




TAKING
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 *Implementation of modePROCON showcasing for karst aquifer - Waidhofen a/d Ybbs, Austria*

 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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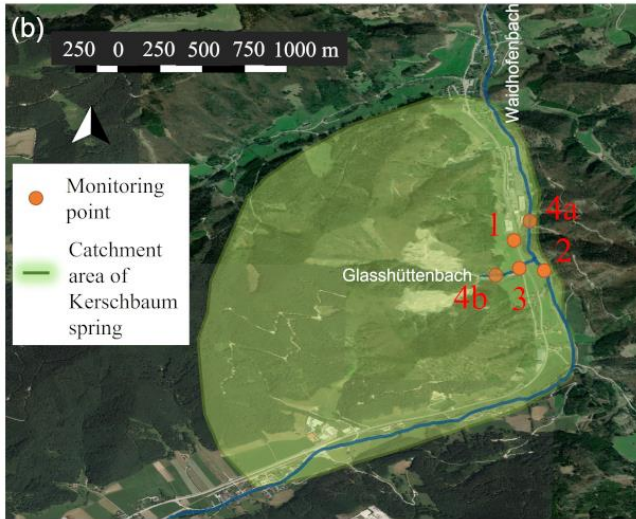
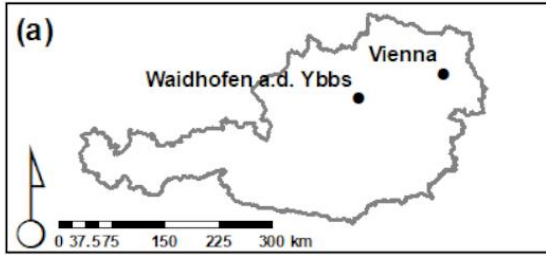
Applying
modePROCON

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Model results



STUDY AREA

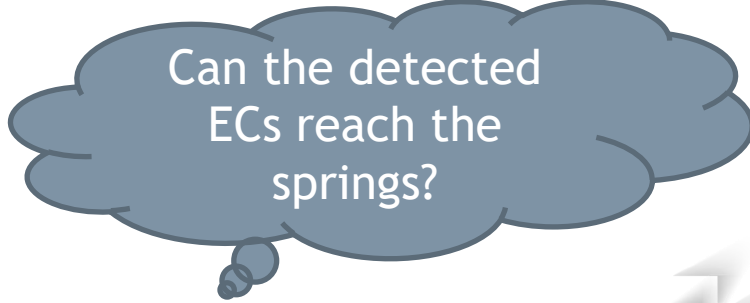


- Investigated aquifers: Waidhofen a/d Ybbs, Austria
- It is composed of the recharge area of one of the main springs exploited for the drinking water supply (Kerschbaum spring)
- Recharge area of the Kerschbaum spring: $\sim 2.5 \text{ km}^2$
- The geology of the study area induced the formation of several karstic springs at different altitudes



DETECTED PPCPs

- The following Emerging Contaminants (ECs) were detected and selected to be modeled in the nearby river and in the groundwater:
 - Diclogenac
 - Methylparaben
 - Valsartan




Can the detected
ECs reach the
springs?



