Estimating pharmaceuticals pollution in river basins with mixed urban-rural land uses

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Introduction

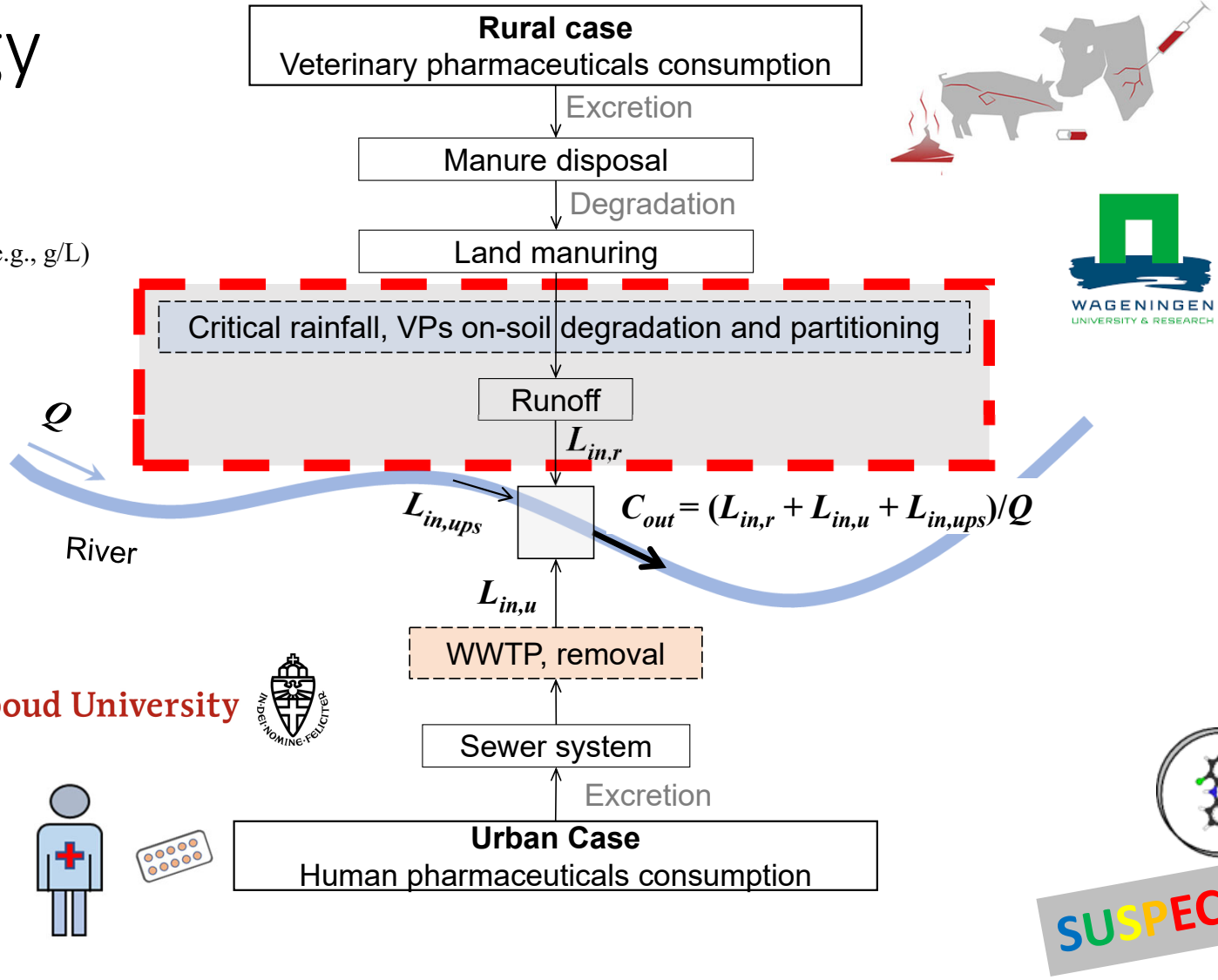
- Thousands of (veterinary-)**pharmaceuticals** are used every day and are **found** in **soils and surface waters**. This **contamination** is mainly originated from **rural** (diffuse sources) and **urban** areas (point sources from waste water treatment plants).

- In the **SUSPECt** research project, we selected an useful **hydrological and water quality** model tool to **integrate** the **rural** and **urban** sources and **predict** the environmental concentration in rivers in **space** and **time**.

- The **goal** is to provide spatial and temporal **exposure information** for **risk assessment and management**.

