online

Implementation of modePROCON showcasing for groundwater – Neufahrn bei Freising, Germany

boDEREC-CE I Chair of Hydrology and River Basin Management

OUTLINE

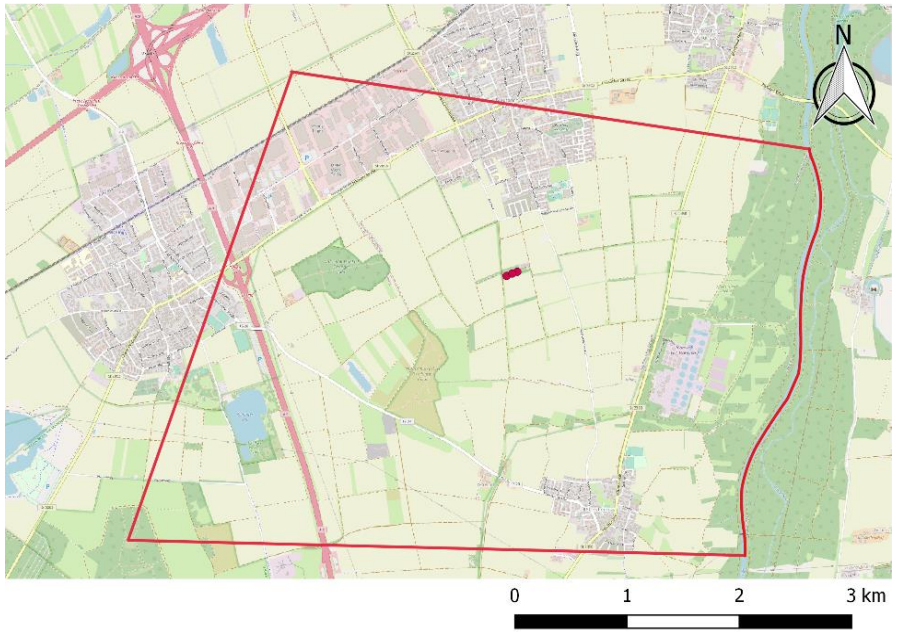
1 Study area

2 Detected PPCPs

3 Applying modePROCON

4 Model results

STUDY AREA

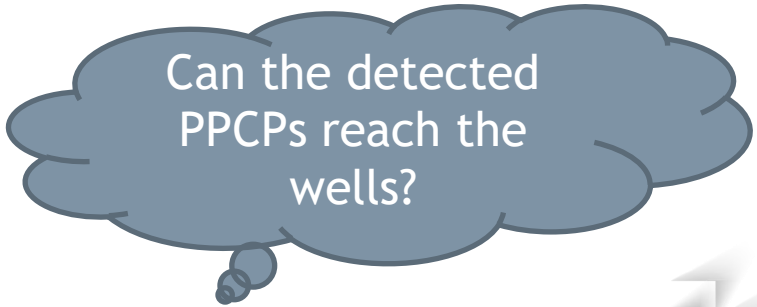


The well field (red dots) in the study area (red framed) is depicted.

- Investigated well field next to “Neufahrn bei Freising”
- Located in the Munich gravel plain
  - Shallow aquifer (~ 4-17 m b.s.)
- Rural area mainly used for agriculture
- WWTP discharging in nearby river “Isar”

