LIÈGE université
Sciences

P&GIRE

Modelling of Micropollutants in Rivers at the Watershed Scale to Assess the Quality of Water and Sediments

Liege, September 9th, 2026
International Meuse Symposium
Aline Grard

Context

Modelling of micropollutants in aquatic ecosystem

Multiclass System of sediment
Distribution Coefficient
Modelling, Results & Validation

MicMod

Discussion

Conclusions & Perspectives

Context

Prerequisite

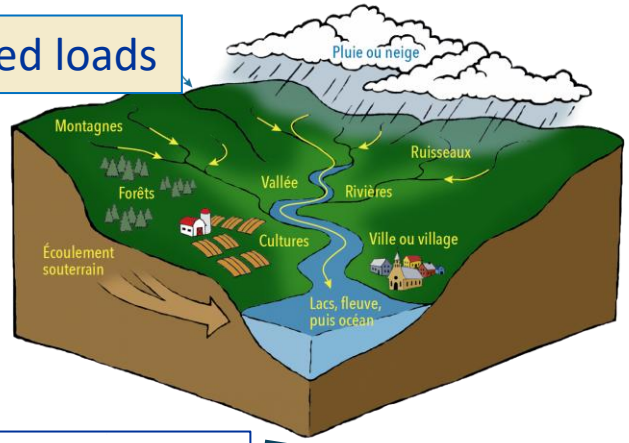
PEGASE Model (developed within our PeGIRE Labo)

- Represents hydrology and hydrodynamics of rivers, phytoplankton production, nutrient fluxes, water temperature…
- Allows the simulation of thousands of rivers in one simulation
- Fine discretisation allowing studies from local scale up to hydrographic districts scale
- …

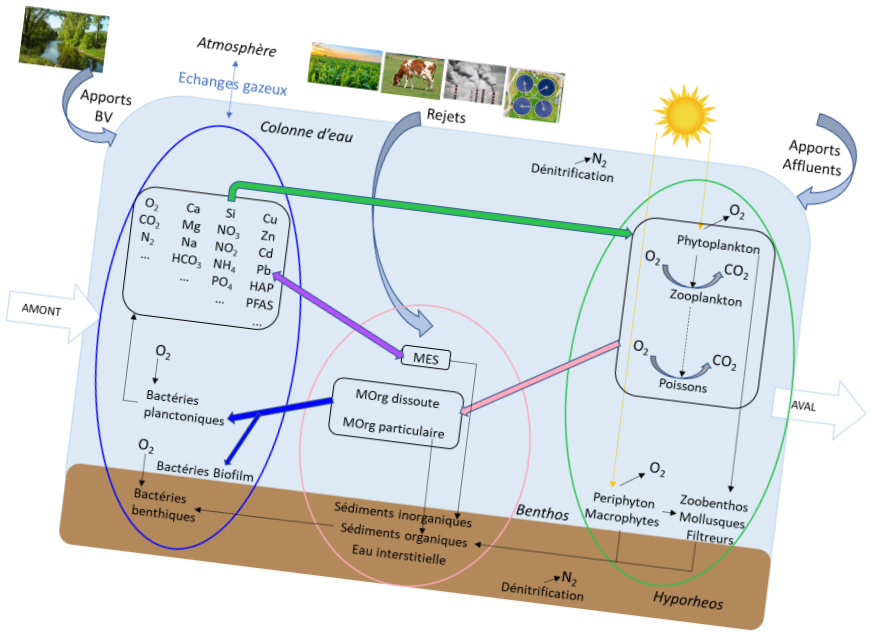
Modelling of Watershed – River Complex

Physically based deterministic modelling of continental aquatic ecosystem - PEGASE

