online

Implementation of modePROCON showcasing for groundwater –Ljubljansko polje aquifer, Slovenia

boDEREC-CE I Chair of Hydrology and River Basin Management

OUTLINE

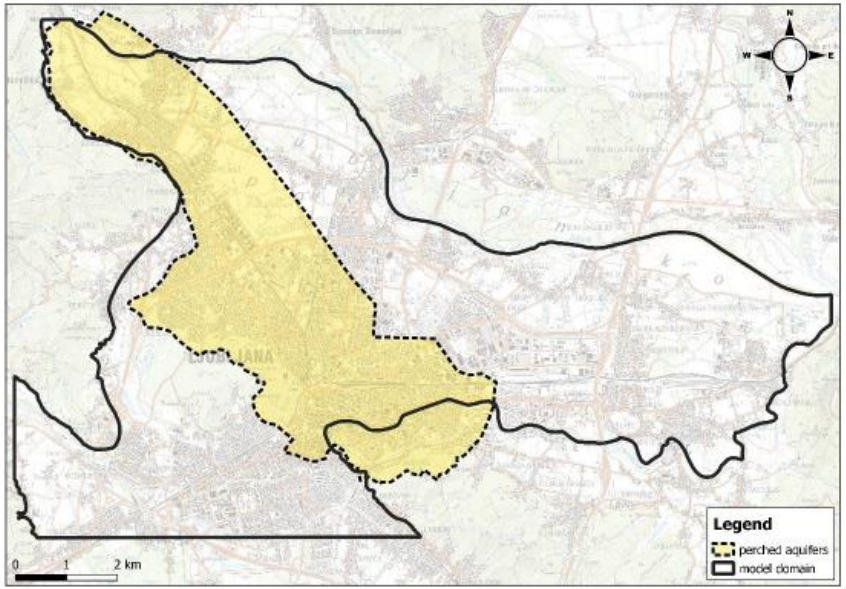
1 Study area

2 Detected PPCPs

3 Applying modePROCON

4 Model results

STUDY AREA

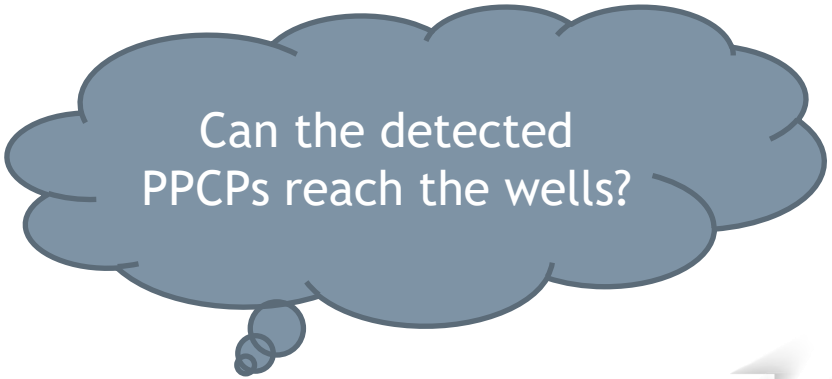


Map of perched aquifers in the model domain

- 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.