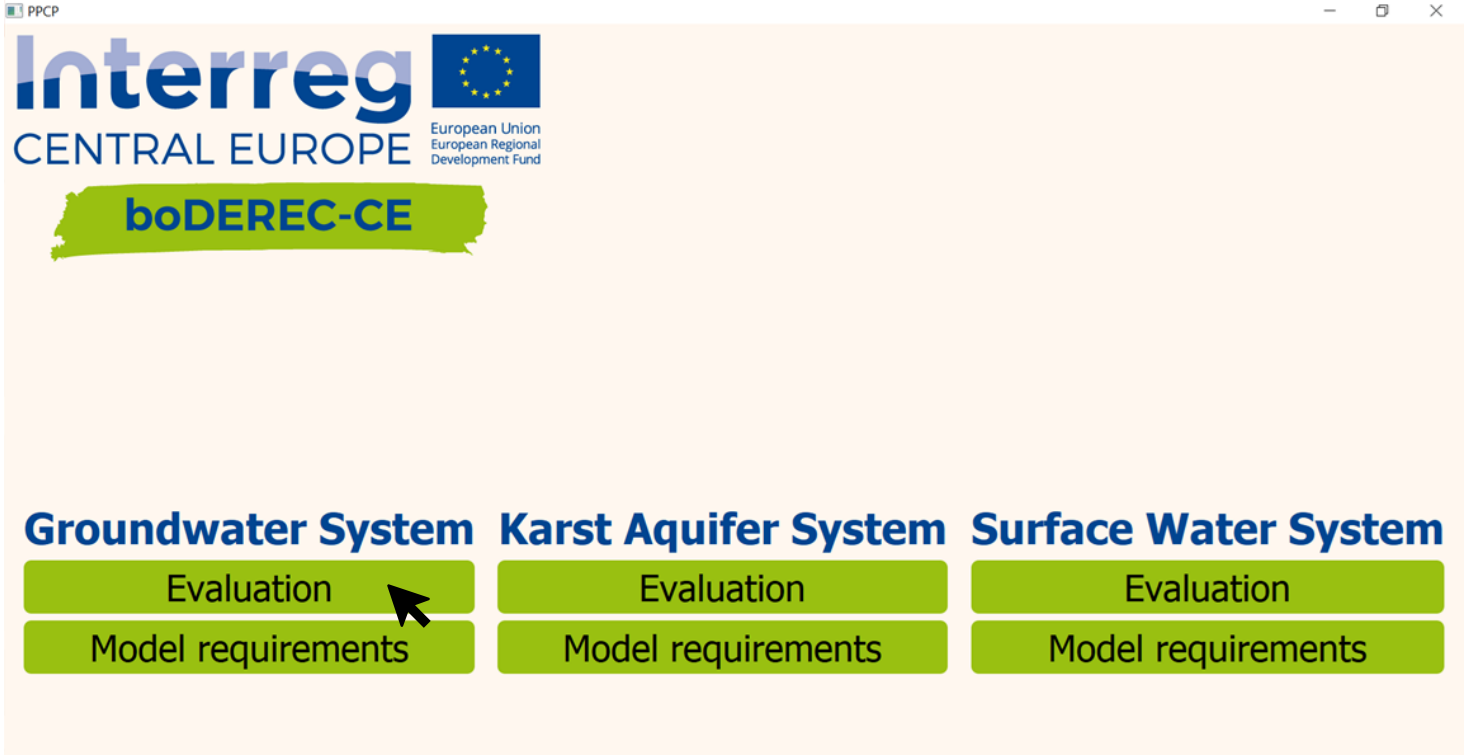
DETECTED PPCPs

- These PPCPs were detected in the nearby river frequently:
  - 4-formylaminoantripyrine (4-FAA)
  - Benzotriazole
  - Diatrizoate
  - Iohexol
  - Iomeprol