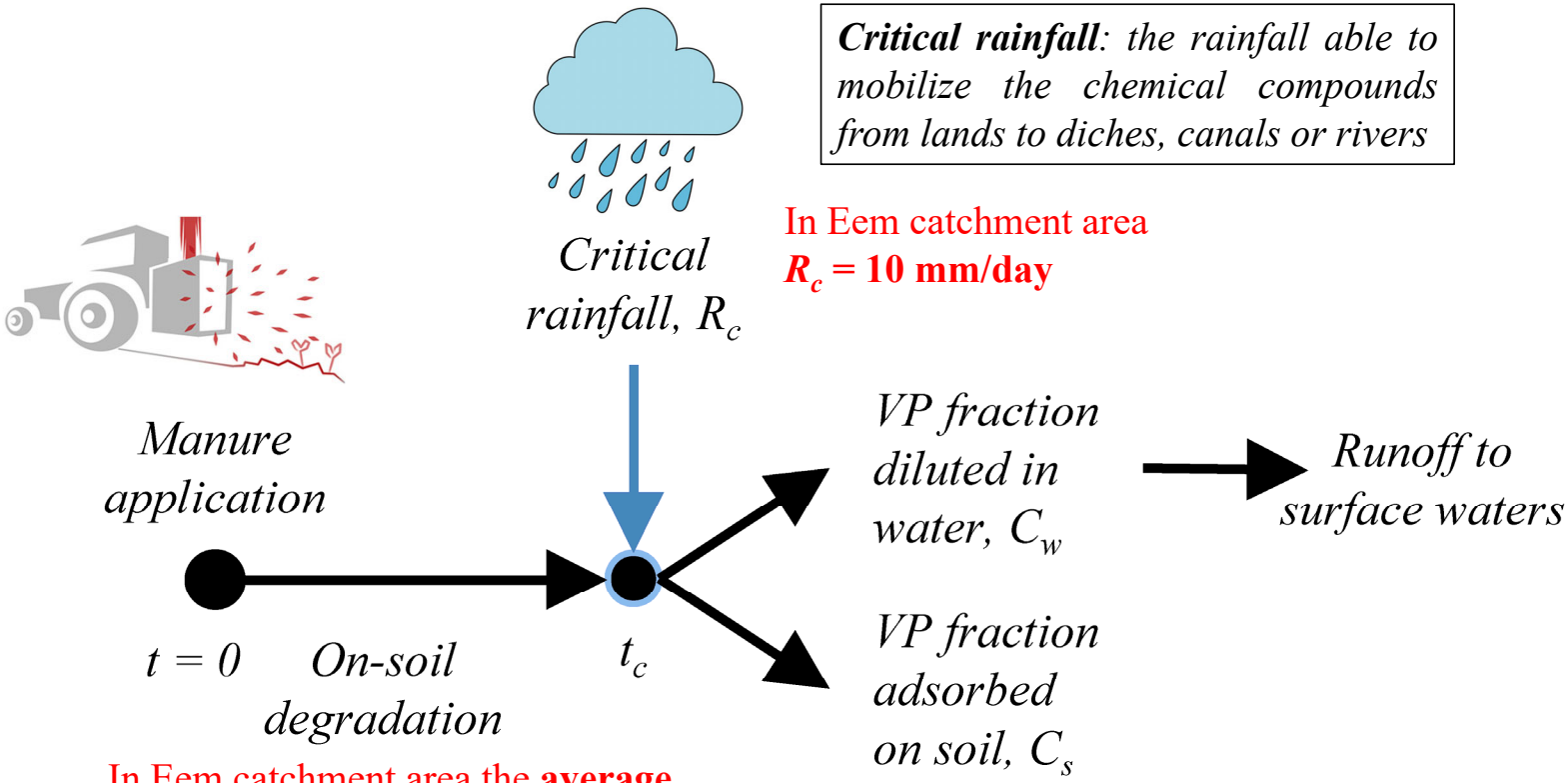
Methodology

Q = river water discharge (e.g., m^3/s)
L = pharmaceuticals load (e.g., g/s)
C = pharmaceuticals concentration (e.g., g/L)
ups: upstream
u: urban
r: rural



Focus on rural effluents

Critical rainfall: *the rainfall able to mobilize the chemical compounds from lands to diches, canals or rivers*



In Eem catchment area
R_c = **10 mm/day**

In Eem catchment area the **average time** between two critical rainfall in Spring is t_c = **15 days**

C_w and C_s is defined by the soil/water partition coefficient $K_d = C_s / C_w$

Case of study – Eem Catchment

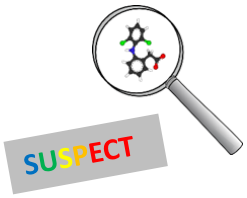
Utrecht and Gelderland provinces, Vallei en Veluwe waterboard

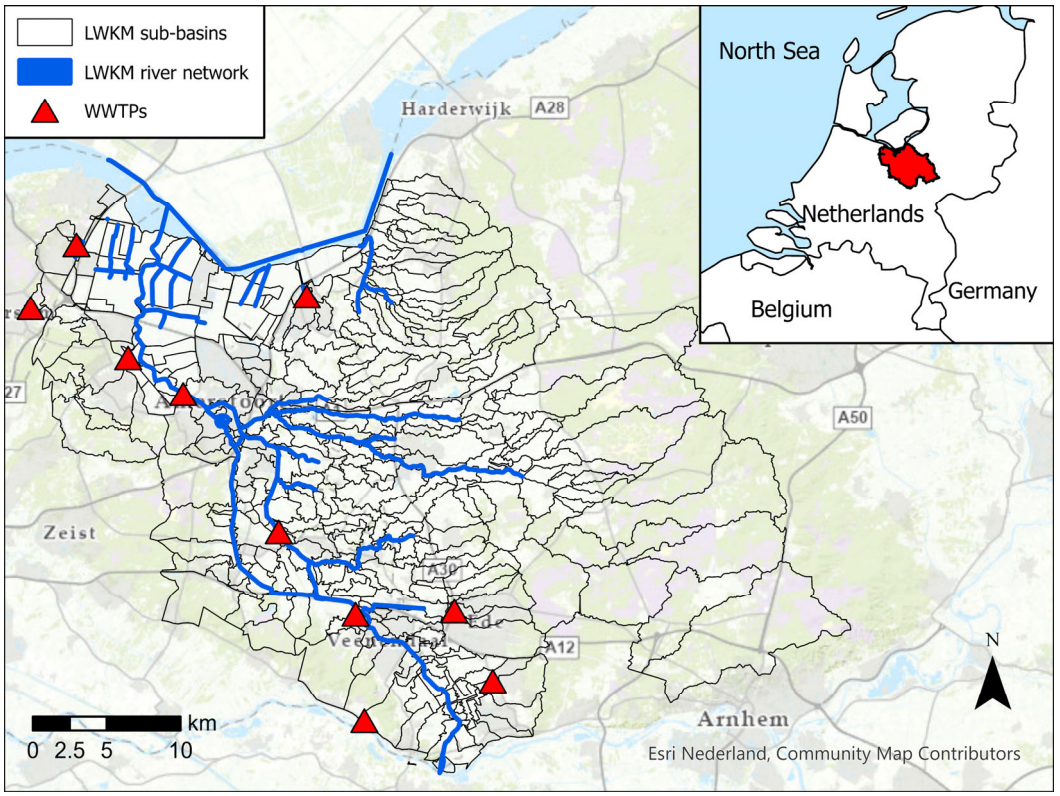
MODELLING TOOL

Deltares

Hydrological and Water Quality model
WFD – LWKM

- Prediction of contaminants concentration in rivers
- **Seasonal**: one prediction per season
- **Point sources** from WWTPs (points)
- **Diffuse sources** from agricultural fields (polygons)





