


TAKING
COOPERATION
FORWARD

 online

 *Implementation of modePROCON showcasing for surface water - Dresden-Hosterwitz, Germany*

 boDEREC-CE | Chair of Hydrology and River Basin Management

OUTLINE

1

Study area

2

Detected
PPCPs

3

Applying
modePROCON

4

Model results



STUDY AREA



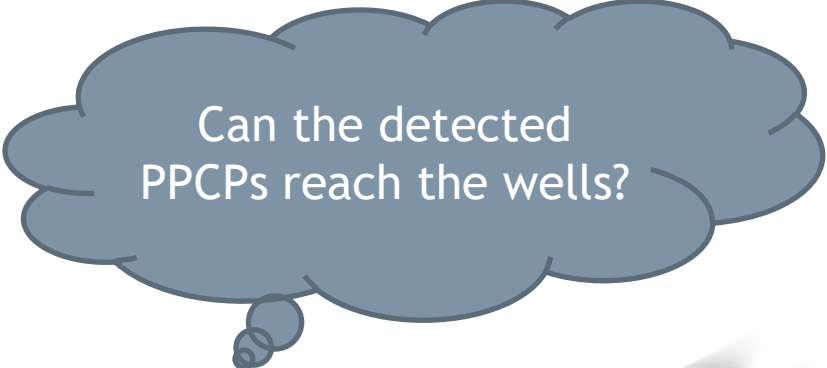
Location of sampling points at Niederpoyritz and Hosterwitz

- Investigated abstraction well for drinking water supply
- A site of riverbank filtration: Dresden-Hosterwitz and -Niederpoyritz
- Riverbank filtration is considered as a showcase of surface water use, but in fact a groundwater water model is applied for the investigation.



DETECTED PPCPs

- The following PPCPs were detected and selected to be modeled in the Dresden-Hosterwitz pilot area are:
 - 4-Formylaminoantipyrine
 - Benzotriazole
 - 5-methyl-1-H-benzotriazole
 - Carbamazepine
 - Lamotrigine
 - Oxypurinol



Can the detected PPCPs reach the wells?



APPLYING modePROCON

Selecting the water source

PPCP

Interreg 
CENTRAL EUROPE European Union
European Regional
Development Fund
boDEREC-CE

Groundwater System	Karst Aquifer System	Surface Water System
Evaluation	Evaluation	Evaluation
Model requirements	Model requirements	Model requirements



APPLYING modePROCON

Selecting the PPCPs

PPCP

PPCP Data

Units:

- Solubility: mg/L
- Sorbability (logKow): Unitless
- Volatility (Henry's constant): atm*m³/mol
- Degradability (DT50): Day
- pKa: Unitless

Data-Reference:

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

	Name	CAS	Solubility	Sorbability	pKa	Volatility	Degradability	Re
1	<input type="checkbox"/> 17a-ethynilestradiol	57-63-6	3.9	4.11	10.24	9.44e-08	97.8	Solubility and
2	<input type="checkbox"/> 17-alpha-estradiol	57-91-0	3.0	4.15	10.27	3.75e-06	97.2	Solubility and
3	<input type="checkbox"/> 17-beta-estradiol	50-28-2	3.0	4.15	10.27	3.75e-06	97.2	Solubility and
4	<input checked="" type="checkbox"/> 4-formylaminoantipyrine	1672-58-8	14000.0	-0.06	12.72	6.98e-09	5.15	Solubility and
5	<input type="checkbox"/> Acetubutolol	37517-30-9	340000.0	1.77	13.78	8.73e-10	3.35	Solubility and
6	<input type="checkbox"/> Acesulfam	33665-90-6	1000000.0	-0.88	-0.28	6.27e-05	4.29	Solubility and
7	<input type="checkbox"/> Alfuzosin	81403-80-7	4300.0	1.27	14.8	2.59e-11	4.29	Solubility and

Buttons: Back, Delete all user input, Add new data, Evaluate

- All the 6 detected and selected to be modelled PPCPs are contained in the database
- But only 5 can be selected simultaneously in modePROCON.



