SUN

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Sustainable Nanotechnologies

European SUN project on “Sustainable Nanotechnologies” of the EU 7th Framework funding.

Stochastic software for (env.)exposure, (eco)tox and (env.)risk

Fadri Gottschalk

ENM Basel 10.02.2016

Outline

Ecotox

- User tool on PSSD (probabilistic species sensitivity distributions)

  Briefly something to the method

  R-package (incl. version for Excel users)

  GUI (graphical user interface)

Environmental release/exposure/(risk)

- User tool on PMFA (probabilistic material flow analysis)

  Briefly something to the method

  R-package (incl. version for Excel users)

  GUI

- Discussion on strengths and next improvement steps, terms of use

PSSD tools

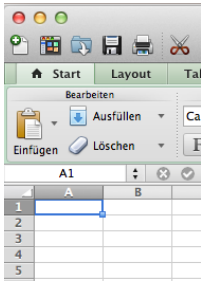
Probabilistic Species Sensitivity Distribution (PSSD) Package

Documentation for package ‘PSSD’ version 1.0.0

- DESCRIPTION file.

Help Pages

createPNECModell	createPNECModell
createPSSDModell	createPSSDModell
loadSpeciesDataFromExcel	loadSpeciesDataFromExcel
plotCdf	plotCdf
plotPdf	plotPdf
plotPdfPNEC	plotPdfPNEC
rawSpeciesData	rawSpeciesData
triangulsimleft	triangulsimleft
triangulsimright	triangulsimright



PSSD input

Add Species

Name of species

Select endpoint

NOEC

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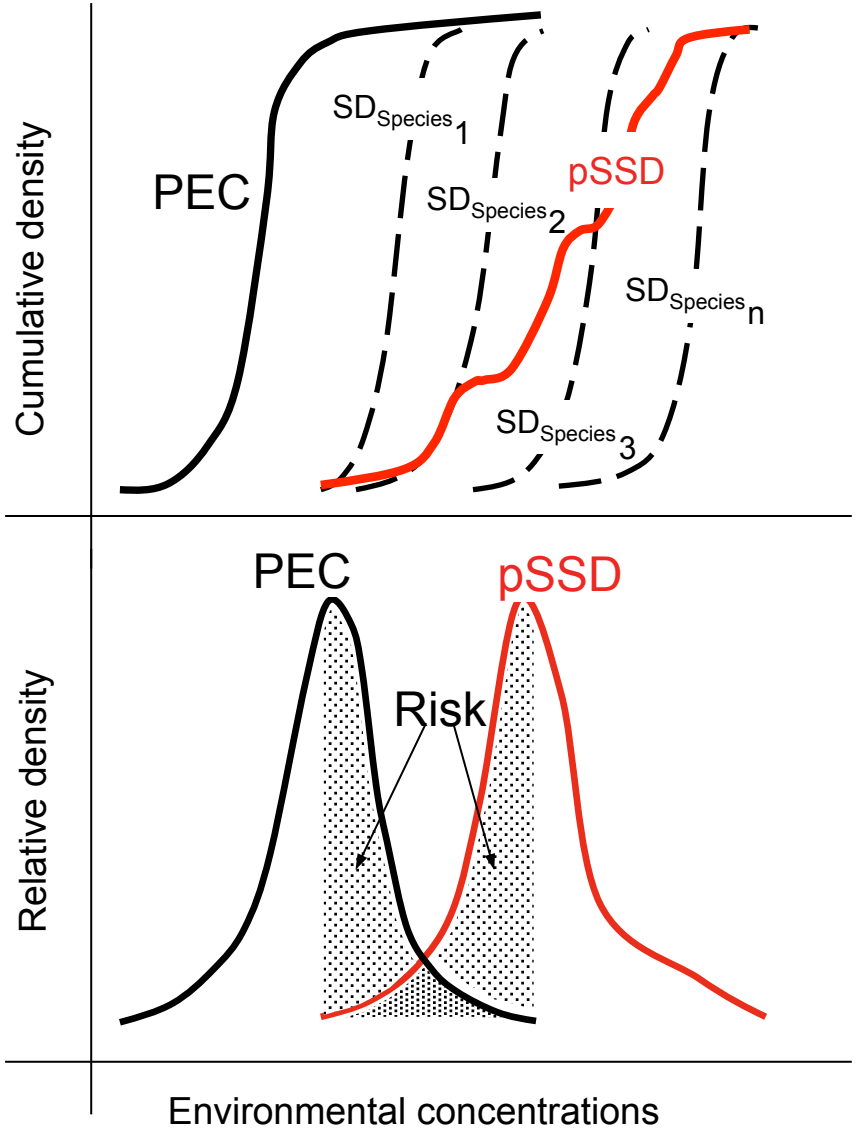
Probabilistic Species Sensitivity Distributions (PSSD) modeling: for risk calculation



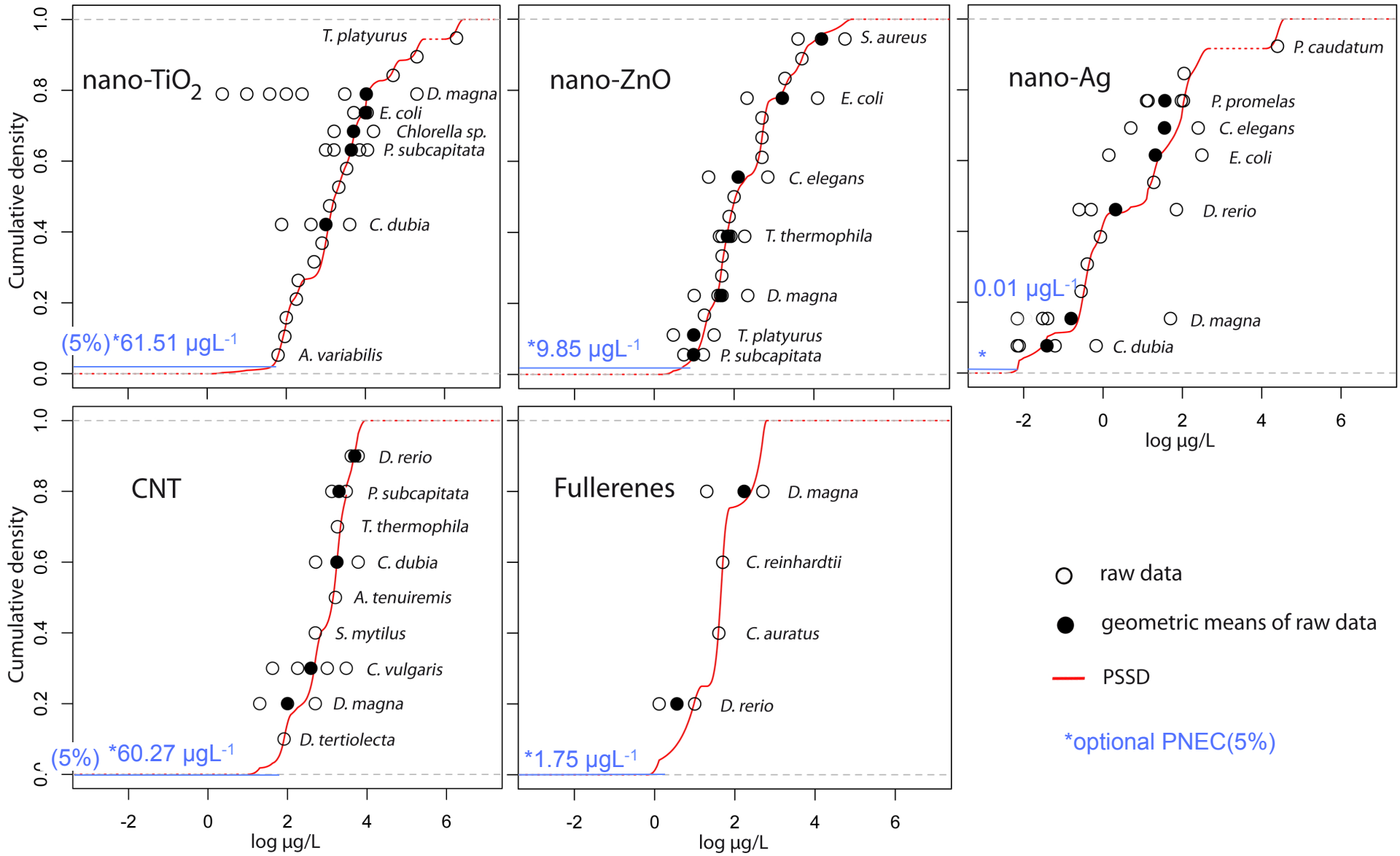
Wang et al. 2016. Science of the Total Environment.

Coll et al. 2015. Nanotoxicology.