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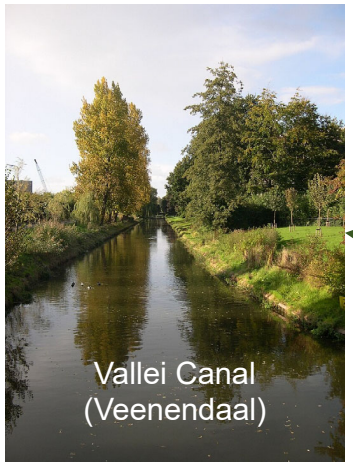
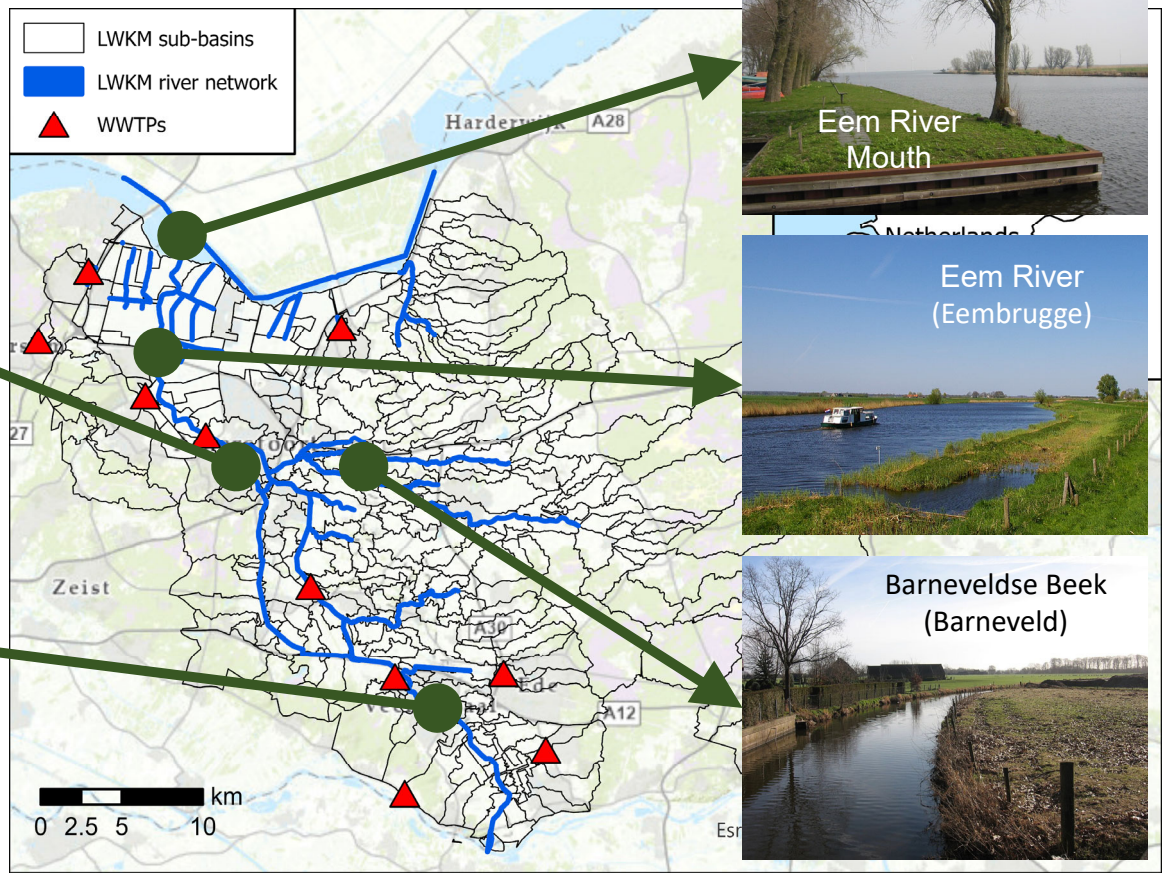
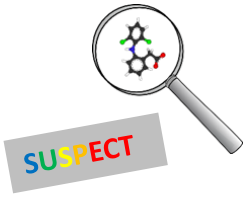






Focus on the LWKM model structure

LWKM model

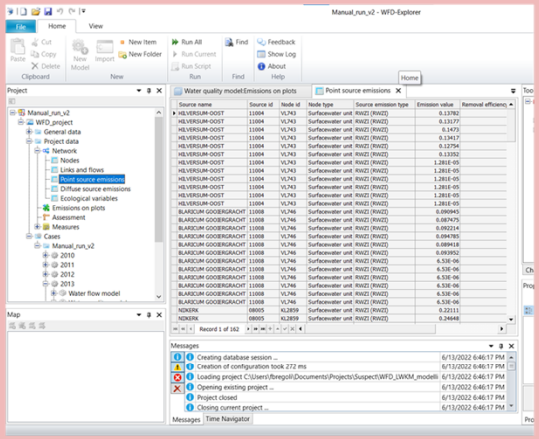
Rural model input

Sourceid	Emission type	Variable	Load (g/s)	Year	Period
151379	AGRIC	Sulfamethoxazol	0.00000342	2015	1
151379	AGRIC	Sulfamethoxazol	0.00000418	2015	2
151379	AGRIC	Sulfamethoxazol	0	2015	3
151379	AGRIC	Sulfamethoxazol	0	2015	4
151381	AGRIC	Sulfamethoxazol	0.0000123	2015	1
151381	AGRIC	Sulfamethoxazol	0.000015	2015	2
151381	AGRIC	Sulfamethoxazol	0	2015	3
151381	AGRIC	Sulfamethoxazol	0	2015	4
…	…	…	…	…	…

Urban model input

Sourceid	Emission type	Variable	Load (g/s)	Year	Season
NL08005	RWZI	Sulfamethoxazol	7E-05	2015	0
NL08019	RWZI	Sulfamethoxazol	8.68E-06	2015	0
NL08021	RWZI	Sulfamethoxazol	6.5E-05	2015	0
NL10010	RWZI	Sulfamethoxazol	7E-05	2015	0
NL10020	RWZI	Sulfamethoxazol	1.82E-05	2015	0
NL10021	RWZI	Sulfamethoxazol	6.5E-05	2015	0
…	…	…	…	…	…

Python script
Or
"WFD – explorer" graphic user interface



CECs Physic-chemical parameters

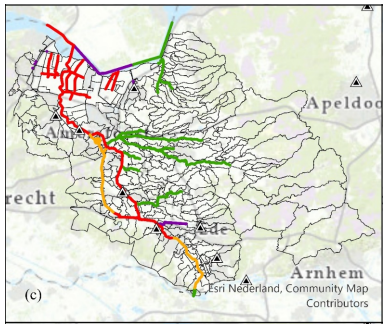
Model Output

Risk Assessment

time [-]	Node [-]	Variable [mg/L]
1/1/2015 0:00	TN1	0.000294159
1/1/2015 0:00	VL742	0.000312031
1/1/2015 0:00	VL743	0.000352724
1/1/2015 0:00	VL746	0.000312036
1/1/2015 0:00	LSM3407	0
1/1/2015 0:00	KL2859	0
1/1/2015 0:00	KL619	0
1/1/2015 0:00	KL620	2.36E-16
1/1/2015 0:00	KL621	3.72E-15
…	…	…

