Global Sensitivity Analysis for a MACRO meta-model for Swedish drinking water abstraction zones

Thorsten Pohlert[1], **Stefan Reichenberger**[2], Sebastian Multsch[1*],
Nicholas Jarvis[3], Mikaela Gönczi[3]

[1] knoell Germany GmbH, [2] knoell France SAS, [3] Swedish University of Agricultural Sciences (SLU), * present affiliation: BASF SE

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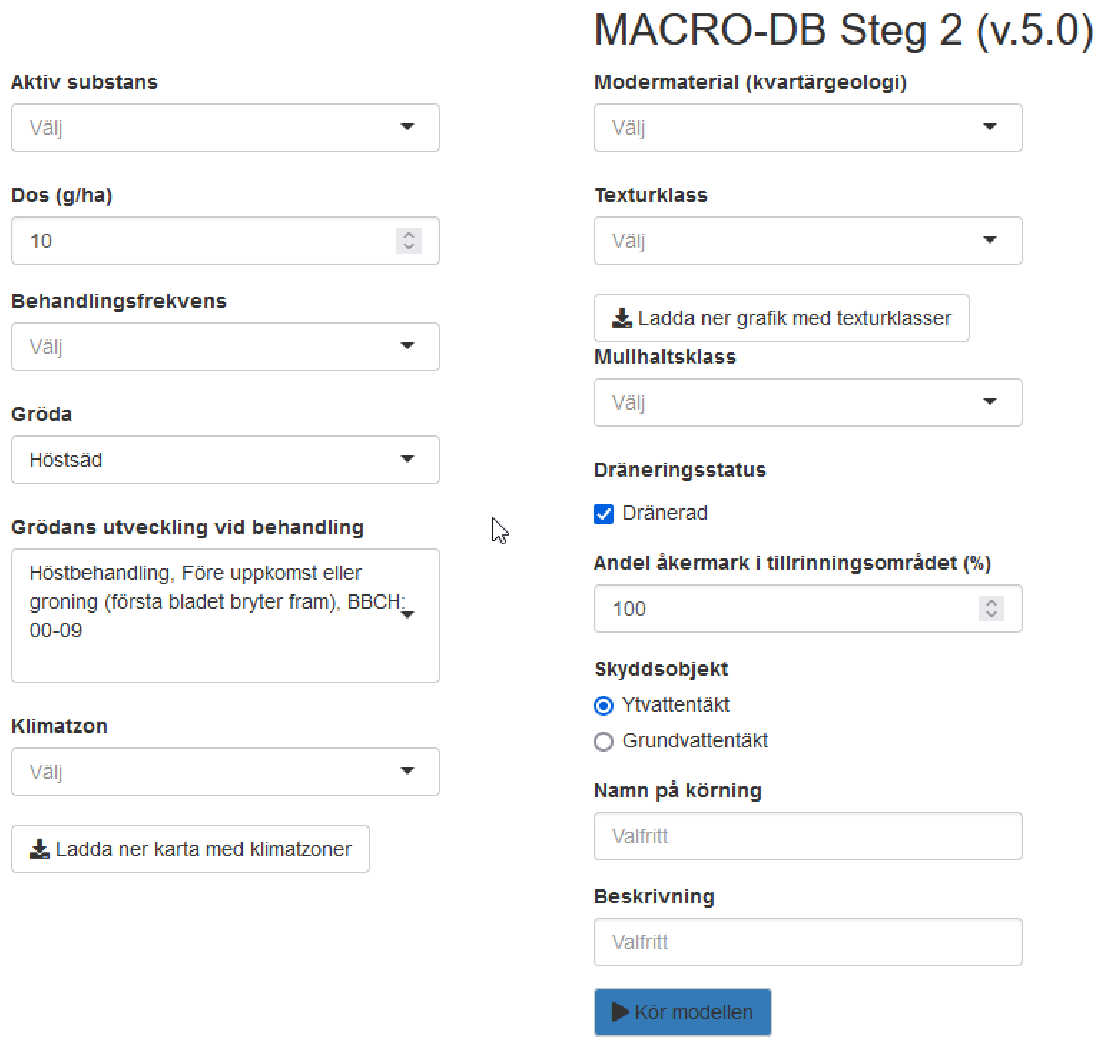
Background

- In Sweden farmers are legally obliged to apply for permits for pesticide use if their land lies within a drinking water abstraction zone.
- The standalone modelling tool MACRO-DB 4 by SLU is available for risk assessment and decision support.
- MACRO-DB 4 is based on the well-established leaching model MACRO 5.2 (Larsbo and Jarvis, 2003).
- Recently, a robust meta-model of MACRO-DB 4 was developed and integrated in a web-based tool (MACRO DB Steg2 v.5).

