

TAKING
COOPERATION
FORWARD

 online

 *Implementation of modePROCON showcasing for groundwater -Káraný, Czechia, Czech Republic*

 boDEREC-CE | Chair of Hydrology and River Basin Management

OUTLINE

1

Study area

2

Detected
PPCPs

3

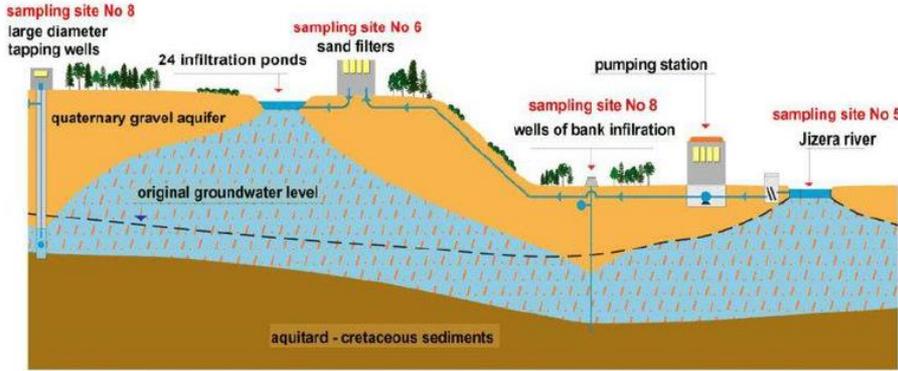
Applying
modePROCON

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Model results



STUDY AREA



Groundplan of the aquifer with representative cross-sections

- Investigated aquifer: Káraný waterworks aquifer (Czech Republic)
- Catchment area: 894 hectares
- It supplies drinking water to about one-third of Prague and its surroundings.
- The groundwater is recharged through nearby river Jizera and artificial infiltration reservoirs.



DETECTED PPCPs

- The following Emerging Contaminants (ECs) were detected in the nearby river and in the groundwater:
 - Lamotrigin
 - Karbamazepin (CBZ)
 - Acesulfam
 - Sulfamethoxazol, Sulfamerazin a Sulfamethazin
 - Oxypurinol metabolite of Alopurinolu

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
99	<input checked="" type="checkbox"/> Sulfamerazine	127-79-7	950.0	0.11	7.35	7.38e-11	3.36	Solubility and
100	<input checked="" type="checkbox"/> Sulfamethazin	57-68-1	420.0	0.3	7.89	7.19e-11	3.36	Solubility and
101	<input checked="" type="checkbox"/> Sulfamethoxazol	723-46-6	2800.0	0.66	5.81	1.72e-10	3.35	Solubility and
102	<input type="checkbox"/> Sulfanilamide	63-74-1	11000.0	-0.67	10.1	8.16e-11	3.87	Solubility and
103	<input type="checkbox"/> Sulfapyridin	144-83-2	850.0	0.47	8.54	3.95e-11	3.36	Solubility and
104	<input type="checkbox"/> Telmisartan	144701-48-4	13.0	6.48	3.86	2.16e-08	37.0	Solubility and
105	<input type="checkbox"/> Testosterone	58-22-0	20.0	3.18	15.06	7.05e-08	97.4	Solubility and

Back Delete all user input Add new data Evaluate

All the 7 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:

- Solubility: mg/L
- Sorbability (logKow): Unitless
- Volatility (Henry's constant): atm*m³/mol
- Degradability (DT50): Day
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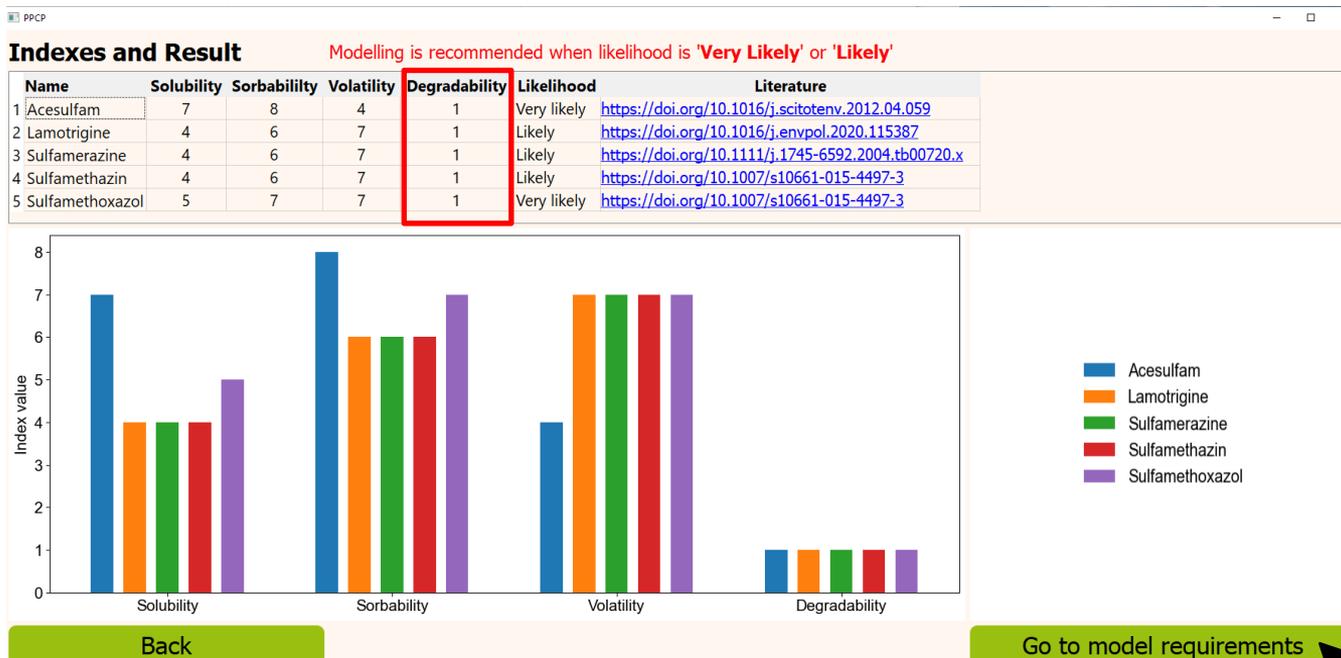
Back Delete all user input Add new data Evaluate

- 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



- All the investigated compounds are easily biodegradable.



APPLYING modePROCON

Probability Estimation

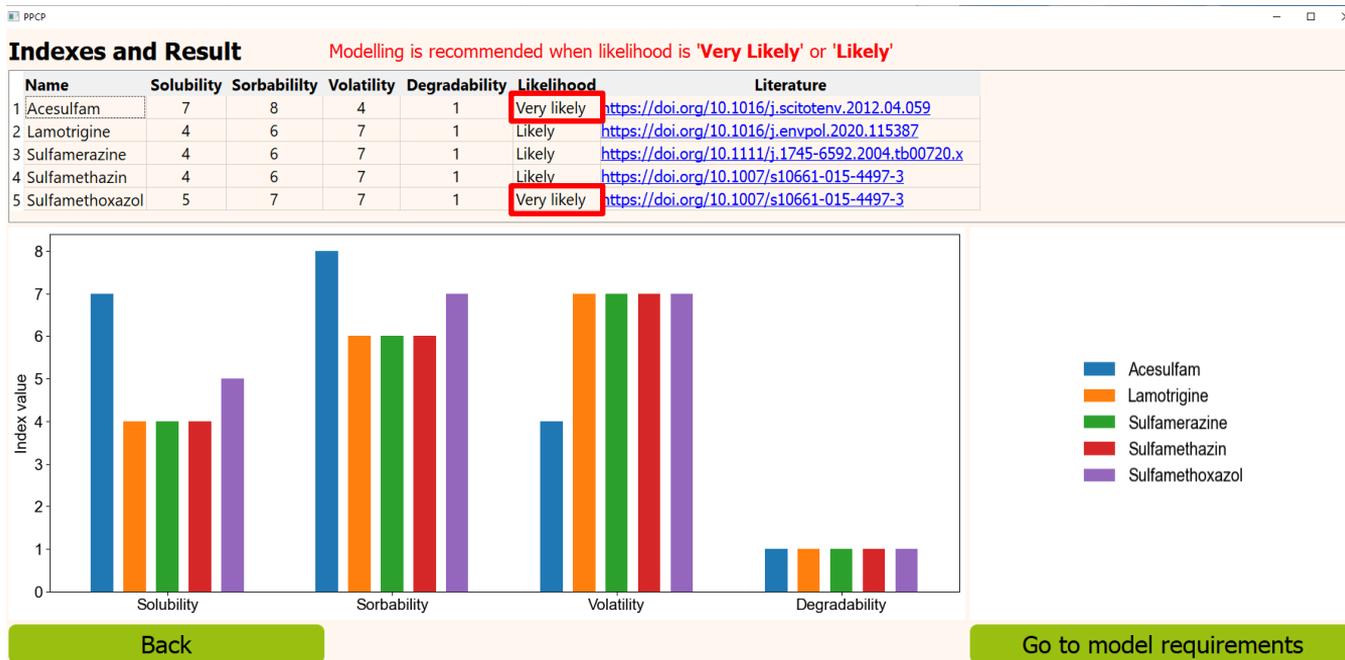


- Due to the high index values, the detection probabilities of **Lamotrigine, Sulfamerazine and Sulfamethazin** are likely.
- This is related to the high solubility.