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
64	<input type="checkbox"/> Ketoprofen	22071-15-4	58000.0	2.91	4.23	1.34e-09	4.64	Solubility and logKow and pKa [1...
65	<input type="checkbox"/> Lamotrigine	84057-84-1	150.0	1.24	5.39	1.13e-09	6.23	Solubility and logKow and pKa [1...
66	<input type="checkbox"/> Lovastatin	75330-75-5	8.1	4.31	13.49	3.17e-08	7.6	Solubility and logKow and pKa [1...
67	<input type="checkbox"/> Memantine	19982-08-2	396000.0	3.0	10.79	1.69e-05	802.0	Solubility and logKow and pKa [1...
68	<input type="checkbox"/> Metformin	657-24-9	1000000.0	-1.25	12.27	3.54e-09	4.76	Solubility and logKow and pKa [1...
69	<input checked="" type="checkbox"/> Methylparaben	99-76-3	5600.0	1.88	8.31	2.96e-09	3.56	Solubility and logKow and pKa [1...
70	<input type="checkbox"/> Metoprolol	51384-51-1	1000000.0	1.63	13.89	2.7e-08	4.47	Solubility and logKow and pKa [1...
71	<input type="checkbox"/> Mirtazapine	85650-52-8	9800.0	0.89	8.1	1.51e-06	30.8	Solubility and logKow and pKa [1...
72	<input type="checkbox"/> Naproxen	22204-53-1	15000.0	2.88	4.84	1.06e-09	3.53	Solubility and logKow and pKa [1...
73	<input type="checkbox"/> Naproxen-O-desmethyl	52079-10-4	50000.0	2.25	4.87	1.44e-09	4.51	Solubility and logKow and pKa [1...
74	<input type="checkbox"/> Norfloxacin	70458-96-7	350.0	1.74	0.16	6.03e-11	3.35	Solubility and logKow and pKa [1...
75	<input type="checkbox"/> Norverapamil	67018-85-3	4800.0	3.67	9.79	2.74e-09	8.74	Solubility and logKow and pKa [1...
76	<input type="checkbox"/> Octyl methoxycinnamate (OMC)	5466-77-3	6.4	5.92	nan	1.07e-07	4.9	Solubility and logKow [1] pKa [N...
77	<input type="checkbox"/> Ofloxacin	82419-36-1	180.0	1.86	5.19	1.16e-09	2.26	Solubility and logKow and pKa [1...

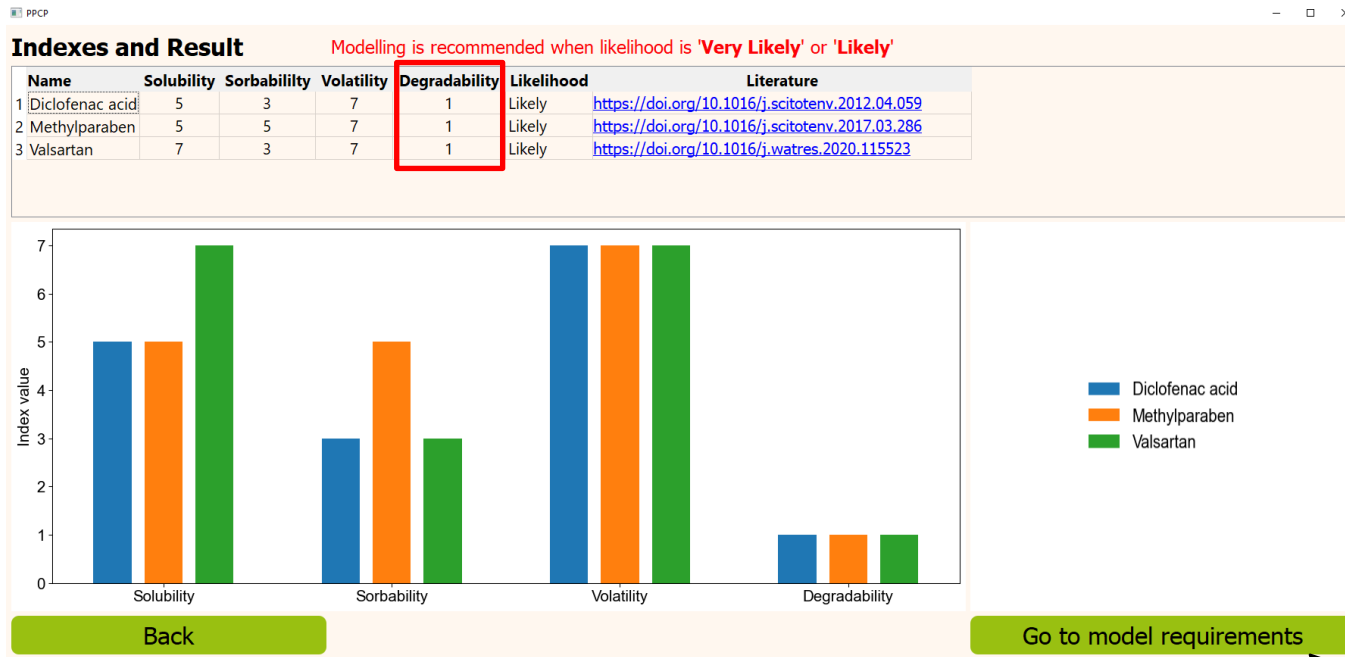
Back Delete all user input Add new data Evaluate

The detected PPCPs Diclogenac, Methylparaben and Valsartan are contained in the database and can be selected simultaneously.