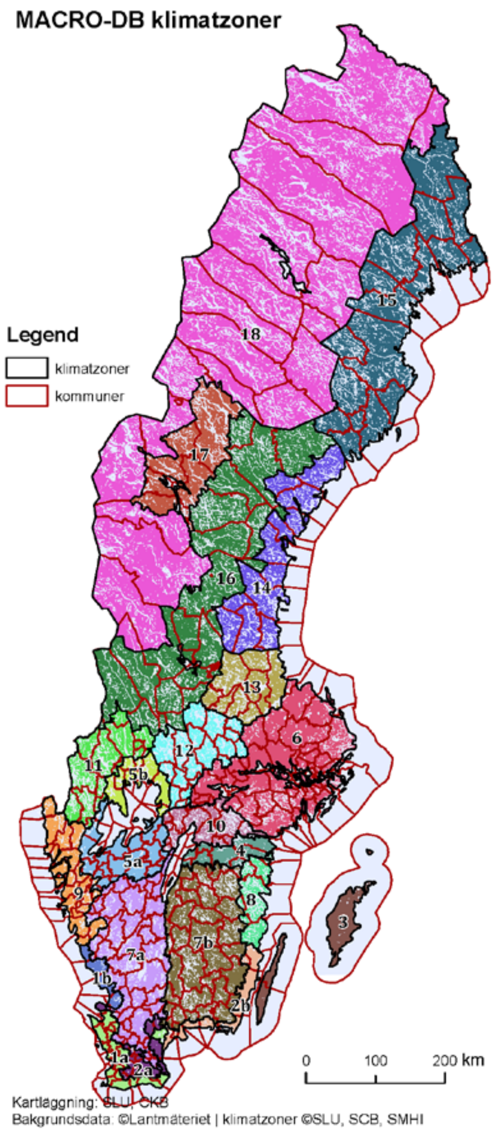


The MACRO meta-model

- The meta-model (Reichenberger et al., 2021) is based on 583200 MACRO simulations for the whole agriculturally relevant area of Sweden.

- The simulations comprised
  - 18 climates
  - 72 soils,
  - 1 typical crop,
  - 3 application seasons, and
  - 150 dummy compounds.

- The meta-model performs a trilinear interpolation (in the space of Koc, DT50 and nf) for log10 of Predicted Environmental Concentrations (PEC) in groundwater or surface water, respectively.



Objective

- The objective of this study was to determine the most important factors influencing predicted pesticide concentrations in drinking water resources in Sweden.

- For this aim, a Global Sensitivity Analysis (GSA) was conducted for the MACRO meta-model.

Materials and Methods

- A variance-based GSA was performed using the Sobol' method (Sobol', 1993; Gatel et al., 2019).
- This method works also for non-linear, non-monotonic and non-additive models and allows
  1) identification of first-order (direct) and higher-order (interaction) effects for each input factor, and
  2) ranking of the input factors according to their importance.

- All calculations were done in R.

- For Sobol' quasi-random sampling and calculating Sobol' sensitivity indices we used the script sobol_sensitivity from JRC (Zambrano-Bigiarini, 2013).

GSA setup: Target variables and constant factors

- Target variables
  - Groundwater: 20-year mean leaching flux concentration at 2 m depth

    PECgw = (total pesticide leaching)/(total percolation)

  - Surface water: 20-year mean concentration in water entering surface water

    PECsw = (total losses via drainage and leaching)/(total drainflow and percolation)