Watershed loads



PRESSURES
Agriculture
Industries
Urban
…



Pressure-Impact Relationships

IMPACTS
Concentrations
Pollutant Fluxes

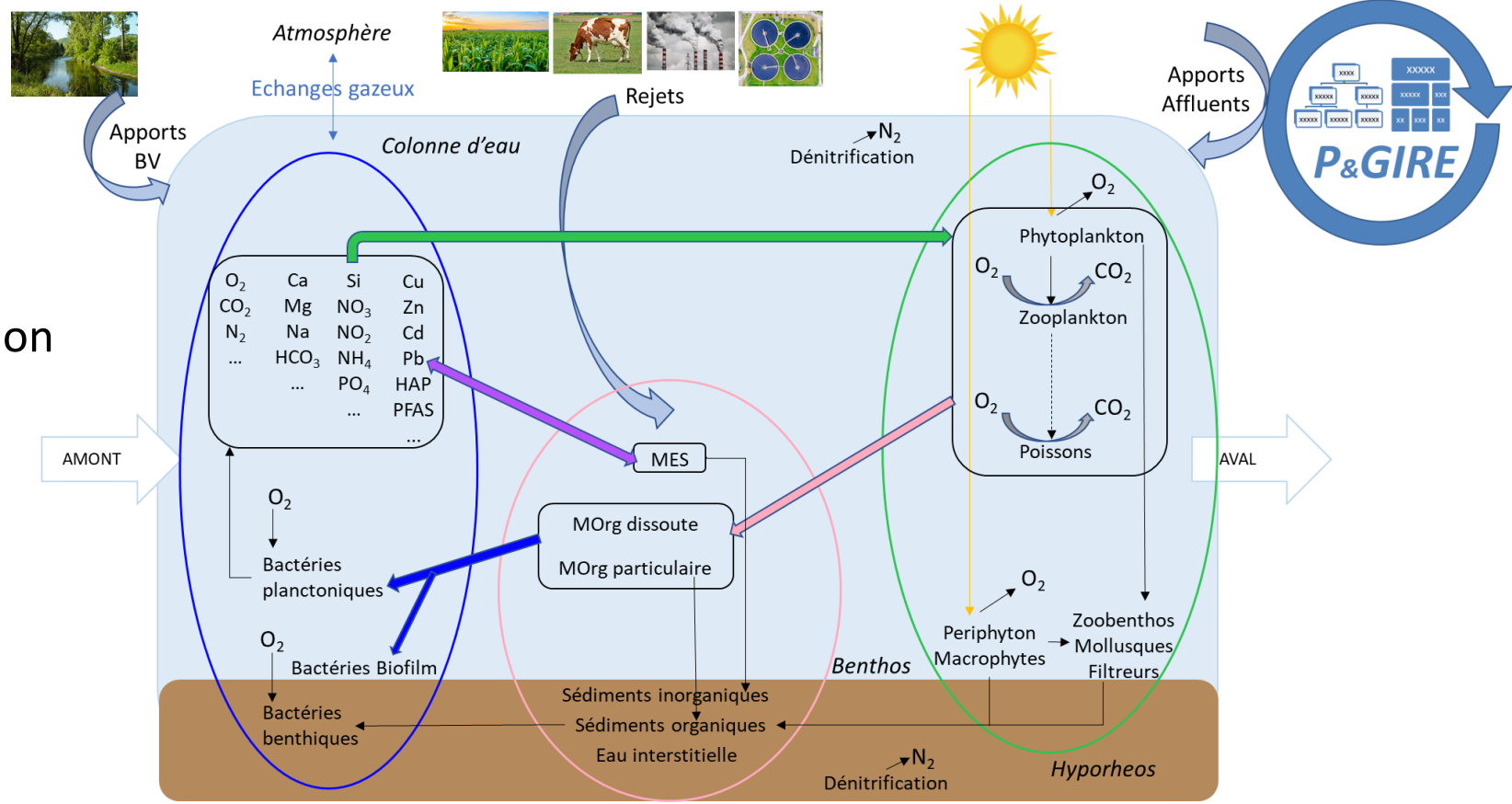
⬇

Water Quality
Balance Sheets
Results per Water Body

Pegase

Processes

- Primary production
- Mortality, biomasses respiration
- Degradation organic matter
- Nitrification, denitrification
- Reaeration
- Sedimentation



Variables

- Flows, velocities, transfer time in the hydrographical network
- Temperature
- Concentrations : OM, DOC, POC, COD, BOD, NH_4, NO_2, NO_3, N_{Kj}, P_{tot}, PO_4, dissolved O_2 (daily average, min, max), biomasses (bacteria, plankton…), macroelements (Ca, Mg, SO_4, …), pH

Results

- Flow, temperature, concentrations (daily average) at each Pegase node (several thousands)
- Globalisation of results per river, per waterbody, per subbasin, … : fluxes, balance sheets
- Curves along the river, time series, maps : statistics (p90, …), quality indices SEQEau