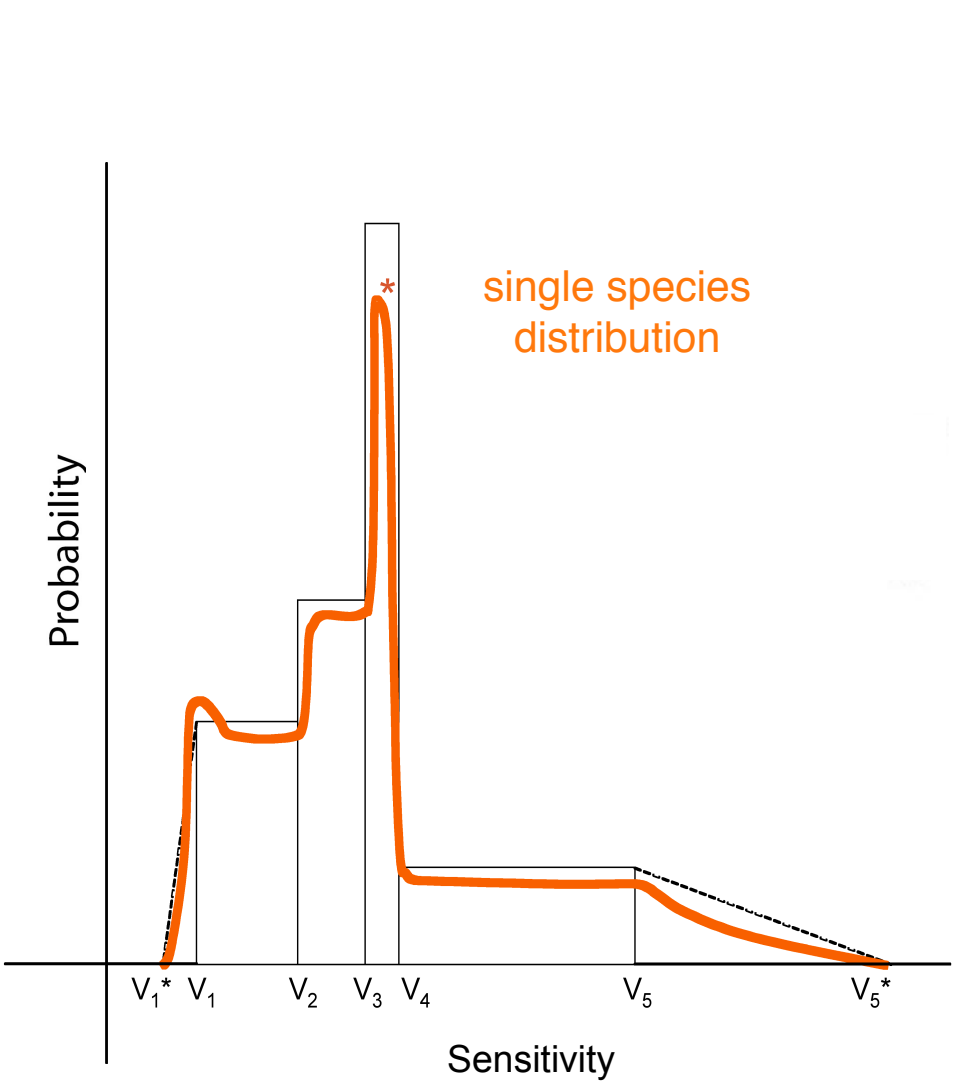
Gottschalk & Nowack 2013. Integrated Environmental Assessment and Management.

Gottschalk et al. 2013. Environ. Toxicol. Chem.

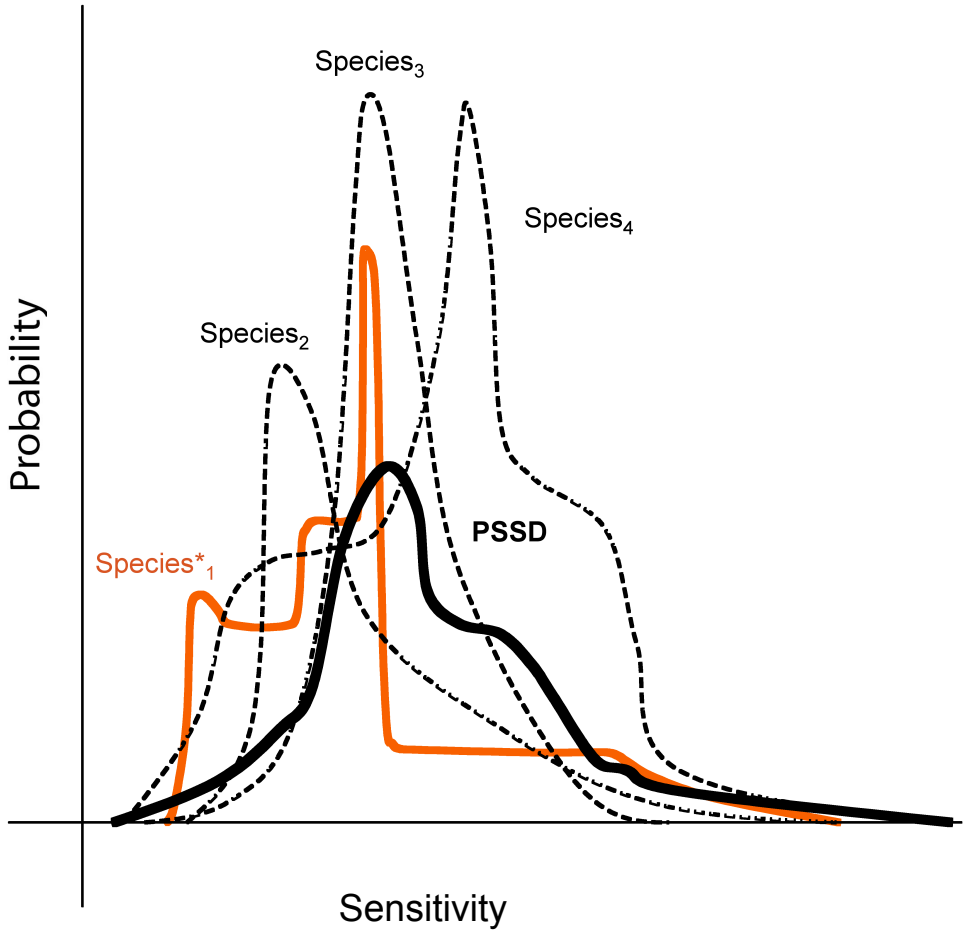
First PSSD simulations in 2013



Modeling procedure



PSSD for species (representing an environmental compartment)



Data needed for PSSD

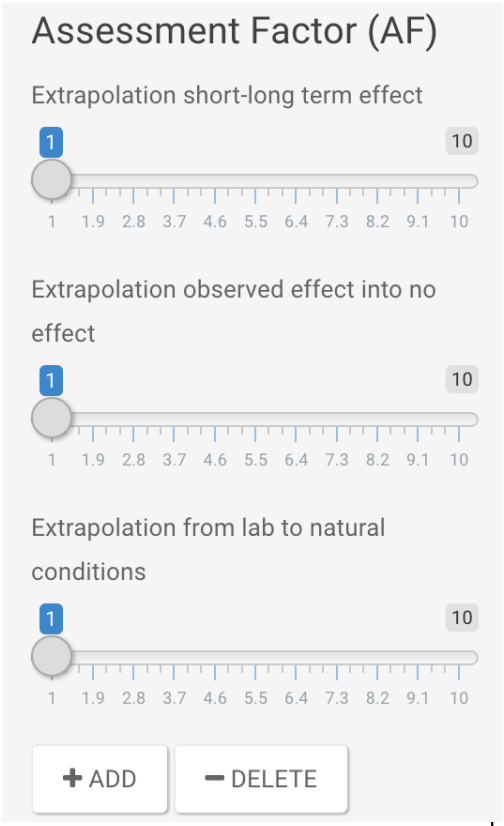
1. Toxicological endpoints and assessment factors (AF)