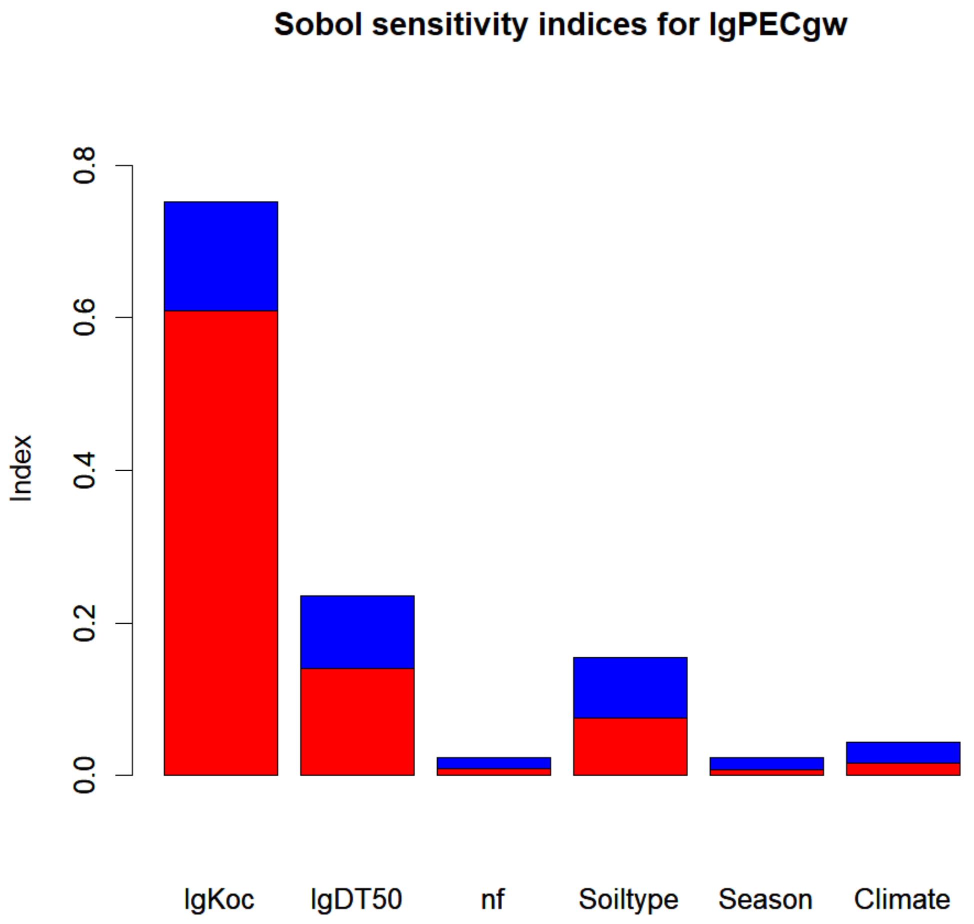
- Constant factors
  - application rate: 1000 g/ha
  - application frequency: 1 application every year
  - proportion of arable land in the catchment: 100 %
  - pesticide interception fraction: 0