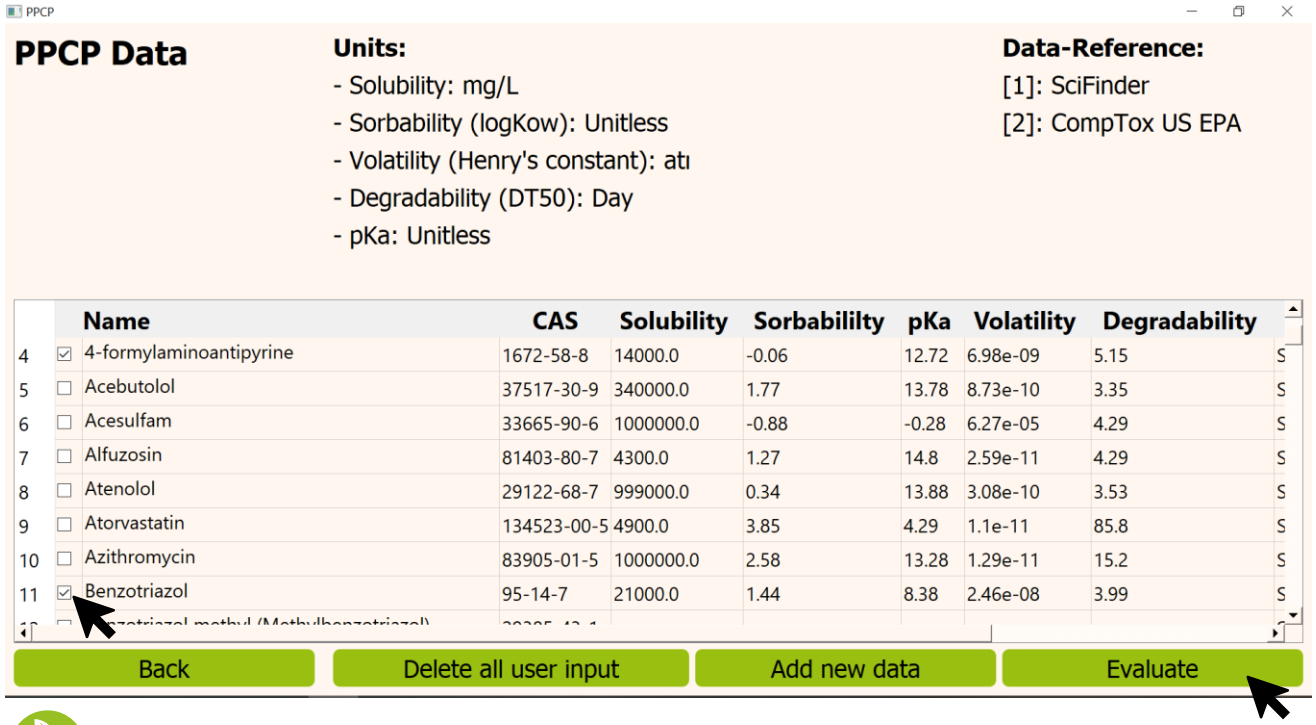


APPLYING modePROCON

Selecting the water source



APPLYING modePROCON
Selecting the PPCPs



	Name	CAS	Solubility	Sorbabililty	pKa	Volatility	Degradability	
4	☑ 4-formylaminoantipyrine	1672-58-8	14000.0	-0.06	12.72	6.98e-09	5.15	S
5	☐ Acebutolol	37517-30-9	340000.0	1.77	13.78	8.73e-10	3.35	S
6	☐ Acesulfam	33665-90-6	1000000.0	-0.88	-0.28	6.27e-05	4.29	S
7	☐ Alfuzosin	81403-80-7	4300.0	1.27	14.8	2.59e-11	4.29	S
8	☐ Atenolol	29122-68-7	999000.0	0.34	13.88	3.08e-10	3.53	S
9	☐ Atorvastatin	134523-00-5	4900.0	3.85	4.29	1.1e-11	85.8	S
10	☐ Azithromycin	83905-01-5	1000000.0	2.58	13.28	1.29e-11	15.2	S
11	☑ Benzotriazol	95-14-7	21000.0	1.44	8.38	2.46e-08	3.99	S

- The detected PPCPs **4-FAA, benzotriazole, diatrizoate, iohexol and iomeprol** are contained in the database and can be **selected simultaneously.**

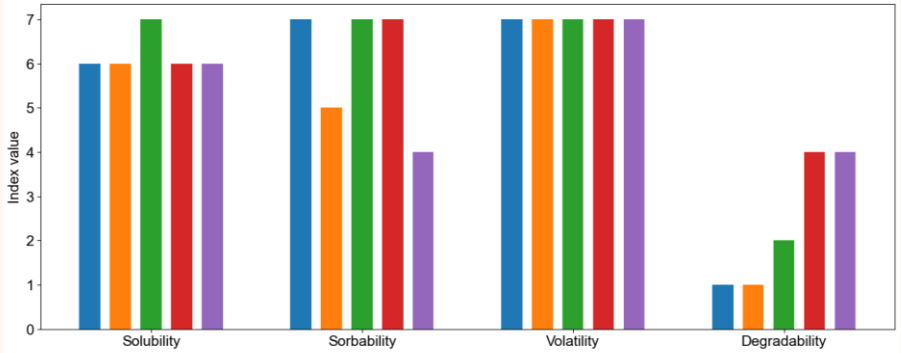
APPLYING modePROCON
Probability Estimation

PPCP

Indexes and Result

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

	Name	Solubility	Sorbabililty	Volatility	Degradability	Likelihood	Literature
1	4-formylaminoantipyrine	6	7	7	1	Very likely	https://doi.org/10.1016/j.watres.20
2	Benzotriazol	6	5	7	1	Likely	https://doi.org/10.1016/j.watres.20
3	Diatrizoate	7	7	7	2	Very likely	https://doi.org/10.1016/j.scitotenv.
4	Iohexol	6	7	7	4	Very likely	https://doi.org/10.1016/j.jconhyd.2
5	Iomeprol	6	4	7	4	Very likely	https://doi.org/10.1016/j.watres.20



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Go to model requirements

- Although the **volatility** and the **solubility** of all PPCPs is in the **same range**, **different likelihoods** can be obtained.