APPLYING modePROCON

Selecting the PPCPs

PPCP

PPCP Data

Units:

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Buttons: Back, Delete all user input, Add new data, Evaluate

- In this showcase, we focus on 5 depending on their importance for the stakeholders and the others can be analysed successively.



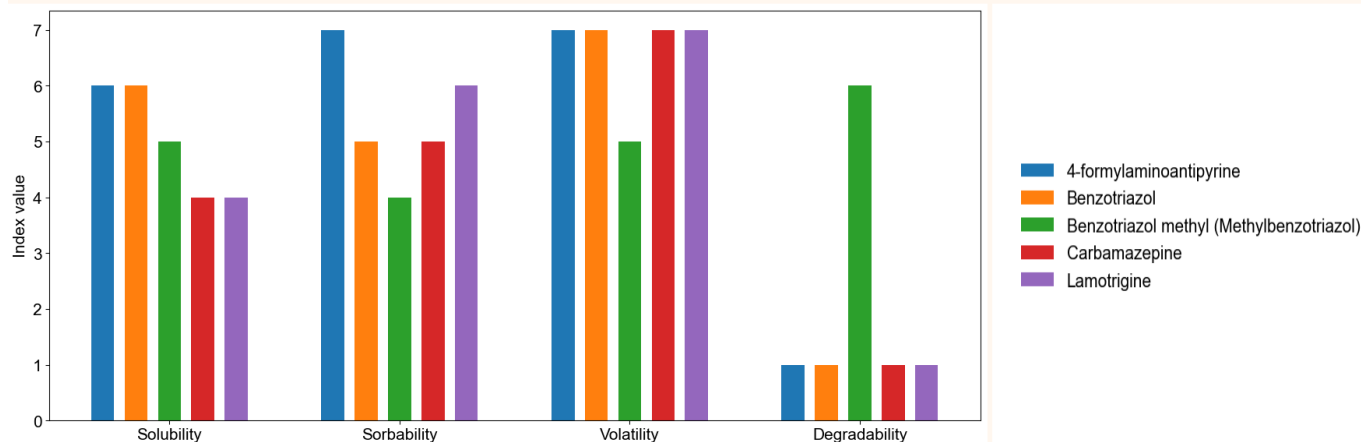
APPLYING modePROCON

Probability Estimation

PPCP

Indexes and Result Modelling is recommended when likelihood is 'Very Likely' or 'Likely'

Name	Solubility	Sorbability	Volatility	Degradability	Likelihood	Literature
1 4-formylaminoantipyrine	6	7	7	1	Very likely	https://doi.org/10.1016/j.watres.2020.115523
2 Benzotriazol	6	5	7	1	Likely	https://doi.org/10.1016/j.watres.2020.115523
3 Benzotriazol methyl (Methylbenzotriazol)	5	4	5	6	Very likely	https://doi.org/10.1016/j.scitotenv.2012.04.059
4 Carbamazepine	4	5	7	1	Likely	https://doi.org/10.1016/j.scitotenv.2012.04.059
5 Lamotrigine	4	6	7	1	Likely	https://doi.org/10.1016/j.envpol.2020.115387



Although the degradability of most PPCPs is very high, 5-methyl-1-H-benzotriazole has a very low degradability.