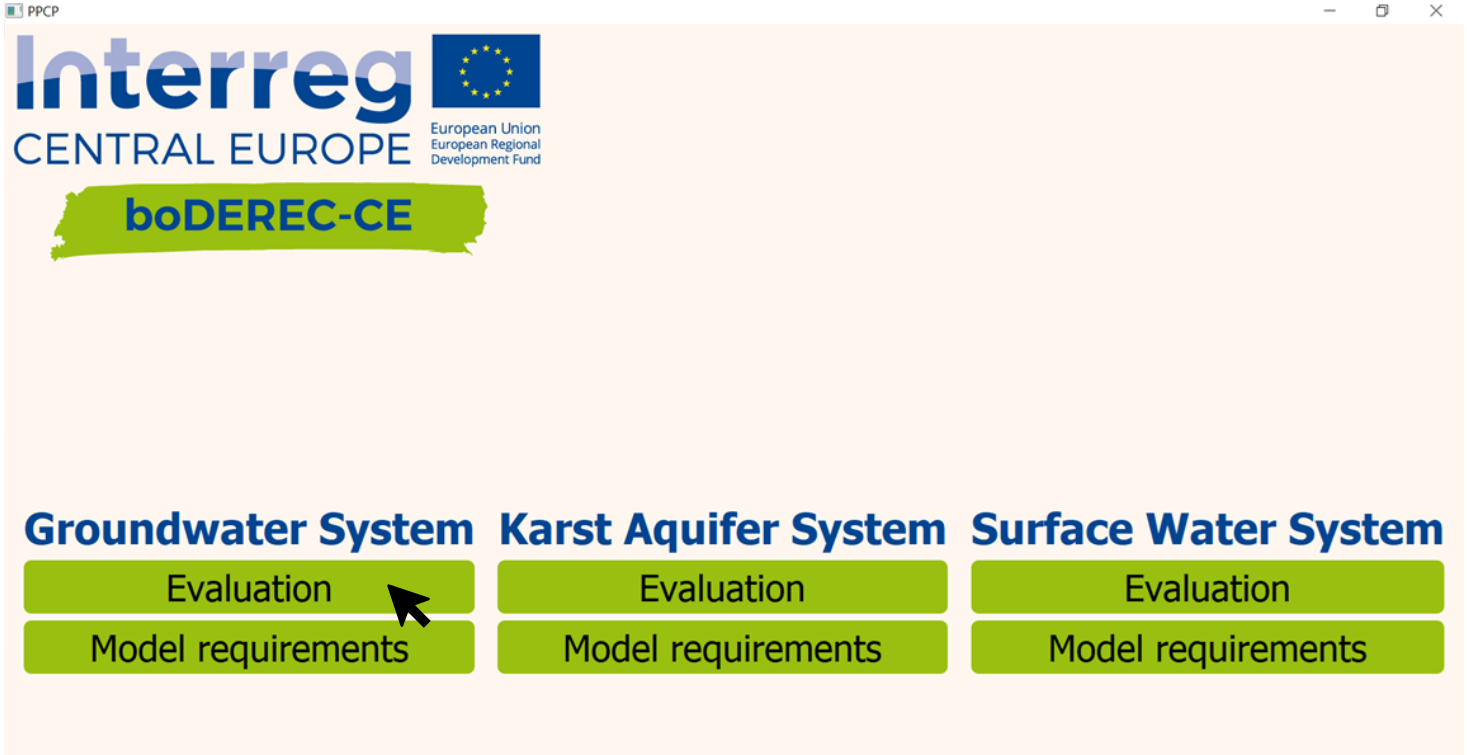
DETECTED PPCPs

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

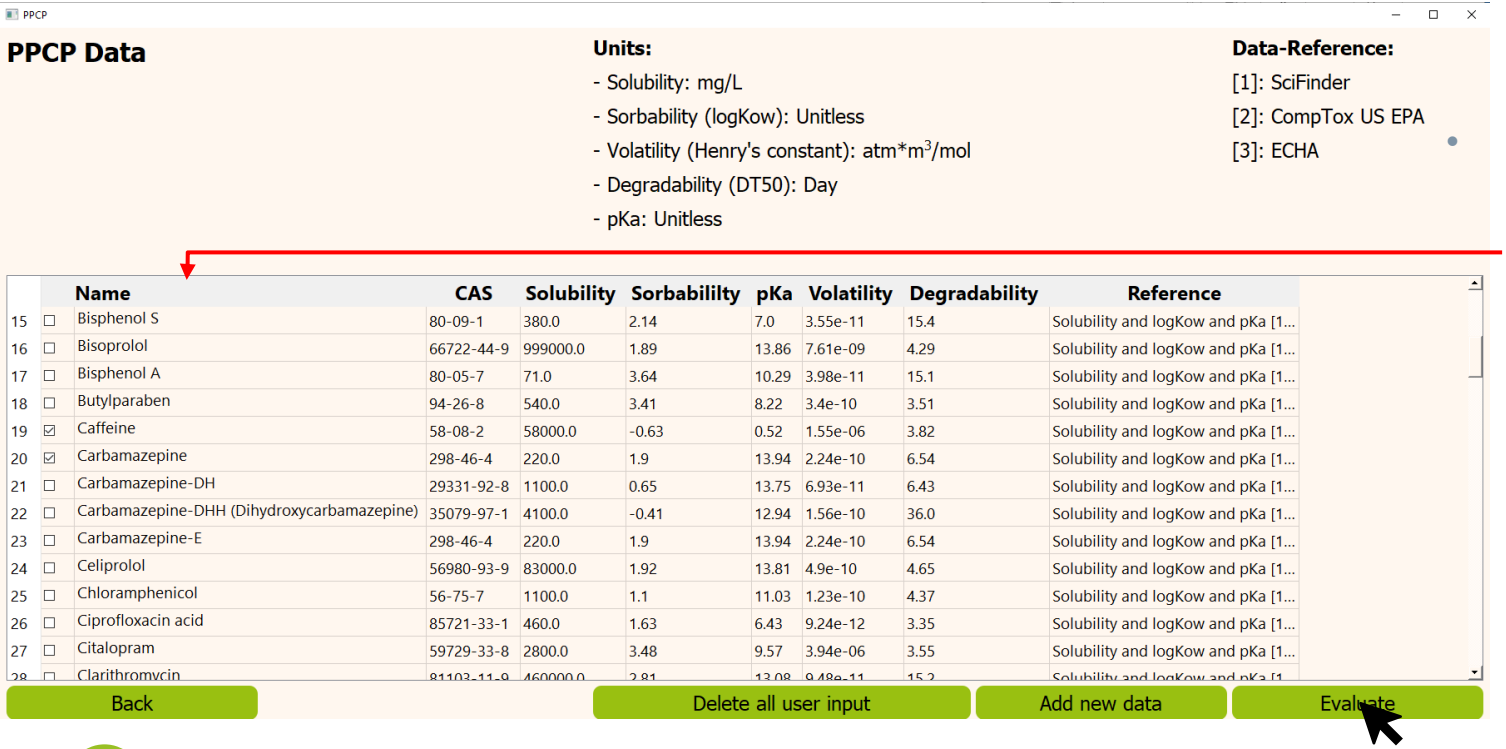


APPLYING modePROCON

Selecting the water source



APPLYING modePROCON