APPLYING modePROCON
Probability Estimation

PPCP

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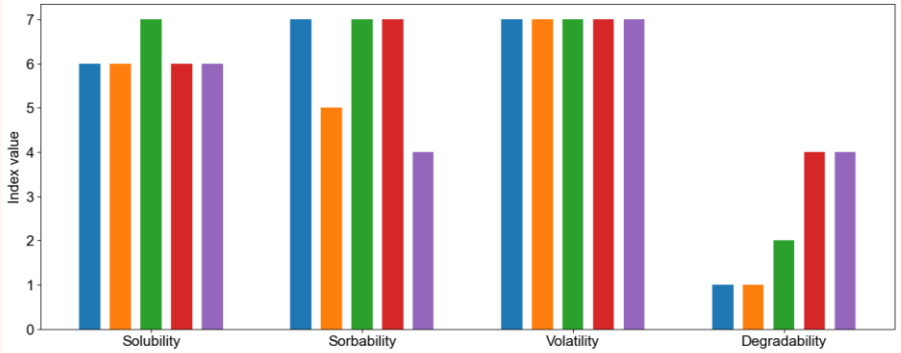

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Go to model requirements

- The detection probabilities of **4-FAA, diatrizoate, iomeprol and iohexol** are very likely.
- This is due to relatively **high index values** of the compounds for each parameter.

APPLYING modePROCON
Probability Estimation

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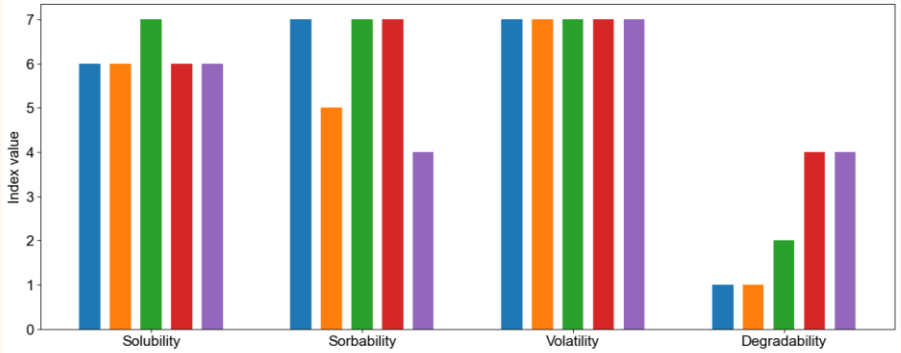

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Go to model requirements

- For **iomeprol** and **iohexol** the **very likely** probability results from the little **biodegradability**.
- **4-FAA** and **diatrizoate** are indeed better **biodegradable** but show a very low **adsorption capability**.

APPLYING modePROCON
Probability Estimation

PPCP

Indexes and Result

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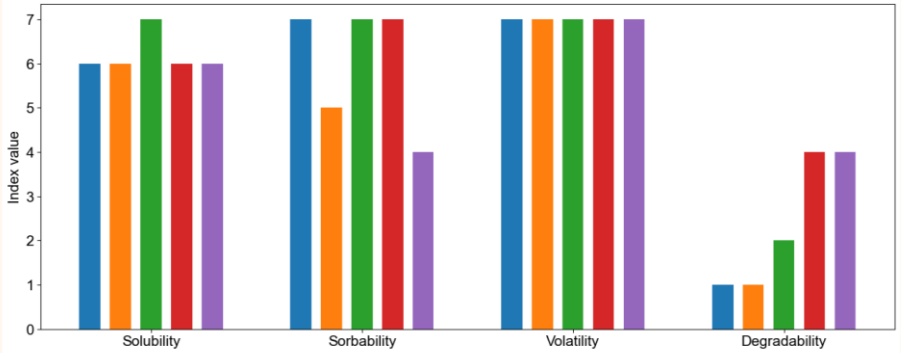

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Go to model requirements

- The detection probability of **benzotriazole** is only likely.
- This is related to its higher **capability** to **adsorb** to organic soil material and its increased **degradability**, compared to the other compounds.