MicMod

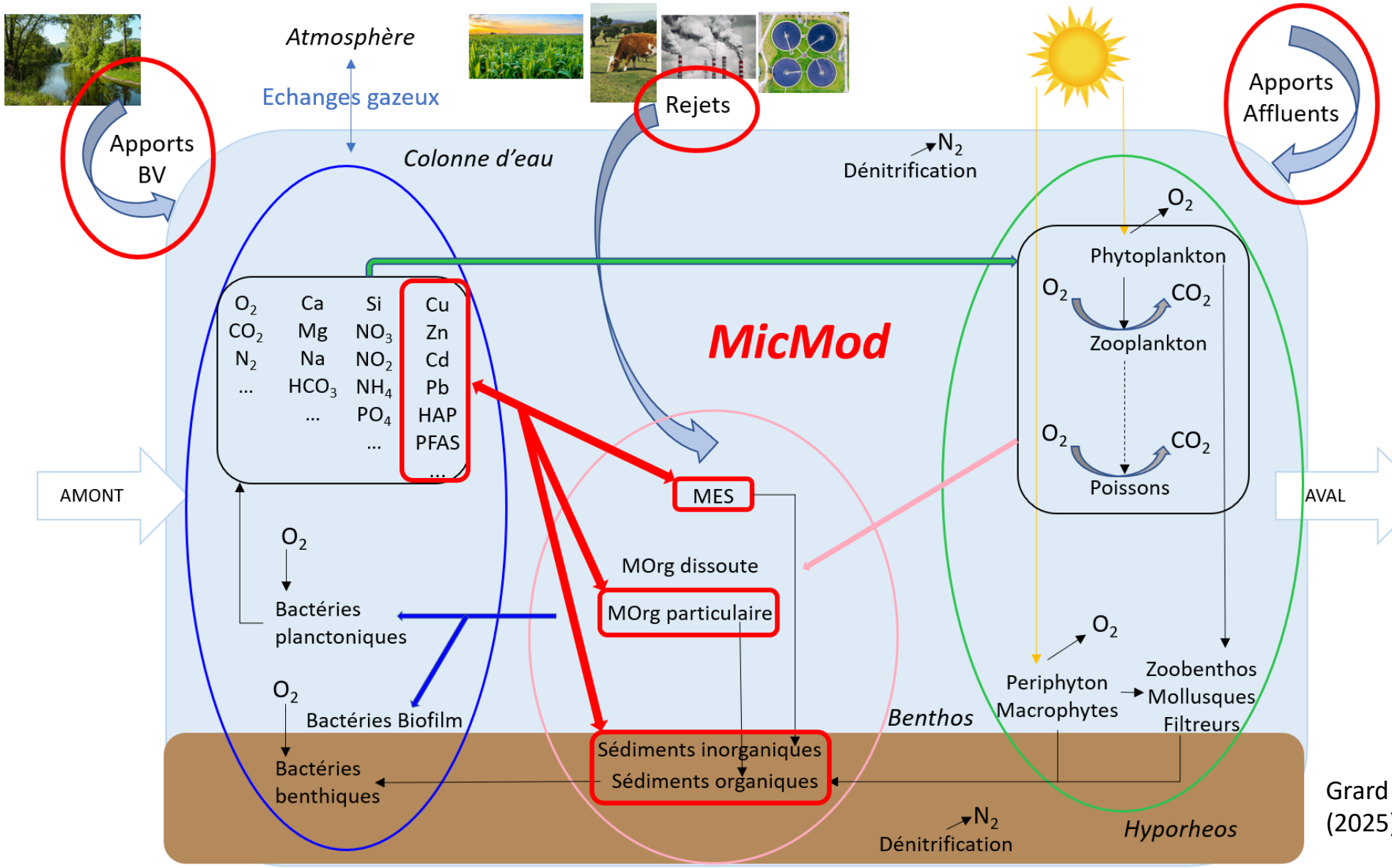
Sediments & Micropollutants

Multiclass sediment system

Knowledge of distribution between liquid and solid phases

MicMod

MicMod

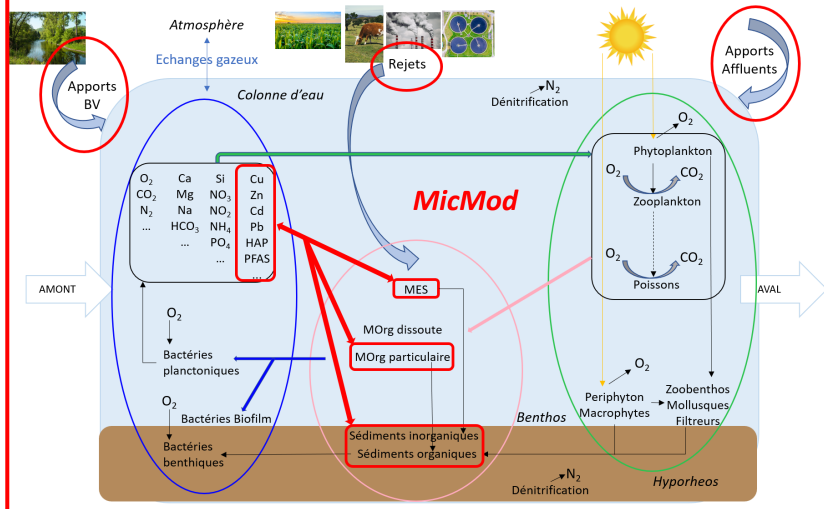


Grard & Deliège (2025)

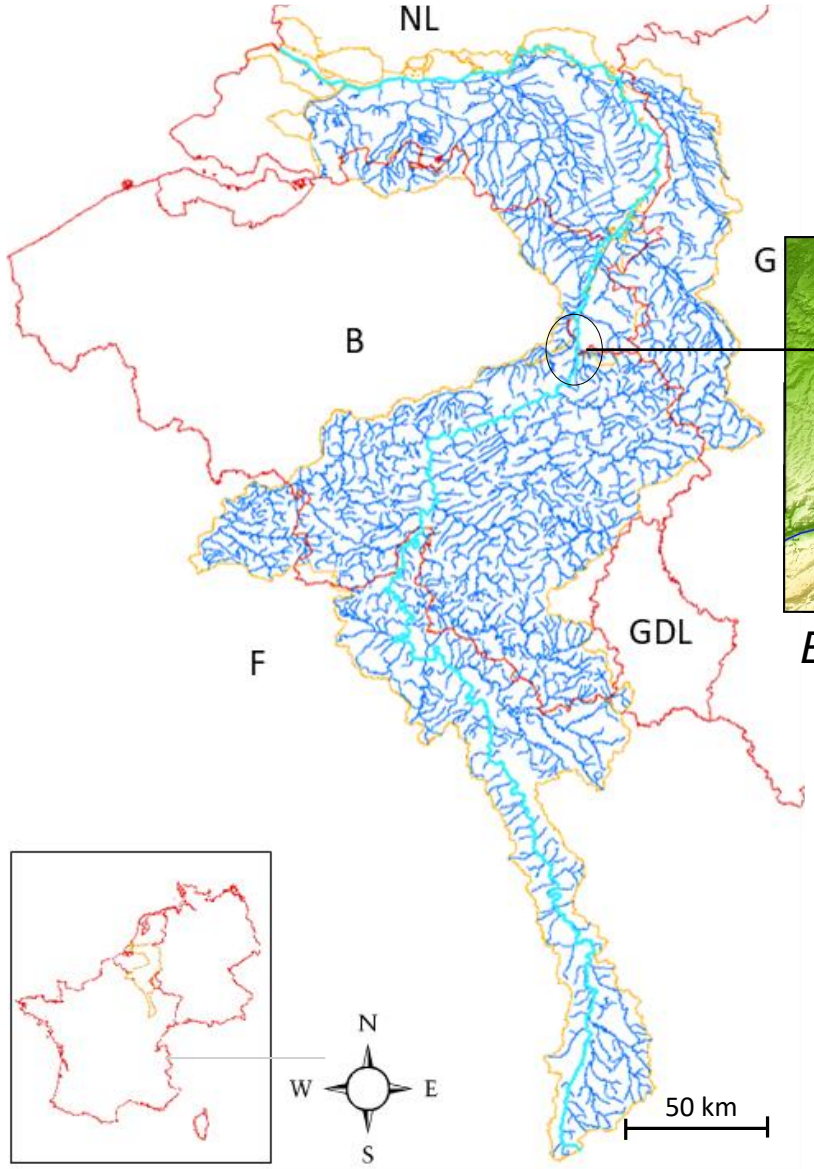
Processes Modelled in MicMod

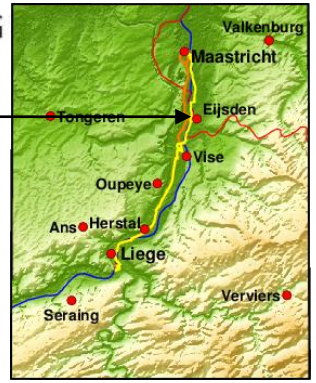
MicMod

1. Micropollutants are transported in water (liquid phase) and on Suspended Matter (solid phase)
2. **Adsorption on SS**
3. **Desorption from SS to Water Column**
4. Adsorption on bottom sediment
5. Desorption from bottom sediment to water column
6. Sedimentation of SS with adsorbed micropollutant
7. Resuspension of bottom sediments with adsorbed micropollutants
8. Biodegradation, volatilisation, photodissociation…



Data collection





Eijsden Data

Meuse River Basin

34 564 km², 905 km

Eijsden : 20 554 km², 617 km

Meuse (Eijsden) : **SS Measured** Concentration

Description hydro-sedimentary

- Concentration of total SS
- Granulometry of SS particles: % < 2µm, % < 16 µm, % < 63 µm (1x / week)

→ *Multi-class particles system (4 classes of mineral SS)*

Classes	Diameter (µm)	Average Diameter (µm)	Acronym
Clay	< 2	1	C_MES1
Fine Silt	2 → 16	9	C_MES9
Coarse Silt	16 → 63	40	C_MES40
Sand	63 → 250	157	

$S = 4 \pi r^2$
$V = 4/3 \pi r^3$
$S/V = 3/r$

The ratio surface/volume is inversely proportional to the diameter

Method to Assess Micropollutant Concentration per Granulometry

Micropollutants

Meuse River in Eijsden

With concentration of particulate micropollutant adsorbed on total SS,

How to assess the distribution of micropollutants within granulometry classes ?