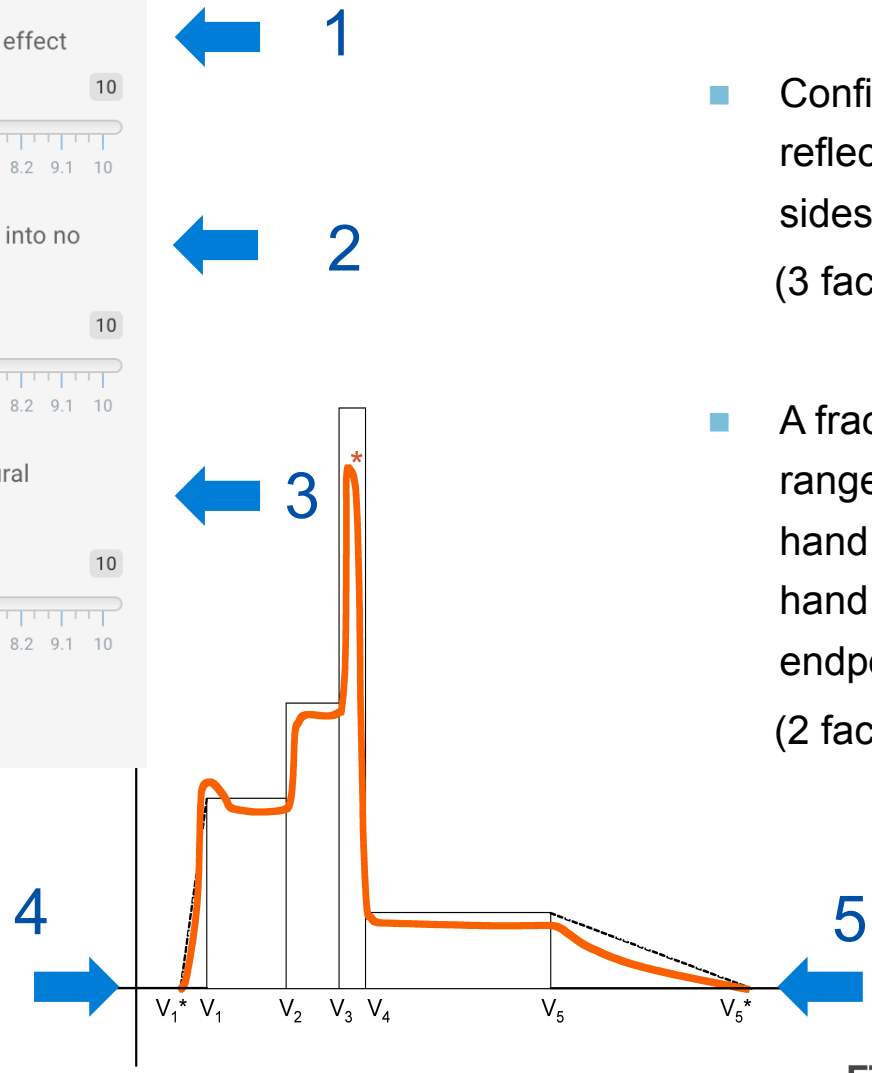
Data Table | Plot VPSSD | Plot VPNEC

	Species name	Toxic Endpoint	Concentration	Unit of Endpoint	AF short-long	AF observed-effect	AF lab-nature	Species Sensitivity
1	Curcubita pepo, zucchini	HONEC	5000000	micro/l	1	1	1	5e+06
2	Eisenia veneta, earthworm	EC50	176000	micro/l	1	10	1	17600
3	x	LC50		micro/l	1	1	1	
4	x	LC50		micro/l	1	1	1	
5	x	LC50		micro/l	1	1	1	

2. Uncertainty and variability on such data (as shown in the next slide)

Assessment factors (uncertainty/variability factors) for PSSD

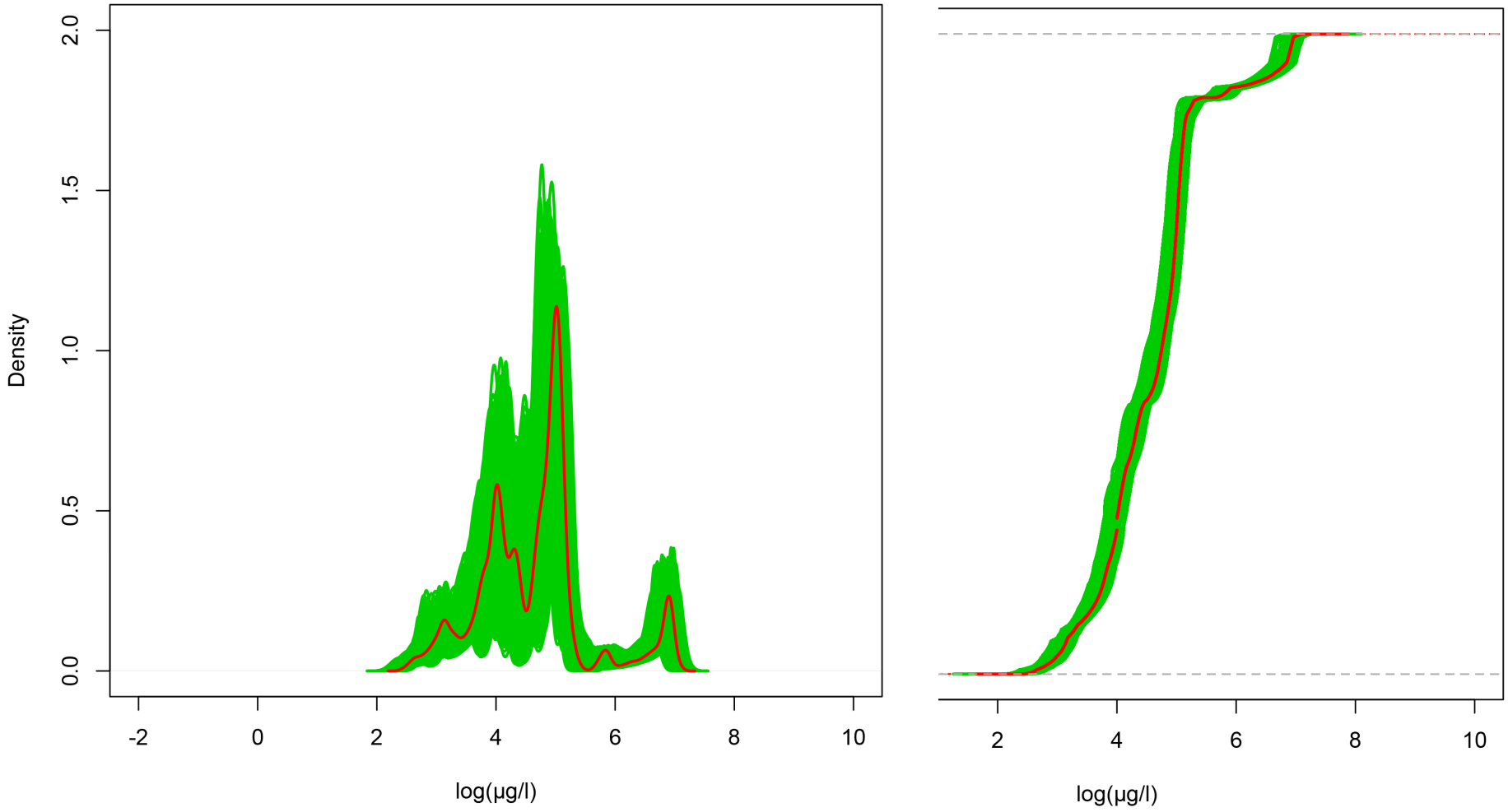




- Confidence intervals as a fraction that reflects the uncertainty range on both sides of the assessment factors (3 factors)
- A fraction that reflects the uncertainty range (confidence interval) on the left hand side of the lowest and the right hand side of the highest toxicological endpoint used for one single species (2 factors)

