





TAKING
COOPERATION
FORWARD

 online

 *Implementation of modePROCON showcasing for groundwater -Ljubljansko polje aquifer, Slovenia*

 boDEREC-CE | Chair of Hydrology and River Basin Management

OUTLINE

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Study area

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Detected
PPCPs

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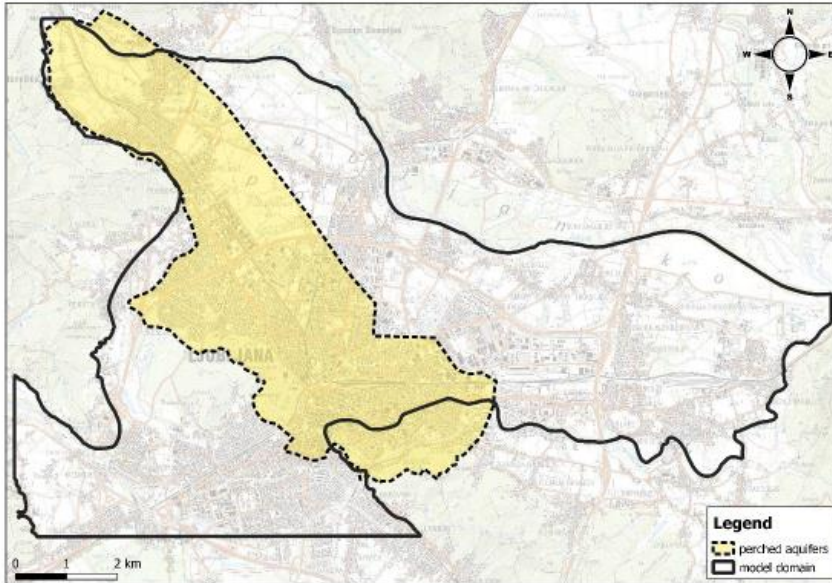
Applying
modePROCON

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Model results



STUDY AREA



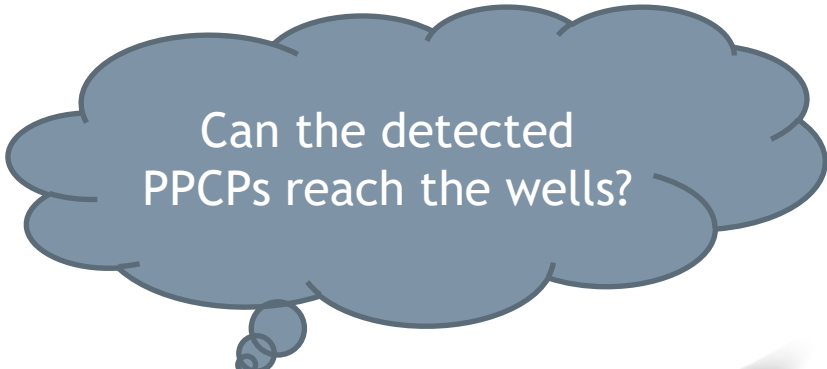
Map of perched aquifers in the model domain

- Investigated aquifer: Ljubljansko polje aquifer, Slovenia
- In the western to central part of the aquifer there is an occurrence of perched groundwater above clayey and silty layers.
- The layers with a minimal thickness of 5 m and hydraulic conductivity 10^{-6} m/s.



DETECTED PPCPs

- The following Emerging Contaminants (ECs) were detected and selected to be modeled in the groundwater system:
 - Propyphenazone
 - Caffeine
 - Carbamazepine