→ <u>Hypotheses</u>

- Micropollutant concentration adsorbed on SS are proportional to the ratio surface/volume
- No differentiating based on SS chemical composition

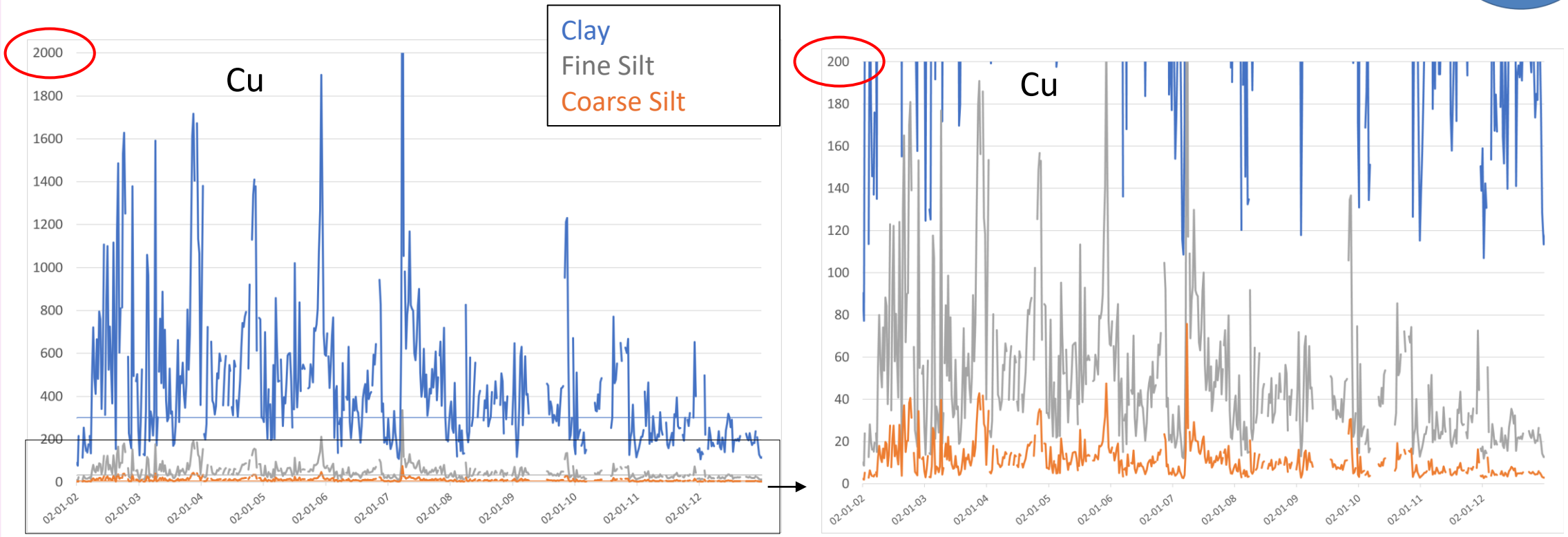
→ Mass Conservation Law

→ Single Unknown Equation

Ratio 9 between C_MES1 & C_MES9 → C_MES9 = C_MES1 / 9
Ratio 40 between C_MES1 et C_MES40 → C_MES40 = C_MES1 / 40
MES * C_MES = MES_1 * C_MES1 + MES_9 * C_MES1 / 9 + MES_40 * C_MES1 / 40
C_MES1 = (MES * C_MES) / (MES_1 + MES_9 / 9 + MES_40 /40)

Micropollutants

Calculated Concentration of **Copper** per Granulometry (Meuse River in Eijsden)



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Mass Concentration of Cu (mg/kg) on SS in Eijsden

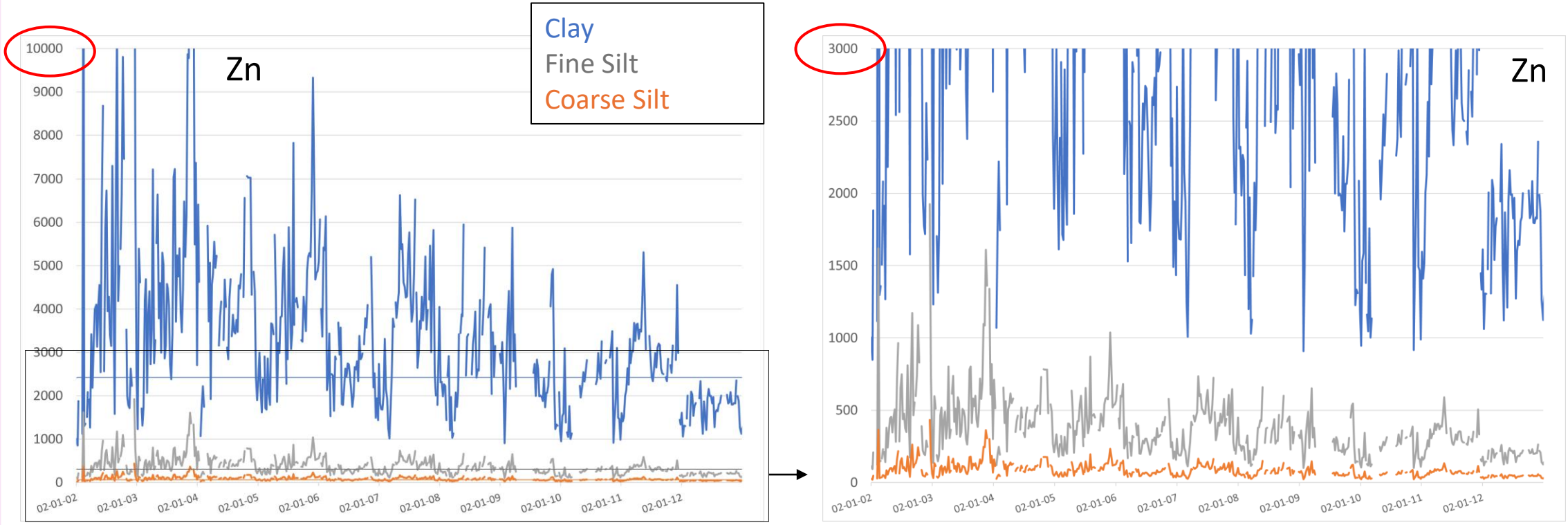
Adsorbed Cu on clay (< 2 µm, mean diameter = 1 µm), fine silt (2 µm to 16 µm, mean diameter = 9 µm) et coarse silt(6 µm to 63 µm, mean diameter = 40 µm)