Selecting the PPCPs



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

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

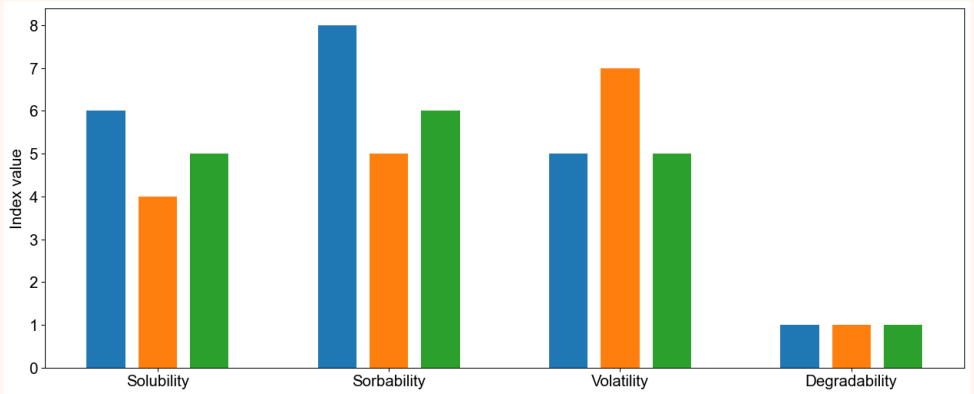
APPLYING modePROCON
Probability Estimation