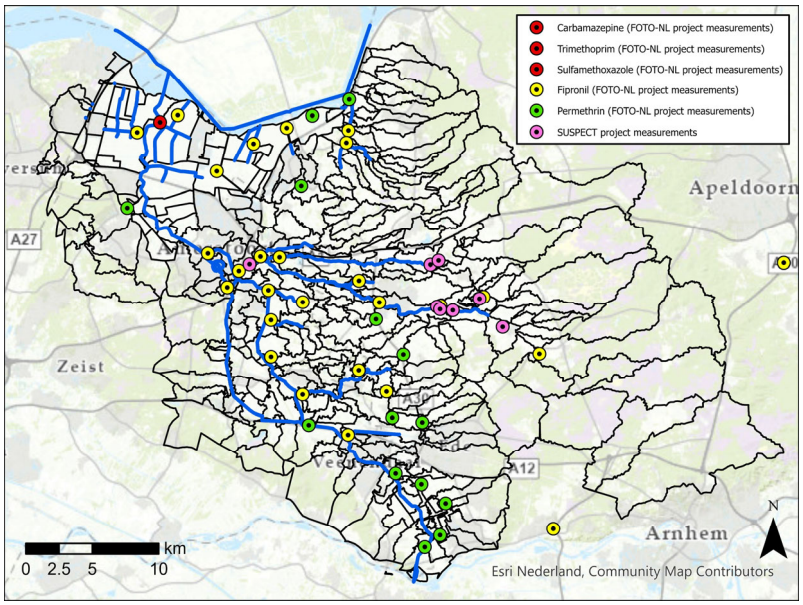
Spreadsheet

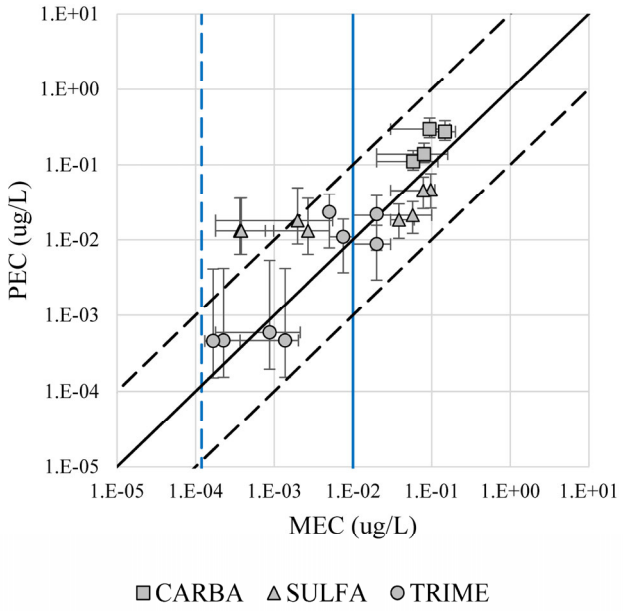
Map



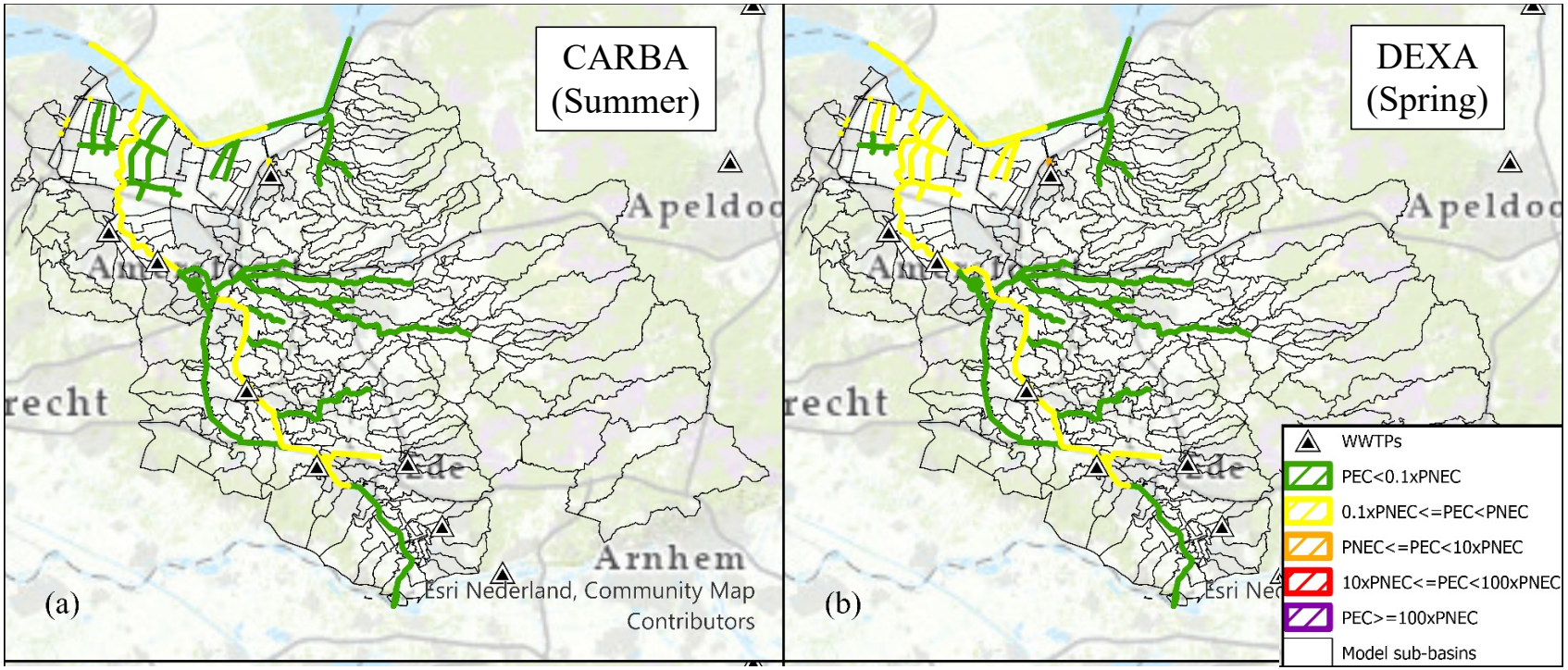
Validation of the methodology

Compound	Source
Carbamazepine	U
Fipronil	U
Trimethoprim	U+R
Sulfamethoxazole	U+R
Permethrin	U+R
Dexamethasone	U+R



