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Implementation of modePROCON showcasing for groundwater –Káraný, Czechia, Czech Republic

boDEREC-CE I Chair of Hydrology and River Basin Management

OUTLINE

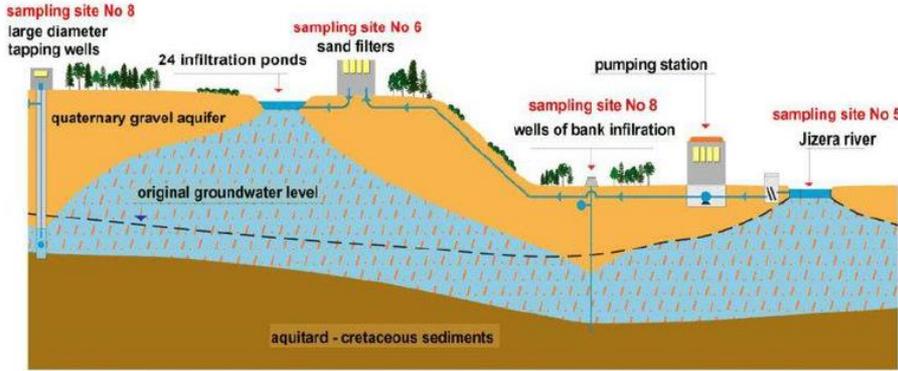| 1	2	3	4
Study area	**Detected PPCPs**	**Applying modePROCON**	**Model results**

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

APPLYING modePROCON
Selecting the PPCPs

PPCP Data

Units:
- Solubility: mg/L
- Sorbability (logKow): Unitless
- Volatility (Henry's constant): atm*m^3/mol
- Degradability (DT50): Day
- pKa: Unitless

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

		Name	CAS	Solubility	Sorbabililty	pKa	Volatility	Degradability	Re
99	☑	Sulfamerazine	127-79-7	950.0	0.11	7.35	7.38e-11	3.36	Solubility and
100	☑	Sulfamethazin	57-68-1	420.0	0.3	7.89	7.19e-11	3.36	Solubility and
101	☑	Sulfamethoxazol	723-46-6	2800.0	0.66	5.81	1.72e-10	3.35	Solubility and
102	☐	Sulfanilamide	63-74-1	11000.0	-0.67	10.1	8.16e-11	3.87	Solubility and
103	☐	Sulfapyridin	144-83-2	850.0	0.47	8.54	3.95e-11	3.36	Solubility and
104	☐	Telmisartan	144701-48-4	13.0	6.48	3.86	2.16e-08	37.0	Solubility and
105	☐	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 Data

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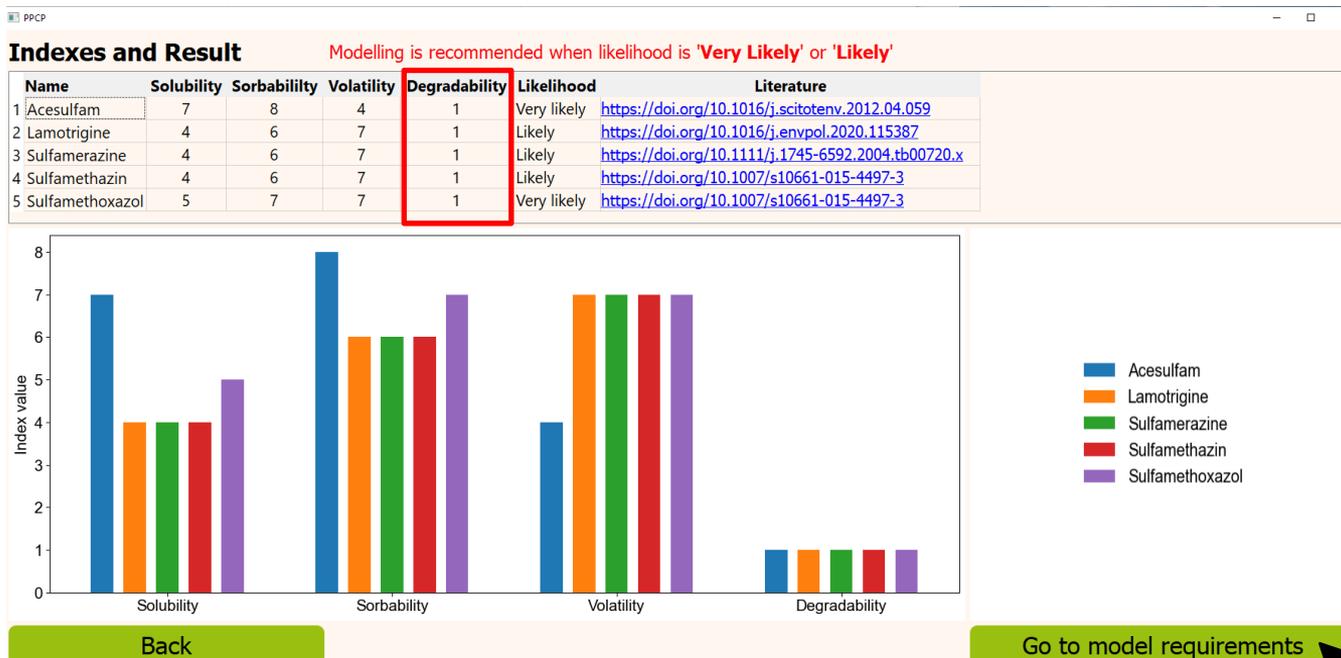
- All the investigated compounds are **easily biodegradable.**