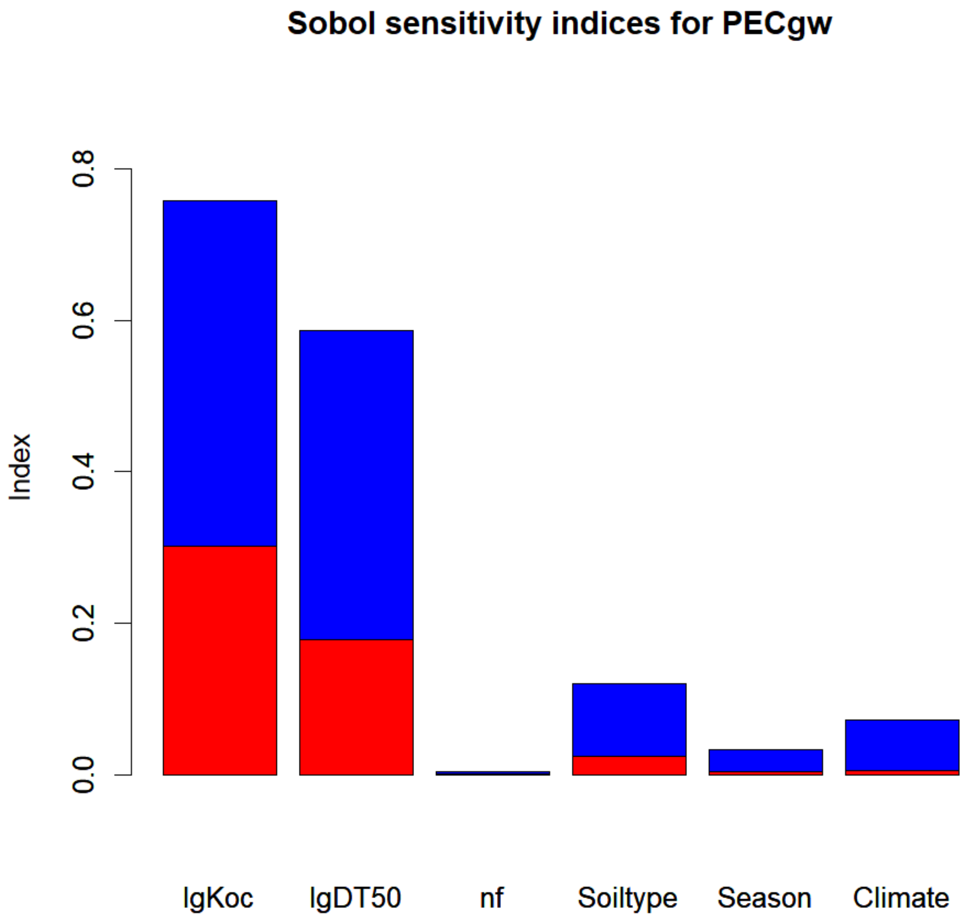
GSA setup: Input factors

Input factors included in the GSA and their distributions

factor	description	type of distribution	range of values
lgKoc	logarithmic normalized Freundlich coefficient	uniform	min = $\log_{10}(3)$; max = $\log_{10}(10000)$
lgDT50	logarithmic degradation half-life in soil at ref. conditions	uniform	min = $\log_{10}(3)$; max = $\log_{10}(200)$
nf	Freundlich exponent	uniform	min = 0.75; max = 1
Soiltype	soil type	discrete uniform	72 soils for SW; 57 for GW