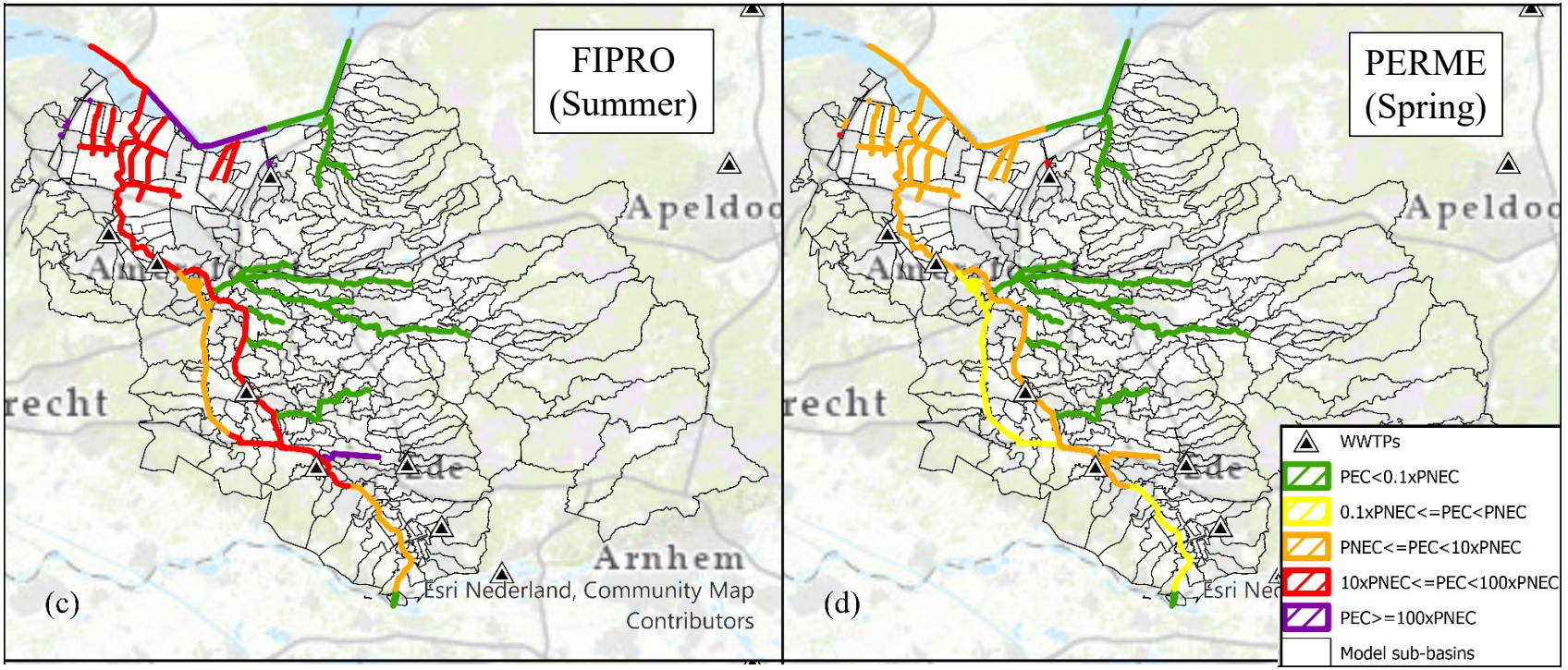


Results



PNEC = Predicted no effect concentration
(EQS = Environmental quality standard)

Results



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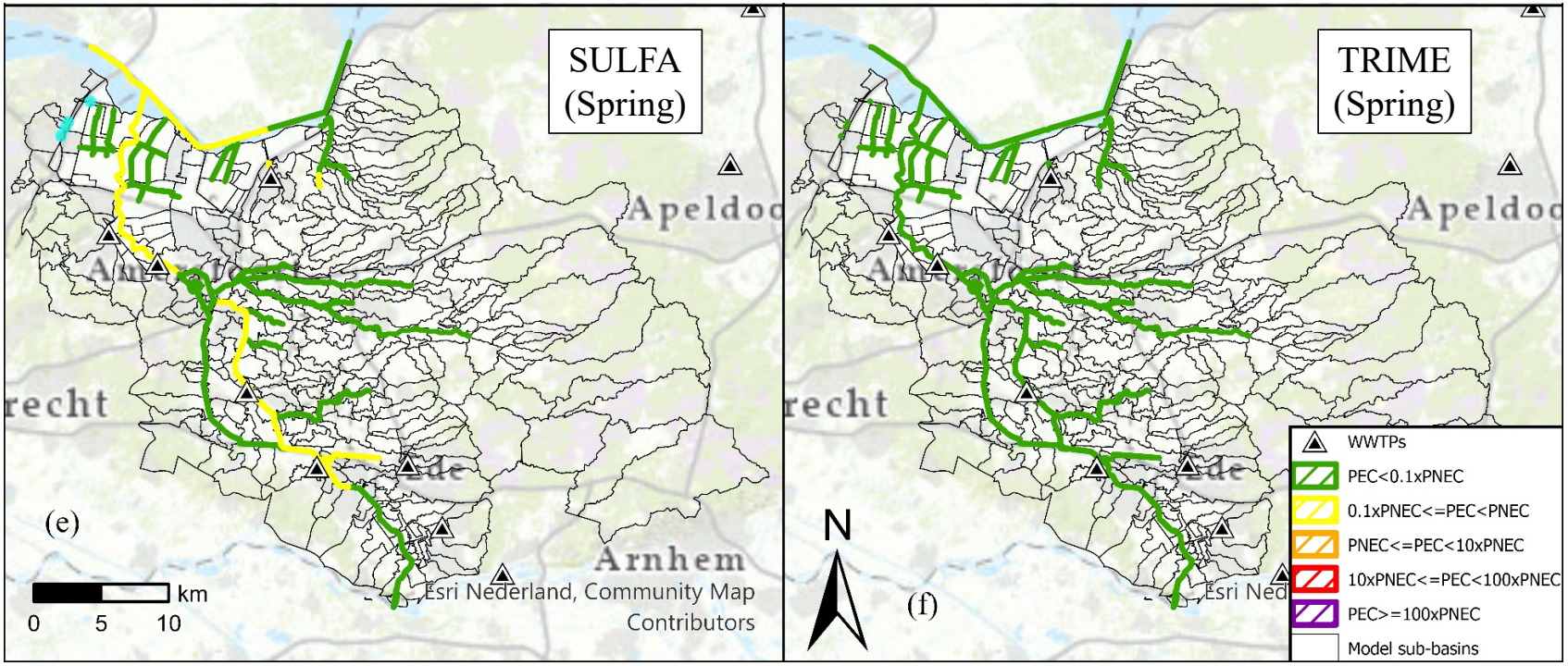
Results



