Reduction of Complexity: Variance-based Sensitivity Analysis for FOCUS STEPS 1-2

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FOCUS STEPS

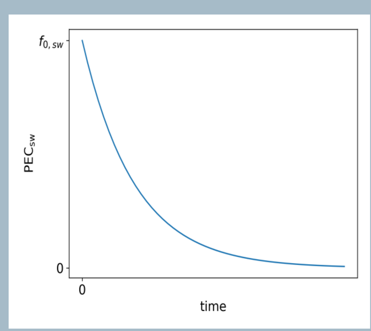
- STEPS (Surface water Tool for Exposure Prediction) [1] is used for derivation of PEC values in water and sediment based upon the chosen scenario
- Requires a minimum of input values. Sorption Koc, Half-life DT50, application methods
- STEPS-1&2 is comprised of a set of analytical formulae

Sensitivity Analysis

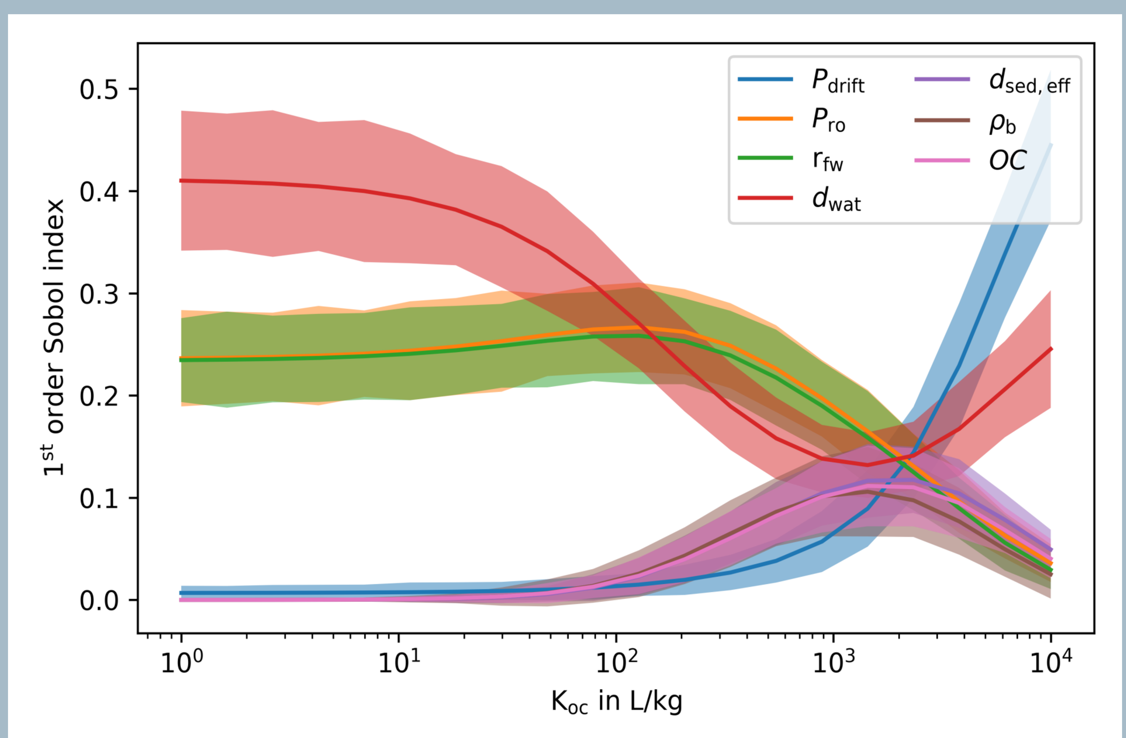
- Variance based sensitivity analysis (SA) examines the impacts of variations of input parameters on the variance of output parameters
- In Sobol' method [2,3], parameters are sampled in a flat distribution within a defined interval
- Sobol indices show the relevance of a parameter on the output variables.
- They are calculated to arbitrary orders by varying sets of parameters
- The 1st order Sobol index measures the impact by varying one parameter alone

STEPS 1: One instant loading via drift and runoff/drainage. Water and sediment are separate. One half-life for the system.

- Solely the sorption constant Koc drives PEC_{max}
- $P_{drift}(crop)$ and $P_{ro} = const$ as fractions of application rate



SA – Parameter impacts on PECmax with varying Koc



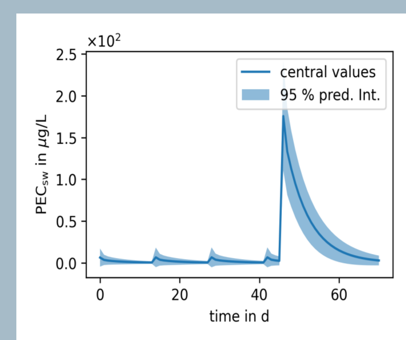
Parameter	Explanation
P_{drift}	Percentages of the substance that enter the water body via drift
P_{ro}	Percentages of the substance that enter the water body via runoff/drainage
d_{wat}	Depth of the water body
$d_{set,eff}$	Effective depth of the sediment
r_{fw}	Ratio of field to water body
ρ_b	Bulk density
OC	Content of organic carbon