PPCP

Indexes and Result

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

	Name	Solubility	Sorbability	Volatility	Degradability	Likelihood	Literature
1	Caffeine	6	8	5	1	Very likely	https://doi.org/10.1007/s11270-010-0532-8
2	Carbamazepine	4	5	7	1	Likely	https://doi.org/10.1016/j.scitotenv.2012.04.059
3	Propyphenazone	5	6	5	1	Likely	https://doi.org/10.1007/s11356-013-2428-9

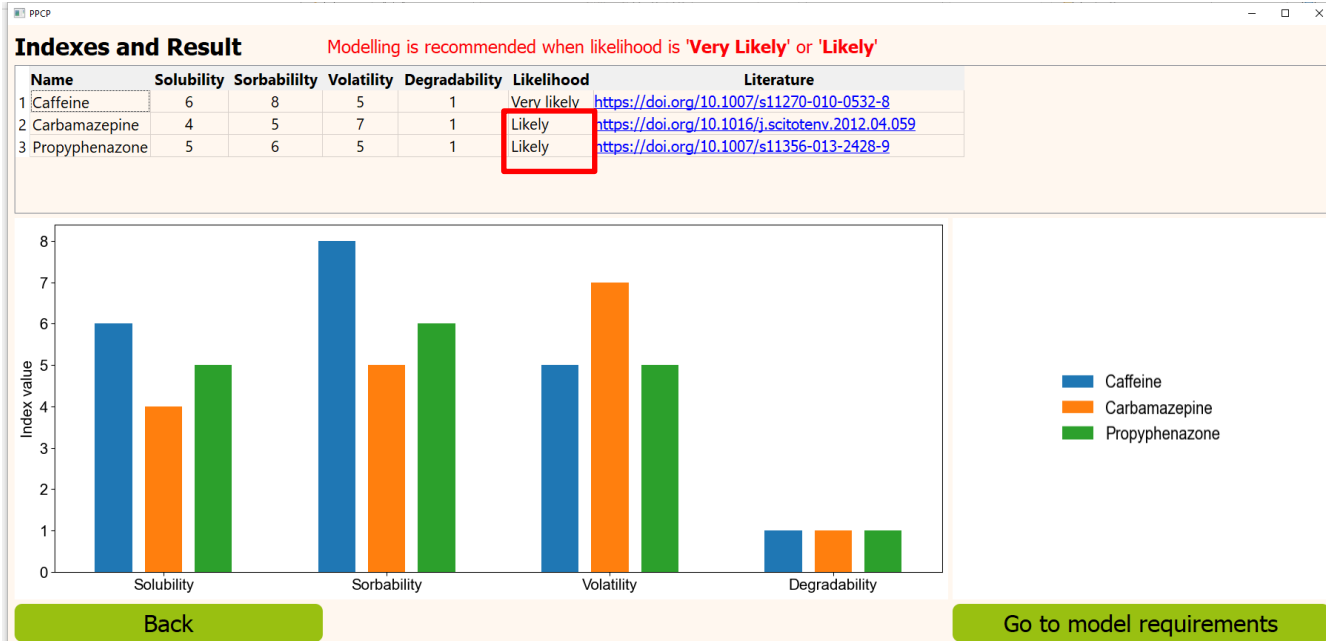


Back

Go to model requirements

- All the investigated compounds are **easily biodegradable.**