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Probability Estimation

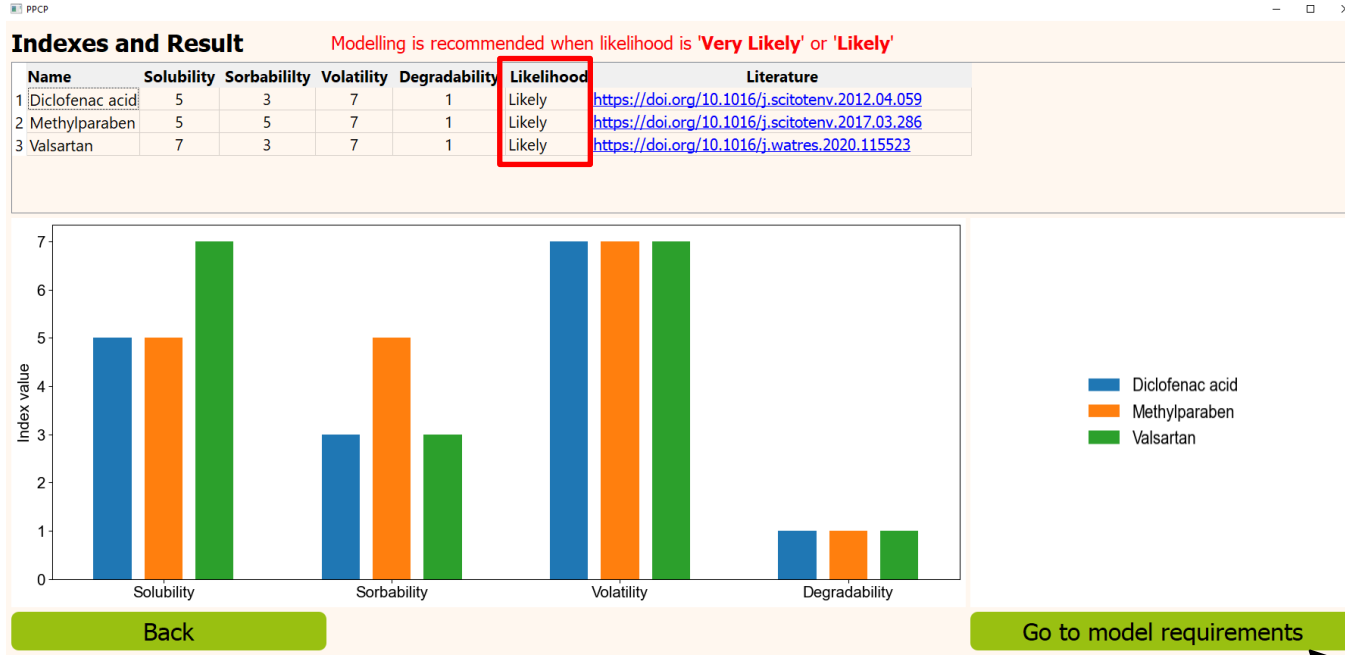


- All the investigated compounds are easily biodegradable.