APPLYING modePROCON
Probability Estimation

PPCP

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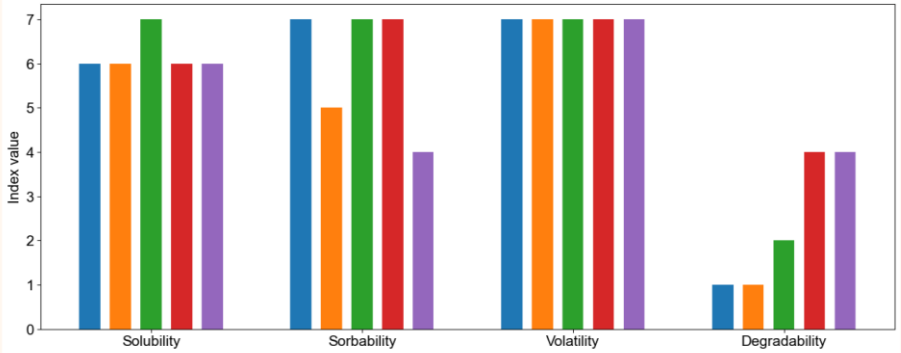

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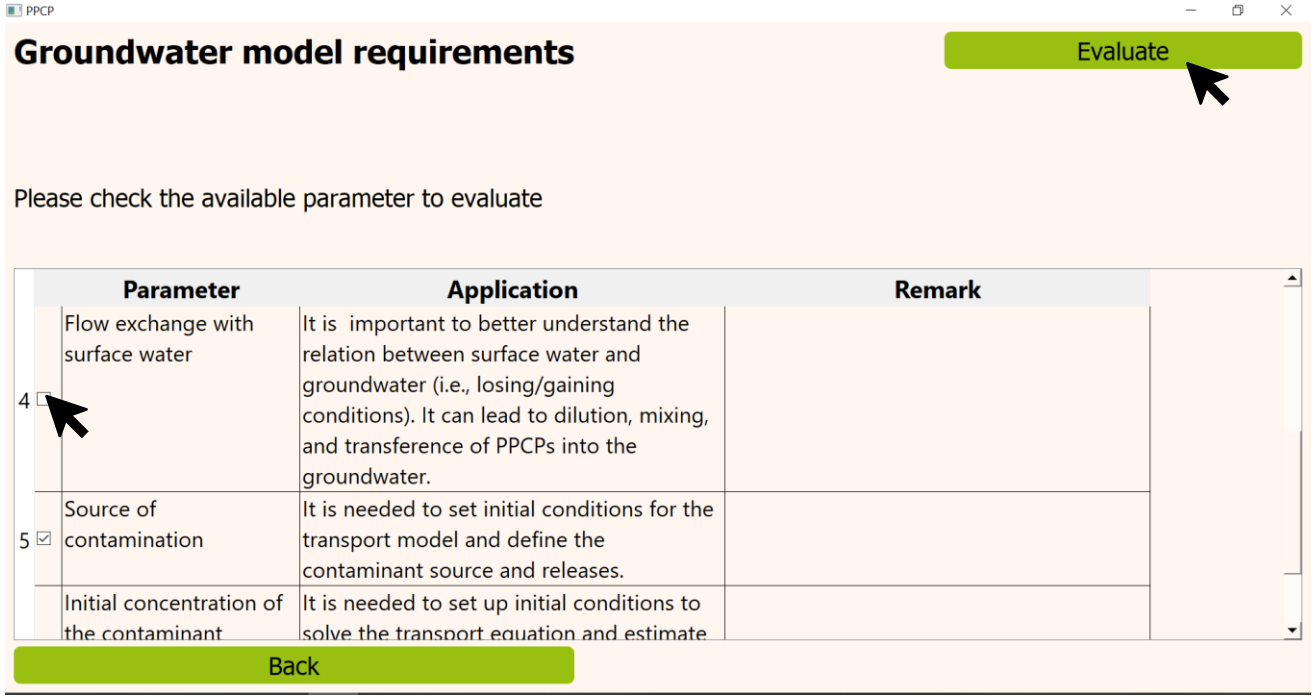
Go to model requirements

