


TAKING
COOPERATION
FORWARD

 online

 *Implementation of modePROCON showcasing for surface water - Brynica River Basin, Poland*

 boDEREC-CE | Chair of Hydrology and River Basin Management

OUTLINE

1

Study area

2

Detected
PPCPs

3

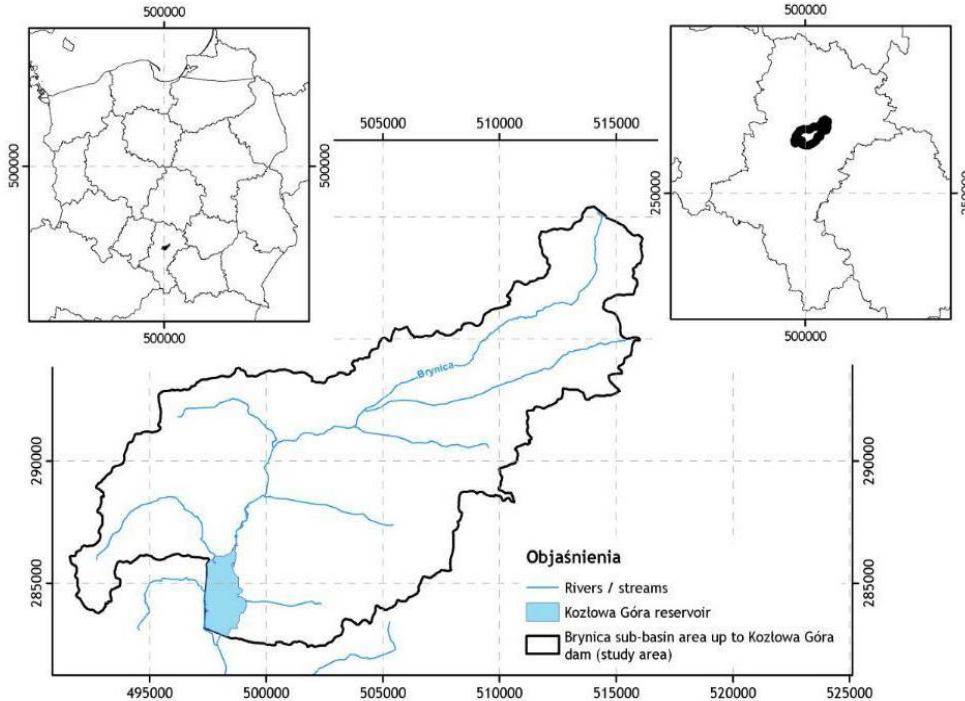
Applying
modePROCON

4

Model results



STUDY AREA

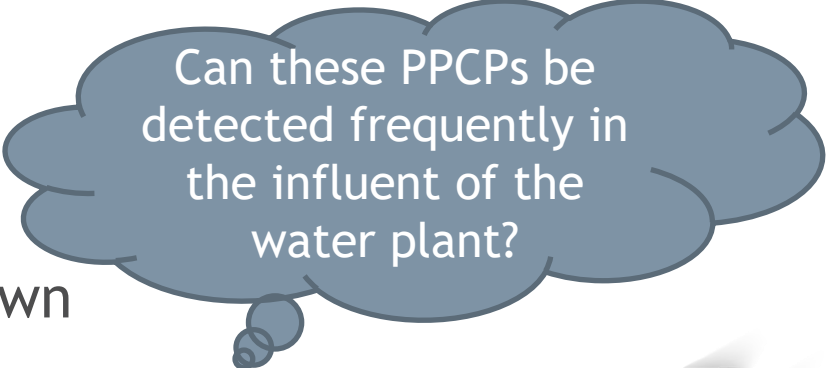


- Investigated drinking water work: Kozłowa Góra
- Brynica river catchment area ~ 193 km²
- Rural area covered by woodland and agriculture
- WWTP discharging in the river



DETECTED PPCPs

- The following PPCPs were detected in the feeding river of the Kozłowa water reservoir:
 - Acesulfame
 - Carbamazepine
 - DEET
 - Oxypurinol
 - PFOS
- Some of the PPCPs were also analyzed in a few samples withdrawn at the inflow of the water work.



Can these PPCPs be detected frequently in the influent of the water plant?