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Go to model requirements



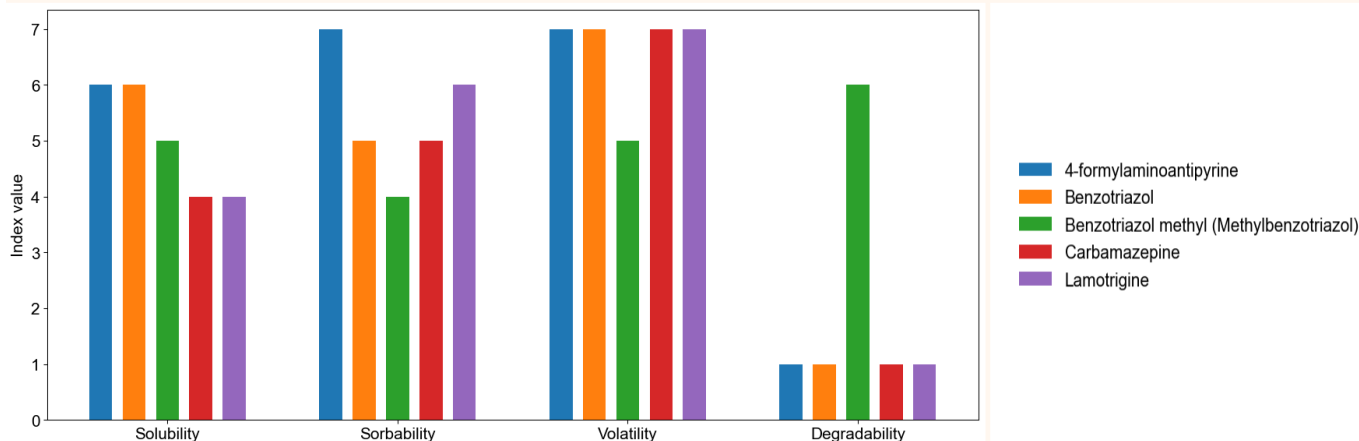
APPLYING modePROCON

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4-
Formylaminoantipyrine and 5-methyl-1-H-benzotriazole are very likely to be detected.



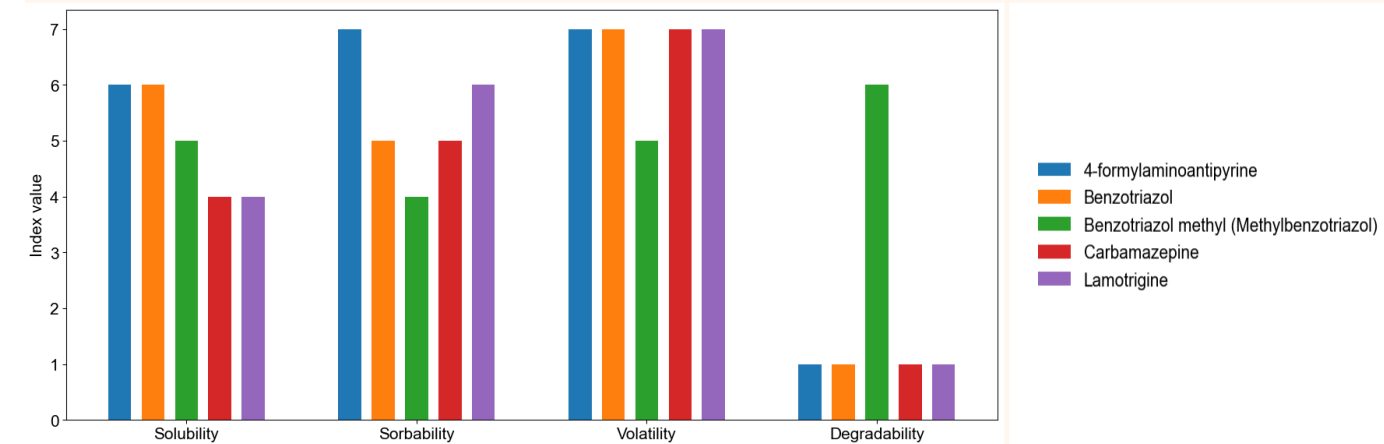
APPLYING modePROCON

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- Benzotriazole, Carbamazepine, and Lamotrigine are likely to be detected in the water, due to the higher solubility.