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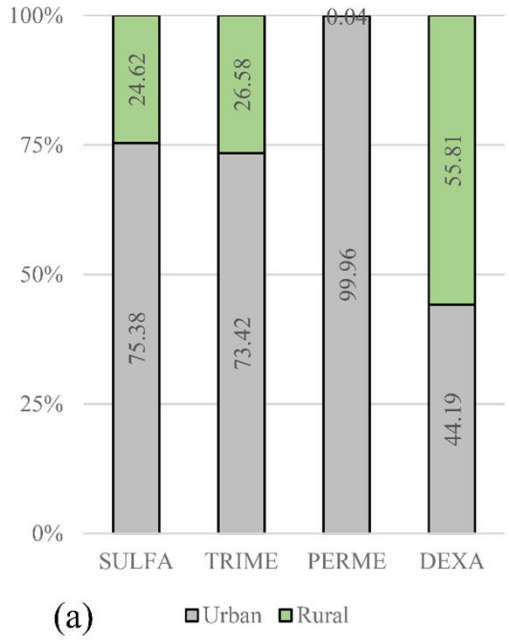
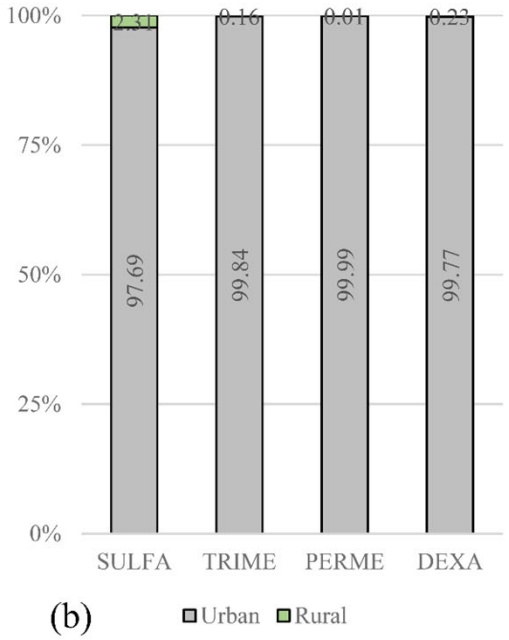
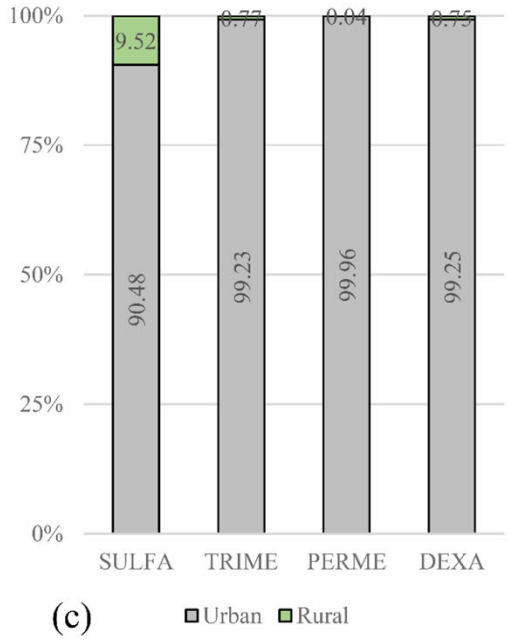
Contribution of sources to river contamination in the Eem Catchment



% of total loads to sewage (urban) or crops (rural)