HSG	hydrological class	discrete uniform	4 values for SW (L, W, U, Y); 3 for GW (L, W, Y)
TXT	texture class	discrete uniform	5 values (1, 2a, 2b, 3, 4)
HR	presence of hard rock in subsoil	discrete uniform	2 values (presence, absence)
OMC	organic matter class	discrete uniform	3 values (low, normal, high)
Season	application season	discrete uniform	3 values (spring, summer, autumn)
Climate	climate zone	discrete uniform	18 climates

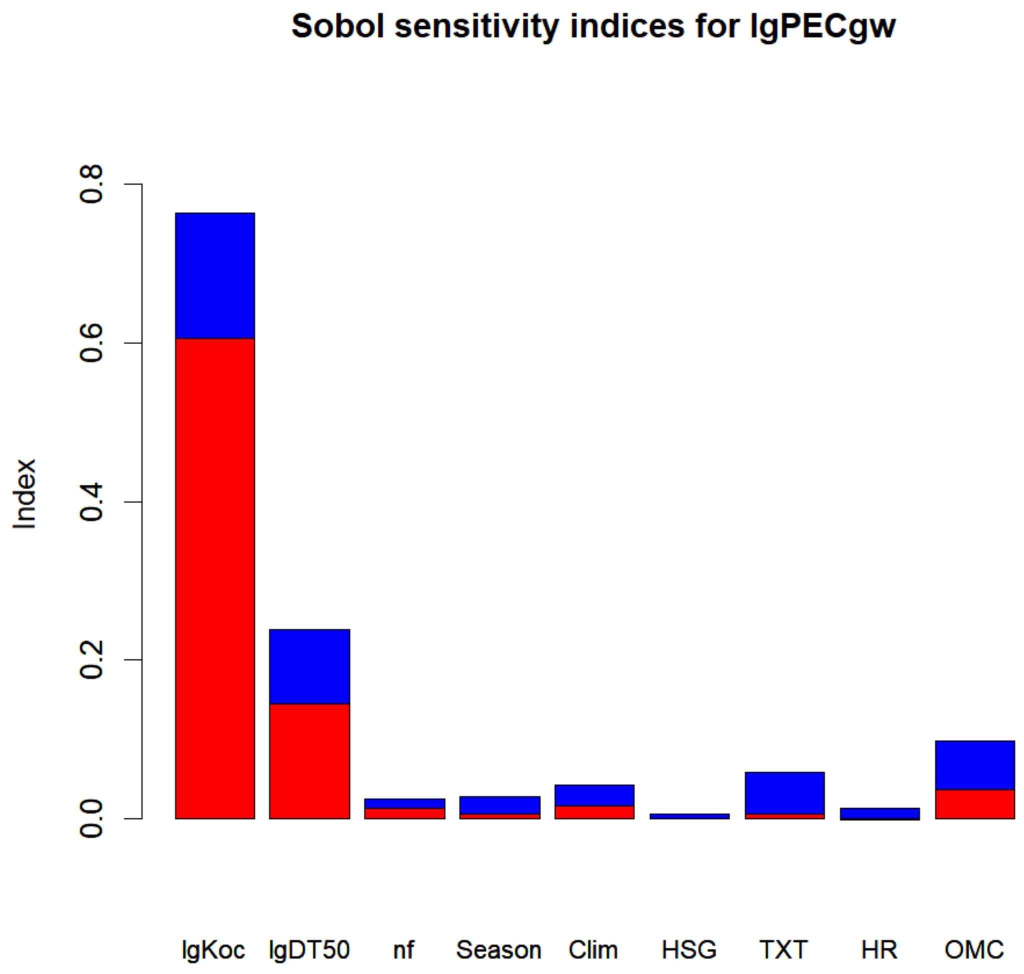
Results: Sobol‘ indices for PECgw using soil IDs