APPLYING modePROCON

Probability Estimation



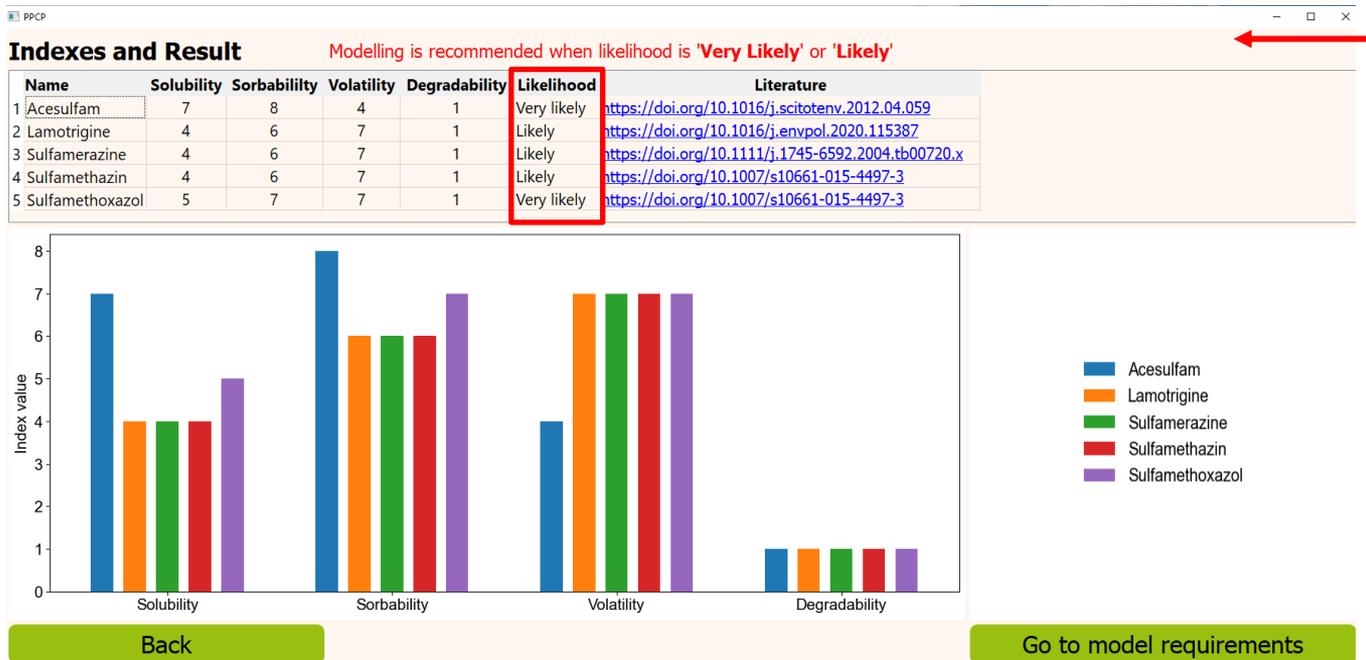
- The detection probabilities of Acesulfam and sulfamethoxazole are very likely.

- For acesulfame, it is related to the low volatility combined with a high solubility.
- For Sulfamethoxazol, it is mainly related to the high solubility.



APPLYING modePROCON

Probability Estimation



As all considered PPCPs are **very likely** or **likely** to be detected in the groundwaters, modePROCON recommends to **model** the situation for further investigation.



APPLYING modePROCON

Model requirements

PPCP

Groundwater model requirements

Evaluate

Please check the available parameter to evaluate

Parameter	Application	Remark
<input checked="" type="checkbox"/>	dynamic viscosity) and medium properties (e.g. grain size and shapes, pore distribution and shape, porosity).	
<input checked="" type="checkbox"/>	Thickness of the aquifer	It is needed to estimate the transmissivity of the aquifer.
<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.
<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.
<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.
<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 initial contamination of the contaminant.**
- 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 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 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.	It can be estimated by collecting groundwater samples from monitoring wells or piezometers. The monitoring wells should be closely spaced along transects across the contaminant plume, and a dense grid of monitoring wells is suggested to have detailed information on the spatial distribution of the contaminant.
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.