Median Cu-mes1 = 300.57 mg/kg

Median Cu-mes9 = 33.40 mg/kg

Median Cu-mes40 = 7.51 mg/kg

Calculated Concentrations of **Zinc** per Granulometry (Meuse River in Eijsden)



Grard & Deliège (2023)

Mass Concentrations of Zn (mg/kg) on SS in Eijsden

Adsorbed Zn on clay (< 2 µm, mean diameter = 1 µm), fine silt (2 µm to 16 µm, mean diameter = 9 µm) et coarse silt (16 µm to 63 µm, mean diameter = 40 µm)

Median Zn-mes1 = 2424.08 mg/kg

Median Zn-mes9 = 303.01 mg/kg

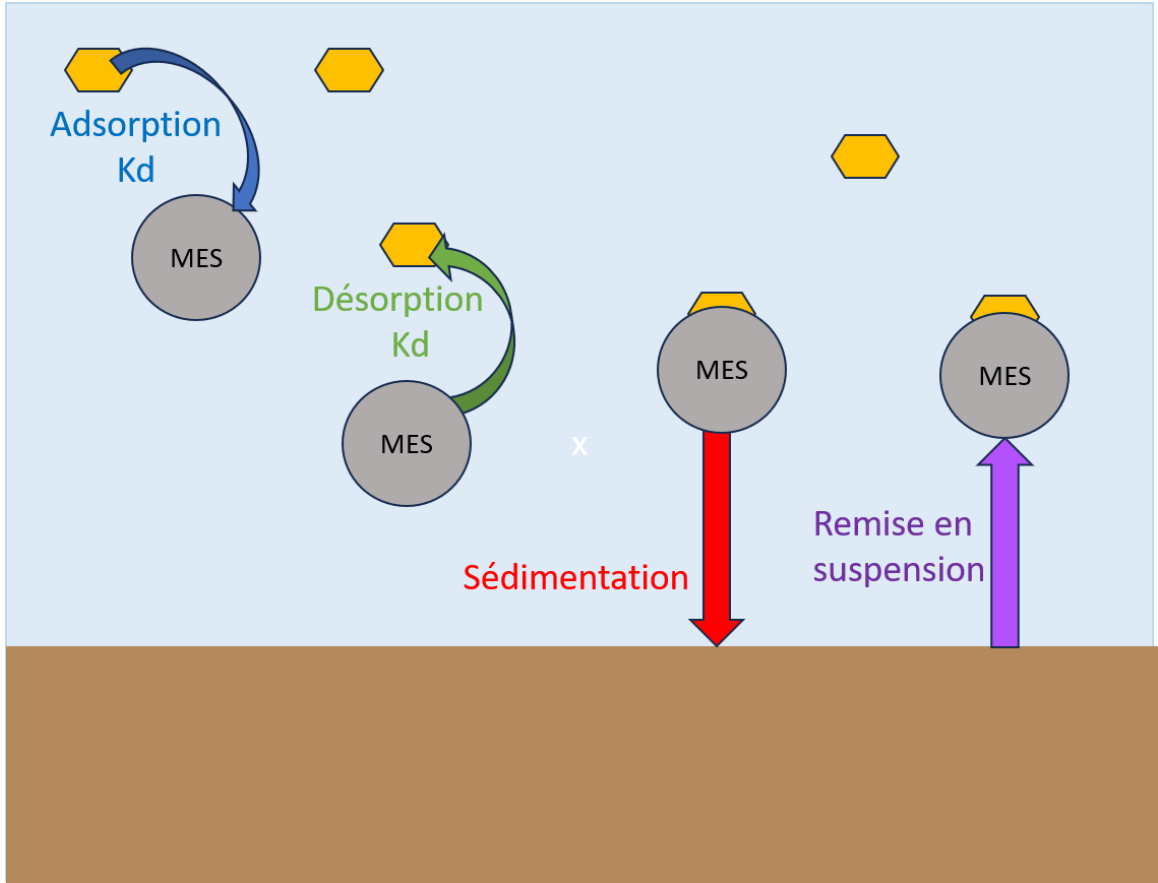
Median Zn-mes40 = 75.75 mg/kg

Distribution Coefficient

- Distribution Coefficient

$$Kd = \frac{\text{Particulate Concentration } [\mu g/g]}{\text{Dissolved Concentration } [\mu g/l]} \rightarrow l/g \text{ or } m^3/kg$$

- This coefficient should be calculated at equilibrium, which is never occurring in natural environment
- The higher the Kd, the more the pollutant is adsorbed on the particles
- We used the collected measurements to assess the Kd