APPLYING modePROCON

Selecting the water source

PPCP

— □ ×



Groundwater System

Evaluation

Model requirements

Karst Aquifer System

Evaluation

Model requirements

Surface Water System

Evaluation

Model requirements



APPLYING modePROCON

Selecting the PPCPs

PPCP

PPCP Data

Units:

- Solubility: mg/L
- Sorbability (logKow): Unitless
- Volatility (Henry's constant): at
- Degradability (DT50): Day
- pKa: Unitless

Data-Reference:

- [1]: SciFinder
- [2]: CompTox US EPA

	Name	CAS	Solubility	Sorbability	pKa	Volatility	Degradability	
79	<input checked="" type="checkbox"/> Oxypurinol	2465-59-0	240.0	-1.05	10.67	1.85e-09	3.53	Si
80	<input type="checkbox"/> Paracetamol	103-90-2	15000.0	0.48	9.86	5.74e-09	3.55	Si
81	<input type="checkbox"/> Paraxanthine	611-59-6	8300.0	-0.94	8.5	2.68e-09	4.63	Si
82	<input type="checkbox"/> Penicillin G	113-98-4	284000.0	0.02	nan	1.49e-11	13.4	Si
83	<input type="checkbox"/> PFOA	335-67-1	13000.0	6.44	0.5	1.92e-10	4.94	Si
84	<input checked="" type="checkbox"/> PFOS	1763-23-1	7500.0	4.51	-3.27	1.8e-11	4.92	Si
85	<input type="checkbox"/> Venazone	60-80-0	15000.0	0.44	0.65	2.65e-06	3.36	Si
86	<input type="checkbox"/> Primidone	125-33-7	1500.0	0.83	12.26	4.26e-10	3.34	Si
87	<input type="checkbox"/> Progesterone	57-82-8	0.1	0.02	12.0	1.2e-09	0.75	Si

Back Delete all user input Add new data Evaluate

The detected PPCPs PFOS, DEET, carbamazepine, acesulfame and oxypurinol are contained in the database and can be selected simultaneously.



APPLYING modePROCON

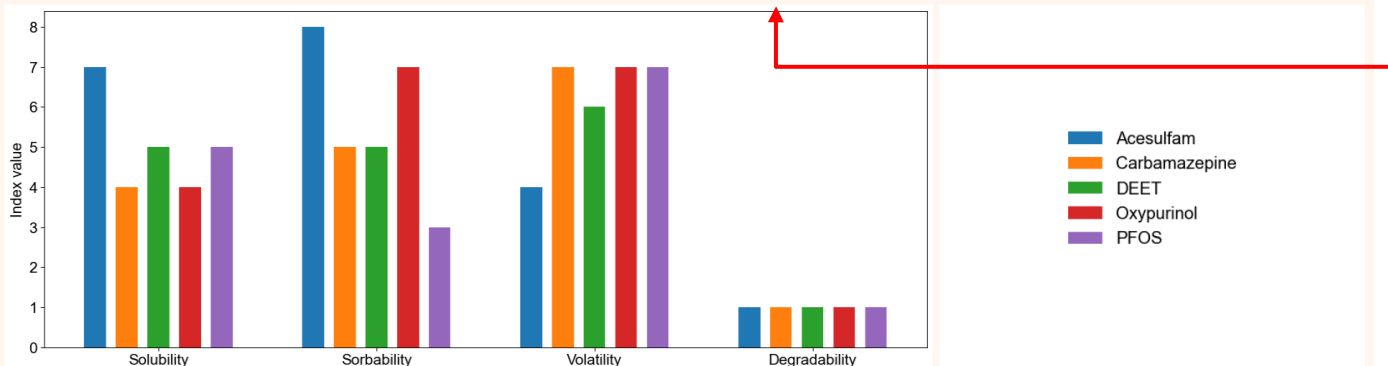
Probability Estimation

PPCP

Indexes and Result

Modelling is recommended when likelihood is 'Very Likely' or 'Likely'

Name	Solubility	Sorbability	Volatility	Degradability	Likelihood	Literature
1 Acesulfam	7	8	4	1	Very likely	https://doi.org/10.1016/j.scitotenv.
2 Carbamazepine	4	5	7	1	Likely	https://doi.org/10.1016/j.scitotenv.
3 DEET	5	5	6	1	Likely	https://doi.org/10.1016/j.watres.20
4 Oxypurinol	4	7	7	1	Likely	https://doi.org/10.1016/j.watres.20
5 PFOS	5	3	7	1	Likely	https://doi.org/10.1016/j.watres.20



Back

Go to model requirements

- Although the degradability of all PPCPs is in the same range, different likelihoods can be obtained.