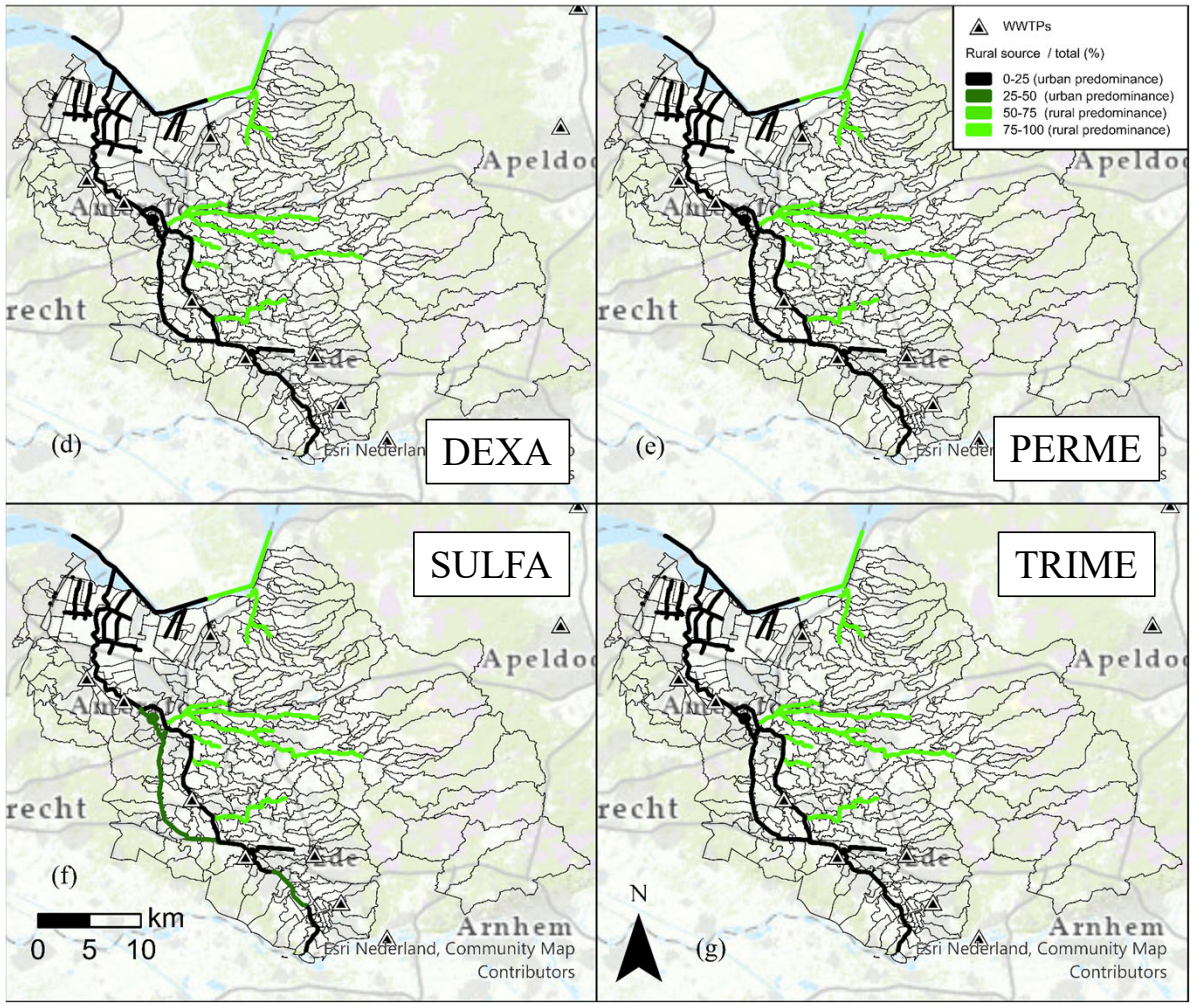


% of total loads to rivers (effluents)



% of total loads at Eem River outlet

Contribution of sources to river contamination



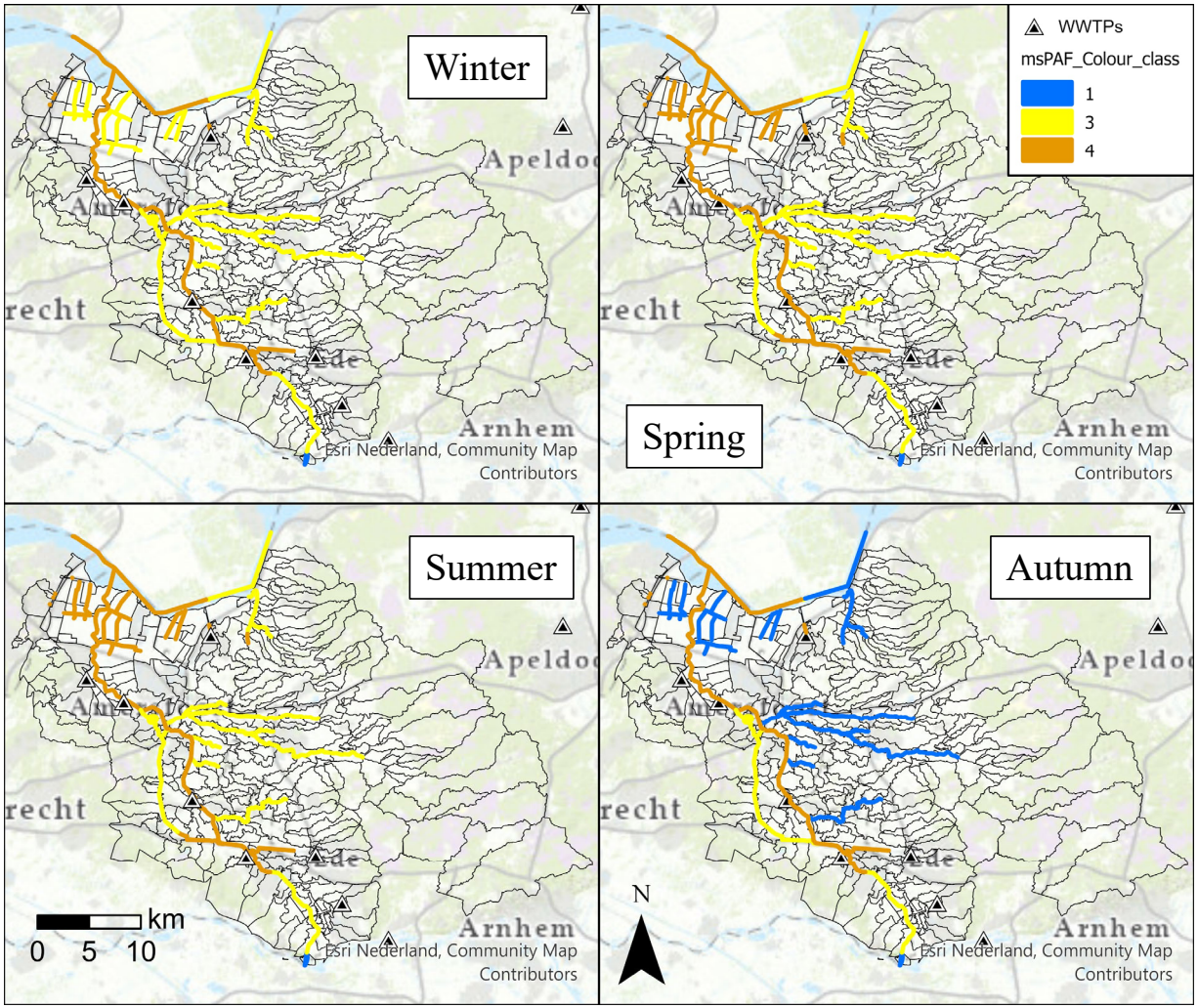
Take home messages

- We showed that our **modelling approach** can **predict** well the **concentration** of **pharmaceuticals** in **space** and **time** (seasons) in surface waters of basins with **mixed rural-urban land uses**.
- In Eem catchment, the results show that predicted concentration **exceeded water quality standards** for some compounds , location and season.
- **Spring** and **Summer** are the most polluted seasons due to higher combined rural-urban input (Spring) and lower dilution in rivers (Summer).
- In the study area, **urban sources contribute notably more** than rural sources to **pharmaceuticals loads** to rivers.
- Our modelling approach can be used to **explore** the **effects of mitigation strategies** or **interventions**.