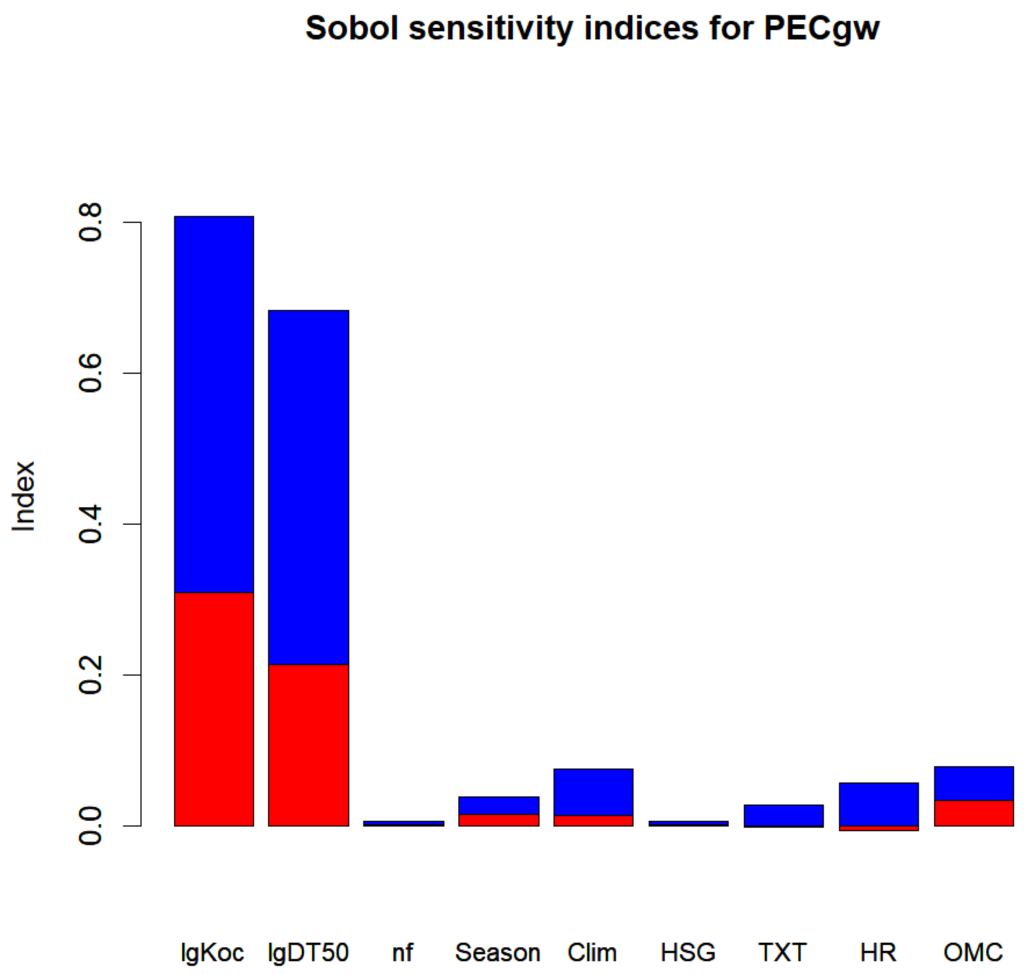




Whole column: total sensitivity index STi; red: first-order sensitivity index Si

Results: Sobol‘ indices for PECgw using soil variables





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Discussion

- Notable difference in Sobol' indices between logarithmic and non-log PEC, but little difference between groundwater and surface water.

- Non-additivity (interactions between input factors) higher for non-log PEC than for logarithmic PEC:
  - non-log PEC : Sum of first-order indices Si < 0.58
  - log PEC: Sum of Si > 0.82

- The most important factors are lgKoc > lgDT50 > soil > climate.

- When the soil ID is split into four variables, the organic matter class (affecting sorption) is the most important of them.