Typical PSSD simulation outputs

Exercise output based on unadjusted Empa data for nano-SiO_2



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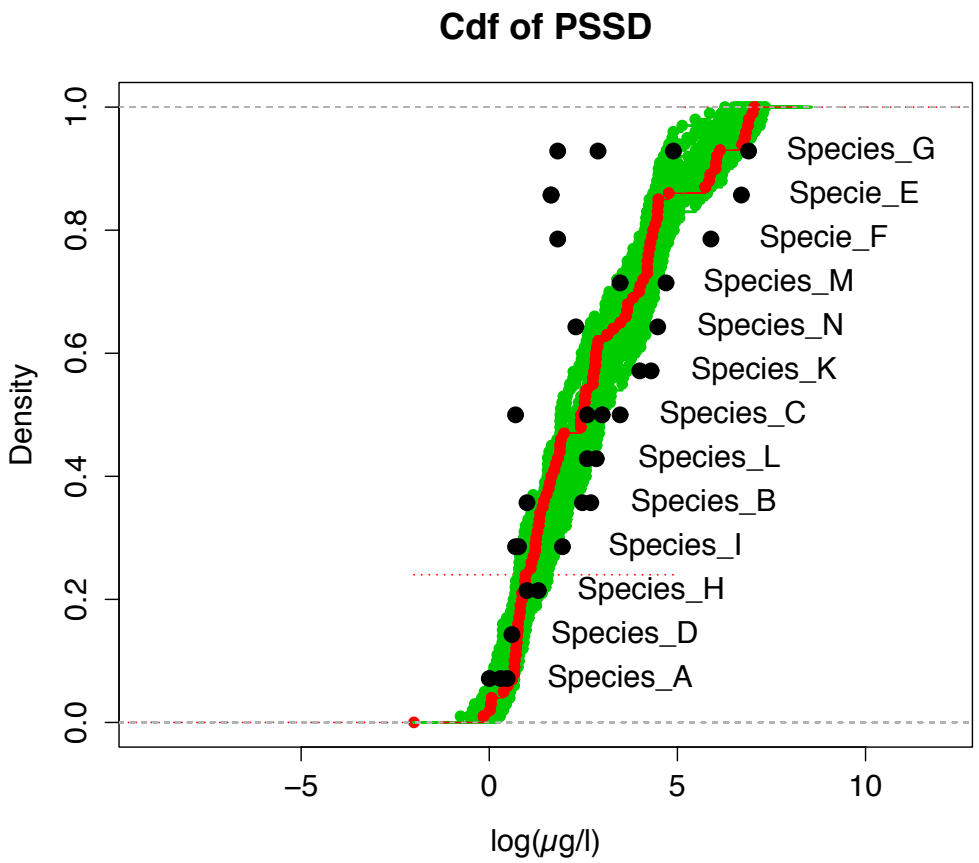
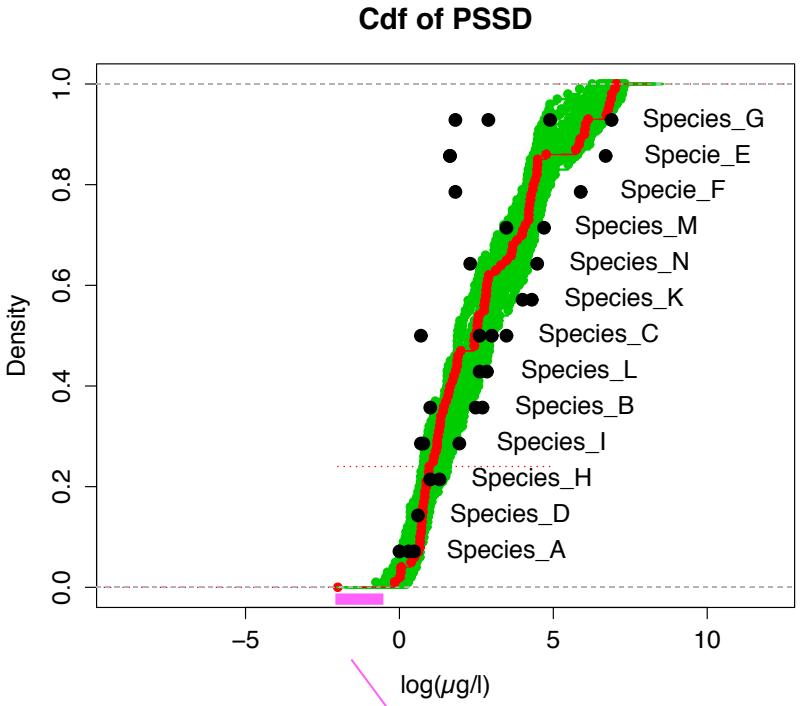
PSSD simulation outputs cont.

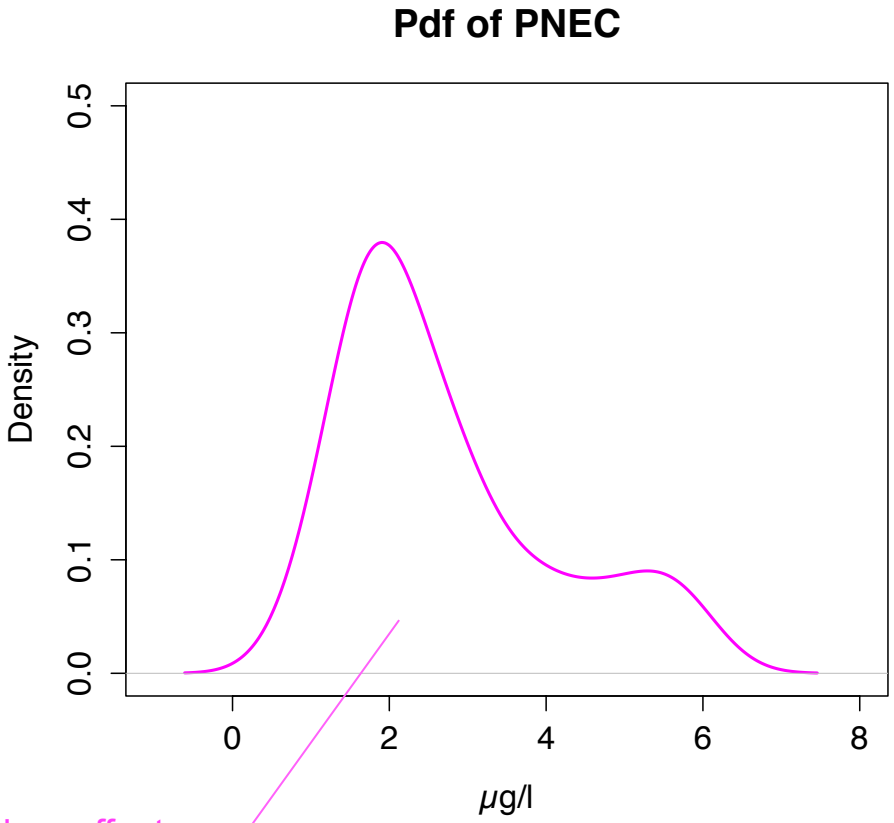
Fictional R-package output



PSSD simulation outputs cont.

Fictional R-package output examples





PNEC= Predicted no effect concentrations = 5% quantile of each PSSD curve

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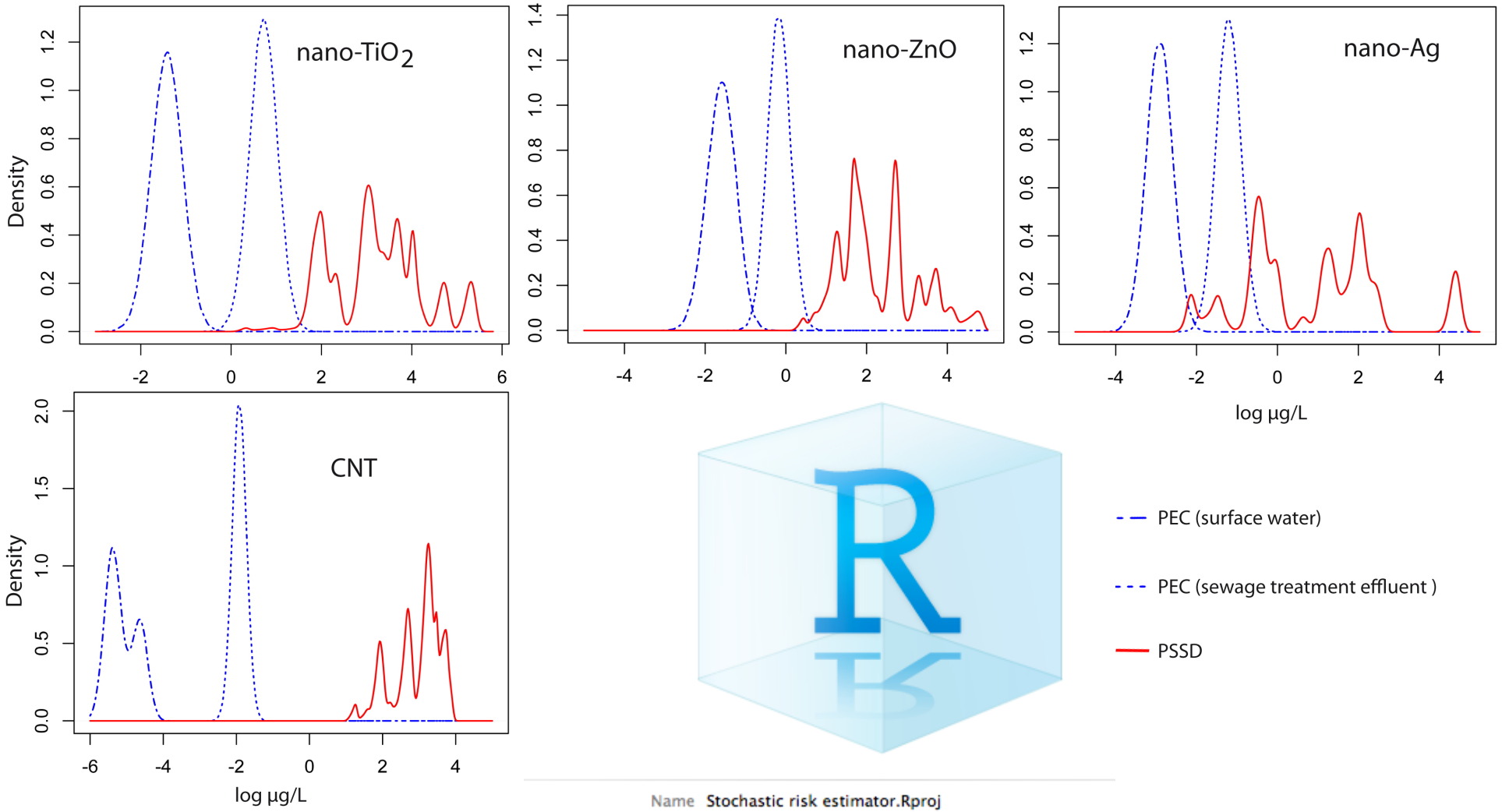
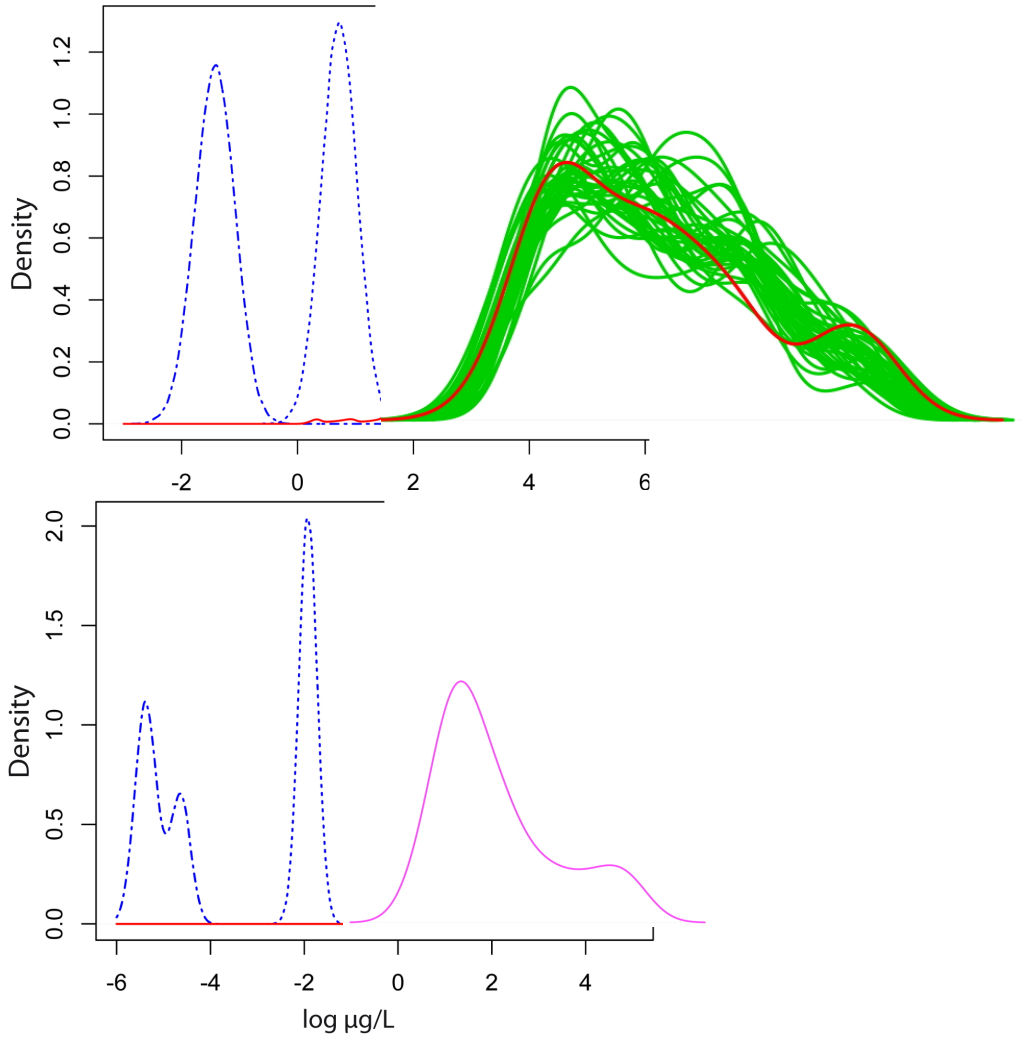
PSSD simulations in risk quantifications

