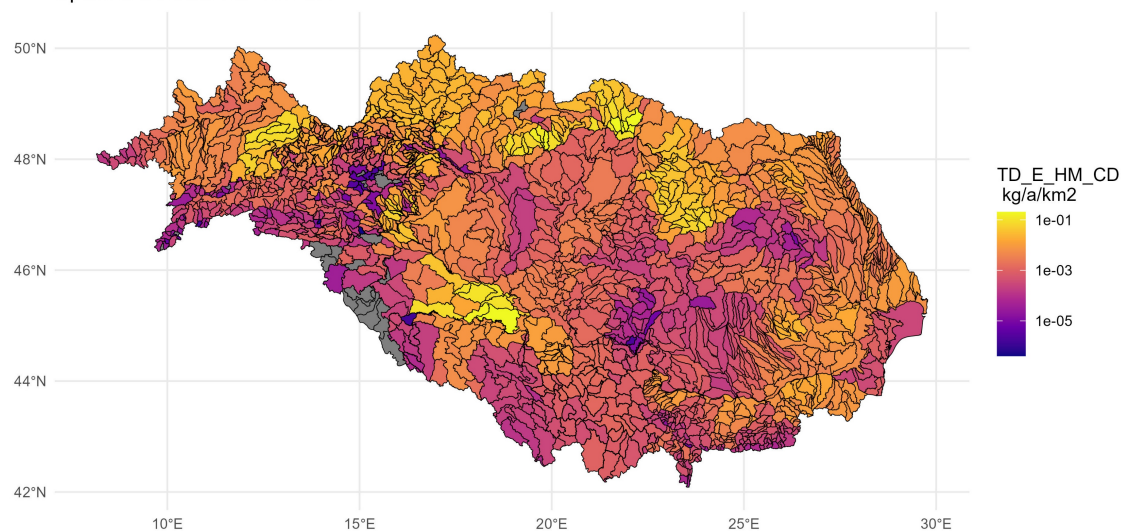
Share of pathways for HM CD



Absolute pathway loads for HM CD



Specific emission of HM CD

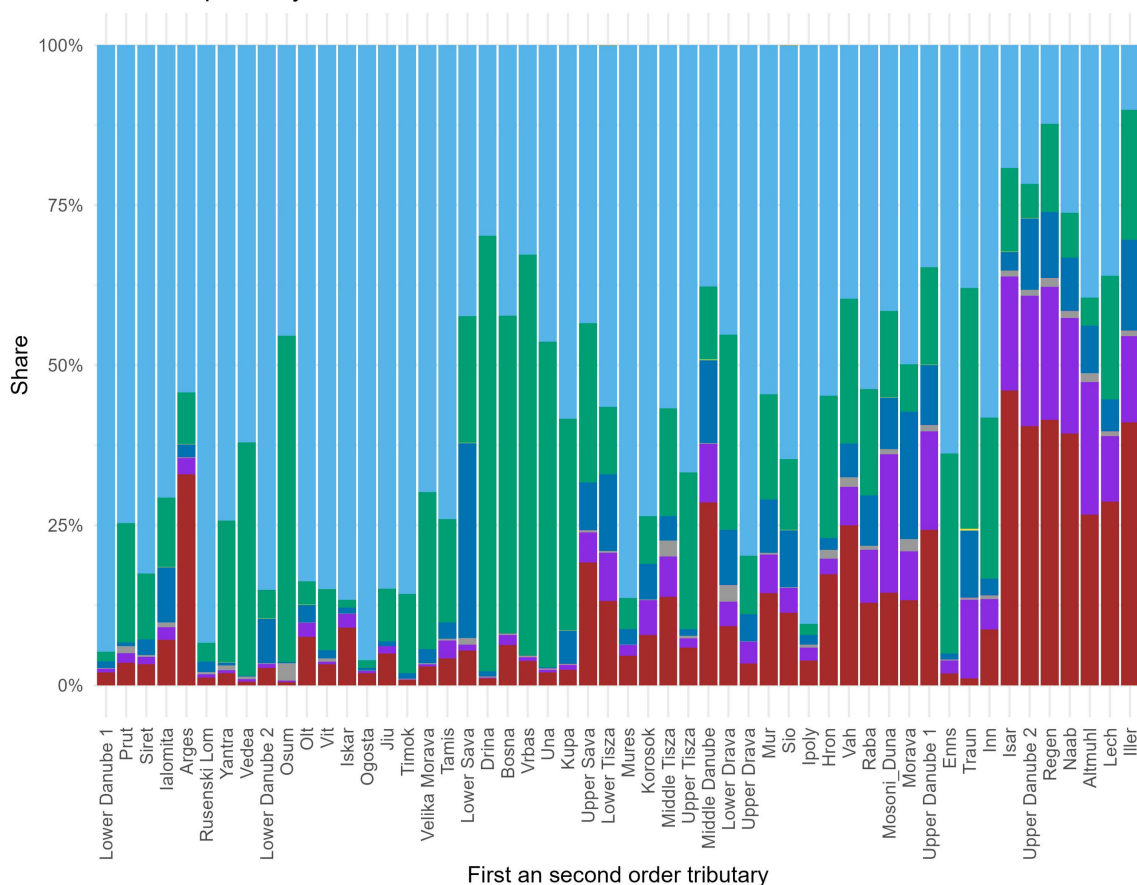


## Main observations

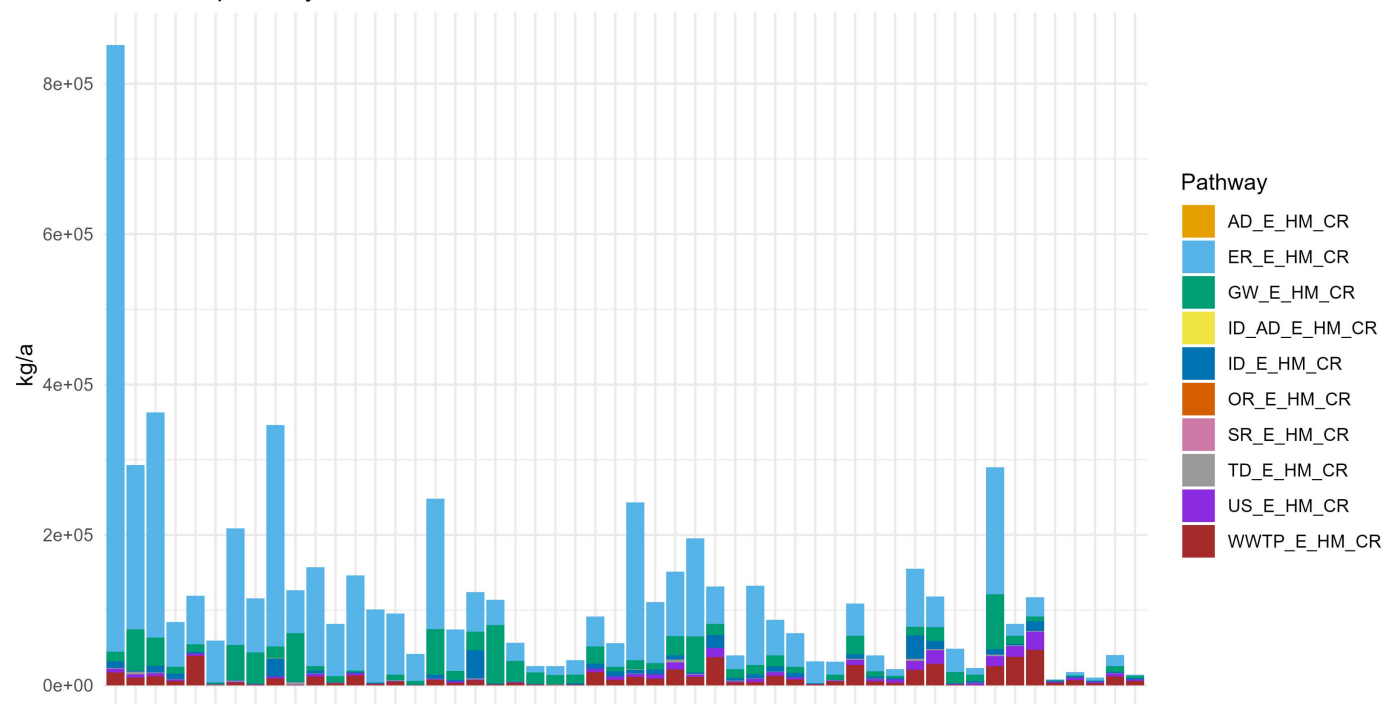
- Industry, erosion and groundwater are the main pathways
- Some hot spot catchments are present (lower Sava, middle and upper-Tisza, Inn)
- Tile drain loads is shown high, but high uncertainty