APPLYING modePROCON
Probability Estimation

- Due to the high index values, the detection probabilities of **Lamotrigin, Sulfamerazine** and **Sulfamethazin** are **likely**.

- This is related to the **high solubility**.
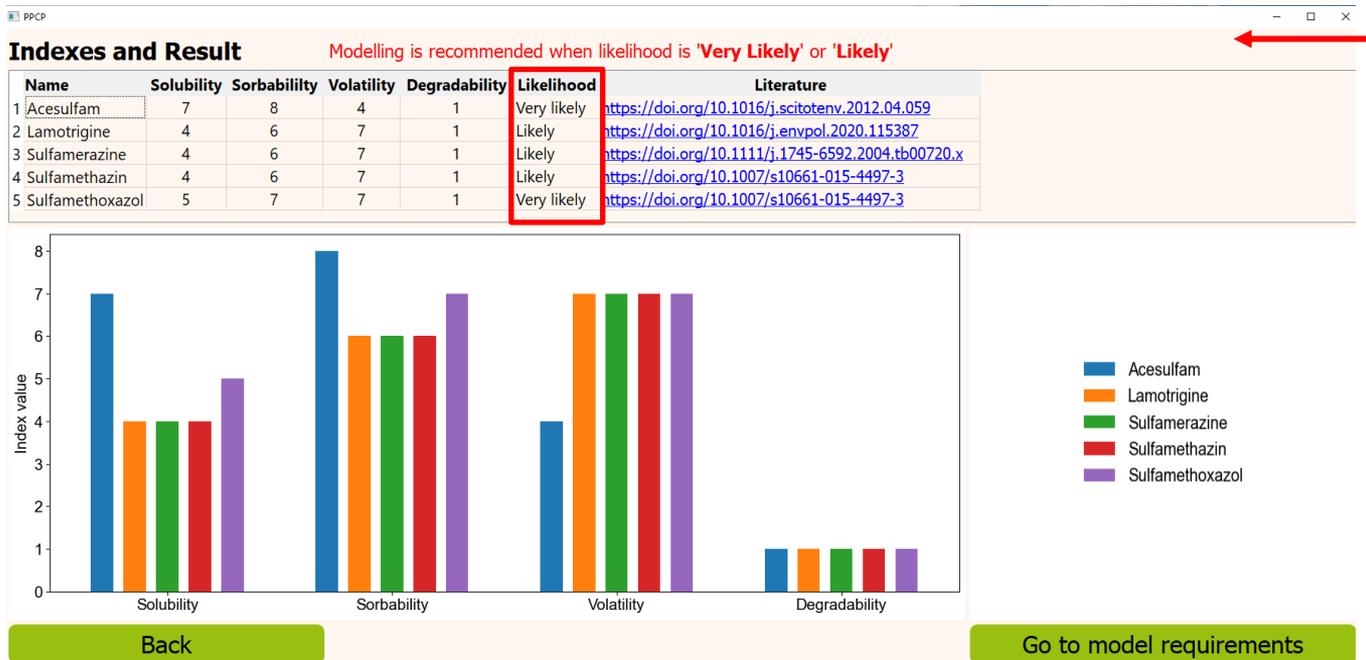
APPLYING modePROCON
Probability Estimation
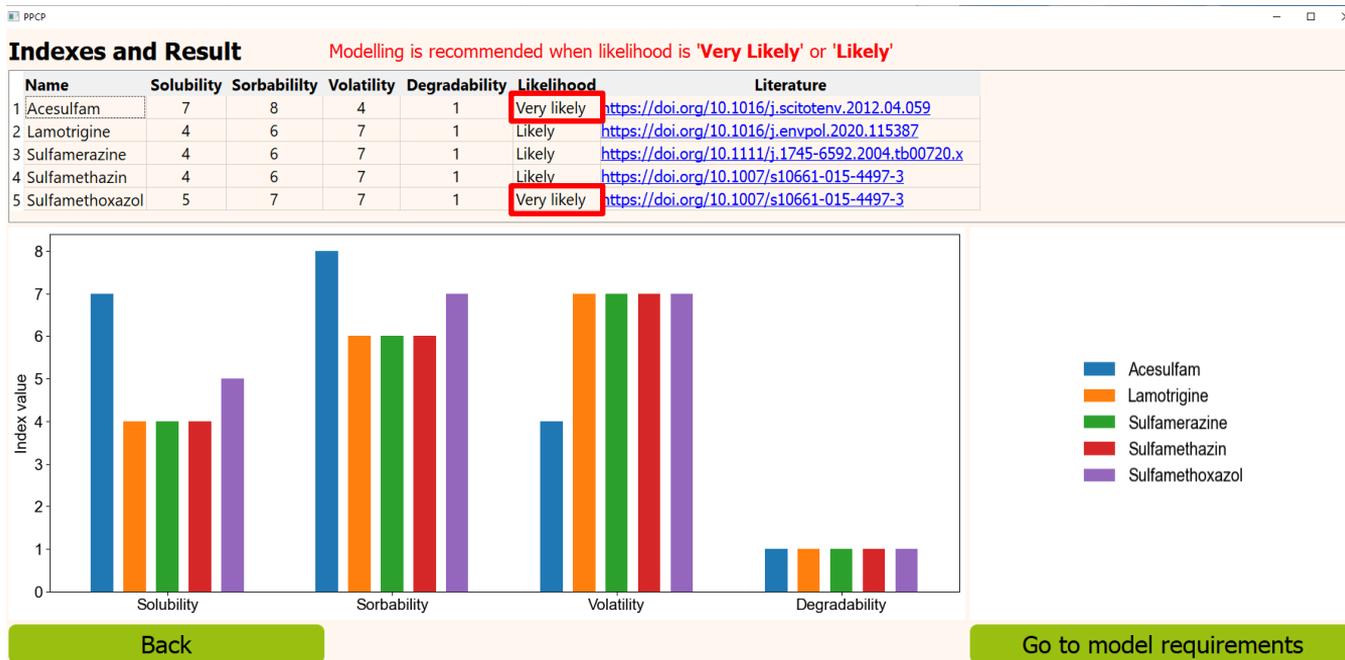
- The detection probabilities of Acesulfam and sulfamethoxazole are **very likely**.

- 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

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

	Name	Solubility	Sorbabililty	Volatility	Degradability	Likelihood	Literature
1	Acesulfam	7	8	4	1	Very likely	https://doi.org/10.1016/j.scitotenv.2012.04.059
2	Lamotrigine	4	6	7	1	Likely	https://doi.org/10.1016/j.envpol.2020.115387
3	Sulfamerazine	4	6	7	1	Likely	https://doi.org/10.1111/j.1745-6592.2004.tb00720.x
4	Sulfamethazin	4	6	7	1	Likely	https://doi.org/10.1007/s10661-015-4497-3
5	Sulfamethoxazol	5	7	7	1	Very likely	https://doi.org/10.1007/s10661-015-4497-3