First quantifications in 2013



PSSD simulations in risk quantifications cont.



PEC (surface water)

PEC (sewage treatment effluent)

PSSD PNEC

Short and simplified demonstration PSSD R-Package

createPSSDModell {PSSD} R Documentation

createPSSDModell

Description

function to create a probabilistic secies sensitivity distribution (PSSD) modell

Usage

```
createPSSDModell(T_data, PSSD_simulations = 1, PSSD_length = 100,
  species_length = 10^2, cv_factor1 = 0.5, cv_factor2 = 0.5,
  cv_factor3 = 0, cv_low_end = 0.5, cv_high_end = 0.5,
  interval_length = 10^2)
```

Arguments

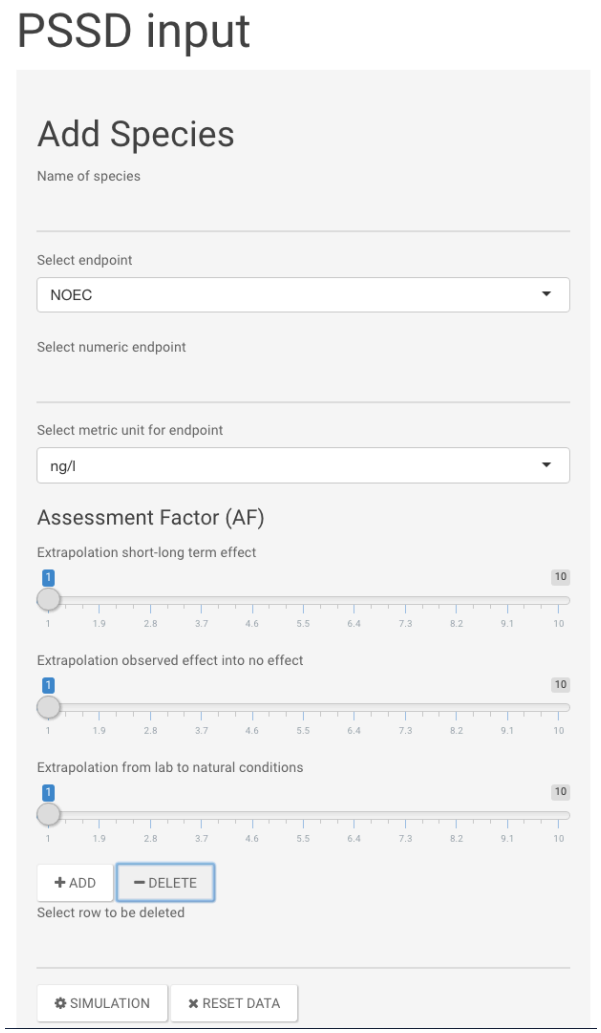
T_data	A nummeric matrix with nrow = 100 and ncol = 100
PSSD_simulations	A number for the quantity of PSSDs to be computed
PSSD_length	A number for the quantity of the model output values for the PSSD
species_length	A number for the quantity of the model output values of the PSSD of one single species
cv_factor1	A fraction that reflects the uncertainty range (confidence interval) on both sides of the first assessment factor (short to long term toxicity)
cv_factor2	A fraction that reflects the uncertainty range (confidence interval) on both sides of the second assessment factor (extrapolation from the observed effect concentrations into no effect concentrations)
cv_factor3	A fraction that reflects the uncertainty range (confidence interval) on both sides of the third assessment factor (expected differences between lab based experimental conditions and natural conditions)
cv_low_end	A fraction that reflects the uncertainty range (confidence interval) on the left hand side of the lowest toxicological endpoint used for one single species
cv_high_end	A fraction that reflects the uncertainty range (confidence interval) on the right hand side of the highest toxicological endpoint used for one single species
interval_lenth	A number for the quantity of the model output values of the interval distributions that are the distributions between all the toxicological endpoints collected for a particular species

Value

a matrix

[Package *PSSD* version 1.0.0 Index]

Short and simplified demonstration PSSD GUI



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PMFA tools

Probabilistic Material Flow Analysis (PMFA)

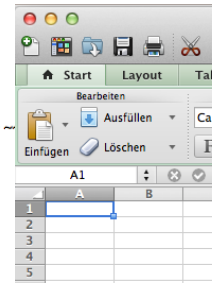
Package

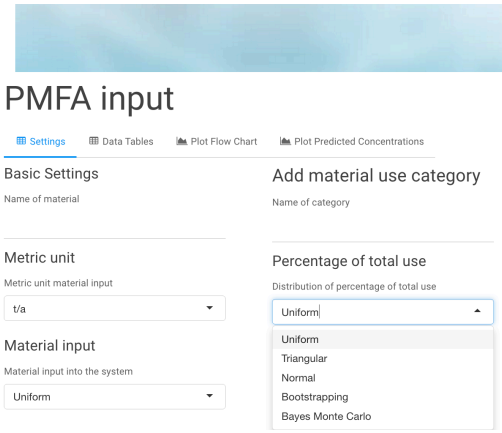
Documentation for package ‘PMFA’ version 1.0.0

- DESCRIPTION file.