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 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	Reference
15	<input type="checkbox"/> Bisphenol S	80-09-1	380.0	2.14	7.0	3.55e-11	15.4	Solubility and logKow and pKa [1...
16	<input type="checkbox"/> Bisoprolol	66722-44-9	999000.0	1.89	13.86	7.61e-09	4.29	Solubility and logKow and pKa [1...
17	<input type="checkbox"/> Bisphenol A	80-05-7	71.0	3.64	10.29	3.98e-11	15.1	Solubility and logKow and pKa [1...
18	<input type="checkbox"/> Butylparaben	94-26-8	540.0	3.41	8.22	3.4e-10	3.51	Solubility and logKow and pKa [1...
19	<input checked="" type="checkbox"/> Caffeine	58-08-2	58000.0	-0.63	0.52	1.55e-06	3.82	Solubility and logKow and pKa [1...
20	<input checked="" type="checkbox"/> Carbamazepine	298-46-4	220.0	1.9	13.94	2.24e-10	6.54	Solubility and logKow and pKa [1...
21	<input type="checkbox"/> Carbamazepine-DH	29331-92-8	1100.0	0.65	13.75	6.93e-11	6.43	Solubility and logKow and pKa [1...
22	<input type="checkbox"/> Carbamazepine-DHH (Dihydroxycarbamazepine)	35079-97-1	4100.0	-0.41	12.94	1.56e-10	36.0	Solubility and logKow and pKa [1...
23	<input type="checkbox"/> Carbamazepine-E	298-46-4	220.0	1.9	13.94	2.24e-10	6.54	Solubility and logKow and pKa [1...
24	<input type="checkbox"/> Celiprolol	56980-93-9	83000.0	1.92	13.81	4.9e-10	4.65	Solubility and logKow and pKa [1...
25	<input type="checkbox"/> Chloramphenicol	56-75-7	1100.0	1.1	11.03	1.23e-10	4.37	Solubility and logKow and pKa [1...
26	<input type="checkbox"/> Ciprofloxacin acid	85721-33-1	460.0	1.63	6.43	9.24e-12	3.35	Solubility and logKow and pKa [1...
27	<input type="checkbox"/> Citalopram	59729-33-8	2800.0	3.48	9.57	3.94e-06	3.55	Solubility and logKow and pKa [1...
28	<input type="checkbox"/> Clarithromycin	81103-11-9	460000.0	2.81	13.08	9.48e-11	15.2	Solubility and logKow and pKa [1...

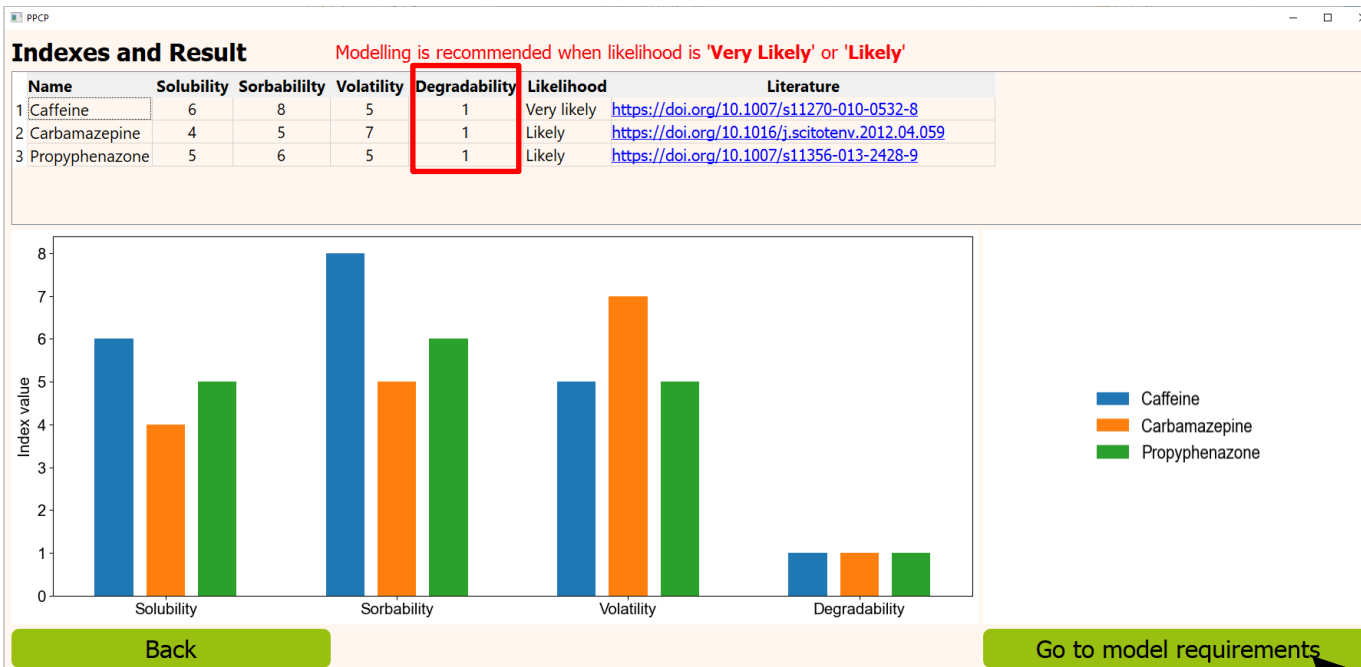
Buttons: Back, Delete all user input, Add new data, Evaluate