# Cr emissions in the DRB

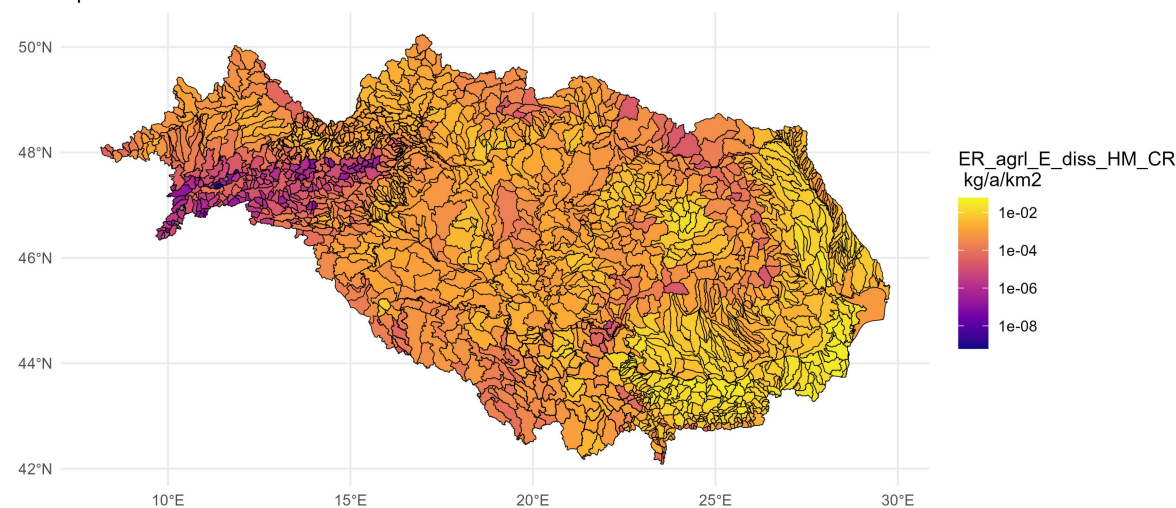
Share of pathways for HM CR



Absolute pathway loads for HM CR



Specific emission of HM CR

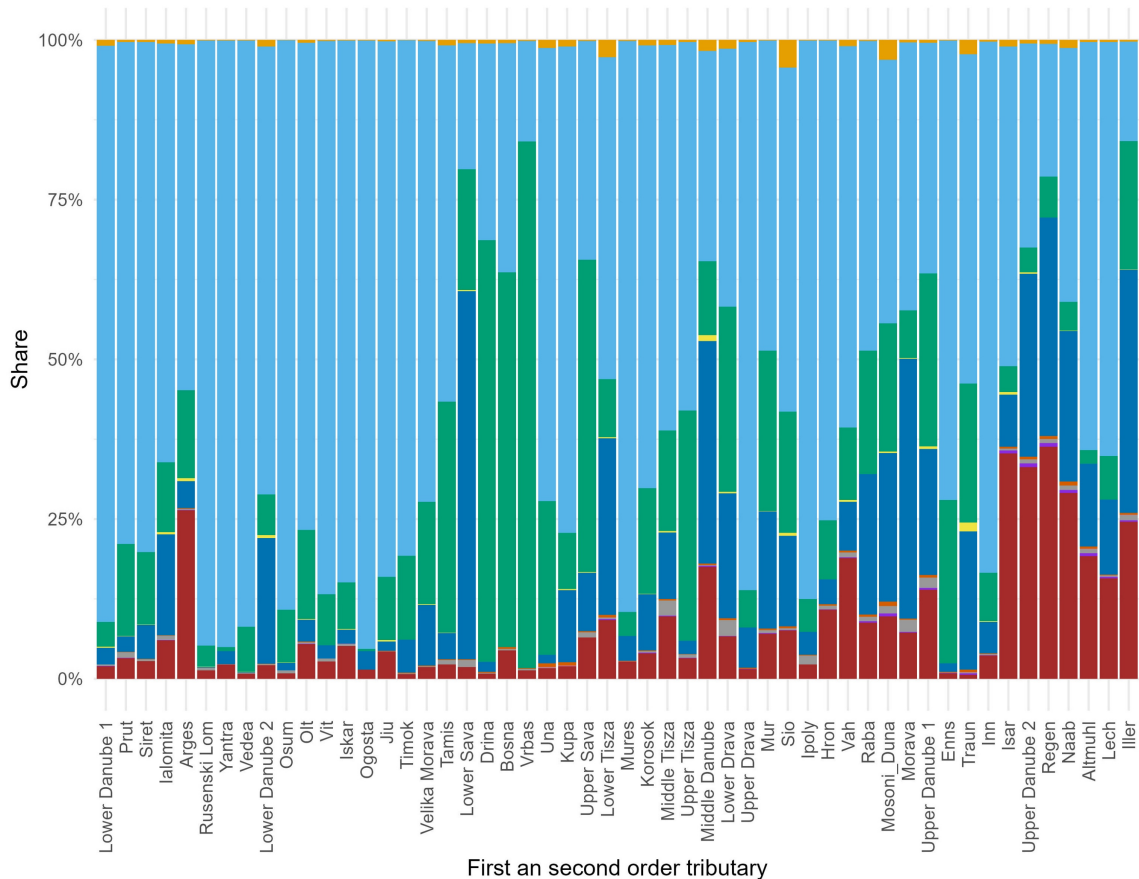


## Main observations

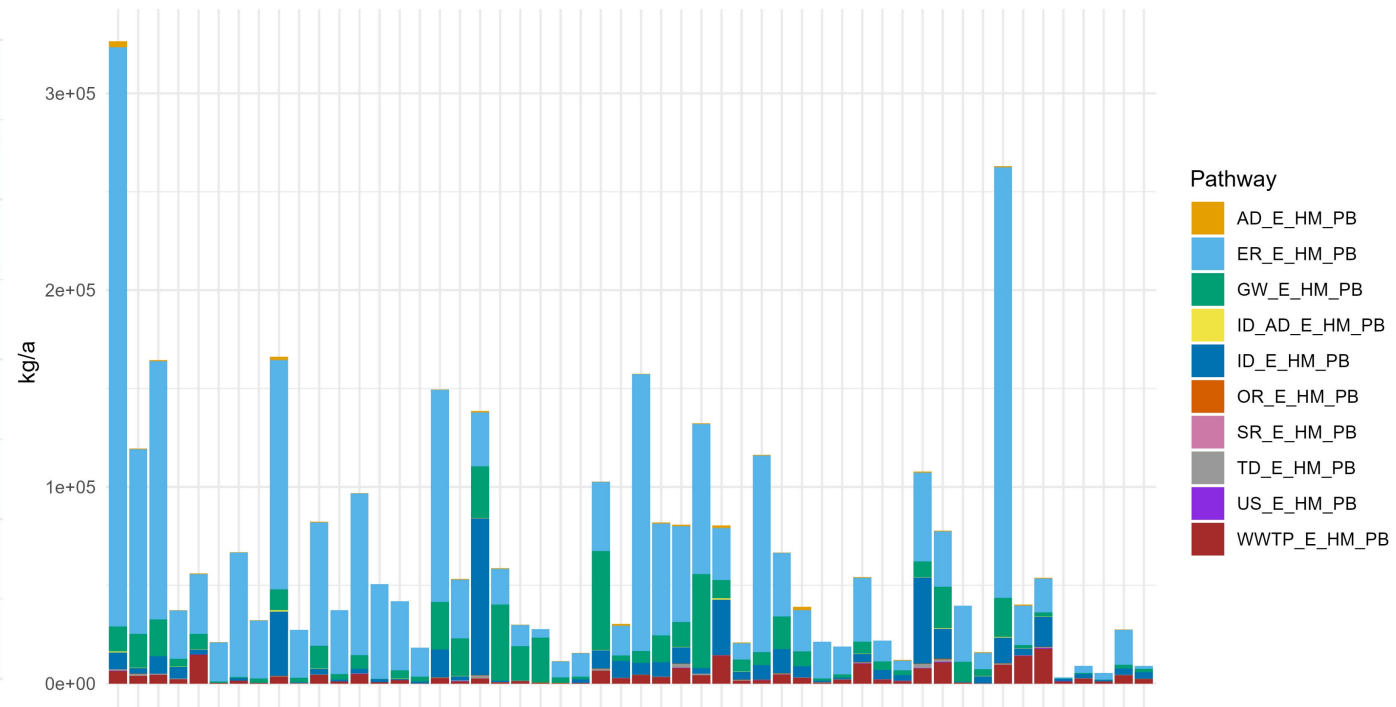
- Strong regional patterns in total loads, highest loads in the lower Danube
- Erosion is the most significant pathway, especially in the lower Danube
- WWTP load is a small share in total terms