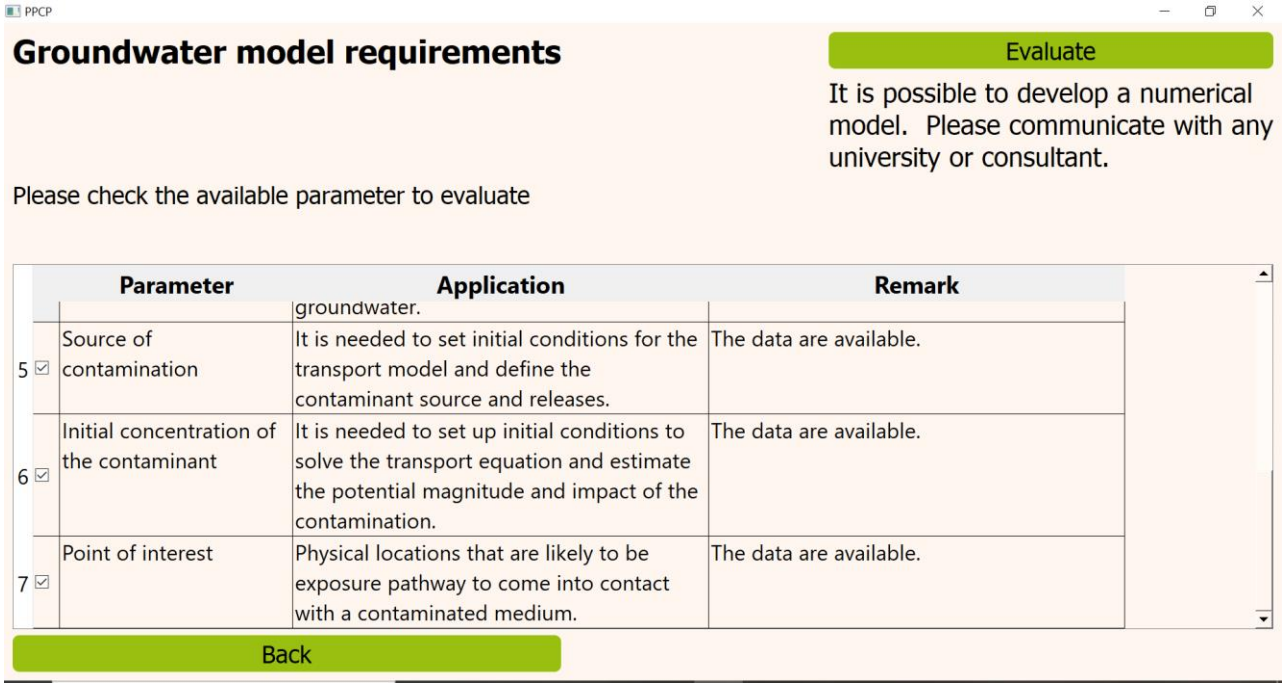
- As the investigated PPCPs are **very likely** or **likely** to be detected in water, modePROCON **recommends to model** the situation for further investigation.

APPLYING modePROCON
Model requirements



- All the **required model parameters** are known in this case.
- modePROCON evaluates the data…