APPLYING modePROCON
Probability Estimation

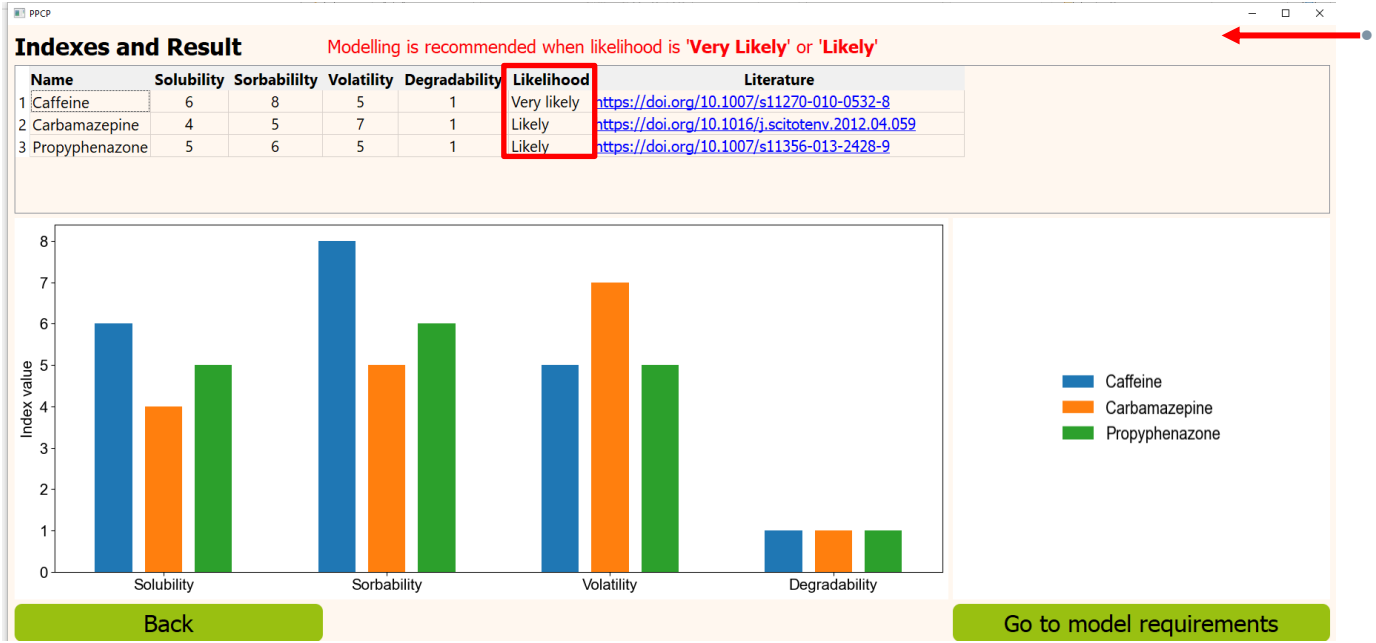


- Due to the high index values, the detection probabilities of **Carbamazepine** and **Propyphenazone** are **likely**.
- This is related to the **high solubility combined**.

APPLYING modePROCON
Probability Estimation

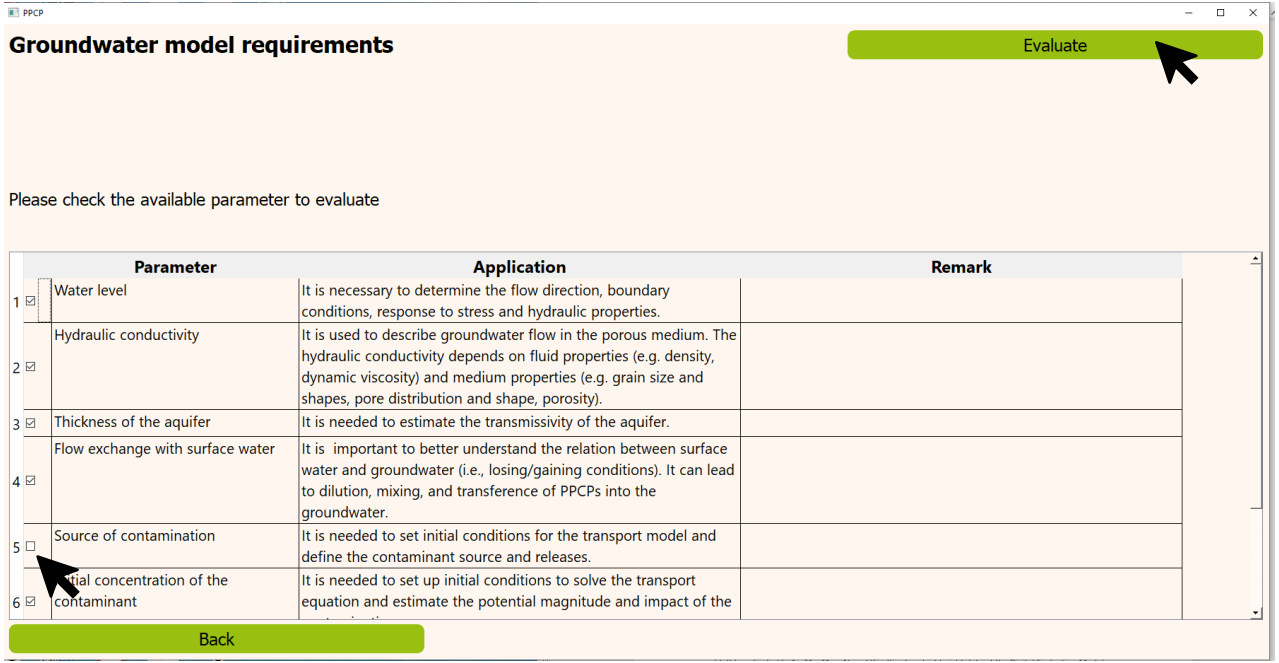
- Due to the high index values, the detection probability of Caffeine is **very likely**.
- This is related to the **high solubility** combined with **low volatility**.