Help Pages

PMFA-package	What the package does (short line) ~~ package title ~~
createFateBox	createFateBox
createInputBox	createInputBox
createPMFAModell	createPMFAModell
createTransferBox	createTransferBox
Fate	Fate
Input	Input
loadExcelData	loadExcelData
Message	Message State of Simulation
PlotStatesVolumesTransfers	PlotStatesVolumesTransfers
PMFA	What the package does (short line) ~~ package title ~~
Transfer	Transfer





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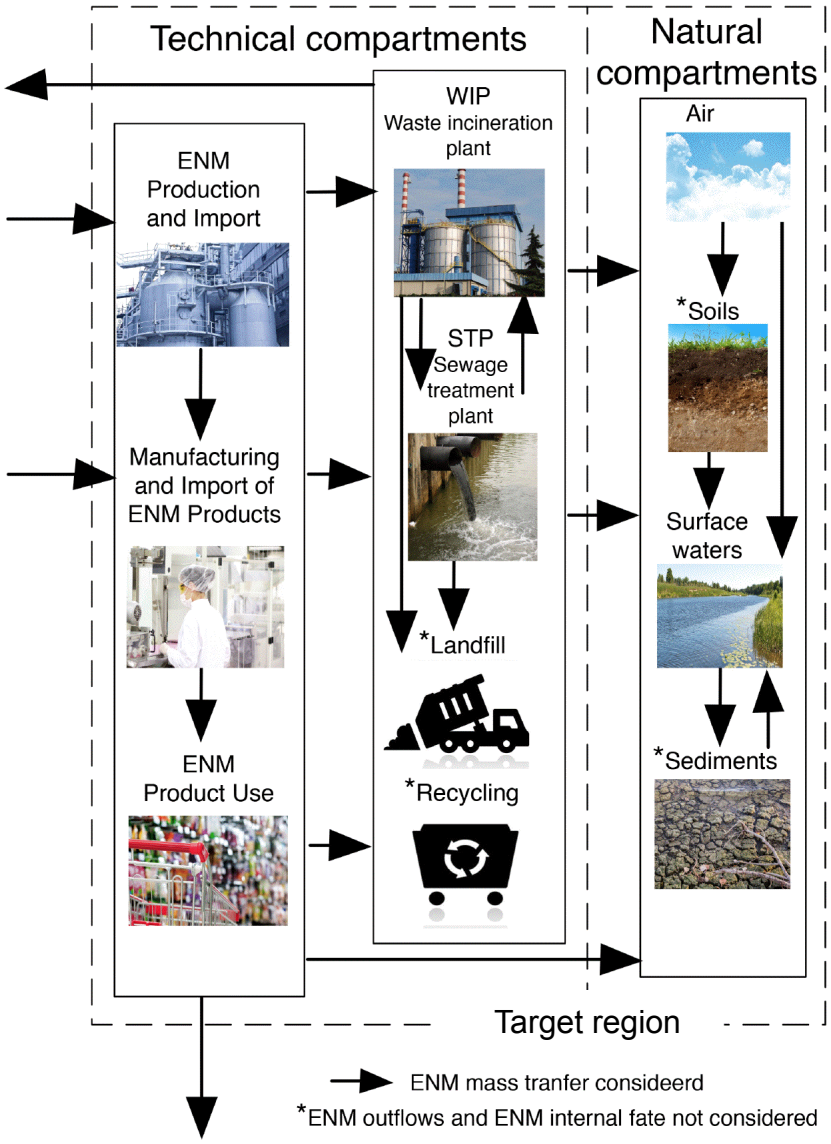
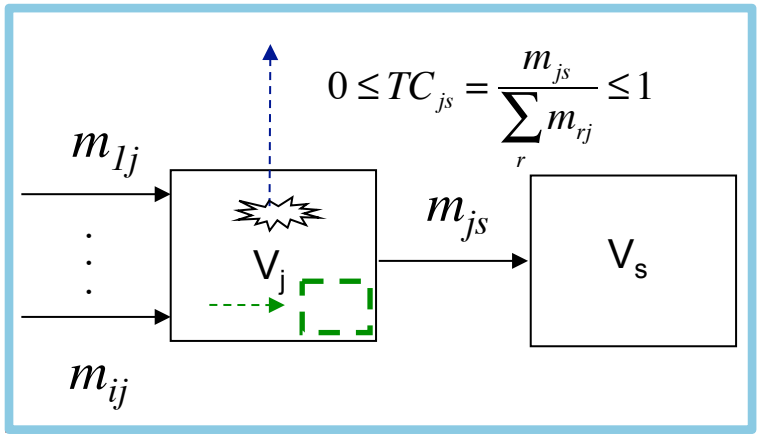
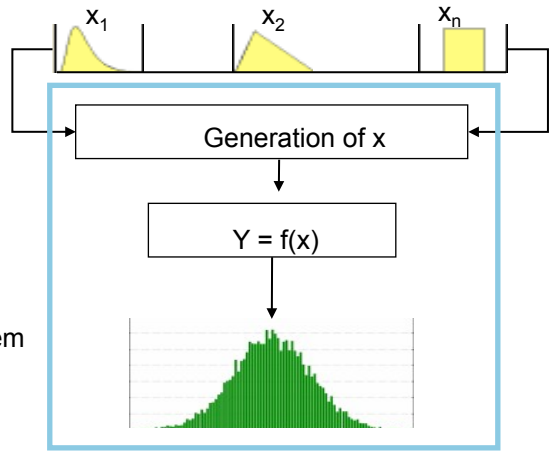
Exposure (mass transfer) model



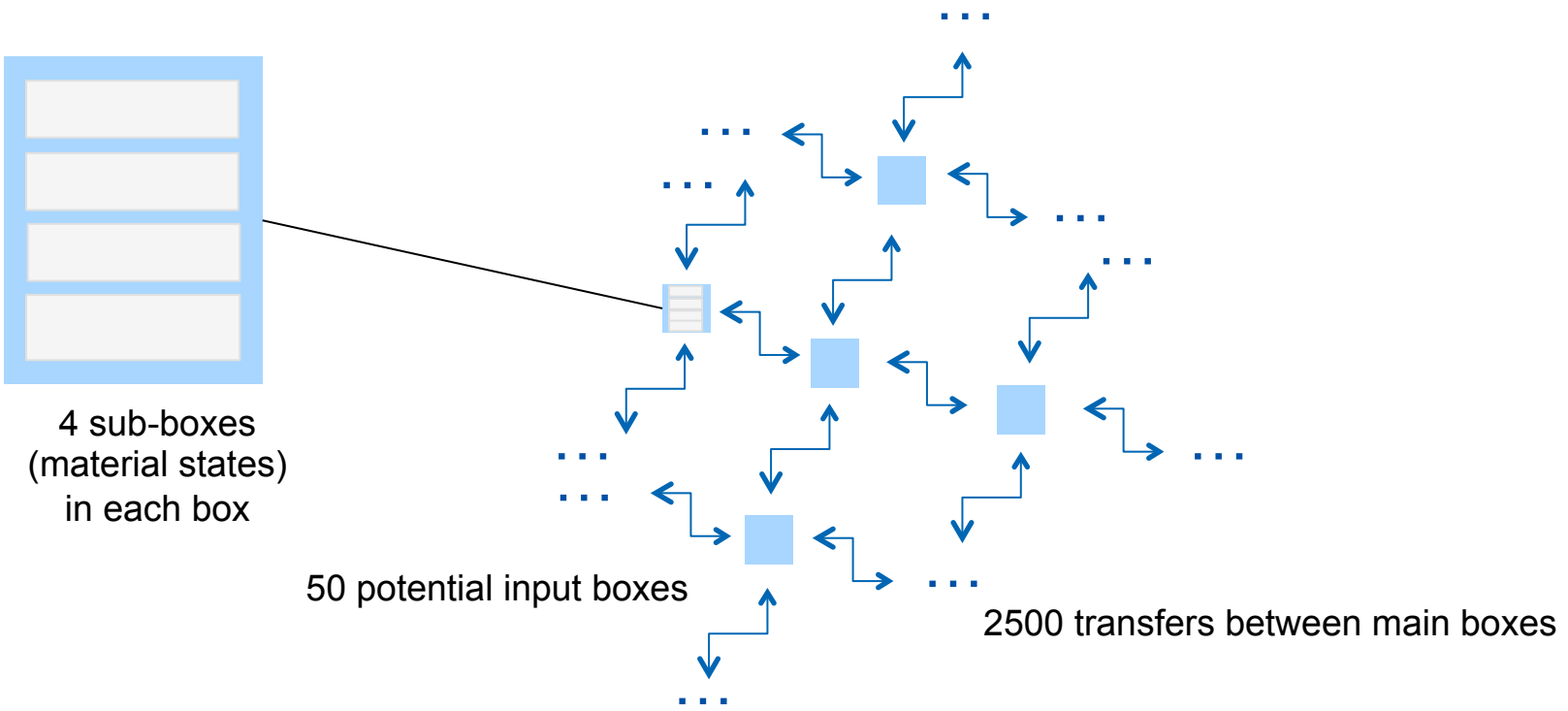
Gottschalk, Nowack et al. 2009-2015
Sun, Bornhöft, Nowack et al. 2014-
and other

Basic idea: transfer coefficients (TC)