# Pb emissions in the DRB

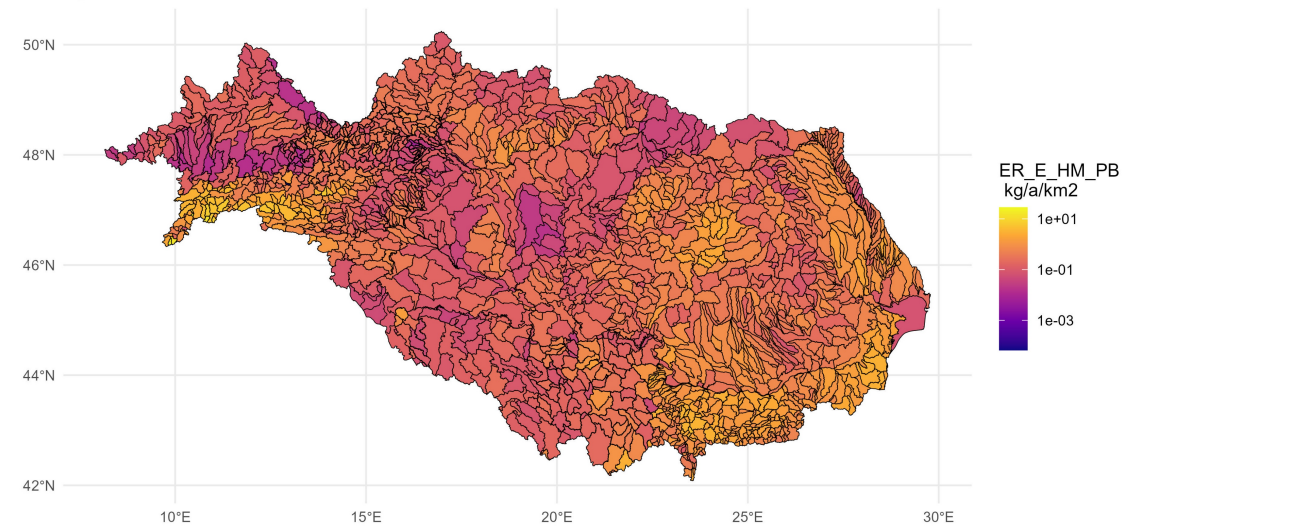
Share of pathways for HM PB



Absolute pathway loads for HM PB



Specific emission of HM PB

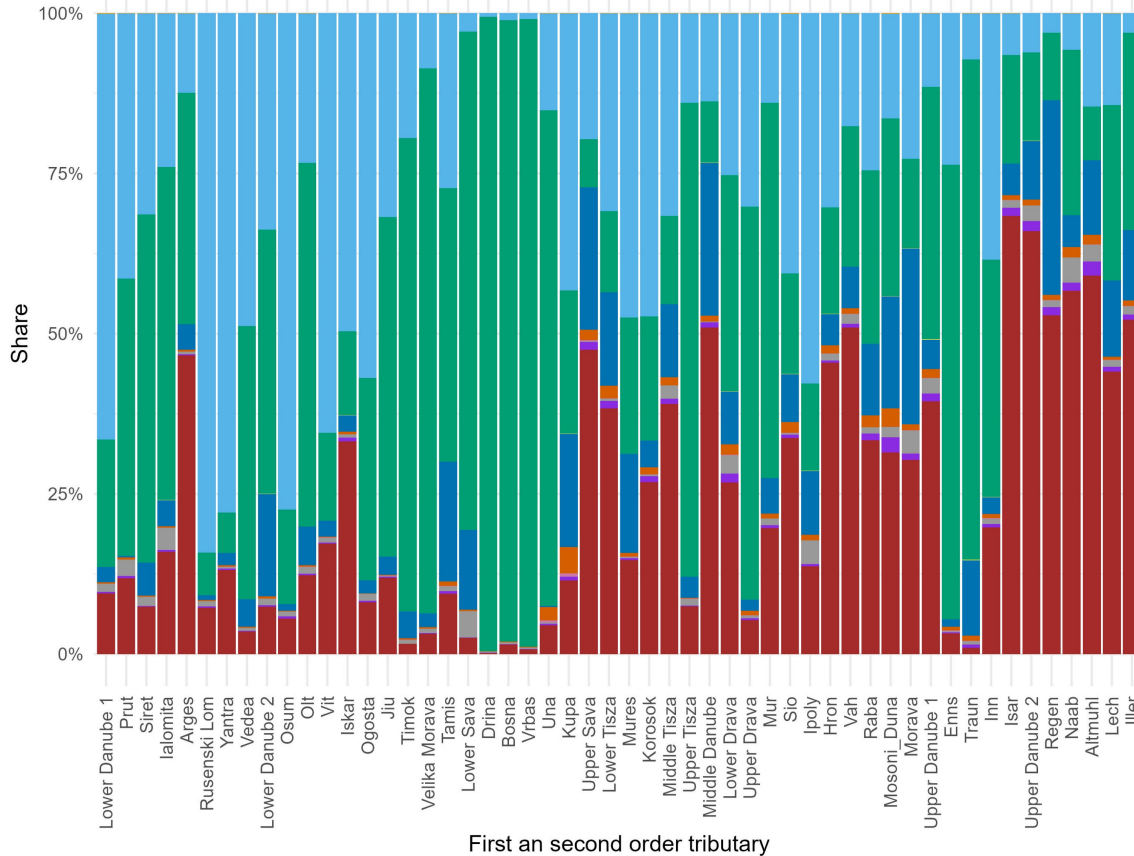


## Main observations

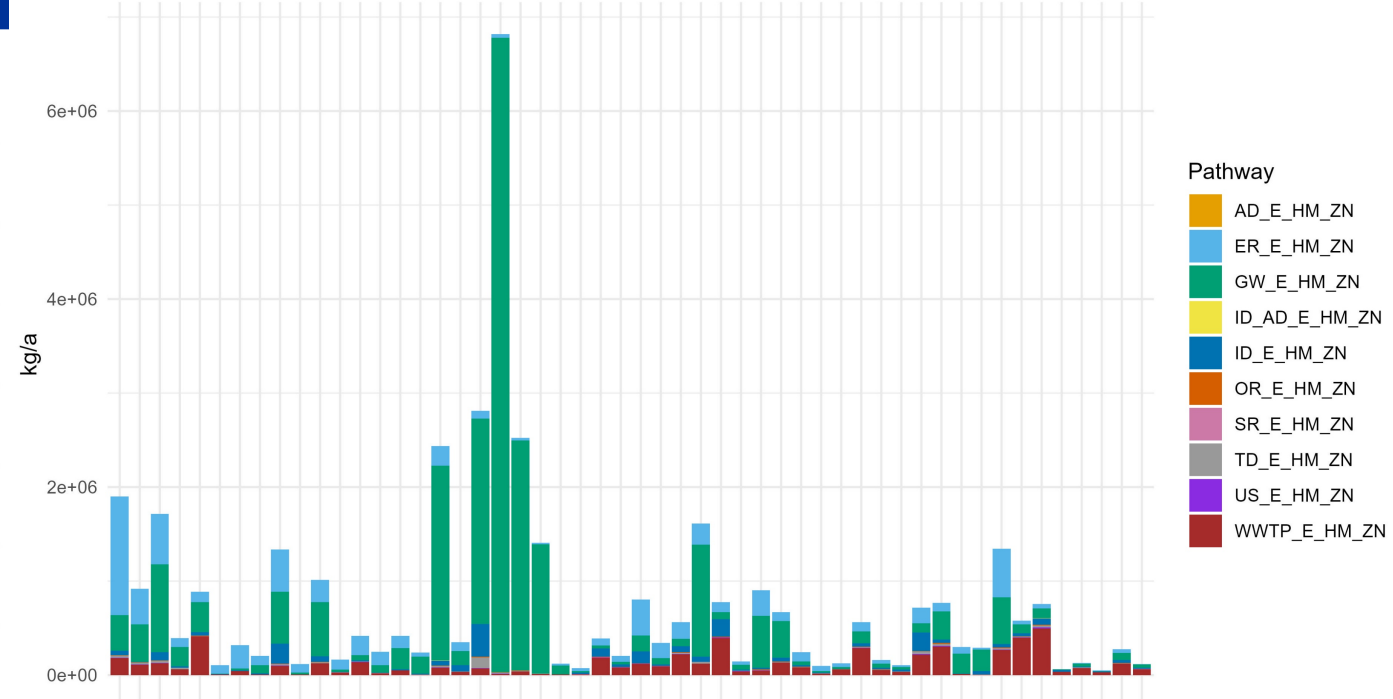
- Uneven distribution of total loads (hot-spot catchments)
- Erosion is the most significant pathway, especially in the lower Danube