- Influence of hydrological class HSG very small. Explanation:
  - The hydrological class mainly affects the proportion of excess water routed to SW vs. GW, not so much concentrations in leachate and drainflow
  - Dilution (mixing) with water originating from other soils not taken into account in calculation of target variables

Conclusions

- The Global Sensitivity Analysis of the MACRO meta-model revealed that substance sorption and degradation parameters were the most important factors influencing Predicted Environmental Concentrations in Swedish drinking water resources.
- Soil type, climate zone and application season were much less important than compound parameters.
- However, the effects of soil hydrology and climate may be underestimated because we did not account for mixing with water from other sources → absolute water and solute fluxes are less important than concentrations in leaching and drainflow.
- Global Sensitivity Analysis combined with meta-modelling is a very useful tool for analyzing complex, non-linear, non-monotonic and non-additive environmental models.

Many thanks for your attention!

Supplementary slides

References

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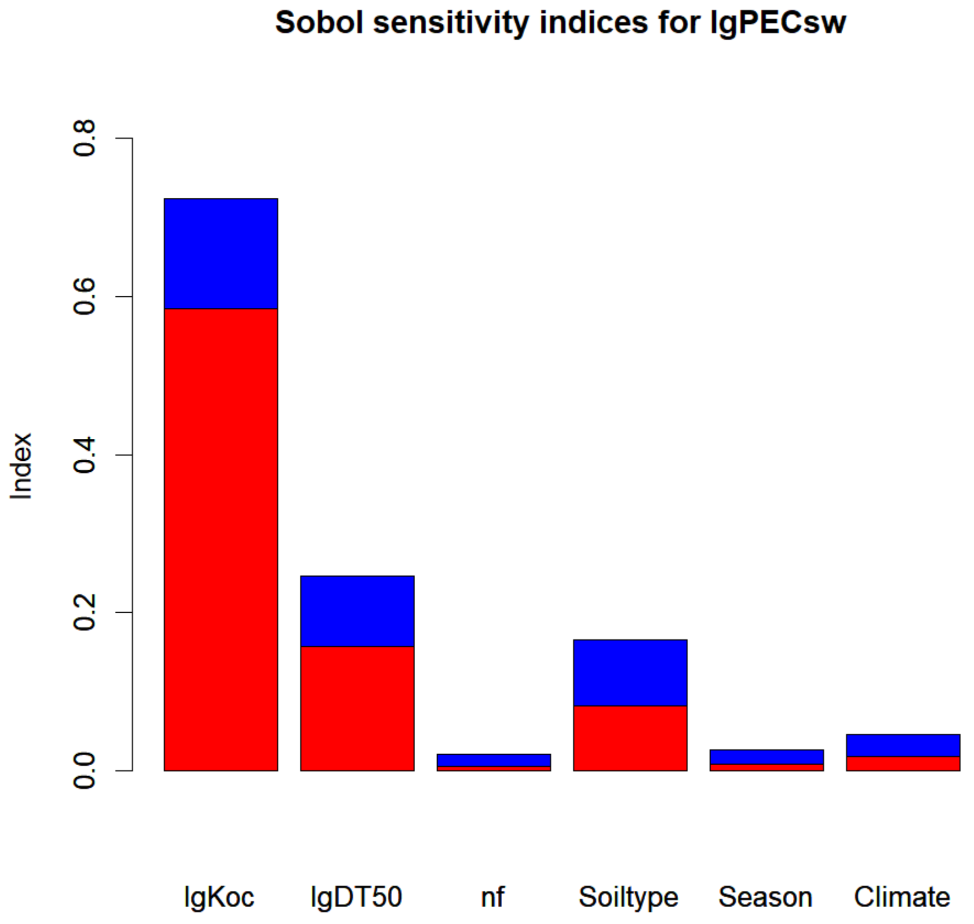
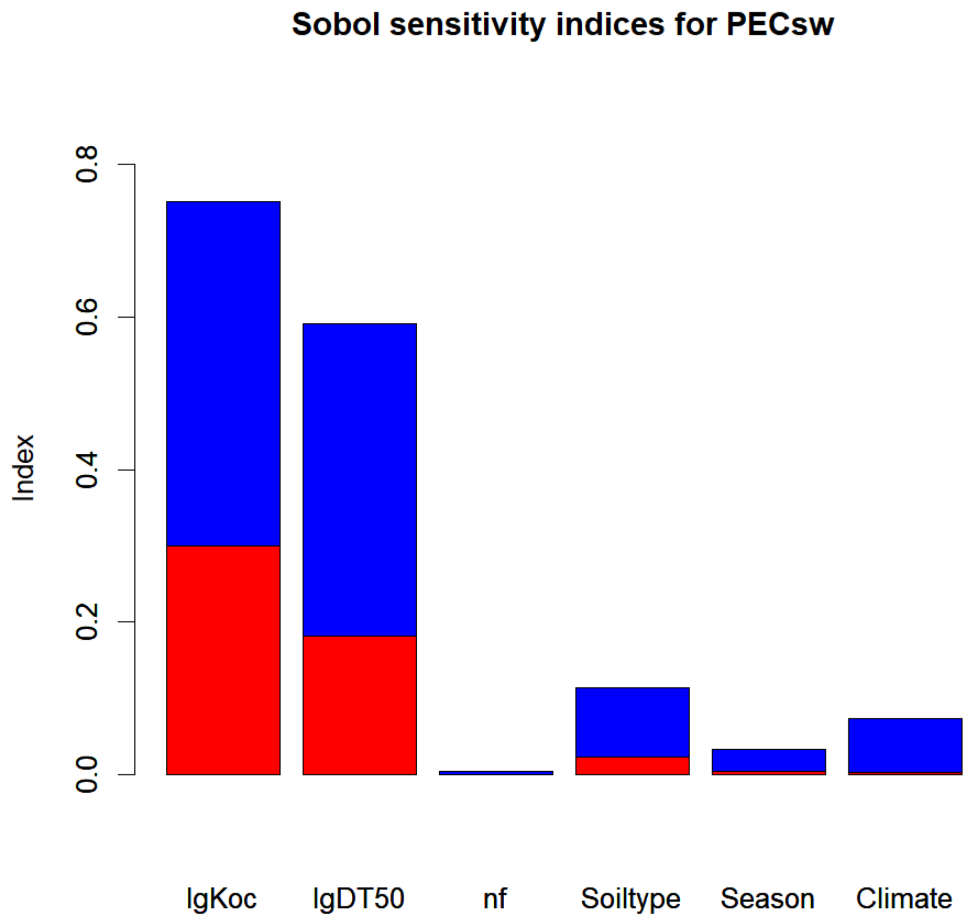
Zambrano-Bigiarini M (2013). sobol_sensitivity.R. https://joint-research-centre.ec.europa.eu/document/download/