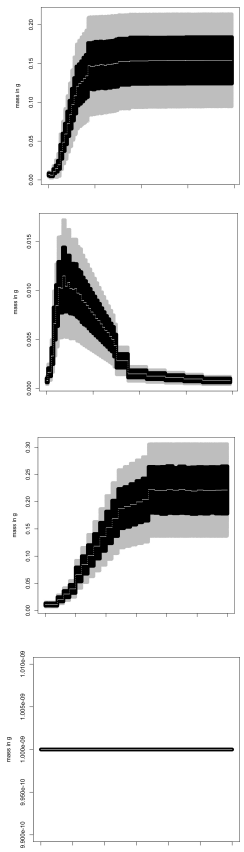


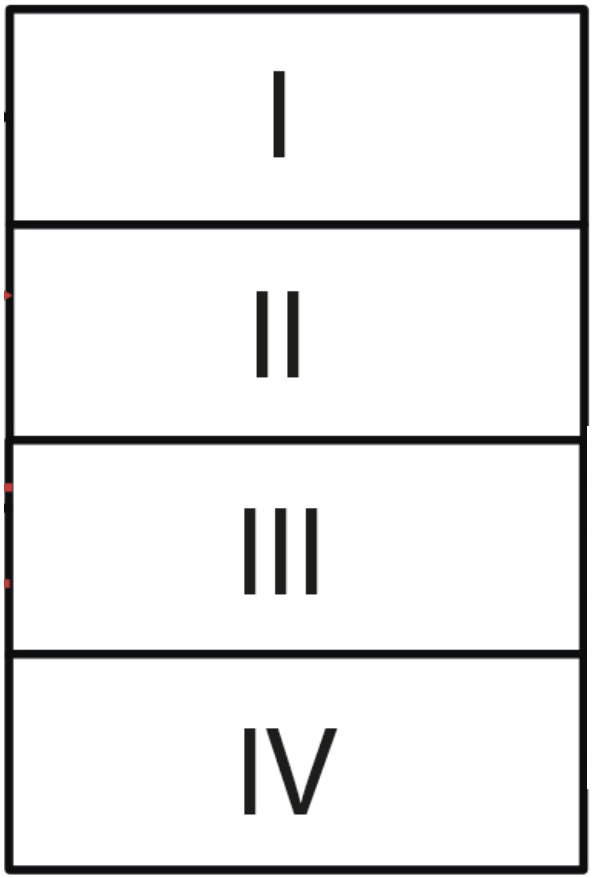
Data needed for PMFA



2750 model input values (needed)

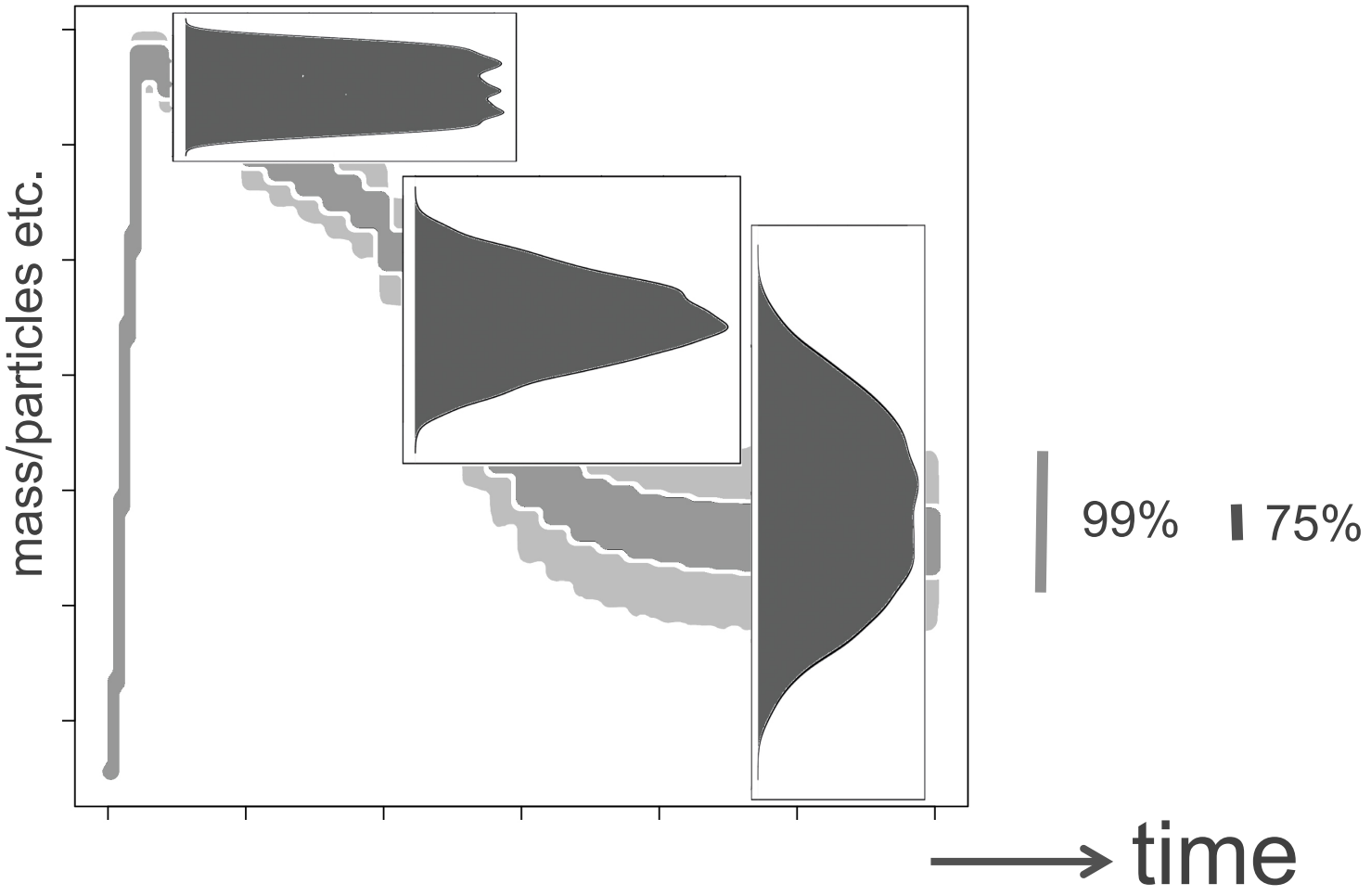
Main boxes



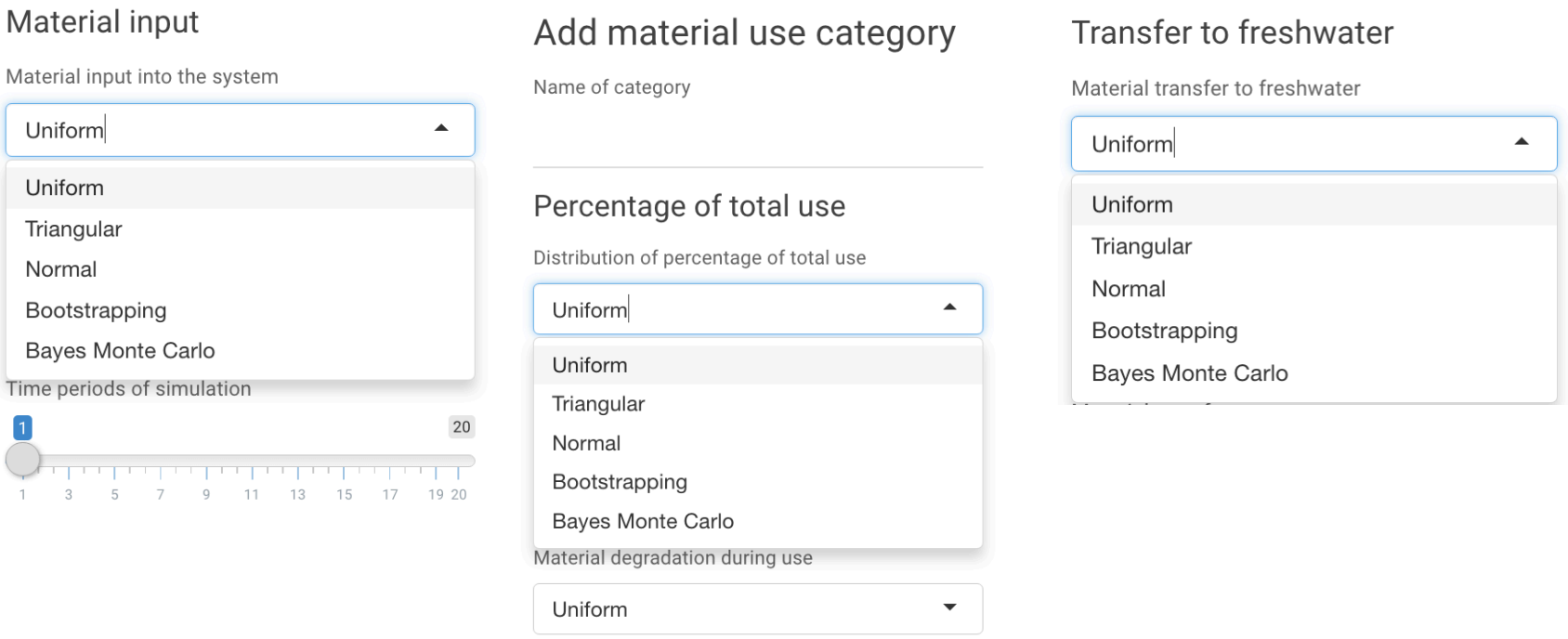


I Not detected
II Not yet transported further
III Dwell time (flow rate)
IV Deposited/transformed