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APPLYING modePROCON

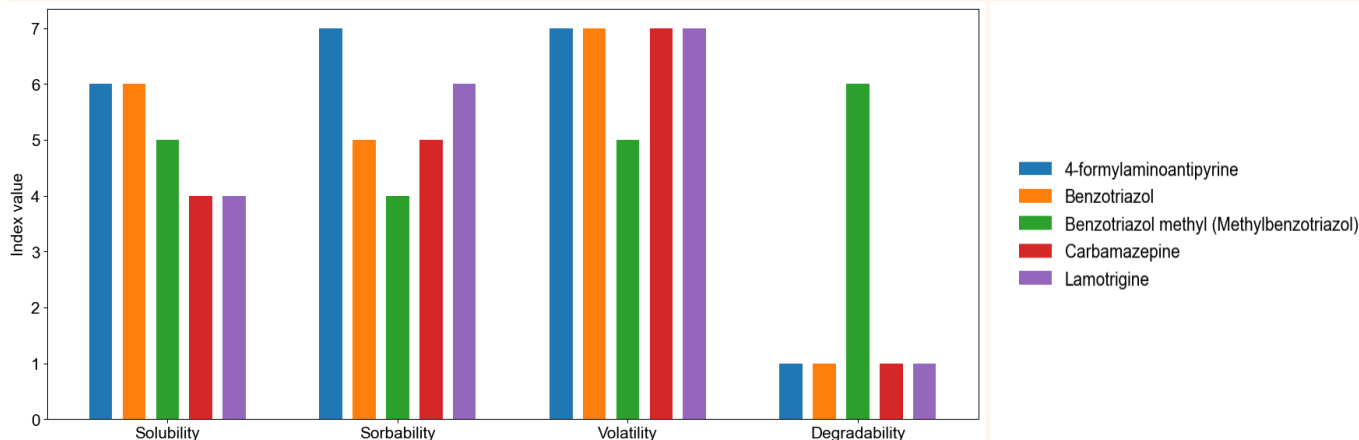
Probability Estimation

PPCP

Indexes and Result

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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

Groundwater model requirements

[Evaluate](#)

Please check the available parameter to evaluate

	Parameter	Application	Remark
1	<input checked="" type="checkbox"/> Water level	It is necessary to determine the flow direction, boundary conditions, response to stress and hydraulic properties.	
2	<input checked="" type="checkbox"/> Hydraulic conductivity	It is used to describe groundwater flow in the porous medium. The hydraulic conductivity depends on fluid properties (e.g. density, dynamic viscosity) and medium properties (e.g. grain size and shapes, pore distribution and shape, porosity).	
3	<input checked="" type="checkbox"/> Thickness of the aquifer	It is needed to estimate the transmissivity of the aquifer.	
4	<input checked="" type="checkbox"/> Flow exchange with surface water	It is important to better understand the relation between surface water and groundwater (i.e., losing/gaining conditions). It can lead to dilution, mixing, and transference of PPCPs into the groundwater.	
5	<input type="checkbox"/> Source of contamination	It is needed to set initial conditions for the transport model and define the contaminant source and releases.	
6	<input checked="" 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	

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- All the required model parameters are known in this case, **except of the source of contamination.**
- modePROCON evaluates the data...



APPLYING modePROCON

Model requirements

PPCP

Groundwater model requirements Evaluate

Model cannot be built. Please collect the missing data.

Please check the available parameter to evaluate

	Parameter	Application	Remark
3	<input checked="" type="checkbox"/> Thickness of the aquifer	It is needed to estimate the transmissivity of the aquifer.	The data are available.
4	<input checked="" type="checkbox"/> Flow exchange with surface water	It is important to better understand the relation between surface water and groundwater (i.e., losing/gaining conditions). It can lead to dilution, mixing, and transference of PPCPs into the groundwater.	The data are available.
5	<input type="checkbox"/> 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 research in the study area is recommended.
5	<input checked="" 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	The data are available.

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COUPON can't be adjusted to 1m*1m*1m. Also, difficulties to adapt height data of the Digital Evaluation Model were

- ... 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

It is possible to develop a numerical model. Please communicate with any university or consultant.