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
		groundwater.	
5 ☑	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 ☑	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 ☑	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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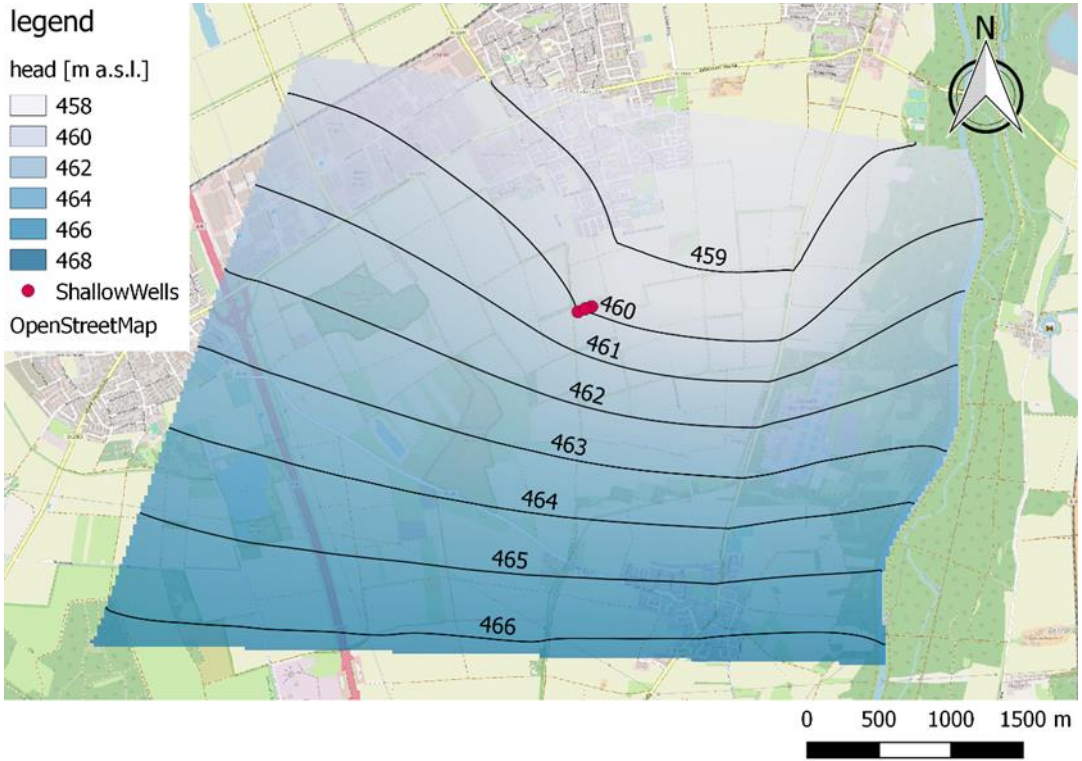
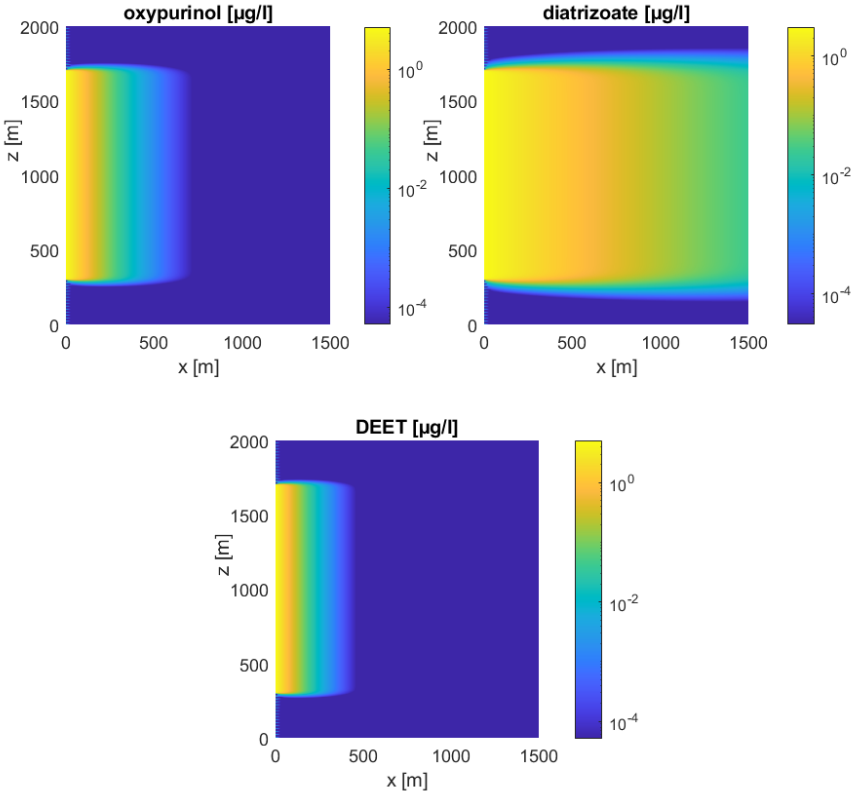
- … and replies that a **model can be built.**
- In a next step, a **university** or a **consultant** should be contacted to set up a transport model.

MODEL RESULTS



- In this case, the evaluation of a **flow model** suggested that the wells are **very unlikely impacted** by the **river** water.
- Even for a **flood** event, the flow regime **remains** the same.
- So, the model **excludes** the **river** as a **potential source** here.

MODEL RESULTS



- Since some **PPCPs** were **detected** during the monitoring campaign also in the **wells**, other potential sources may be present in this case study.
- **Transport modelling** can be used, to further **investigate potential sources** and transport processes.