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Probability Estimation

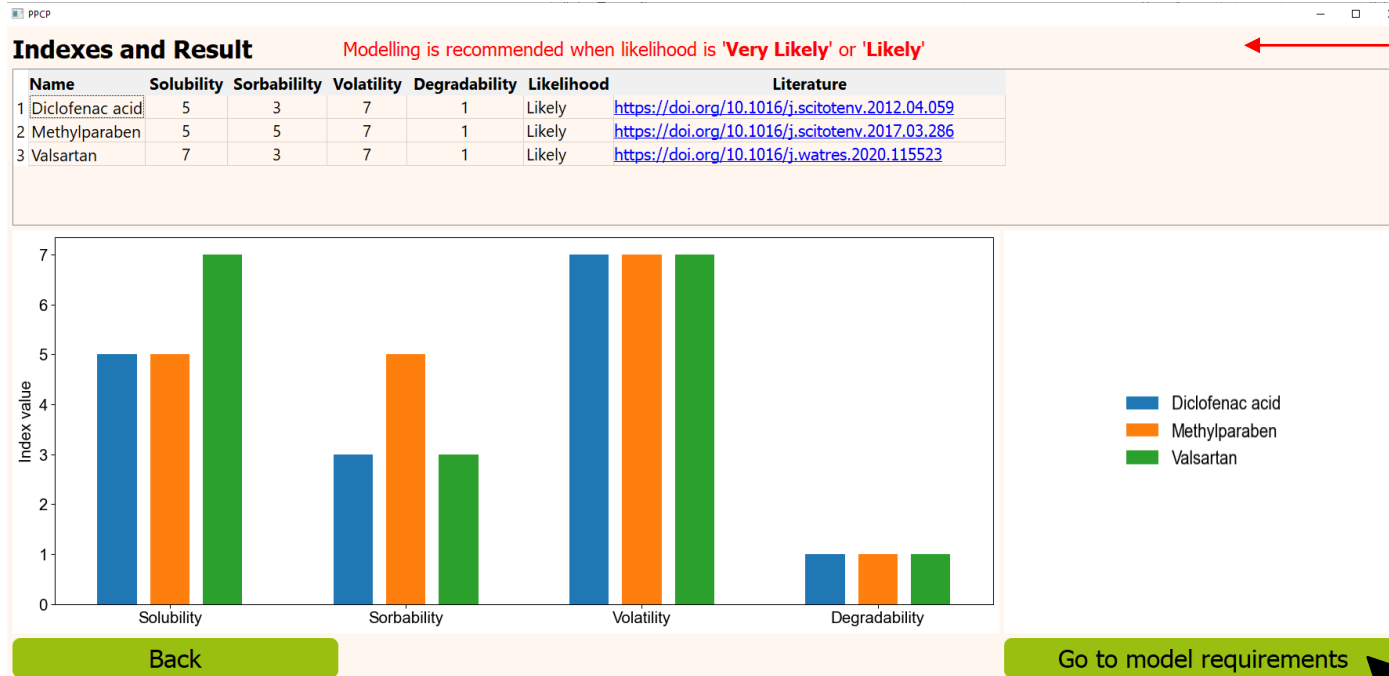


- Due to the high index values, the detection probabilities of **Diclofenac, Methylparaben and Valsartan** are likely.
- This is related to the **low sorption capacity** combined with the **high solubility**.



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Probability Estimation



As all considered PPCPs are likely to be detected in the karst aquifers, modePROCON recommends to model the situation for further investigation.



APPLYING modePROCON

Model requirements

PPCP

Karst aquifer model requirements

[Evaluate](#)

Please check the available parameter to evaluate

	Parameter	Application	Remark
3 <input checked="" type="checkbox"/>		potentially useful information concerning aquifer geometry, recharge, retention time underground and water circulation.	
4 <input checked="" type="checkbox"/>	Air temperature	The spatial-temporal discharge pattern in the conduits, fracture networks and matrix is strongly controlled by temperature variations.	
5 <input checked="" type="checkbox"/>	Precipitation	It influences the infiltration discharge and electrical conductivity and it is a source of recharge. The water levels and spring discharge can change rapidly in response to rainfall.	
6 <input type="checkbox"/>	Source of contamination and initial concentration of the contaminant	They are needed to set initial conditions to solve the transport equation and define the contaminant sources and releases.	
7 <input checked="" type="checkbox"/>	Catchment area	It is required to define the catchment area of a potential contaminant source.	
8 <input checked="" type="checkbox"/>	Point of interest	Physical locations that are likely to be exposure pathway to come into contact with a contaminated medium.	

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- 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.

PPCP

Karst aquifer model requirements

Evaluate

Model cannot be built. Please collect the missing data.

Please check the available parameter to evaluate

	Parameter	Application	Remark
4	<input checked="" type="checkbox"/> Air temperature	The spatial-temporal discharge pattern in the conduits, fracture networks and matrix is strongly controlled by temperature variations.	The data are available.
5	<input checked="" type="checkbox"/> Precipitation	It influences the infiltration discharge and electrical conductivity and it is a source of recharge. The water levels and spring discharge can change rapidly in response to rainfall.	The data are available.
6	<input type="checkbox"/> Source of contamination and initial concentration of the contaminant	They are needed to set initial conditions to solve the transport equation and define the contaminant sources 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.