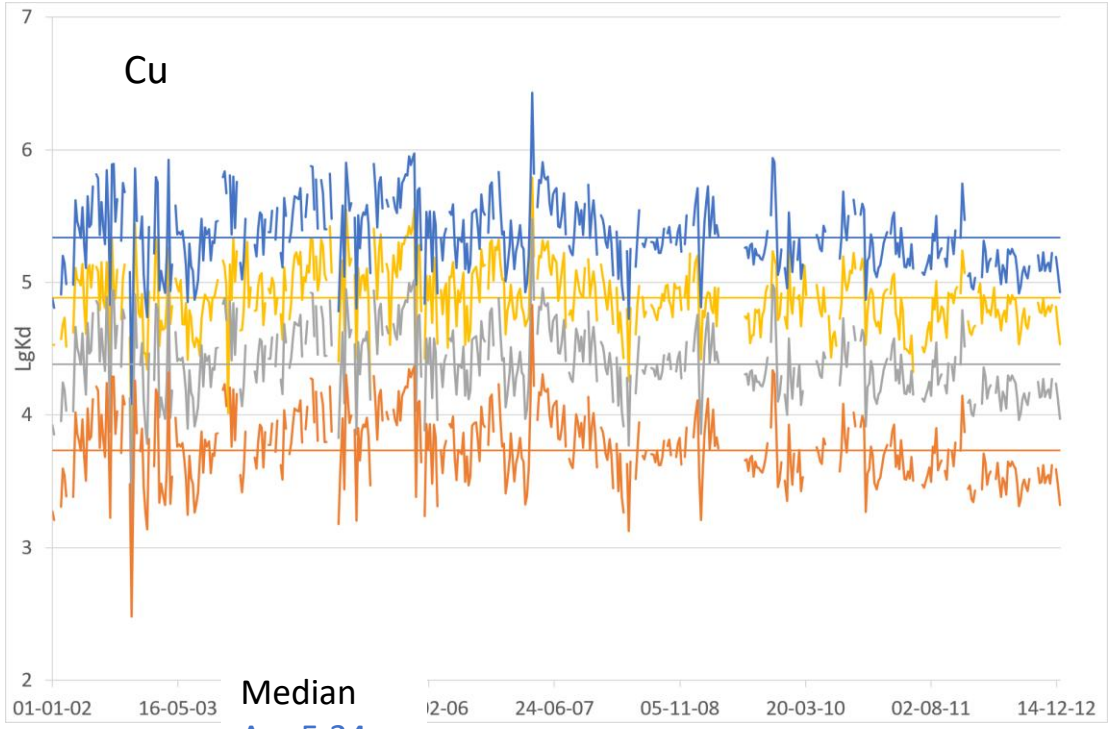


Distribution Coefficient

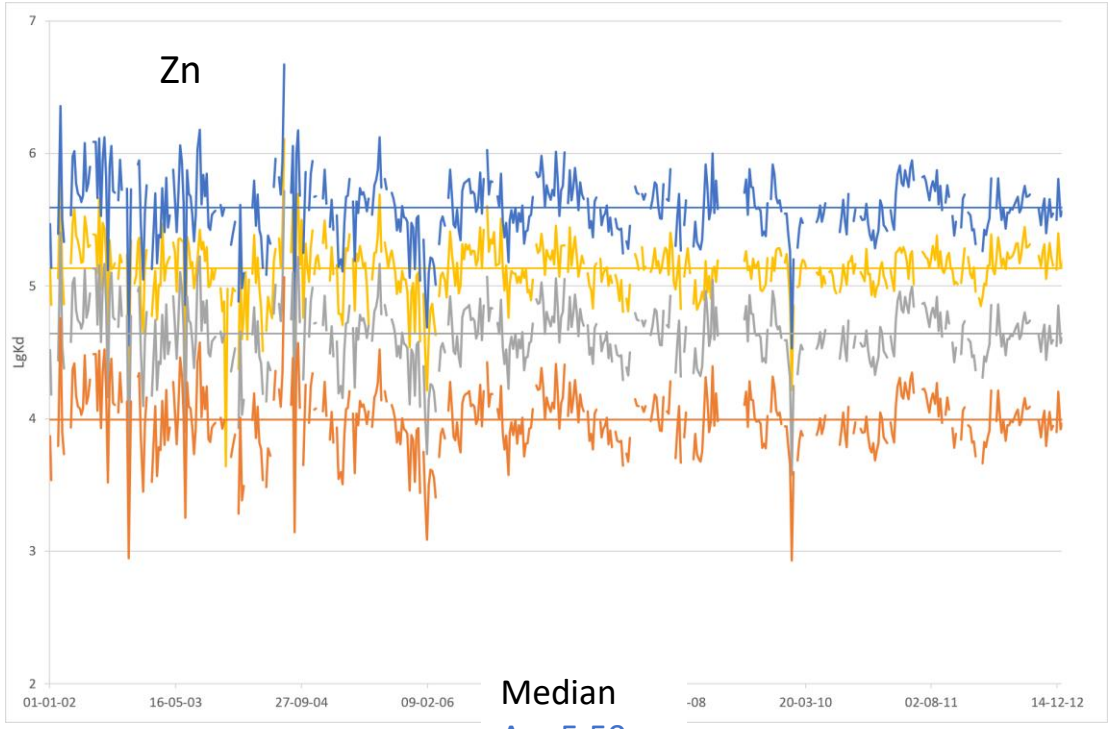
Determination of **Distribution Coefficients** per Granulometry (Meuse River in Eijsden)

Clay
Total
Fine Silt
Coarse Silt

Logarithmic Values (log) : logKd



Median
Arg 5.34
Tot 4.92
Lif 4.38
Lig 3.74



Median
Arg 5.59
Tot 5.14
Lif 4.64
Lig 3.99

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MicMod

Sediment & Micropolluants

Modelling of micropollutants in aquatic ecosystem & Results

Sources of micropollutants & SS

Point Loads

- Main Urban Releases: micropollutants (Wastewater Treatment Plants Releases & Non-Connected Wastewater) & SS
- Main Industrial Releases: micropollutants & SS (based on release directory, industrial emissions inventory, …)