# Zn emissions in the DRI

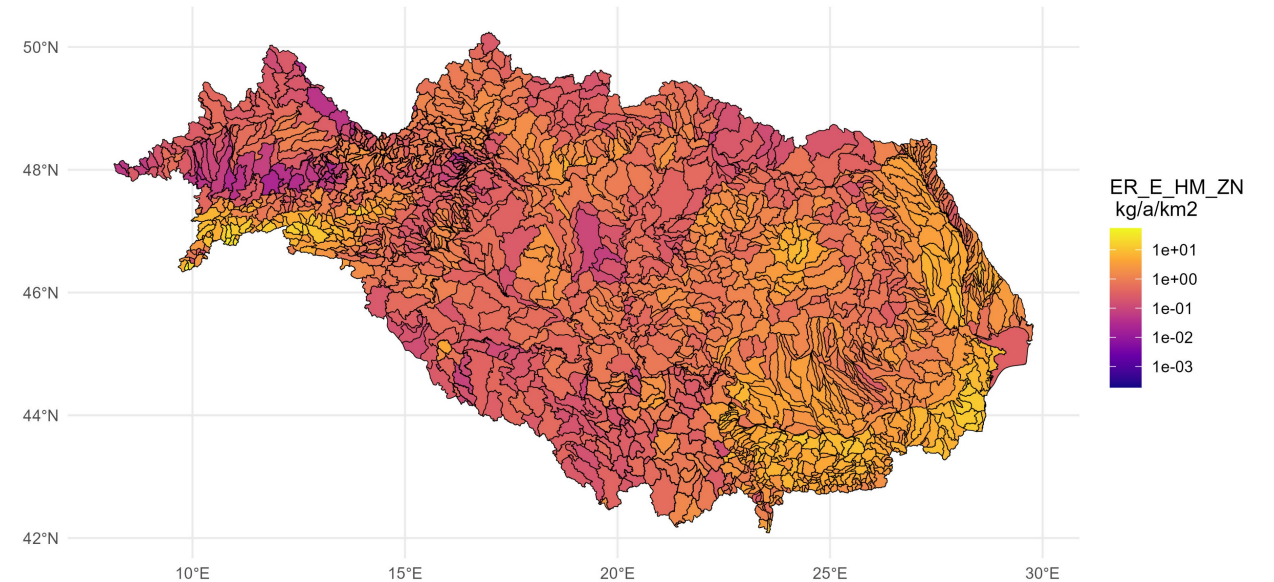
Share of pathways for HM ZN



Absolute pathway loads for HM ZN



Specific emission of HM ZN

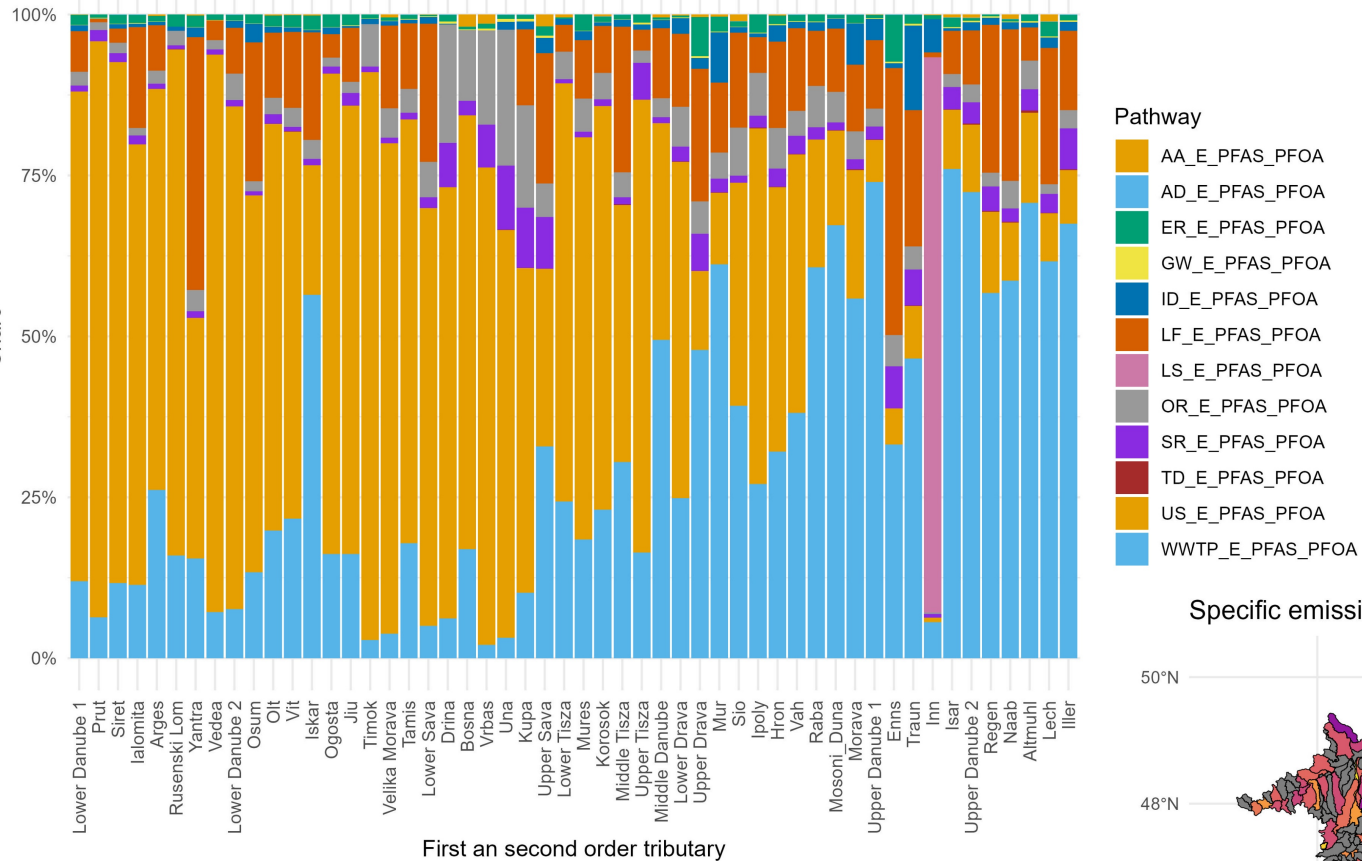


## Main observations

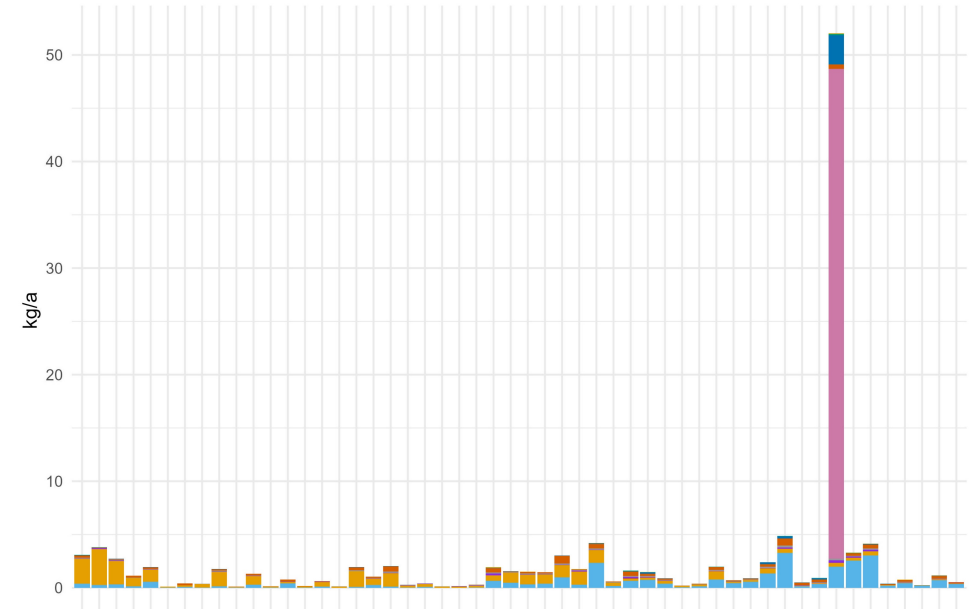
- Overestimation of GW loads in the Bosnian rivers
- Erosion and waste water loads are the most significant
- Groundwater is locally significant.