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.

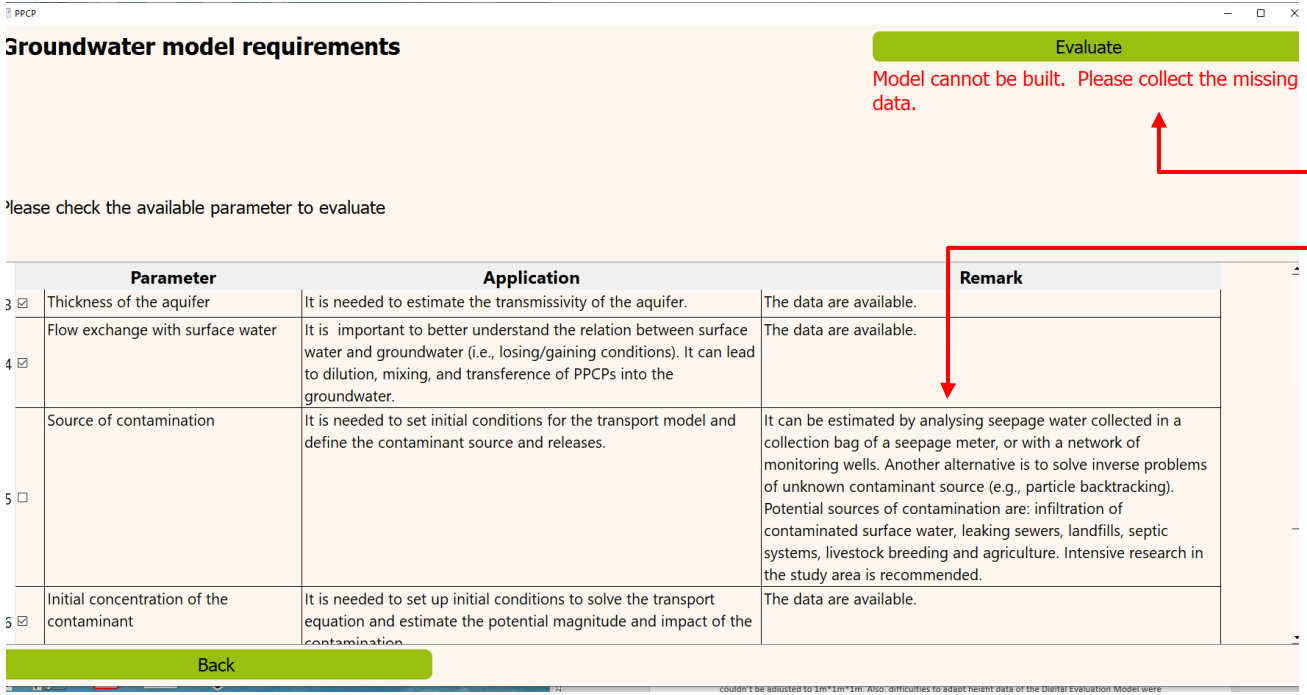
APPLYING modePROCON
Model requirements



	Parameter	Application	Remark
1 ☑	Water level	It is necessary to determine the flow direction, boundary conditions, response to stress and hydraulic properties.	
2 ☑	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 ☑	Thickness of the aquifer	It is needed to estimate the transmissivity of the aquifer.	
4 ☑	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 ☐	Source of contamination	It is needed to set initial conditions for the transport model and define the contaminant source and releases.	
6 ☑	...ial 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	