APPLYING modePROCON

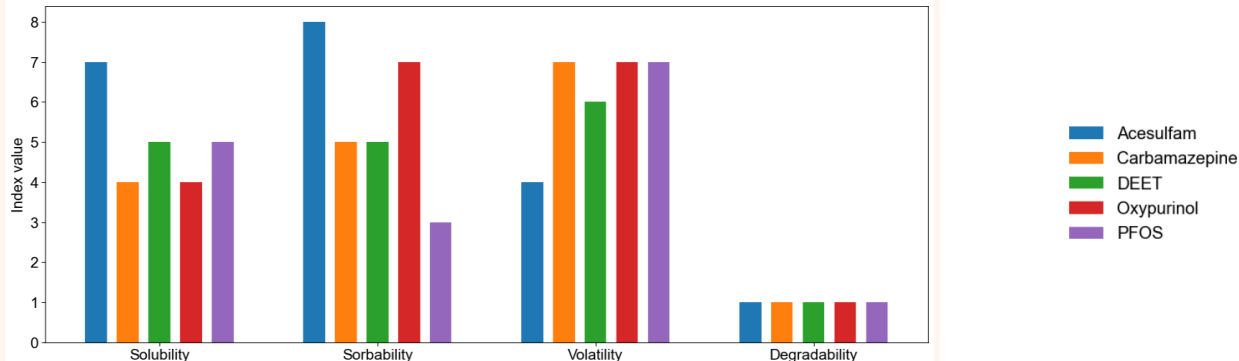
Probability Estimation

PPCP

Indexes and Result

Modelling is recommended when likelihood is 'Very Likely' or 'Likely'

Name	Solubility	Sorbability	Volatility	Degradability	Likelihood	Literature
1 Acesulfam	7	8	4	1	Very likely	https://doi.org/10.1016/j.scitotenv.
2 Carbamazepine	4	5	7	1	Likely	https://doi.org/10.1016/j.scitotenv.
3 DEET	5	5	6	1	Likely	https://doi.org/10.1016/j.watres.20
4 Oxypurinol	4	7	7	1	Likely	https://doi.org/10.1016/j.watres.20
5 PFOS	5	3	7	1	Likely	https://doi.org/10.1016/j.watres.20



Back

Go to model requirements

Acesulfame is very likely to be detected, as it is very soluble in water and does only little adsorb to organic matter.



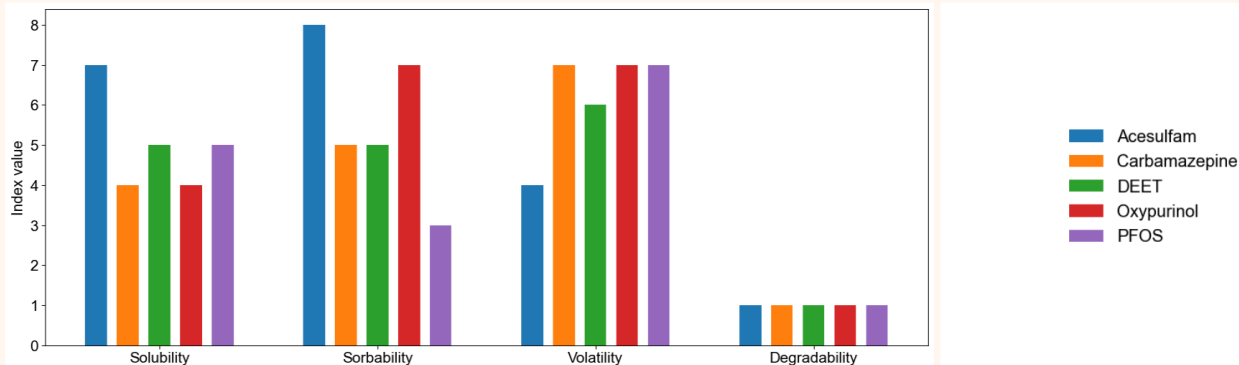
APPLYING modePROCON Probability Estimation

PPCP

Indexes and Result

Modelling is recommended when likelihood is 'Very Likely' or 'Likely'