# PFOA emissions in the DRB

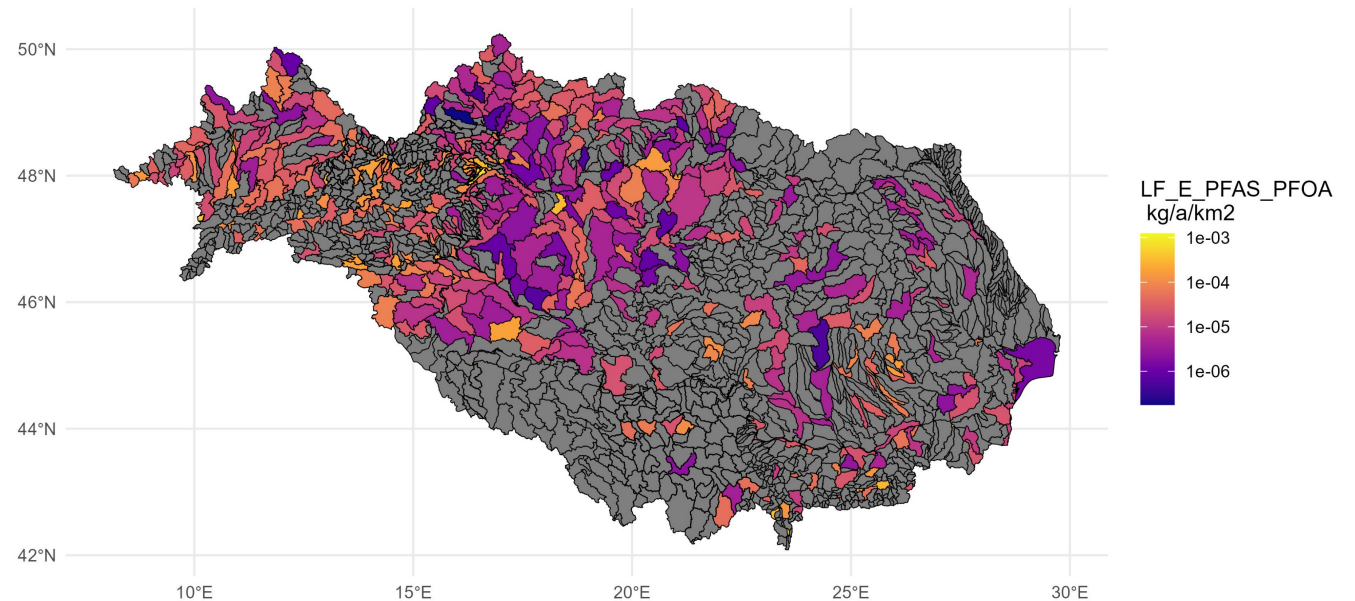
Share of pathways for PFAS PFOA



Absolute pathway loads for PFAS PFOA



Specific emission of PFAS PFOA

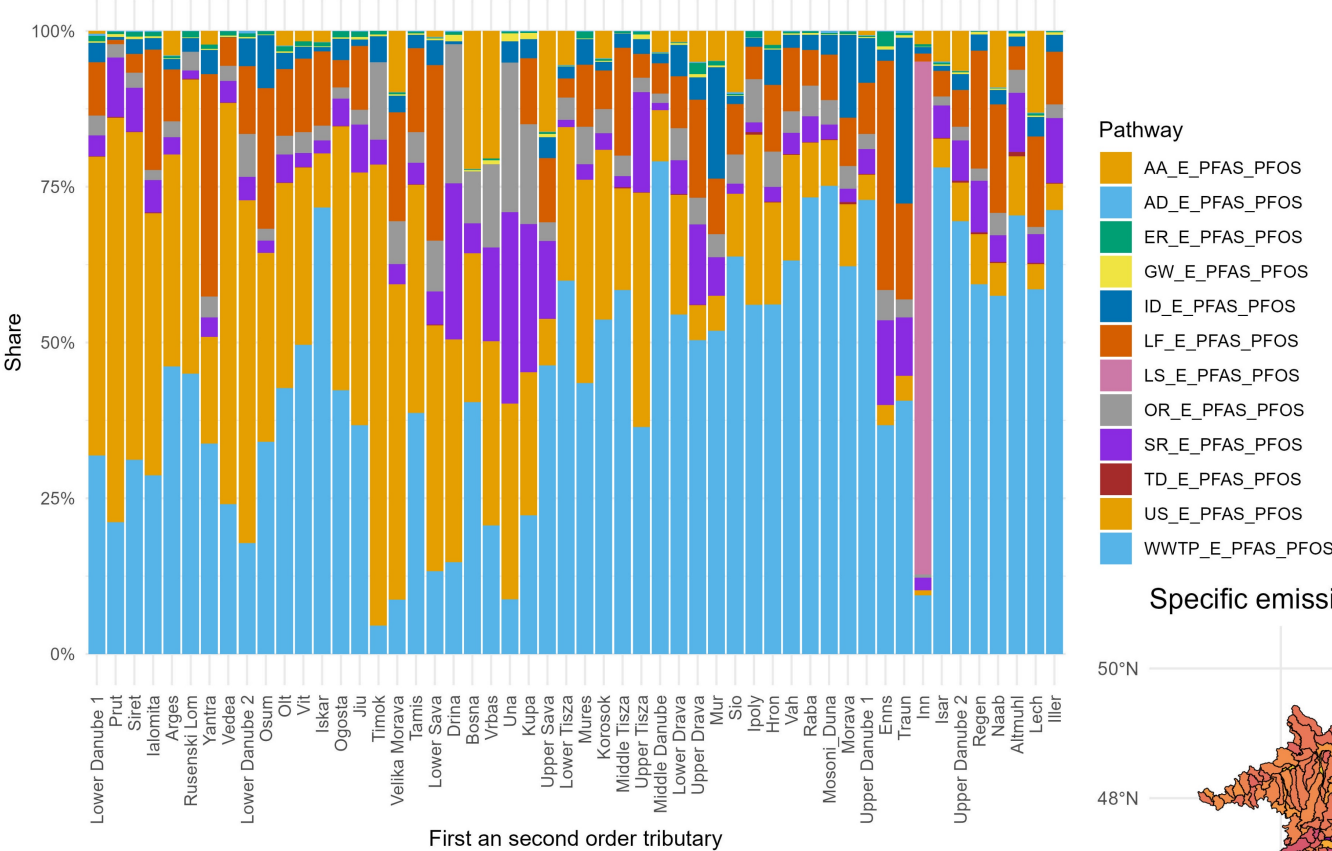


## Main observations

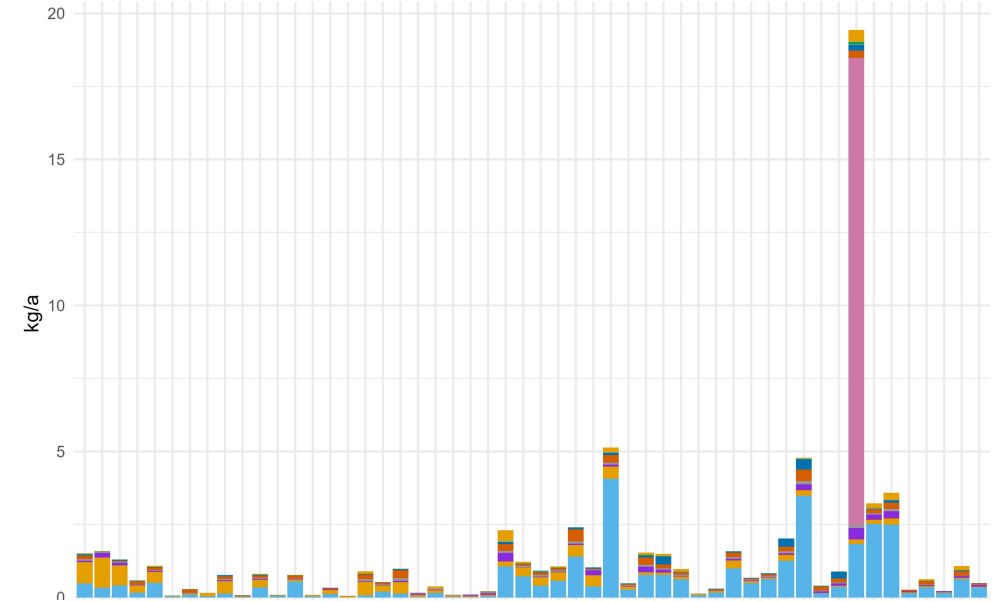
- Gendorf legacy hot spot is a dominant source
- WWTP loads dominate river loads in the upper Danube
- Urban systems related emissions dominate river loads in the middle and lower Danube
- Landfill hot-spots give a significant share (high uncertainty)