Results: Sobol‘ indices for PECsw using soil IDs





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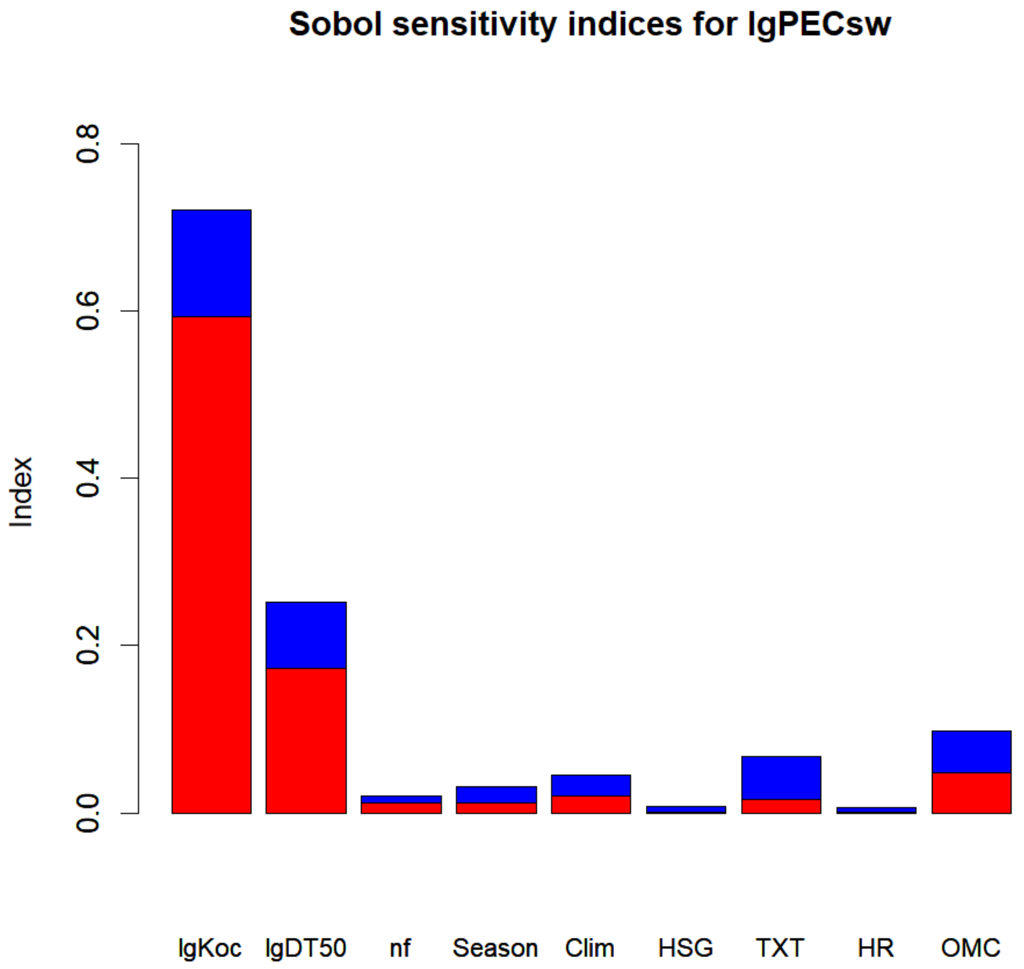
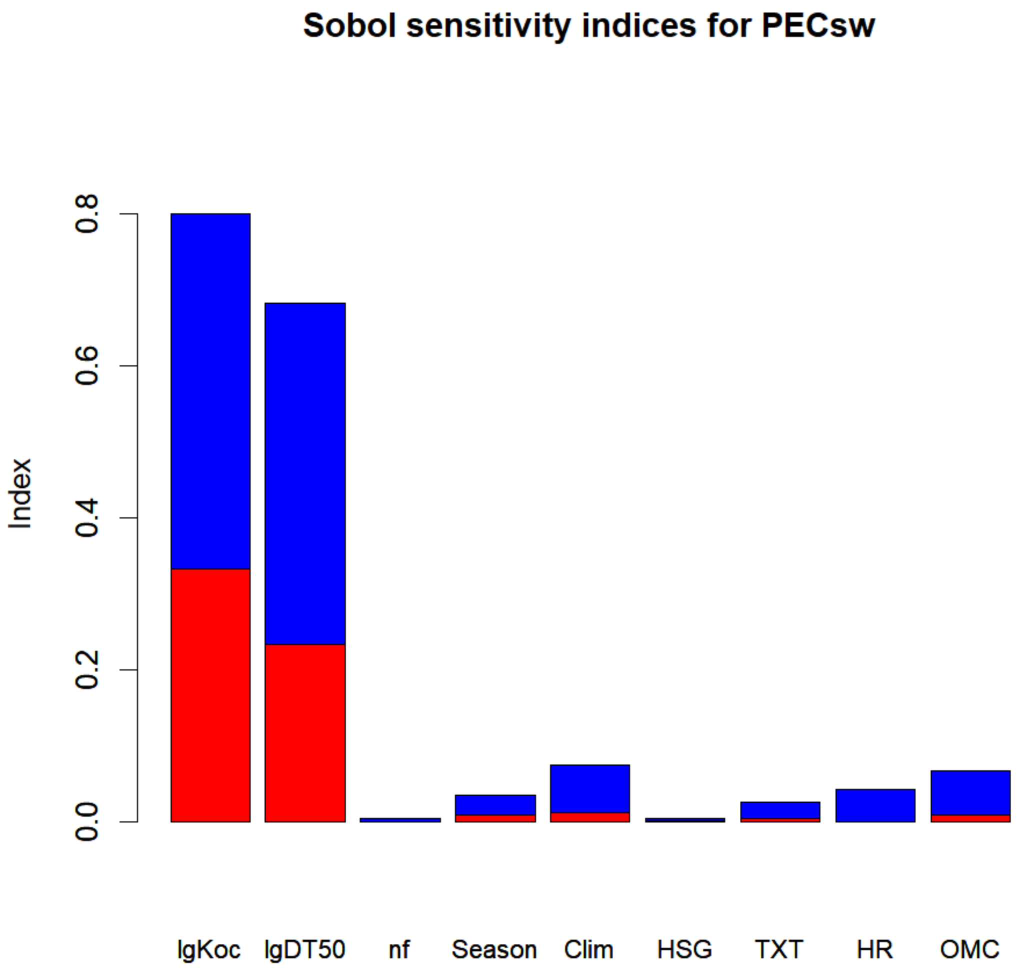
Results: Sobol‘ indices for PECsw using soil variables





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