Name	Solubility	Sorbability	Volatility	Degradability	Likelihood	Literature
1 Acesulfam	7	8	4	1	Very likely	https://doi.org/10.1016/j.scitotenv.
2 Carbamazepine	4	5	7	1	Likely	https://doi.org/10.1016/j.scitotenv.
3 DEET	5	5	6	1	Likely	https://doi.org/10.1016/j.watres.20
4 Oxypurinol	4	7	7	1	Likely	https://doi.org/10.1016/j.watres.20
5 PFOS	5	3	7	1	Likely	https://doi.org/10.1016/j.watres.20



Back

Go to model requirements

Carbamazepine, DEET, oxypurinol and PFOS are likely to be detected in the water, due to a lower solubility and a higher sorbability compared to acesulfame.



APPLYING modePROCON

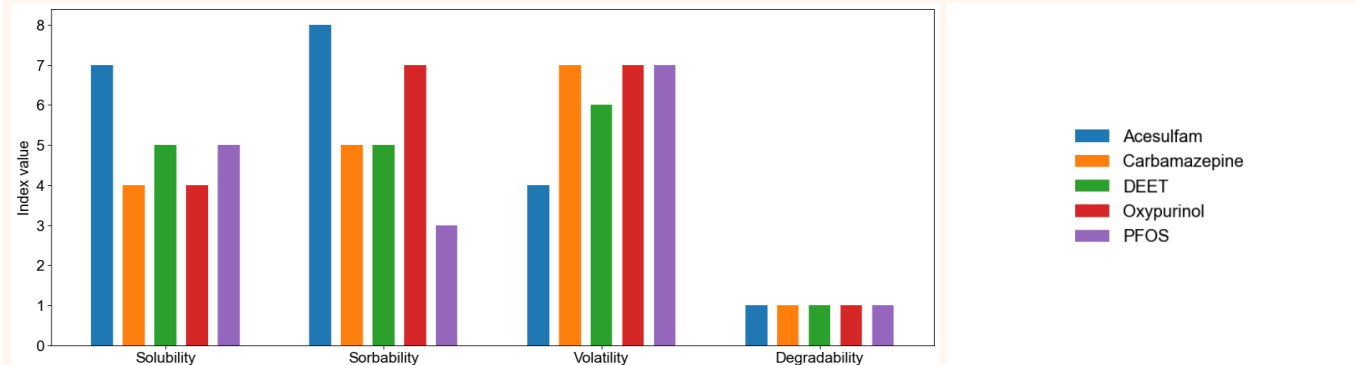
Probability Estimation

PPCP

Indexes and Result

Modelling is recommended when likelihood is **'Very Likely'** or **'Likely'**

Name	Solubility	Sorbability	Volatility	Degradability	Likelihood	Literature
1 Acesulfam	7	8	4	1	Very likely	https://doi.org/10.1016/j.scitotenv.
2 Carbamazepine	4	5	7	1	Likely	https://doi.org/10.1016/j.scitotenv.
3 DEET	5	5	6	1	Likely	https://doi.org/10.1016/j.watres.20
4 Oxypurinol	4	7	7	1	Likely	https://doi.org/10.1016/j.watres.20
5 PFOS	5	3	7	1	Likely	https://doi.org/10.1016/j.watres.20



Back

Go to model requirements

As the investigated PPCPs are very likely or likely to be detected in water, modePROCON recommends to develop a model for further investigation.



APPLYING modePROCON

Model requirements

PPCP

Surface water model requirements

[Evaluate](#)

Please check the available parameter to evaluate

	Parameter	Application	Remark
5	<input type="checkbox"/> Source of contamination	water. It is needed to set initial conditions for the transport model and define the contaminant source and releases.	
6	<input type="checkbox"/> Initial concentration of the contaminant	It is needed to set up initial conditions to solve the transport equation and estimate the potential magnitude and impact of the contamination.	
7	<input checked="" type="checkbox"/> Point of interest	Physical locations that are likely to be exposure pathway to come into contact with a contaminated medium.	

[Back](#)

- All the required model parameters are known in this case, **except of the source's location and the initial concentration.**
- modePROCON evaluates the data...



APPLYING modePROCON

Model requirements

PPCP

Surface water model requirements

Evaluate

Model cannot be built. Please collect the missing data.