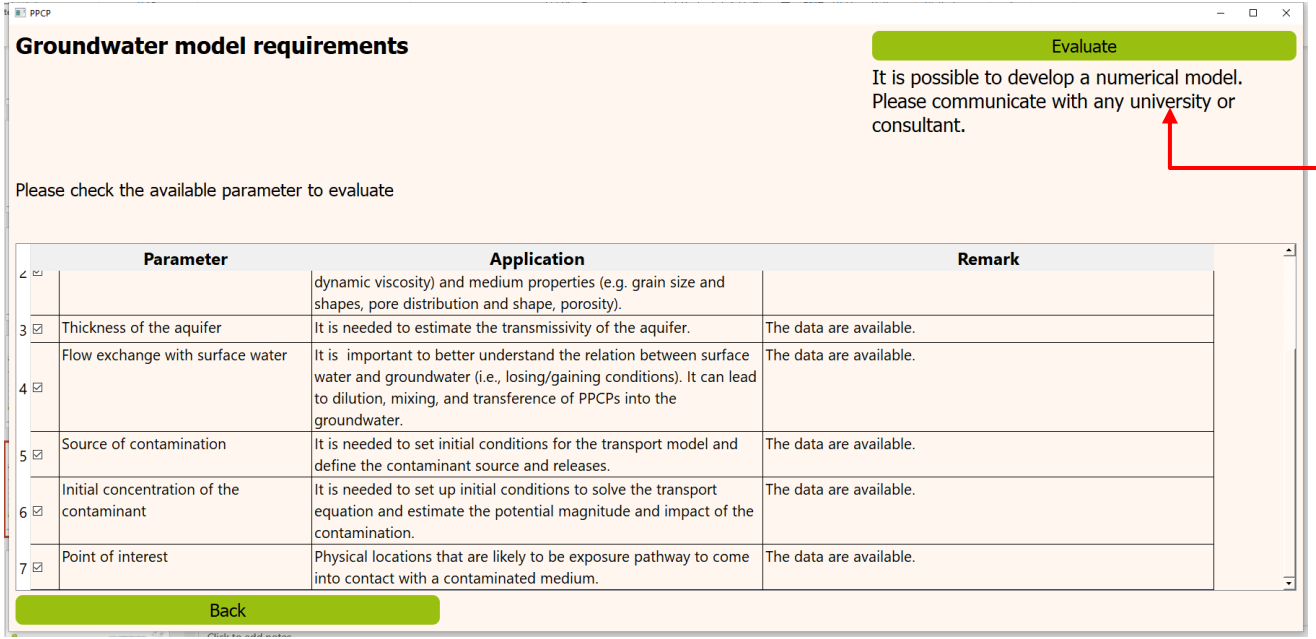
- All the required model **parameters** are known in this case, **except** of the **source of contamination.**
- modePROCON evaluates the data…