# PFOS emissions in the DRB - strongly underestimated!!!!

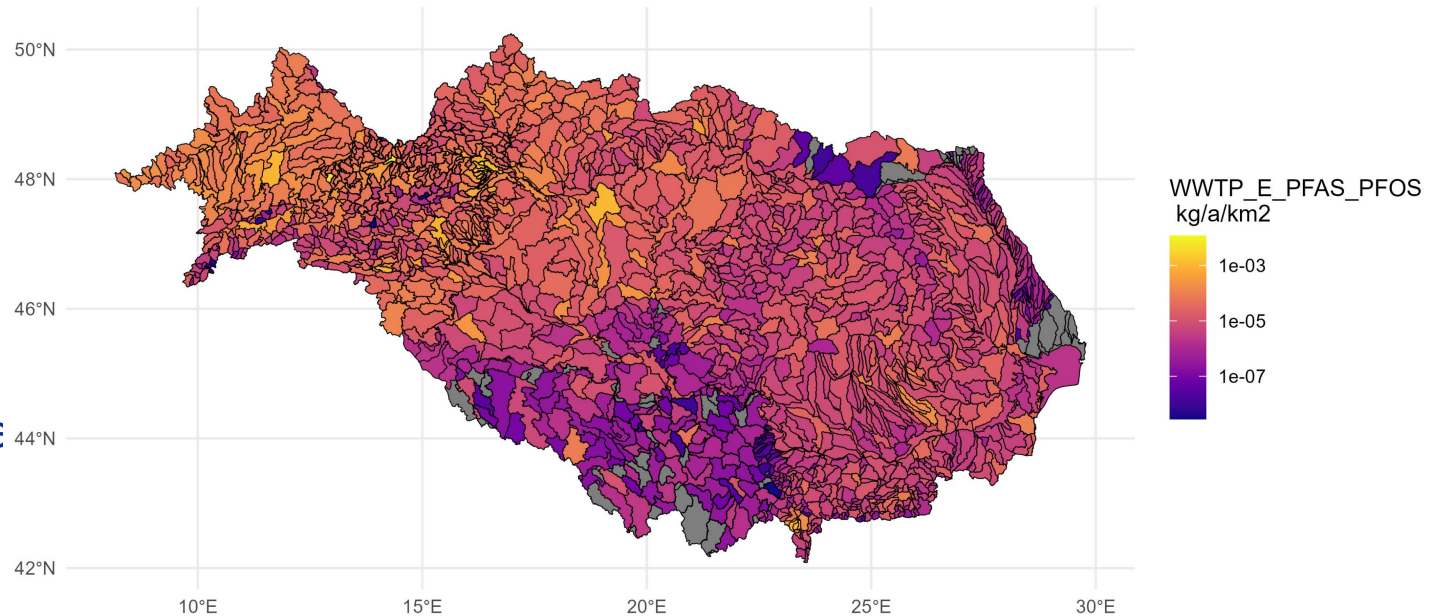
Share of pathways for PFAS PFOS



Absolute pathway loads for PFAS PFOS



Specific emission of PFAS PFOS

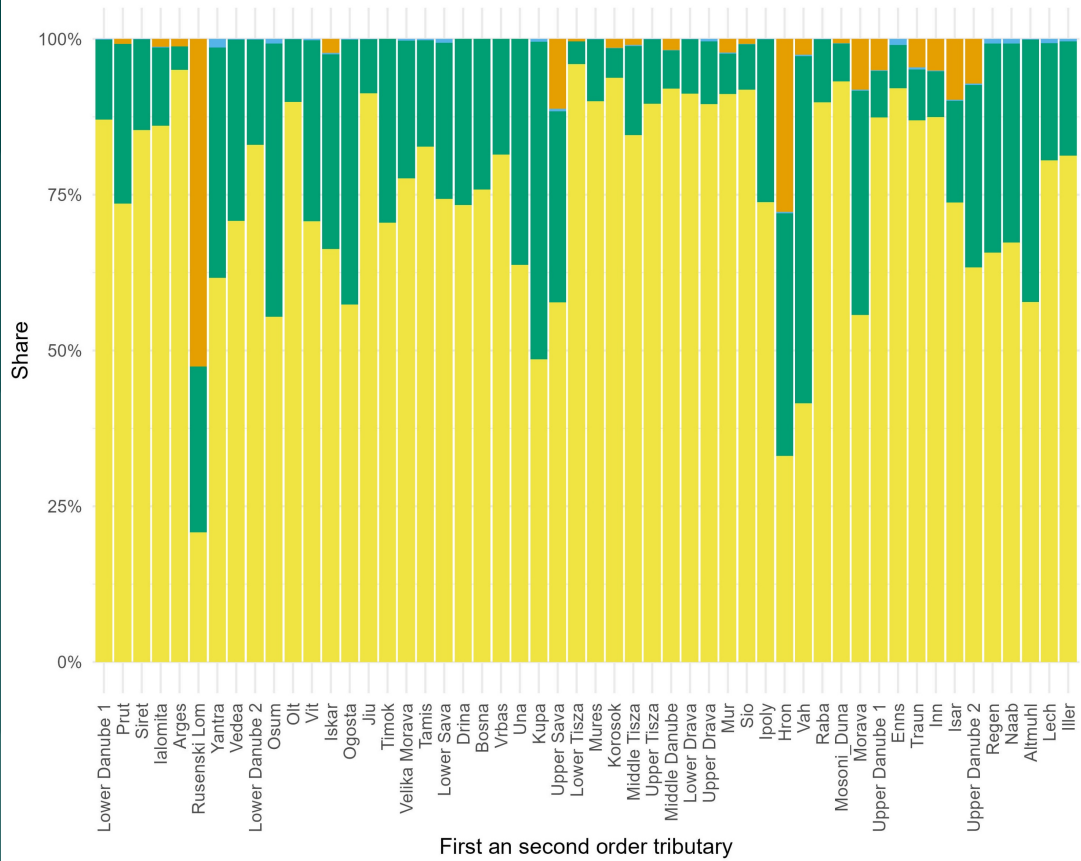


## Main observations

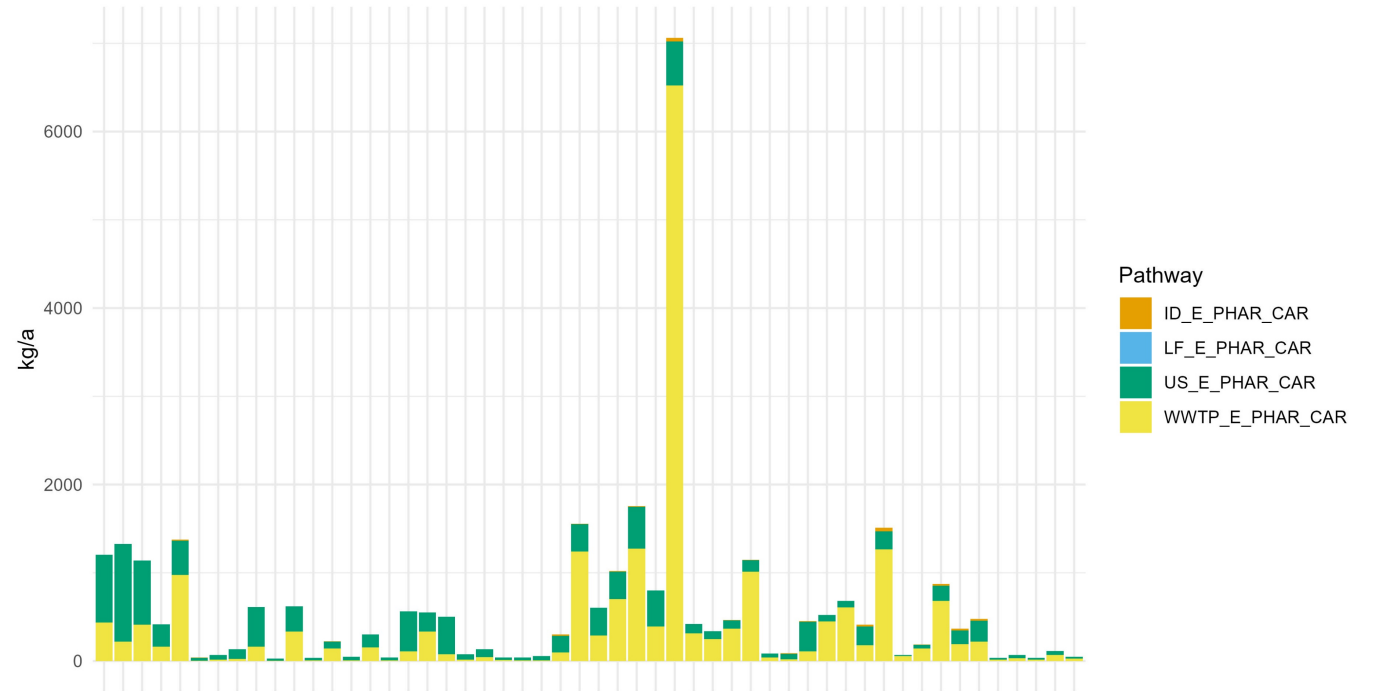
- WWTP loads dominate river loads in the upper Danube
- Loads from urban systems are very relevant in the lower Danube region
- Landfill/Aerodrome hot-spots give a significant share (high uncertainty)