Please check the available parameter to evaluate

Parameter	Application	Remark
Source of contamination	It is needed to set initial conditions for the transport model and define the contaminant source and releases.	It can be estimated by analysing seepage water collected in a collection bag of a seepage meter, or with a network of monitoring wells. Another alternative is to solve inverse problems of unknown contaminant source (e.g., particle backtracking). Potential sources of contamination are: infiltration of contaminated surface water, leaking sewers, landfills, septic systems, livestock breeding and agriculture. Intensive

Back

- ... and replies that a model cannot be built with the available data. modePROCON suggests a possibility to obtain the missing data in the remark column.



APPLYING modePROCON

Model requirements

PPCP

Surface water model requirements

Evaluate

Model cannot be built. Please collect the missing data.

Please check the available parameter to evaluate

Parameter	Application	Remark
Source of contamination	It is needed to set initial conditions for the transport model and define the contaminant source and releases.	It can be estimated by analysing seepage water collected in a collection bag of a seepage meter, or with a network of monitoring wells. Another alternative is to solve inverse problems of unknown contaminant source (e.g., particle backtracking). Potential sources of contamination are: infiltration of contaminated surface water, leaking sewers, landfills, septic systems, livestock breeding and agriculture. Intensive

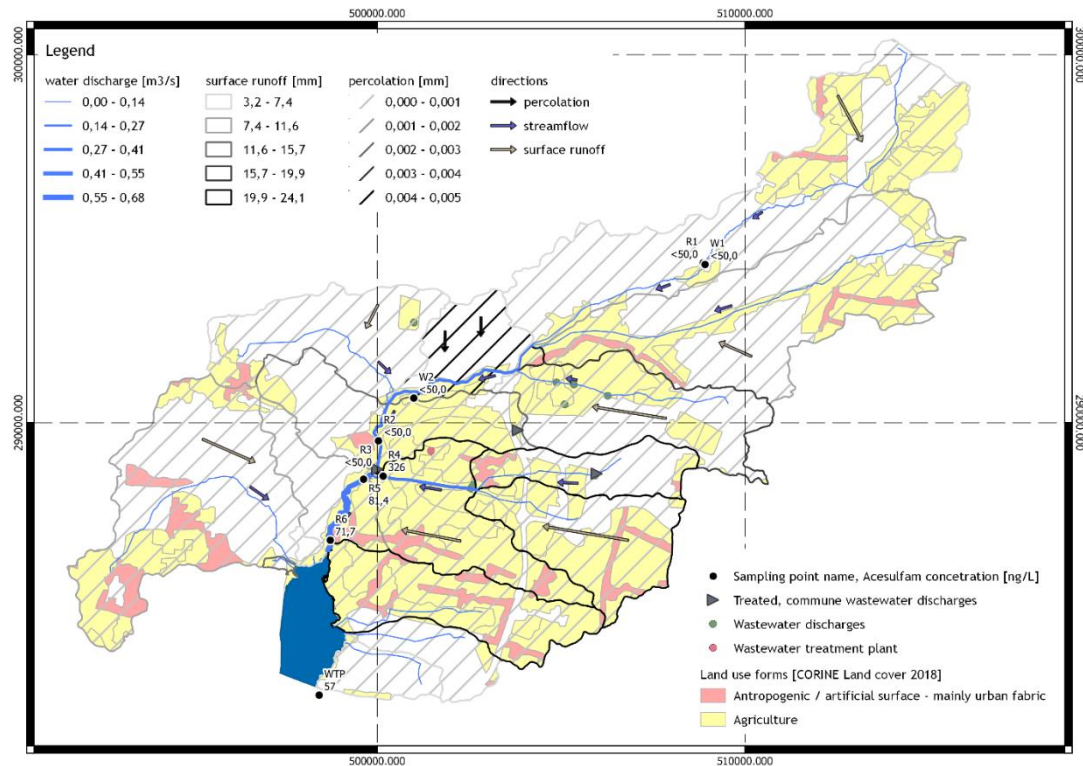
5

Back

- In this case, several potential sources were investigated.
- For this, locations of potential sources were identified, and concentration ranges were estimated.
- The assumptions were studied in a conceptual model.



MODEL RESULTS



• A conceptual transport model (shown here for acesulfame) can investigate potential sources:

- Agricultural run-off
- Wastewater discharges
- Unregistered discharges