Results

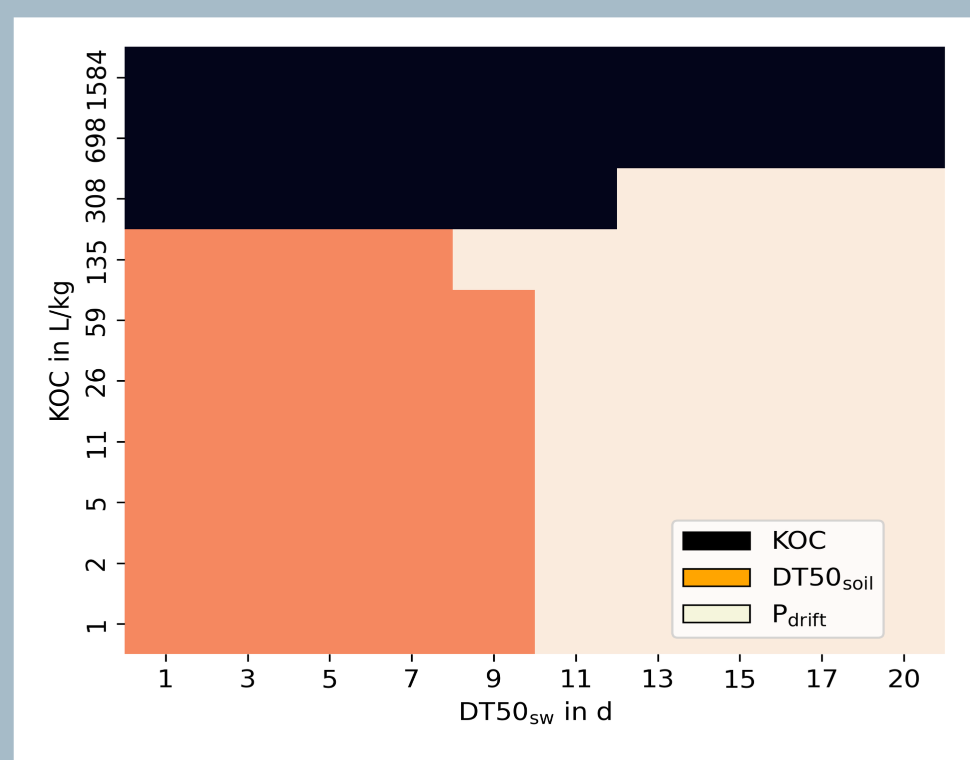
- Vary fixed scenario parameters between 0.5 and 2 times the central value. Vary dependent scenario parameters between their minima and maxima. Only one parameter is varied at a time. Keep Koc as an independent variable
- Depicted are the impacts when PEC_{max} is reached, i.e. at simulation day 1
- For Koc < 100 L/kg: Runoff/drainage parameters are most relevant
- For Koc > 5000 L/kg: Runoff/drainage becomes less relevant and drift more important. Water depth remains relevant as a global parameter
- Foc Koc ≈ 2000 L/kg: no clear dominant parameters can be identified

STEPS 2: Multiple loadings via drift and one via runoff/drainage. Exchange between water and sediment. Individual half-lives.

- Storm event four days after last application triggers runoff/drainage event
- $P_{drift}(crop, N_{app})$ and $P_{ro}(\text{Region/Season})$ as fractions of application rate



SA – 2nd most sensitive parameters in phase space



Results

- Vary central values of Koc and $DT50_{sw}$ to examine different regions in the parameter phase space
- User defined parameters (Koc, $DT50_{sw/sed/soil}$, P_{drift}, P_{ro}) are varied in intervals around central values
- P_{ro} is most relevant parameter in considered phase space (largest 1st order Sobol index)
- High Koc: Koc has a large interval. Large variance results in high relevance
- Low Koc: $DT50_{soil}$ affects runoff input exponentially. For high $DT50_{sw}$, P_{drift} is relevant as drift input is not fully degraded

Conclusions & Outlook

- High sensitivity of a parameter indicates significant influence on the model's response to variations
- STEPS-1&2: Runoff parameters are most relevant for PEC_{max} in most cases
- In phase space regions with high Koc and high $DT50_{sw}$, P_{drift} becomes more relevant
- Mitigating uncertainties of relevant user input parameters becomes crucial
- Spatial distribution of scenario parameters should be considered
- STEPS 3 introduces more parameters and needs more computation time. Partial exploration of the parameter phase space is envisaged.

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[1] FOCUS. 2001. FOCUS Surface Water Scenarios in the EU Evaluation Process under 91/414/EEC. Report of the FOCUS Working Group on Surface Water Scenarios, EC Document Reference SANCO/4802/2001-rev.1. 221 p.
[2]I M. Sobol'. 2001. Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates. Mathematics and Computers in Simulation 55:271-280
[3] A. Saltelli, et al. 2007. Global Sensitivity Analysis. The Primer. Hoboken (NJ), USA: John Wiley & Sons, Ltd. 304 p.

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