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

- 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

- … 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.
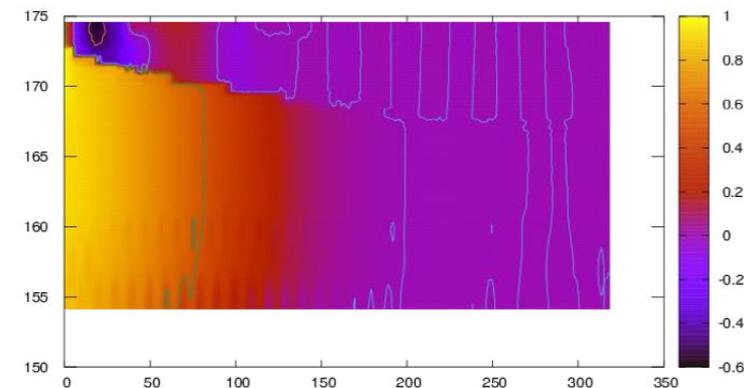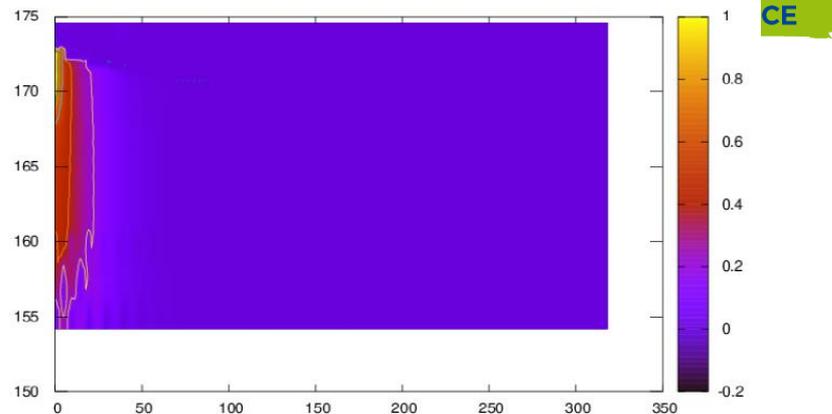
APPLYING modePROCON
Model requirements

- In this case, 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
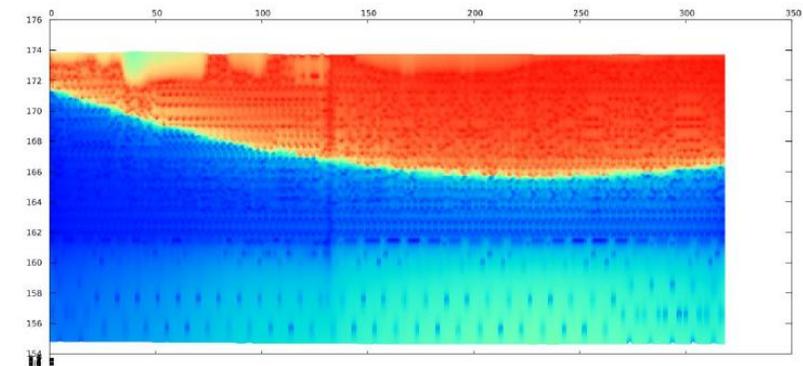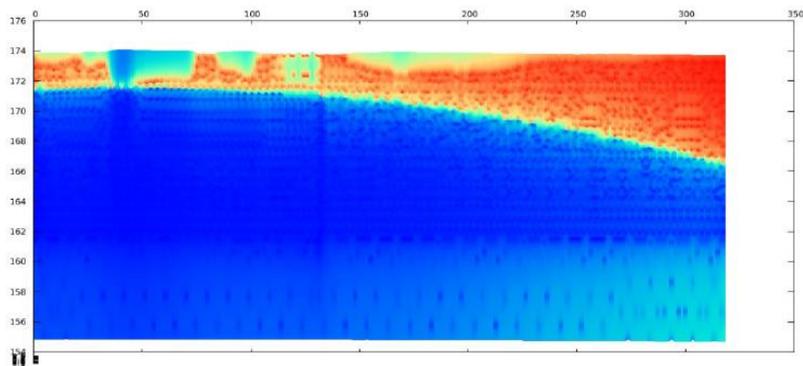
Top: groundwater table during wet periods
bottom: groundwater table during periods of drought

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