The detected PPCPs Propyphenazone, Caffeine and Carbamazepine are contained in the database and can be selected simultaneously.



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Probability Estimation



- All the investigated compounds are easily biodegradable.



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Probability Estimation



- Due to the high index values, the detection probabilities of Carbamazepine and Propyphenazone are likely.
- This is related to the high solubility combined.



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Probability Estimation

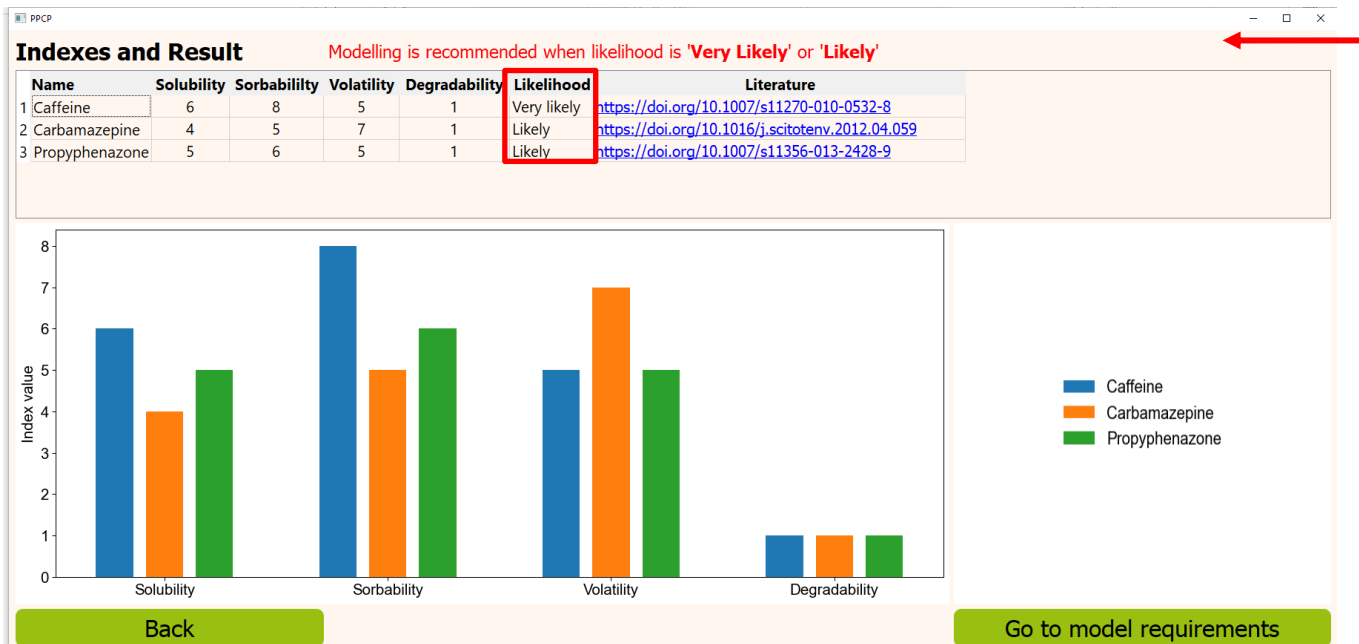


- Due to the high index values, the detection probability of Caffeine is very likely.
- This is related to the high solubility combined with low volatility.



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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
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	

[Back](#)

- 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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couldn'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

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
<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. The data are available.
<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.
<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.
<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.
<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.