APPLYING modePROCON
Model requirements



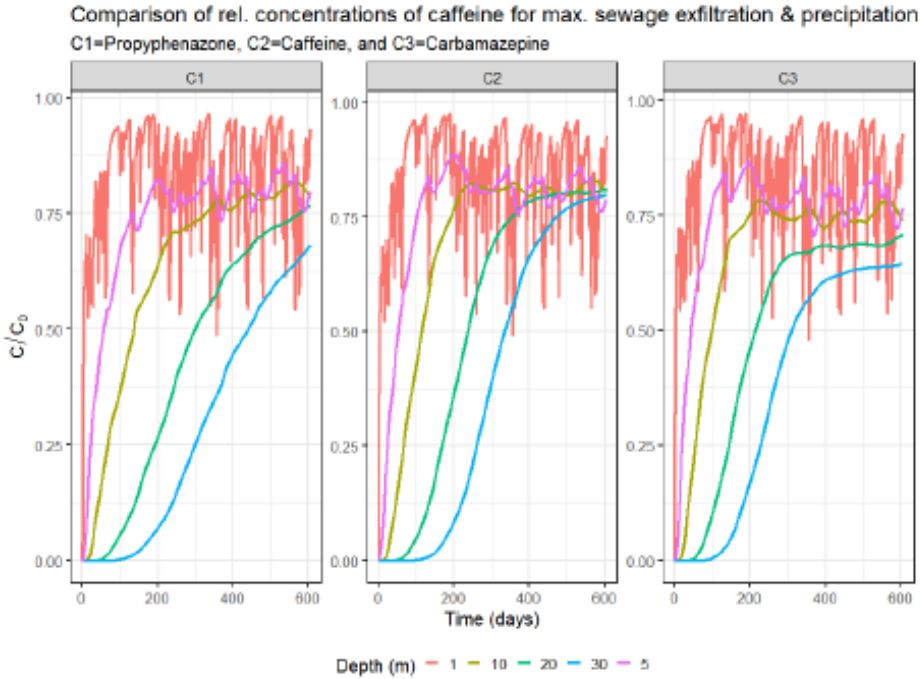
- … and replies that a **model cannot be built** with the available data.
- modePROCON suggests a **possibility to obtain** the **missing data** in the remark column.

APPLYING modePROCON
Model requirements

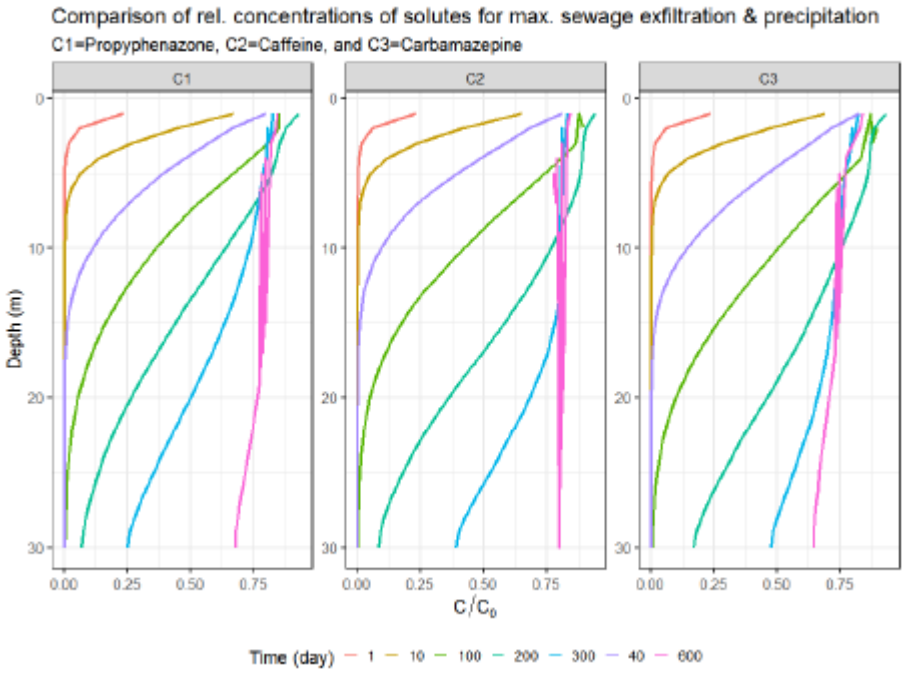


- In this case, only **sewage source** of PPCPs is considered. This was chosen based on the prevailing infrastructure conditions in the area and the characteristics of the chosen ECs' use.
- Now modePROCON replies that a **model can be built**.
- In a next step, a **modelling expert** should be contacted to set up a transport model.

MODEL RESULTS



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



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