Please check the available parameter to evaluate

	Parameter	Application	
4	<input checked="" type="checkbox"/>	water and groundwater (i.e., losing/gaining conditions). It can lead to dilution, mixing and transference of PPCPs into the surface water.	
5	<input checked="" type="checkbox"/>	Source of contamination	It is needed to set initial conditions for the transport model and define the contaminant source and releases. The data are available.
6	<input checked="" 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. The data are available.
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. The data are available.

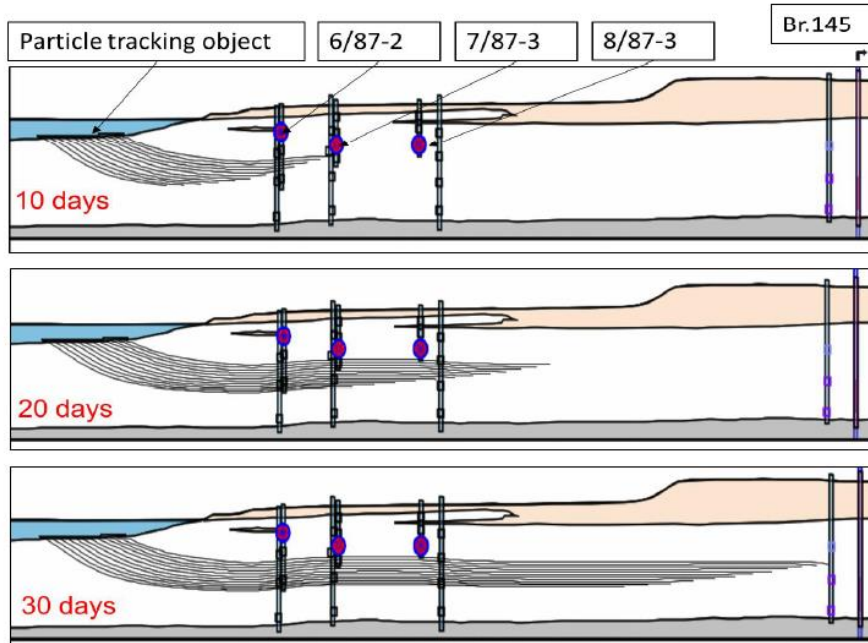
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- In this case, two scenarios were investigated.
- The first scenario simulates the breakthrough curve of 1-day spill of oxypurinol with a concentration of 500 ng/l in the Elbe River on the first day of simulation time. The concentration of 500 ng/l refers from **median value of 526 ng/l from 7 sampling campaigns**.
- The second scenario simulates the change in concentration arriving at OW 9/87-3 next to the abstraction well Br.145. It corresponds to **different spill times of input source** in the Elbe River water.

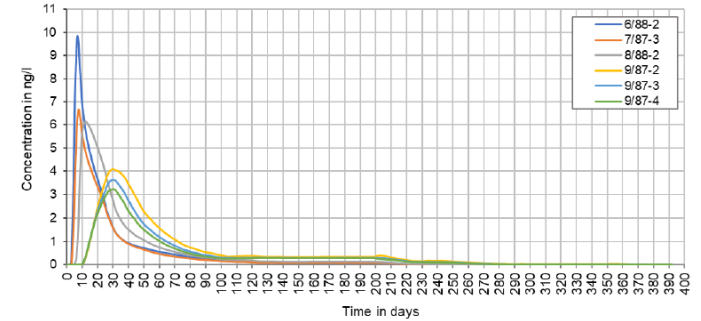


MODEL RESULTS

Travel time and flow paths of particles moving from the river to the abstraction well



Scenario 1: Breakthrough curve after a 500 ng/l oxyprynol input conc. in Elbe River water due to a 1-day spill.



Scenario 2: Change in concentration at OW 9/87-3 after different spill durations in Elbe River water