Outlook - 1

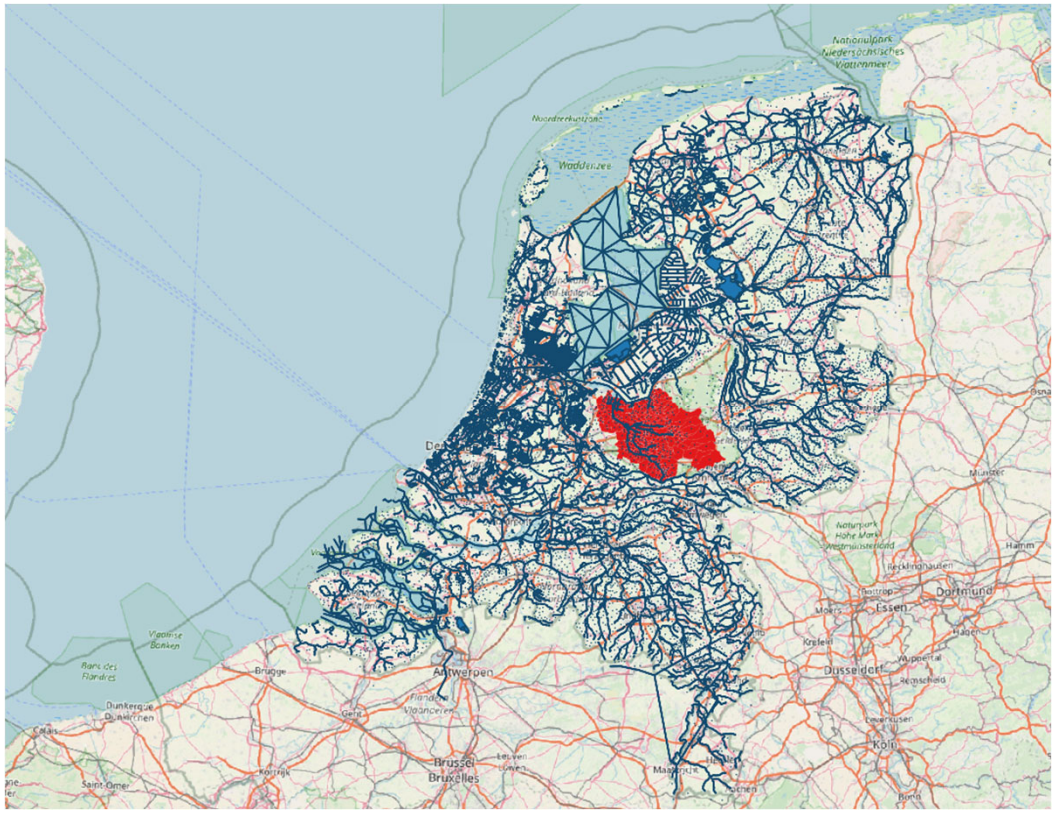
- Run the model for many pharmaceuticals and **assess the risk** due to **mixtures of pollutants**

(example with the 6 compounds)



Outlook - 2

- **Extend** this methodology to the **whole Netherlands** and potentially to other areas.



SUSPECt – onderdeel van:

stowa

KWR Watercycle Research Institute

TOPSECTOR WATER

STW Partnership

connecting innovators

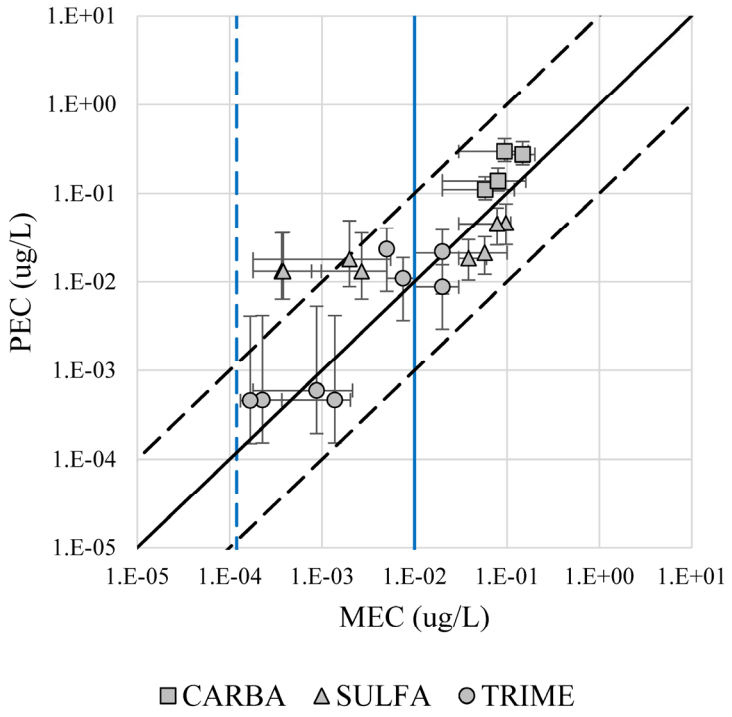
Modelling input and scenarios

Compound	Type	Emission source	n. meas.
Carbamazepine	Anti-epilectic	Urb.	19
Fipronil	Pesticide	Urb.	47
Trimethoprim	Antibiotic	Urb.+Rur.	18
Sulfamethoxazole	Antibiotic	Urb.+Rur.	27
Permethrin	Insecticide	Urb.+Rur.	146
Dexamethasone	Hormon	Urb.+Rur.	16

Emission scenario	Urban source WWTP removal efficiency (specific per WWTP and compound)	Rural source K_{oc} (specific per compound)	Notes
HIGH	Minimum	minimum	Worst case scenario
AVERAGE	average	average	Average case scenario
LOW	maximum	maximum	Best case scenario

Validation

Carbamazepine, Trimethoprim, Sulfamethoxazole



Permethrin, Dexamethasone, Fipronil

below limit of detection

Matrix model (Fawcett, 2006)

		PEC	
		Detected	Not detected
MEC	Detected	True positive	False negative
	Not detected	False positive	True negative

$$\text{Success rate} = \frac{TP + TN}{TP + FP + TN + FN}$$

	Success rate (n)
DEXA	**1** (16)
PERME	**0.99** (146)
FIPRO	**0.91** (47)

Fawcett T (2006), https://doi.org/10.1016/j.patrec.2005.10.010

Environmental quality standard (EQS)

Compound	EQS (µg L^{-1})	Source
Carbamazepine	2.50 10^{0}	AA-QS fw (chronic), (European Commission, 2023)
Dexamethasone	1.00 10^{-3}	PNEC (chronic), (Musee et al., 2021)
Fipronil	7.00 10^{-5}	PNEC (chronic), (Moermond et al., 2020)
Permethrin	2.70 10^{-4}	AA-QS fw (chronic), (European Commission, 2023)
Sulfamethoxazole	1.18 10^{-1}	PNEC (chronic), (Moermond et al., 2020)
Trimethoprim	1.60 10^{1}	PNEC (chronic), (Moermond et al., 2020)