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Model requirements

PPCP

Karst aquifer 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

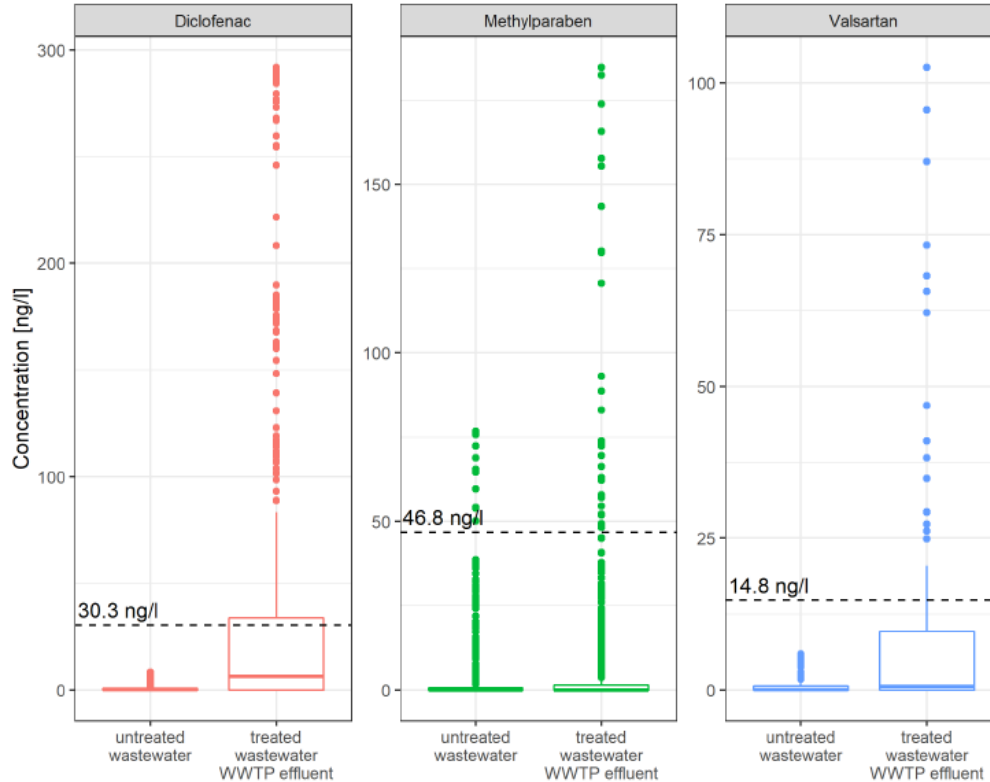
	Parameter	Application	Remark
3	<input checked="" type="checkbox"/> Air temperature	The spatial-temporal discharge pattern in the conduits, fracture networks and matrix is strongly controlled by temperature variations.	The data are available.
4	<input checked="" type="checkbox"/> Precipitation	It influences the infiltration discharge and electrical conductivity and it is a source of recharge. The water levels and spring discharge can change rapidly in response to rainfall.	The data are available.
5	Source of contamination and initial concentration of the contaminant	They are needed to set initial conditions to solve the transport equation and define the contaminant sources and releases.	The data are available.
6	<input checked="" type="checkbox"/> Source of contamination and initial concentration of the contaminant	They are needed to set initial conditions to solve the transport equation and define the contaminant sources and releases.	The data are available.
7	<input checked="" type="checkbox"/> Capture area	It is required to define the catchment area of a potential contaminant source.	The data are available.
8	<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.

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- In this case, two scenarios were assumed.
- Scenario 1: untreated wastewater as contamination source
- Scenario 2: WWTP-effluent as contamination source
- 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



Estimated concentrations in the spring from scenario analysis

- The model results indicate that infiltration of surface water from the Waidhofenbach (contaminated by treated wastewater) is much **more plausible** as a source for the detected concentrations in the Kerschbaum spring compared to the alternative source from leakage of a sewer system or septic tank.