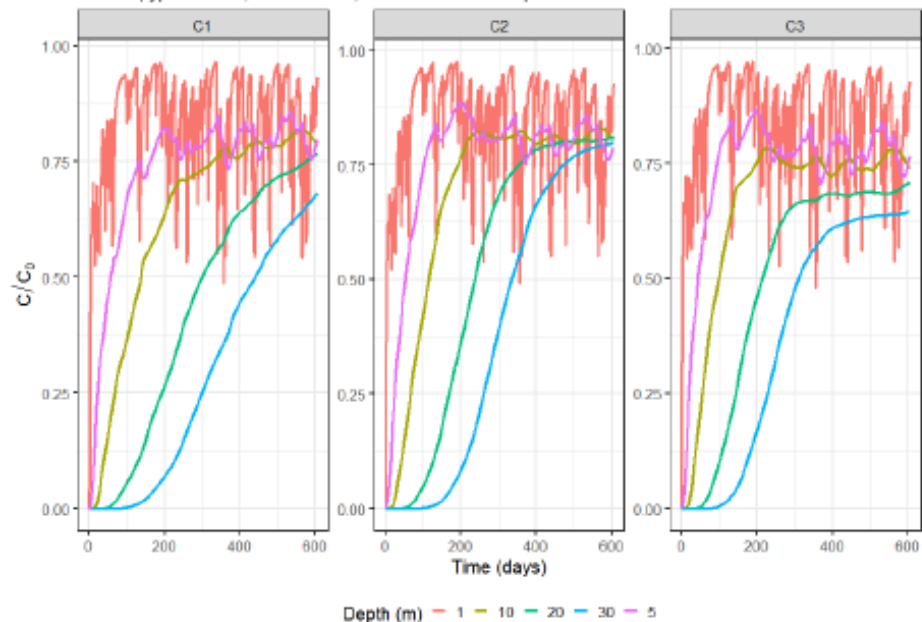
Back

- In this case, only **sewage source** of PPCPs is considered. This was chosen based on the prevailing infrastructure conditions in the area and the characteristics of the chosen ECs' use.
- 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.



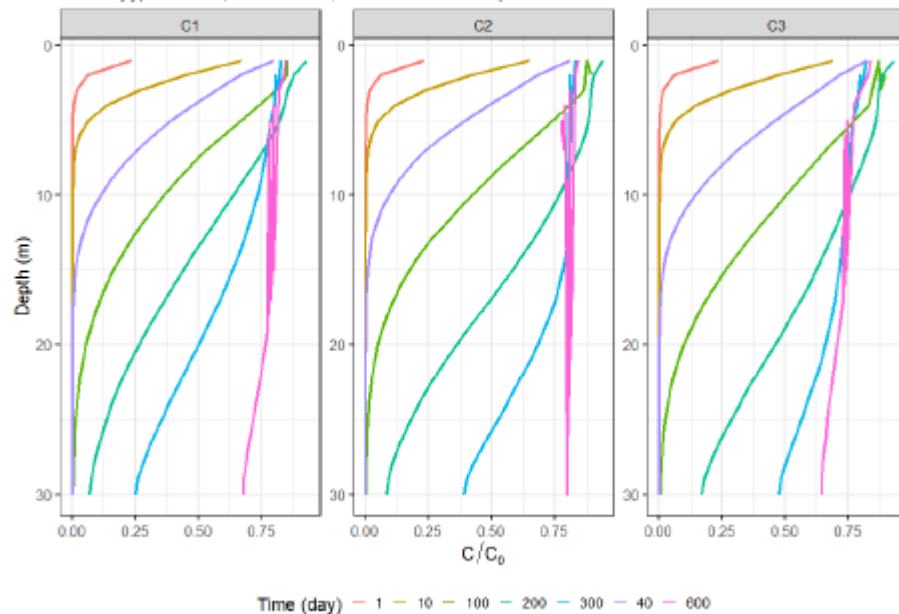
MODEL RESULTS

Comparison of rel. concentrations of caffeine for max. sewage exfiltration & precipitation
C1=Propyphenazone, C2=Caffeine, and C3=Carbamazepine



Relative concentrations of ECs versus time for different depths of the UZ with maximum sewage exfiltration estimation

Comparison of rel. concentrations of solutes for max. sewage exfiltration & precipitation
C1=Propyphenazone, C2=Caffeine, and C3=Carbamazepine



Depth versus relative concentrations of ECs for different times with maximum sewage exfiltration estimation