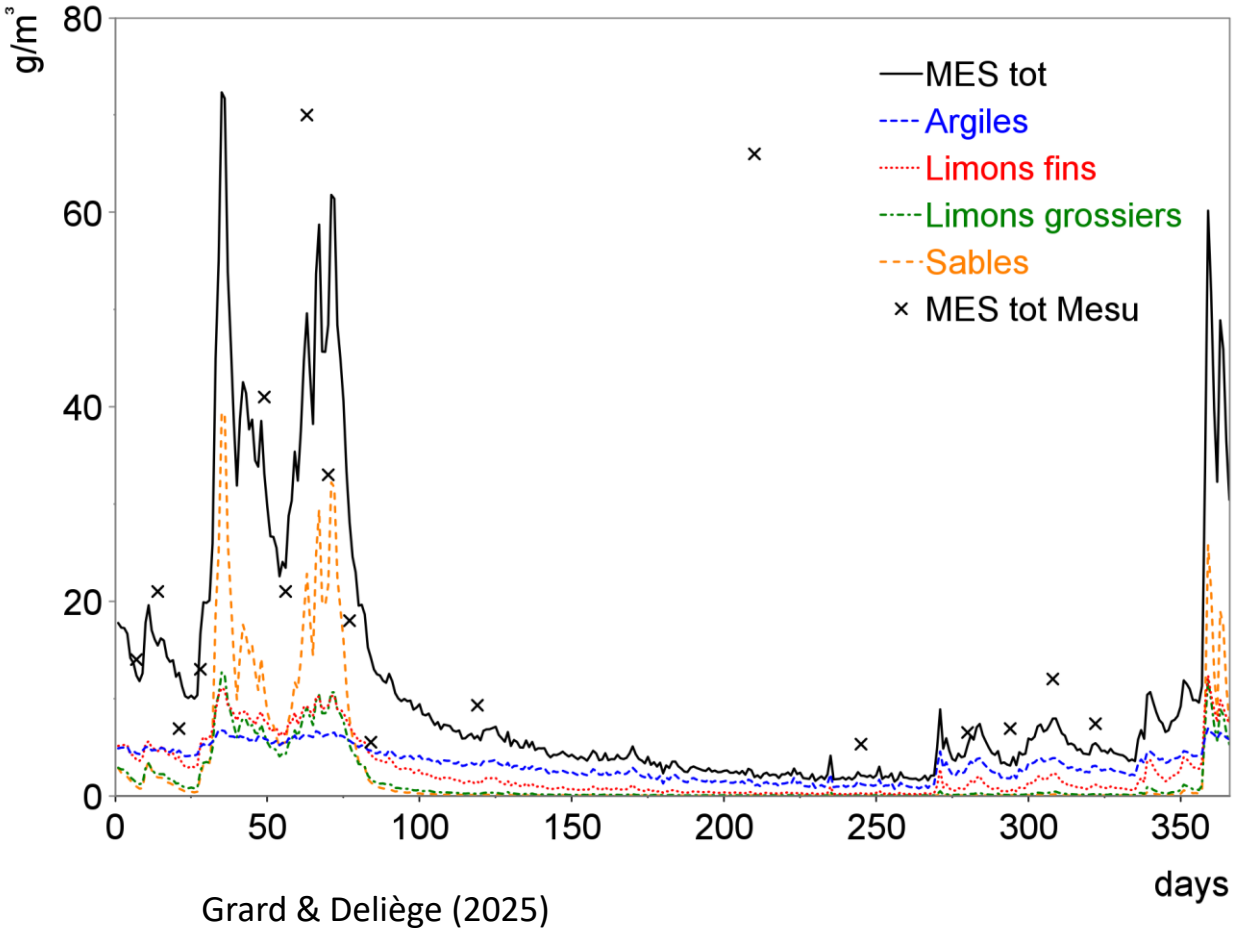
Diffuse Loads

- Micropollutants: calibration based on upstream watershed
- SS: leaching based on a rating curve ($SS = b \times Flow^a$)

Results

Results of MicMod Modelling

Meuse River in Eijsden: distribution of SS per granulometry



Grard & Deliège (2025)

Time series of total SS concentration (g/m^3), clay, fine silt, coarse silt & sand.