# Carbamazepine emissions in the DRB

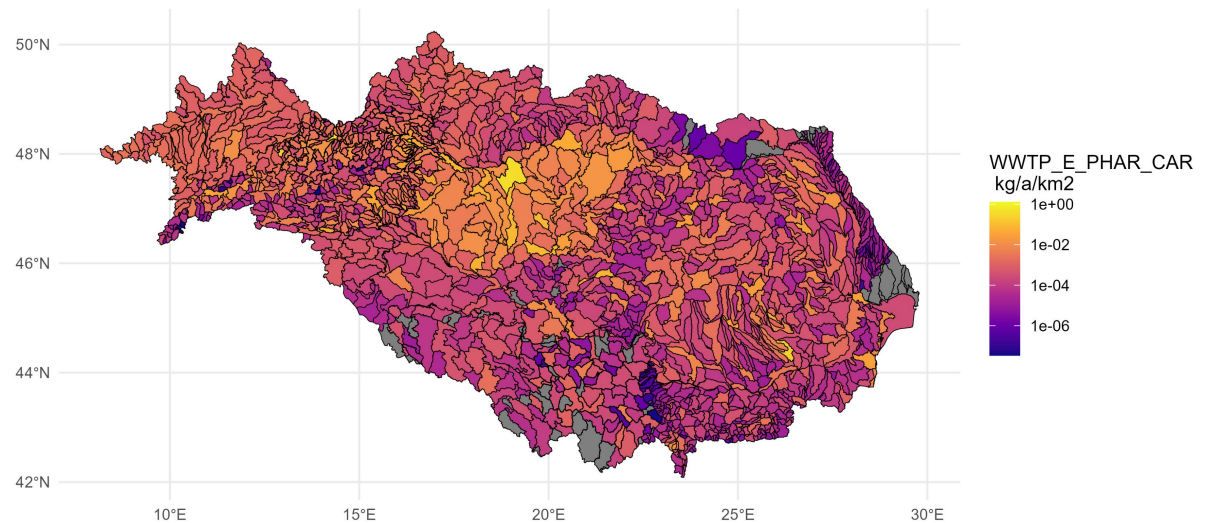
Share of pathways for PHAR CAR



Absolute pathway loads for PHAR CAR



Specific emission of PHAR CAR

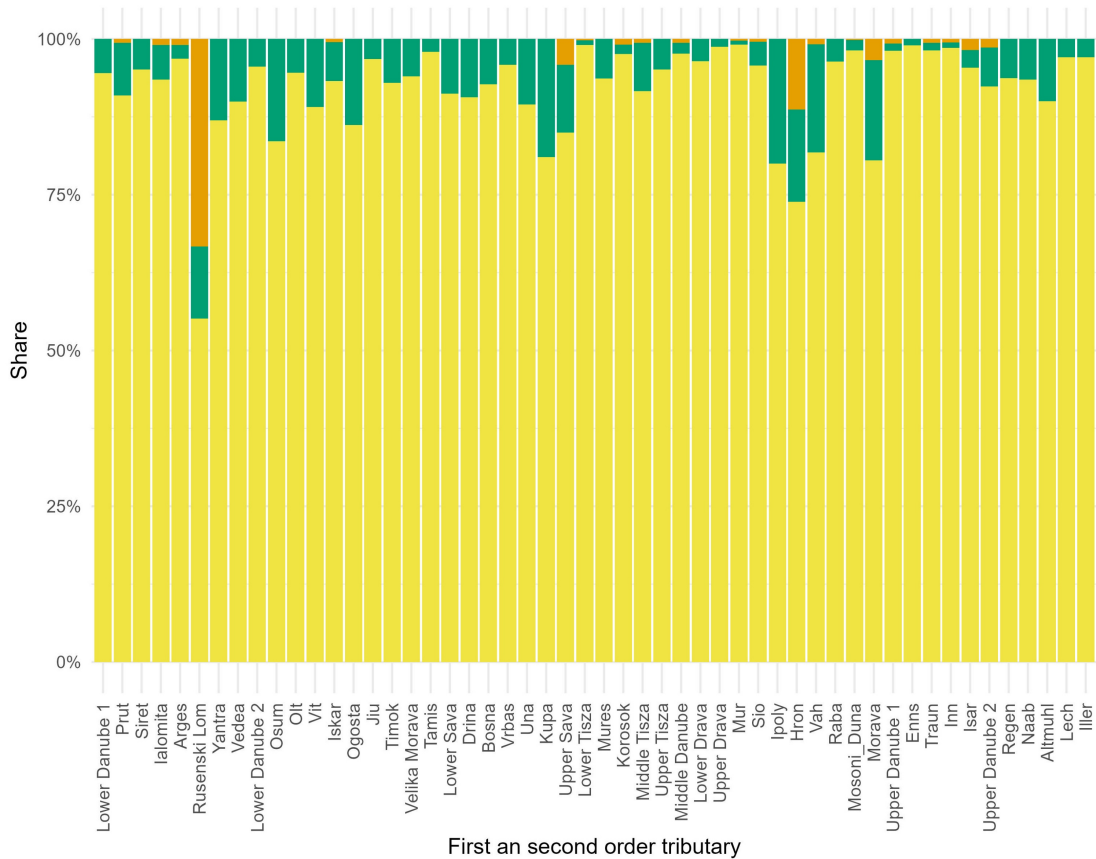


## Main observations

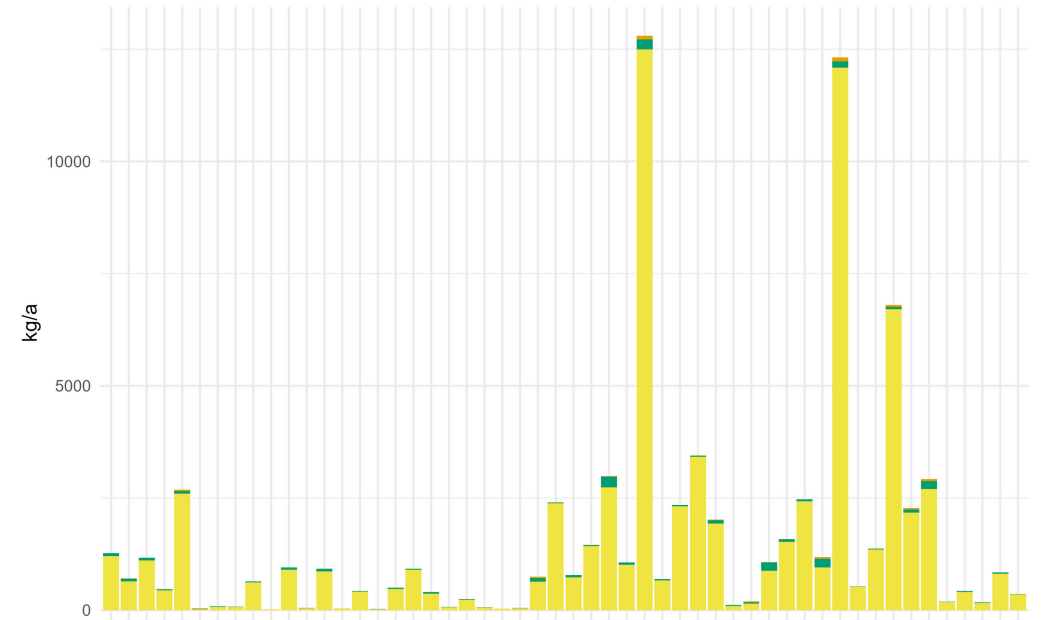
- Beside WWTPs, urban systems play an important part in total loads
- Due to lower share of sewage treatment, share of urban systems related diffuse load might be important in the lower Danube
- Industrial discharges show strong hot-spot loads in a few catchments (only estimated loads!)

# Diclophenac emissions in the DRB

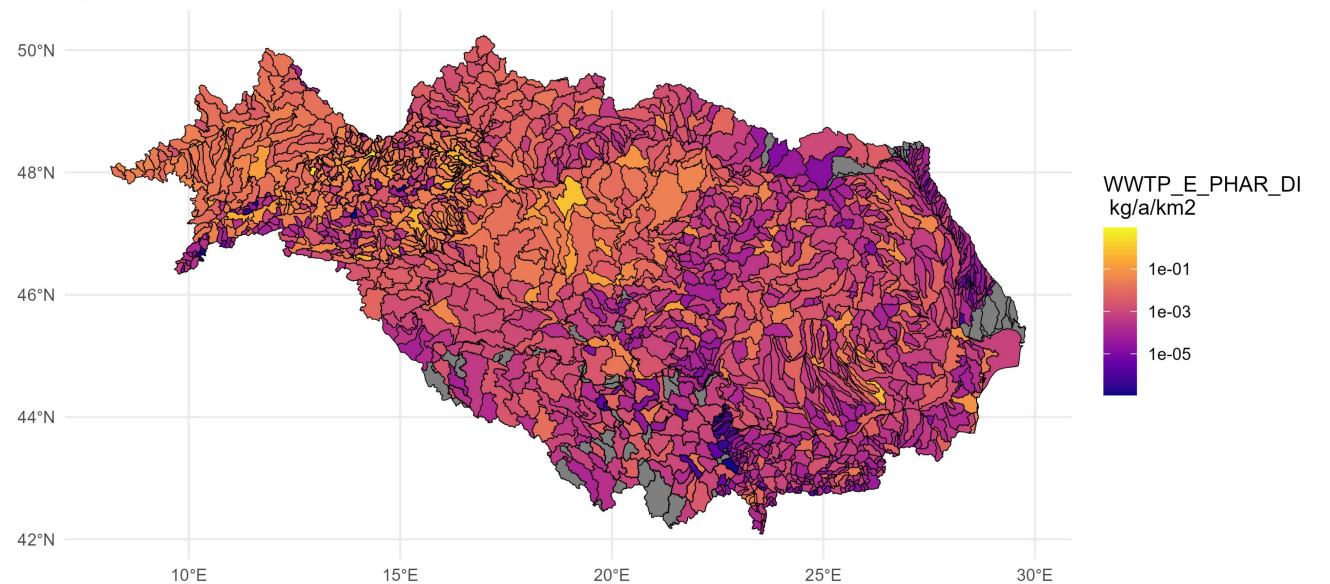
Share of pathways for PHAR DI



Absolute pathway loads for PHAR DI



Specific emission of PHAR DI



## Main observations

- Beside WWTPs, urban systems may play an important part in total loads
- Due to lower share of sewage treatment, share of urban systems related diffuse load might be important in the lower Danube
- Industrial discharges show strong hot-spot loads in a few catchments

# Conclusions

**Model input data:** some regions lack sufficient input data on groundwater concentrations and industrial emissions. Landfills and fire-fighting centre dataset is needed for PFAS substances.

**Validation data:** data frequency needs to be increased for emerging substances to improve validation load estimation.

**Model validation:** Validation performance vary between substances. Strong regional pattern is shown in validation performance for metalloids.

## Emission patterns:

- **PFAS** loads are strongly dominated by the upper Danube (linked to GDP in soil and WWTP concentrations);
- **Pharma** emissions levels from WWTP are strongly country specific; urban diffuse loads might be important.
- For **metalloids**, groundwater and agricultural erosion are dominating the overall loads, but regional differences are significant.

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# Thank you for your attention!



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