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

Groundwater 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

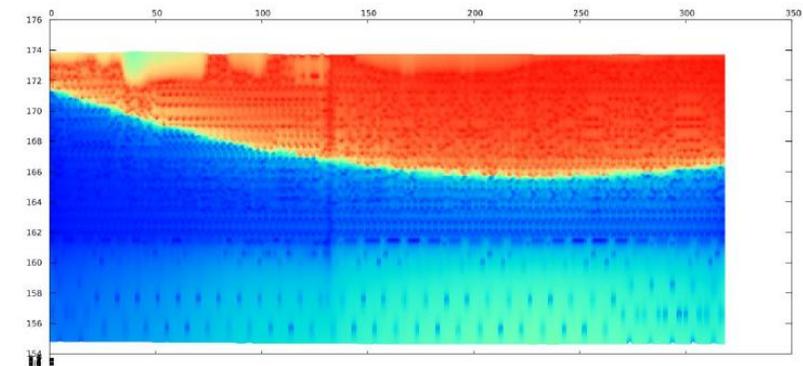
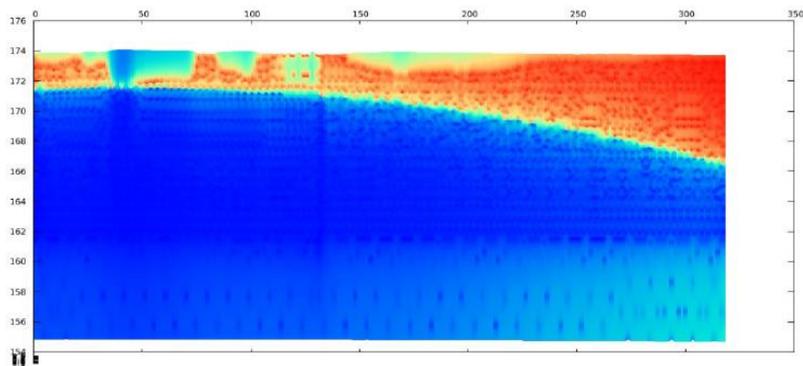
Parameter	Application	Remark	
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<input checked="" type="checkbox"/>	Flow exchange with surface water	It is important to better understand the relation between surface water and groundwater (i.e., losing/gaining conditions). It can lead to dilution, mixing, and transference of PPCPs into the groundwater.	The data are available.
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<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.

Back

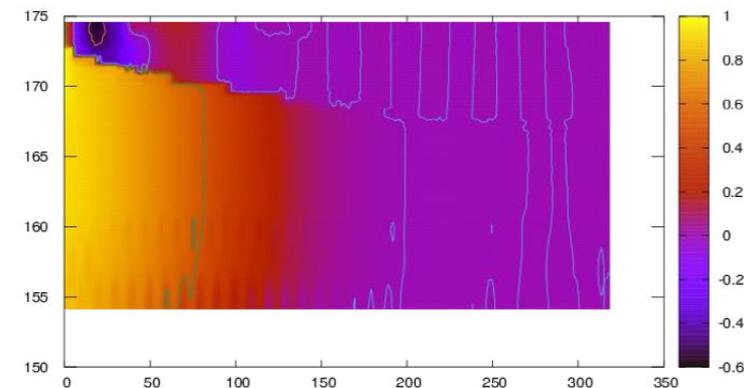
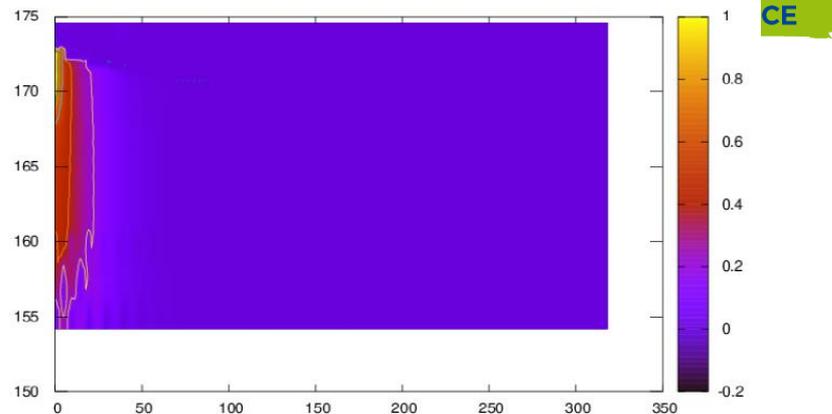
- In this case, the initial concentration was assumed as zero.
- Now modePROCON replies that a model can be built.
- In a next step, a modelling expert should be contacted to set up a transport model.



MODEL RESULTS



Top: groundwater table during wet periods
bottom: groundwater table during periods of drought



Top: contamination after 2 days
bottom: contamination after 20 days.