Measured total SS concentration (cross) in the Water column

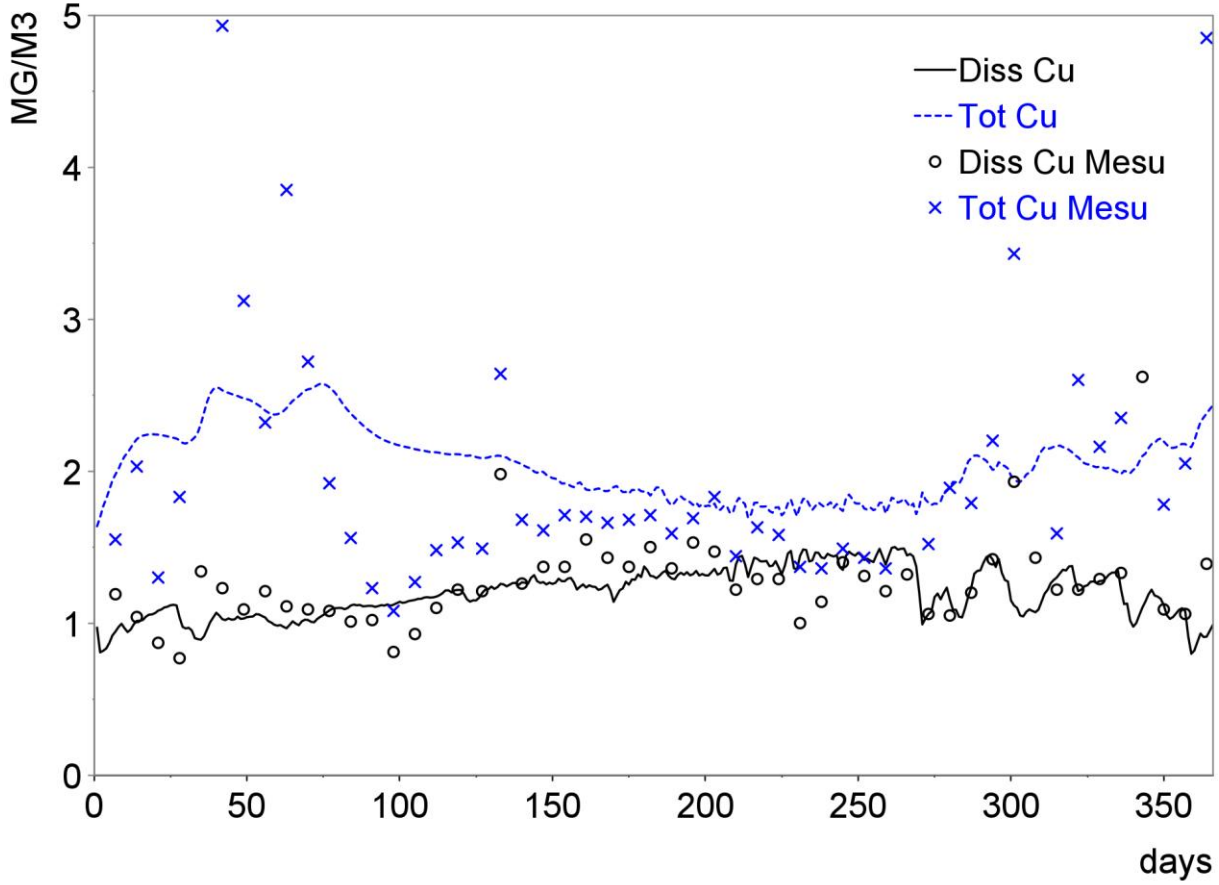
Eijsden, 617 km, Meuse River, year 2020

Validation

Results

Results of MicMod Modelling

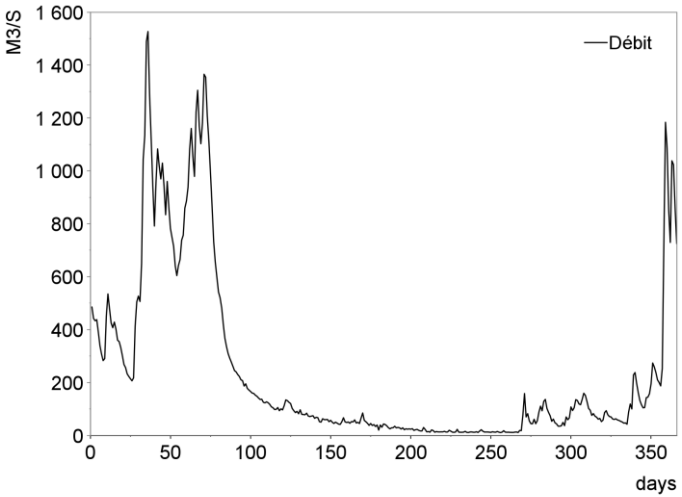
Meuse River in Eijsden: dissolved & total fractions of copper



Grard & Deliège (2025)

Validation

Time series of calculated and measured concentration in dissolved Cu and total Cu (mg/m³)
Eijsden, 617 km, Meuse River, year 2020



Time series of flows (m³/s)
Eijsden, Meuse River, year 2020

Conclusions

MicMod

Conclusion

- Hydro-sedimentary Description → development of a multiclass system of particles (4 classes)
- Determination of distribution coefficients per granulometry
- Implementation of multiclass system: 4 classes of particles model properly the targeted phenomena (ads°/désorp°, sed°/resusp°)
- Clay class is essential to model the fate of micropollutants

Challenges

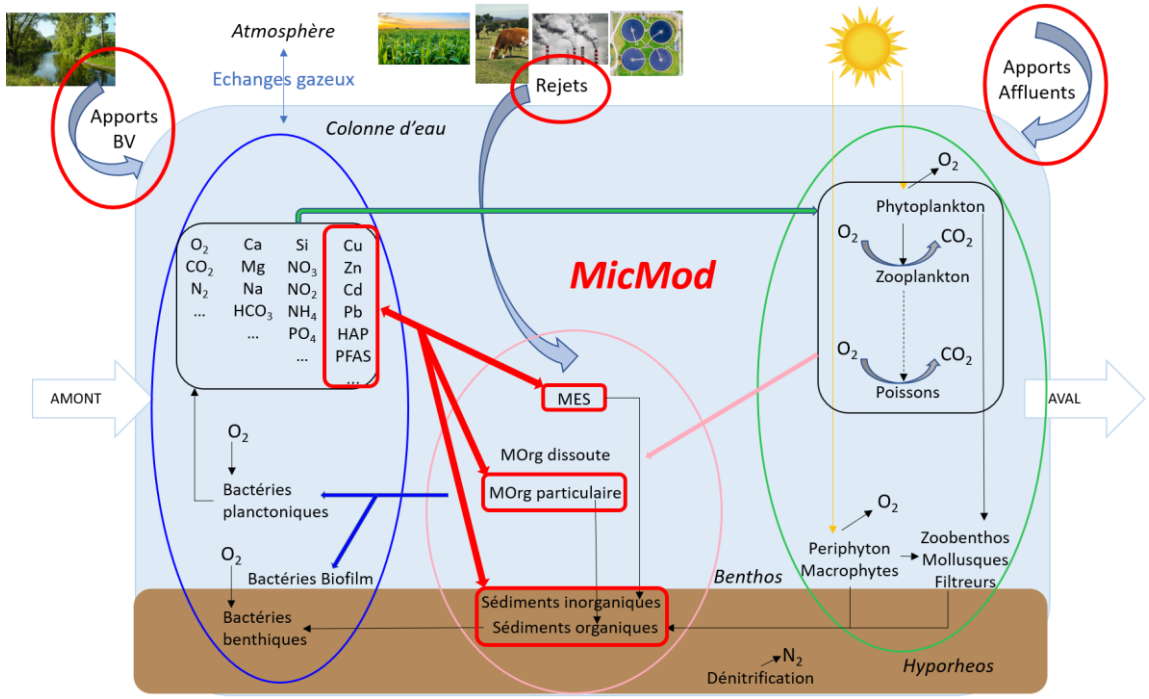
MicMod is physically based

→ Transposability of MicMod to other national and transnational basins

→ Transposability of MicMod to other substances

- Sources / Loads
- Measurements
- Behaviour in aqueous solution

Thanks for your attention



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