Output interpretation

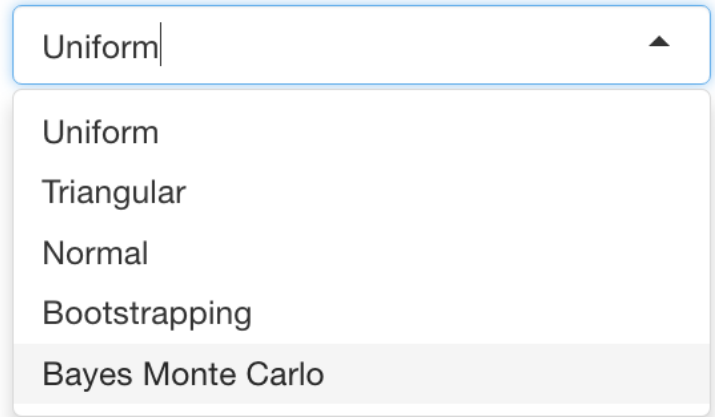


Model input data and distributions



Basically, we need only two different types of data:
I) Material input into (internal/external in/to each main box) the system and II) transfer (covers geographical translocation, elimination, dissolution etc.) inside the system.

Choice of probability distributions

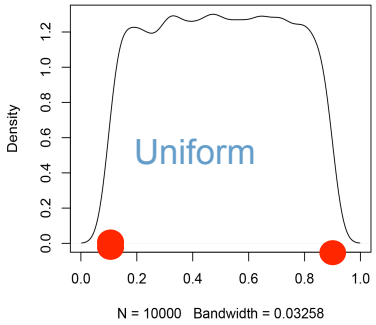


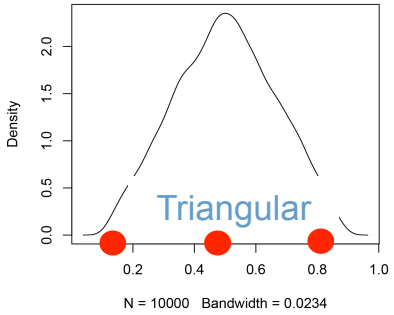
interacts with data quality and quantity,
for the selection a decision tree approach helps (next slide)

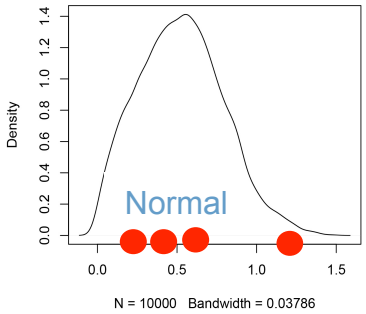
Data needed for PSSD

Shaping distributions

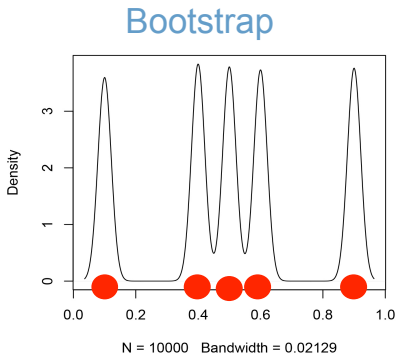
Less informativ distribution

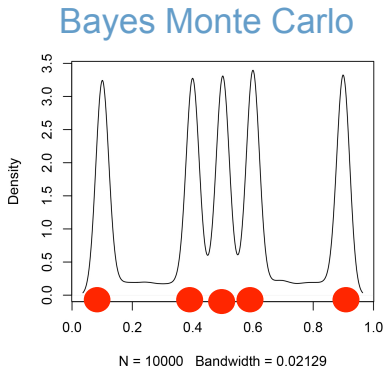






Emprical distributions





Chose … if… (very simplified version of decision support, some basis for a decision tree that can be developed)

Uniform: the minimal and the maximal must be taken as extremes … other values can be ignored…

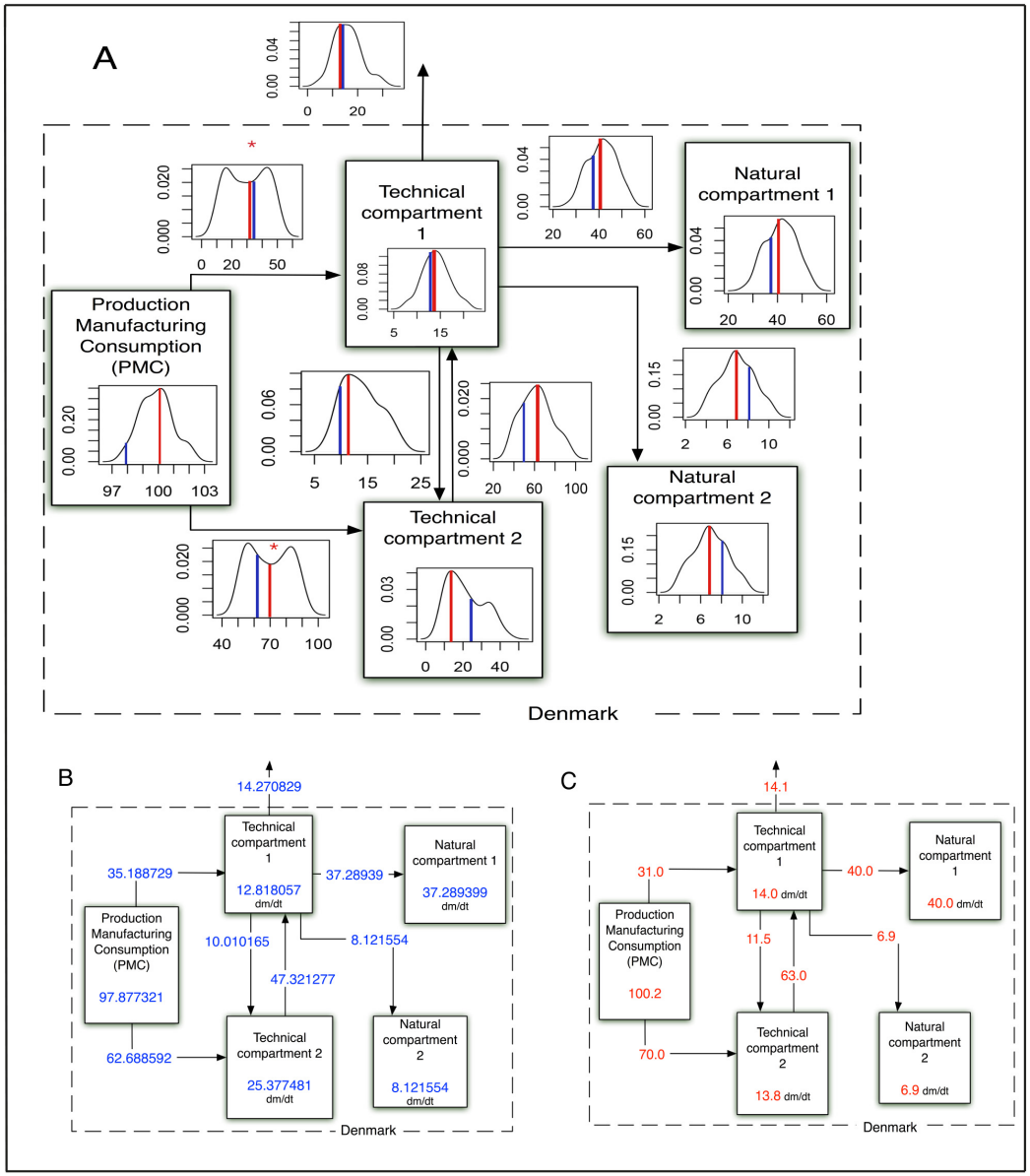
Triangular: the minimal and the maximal value are taken as extremes, the median/mean value computed as the peak (most frequent), other values can be ignored….

Normal: if you have some data, … need to account for very high and very low values … with low probability (that however cannot be excluded)…

Bootstrapping: only the raw values should be fed into the model (randomly, equally and repetitively) and taken to compute an empirical distribution, no evidence that other values (between data points) should be considered

Bayes Monte Carlo: combine bootstrapping (see above) with some expert based prior distribution (assumption) that ranges from 0 to 1 for example

Exposure (mass transfer) model cont.



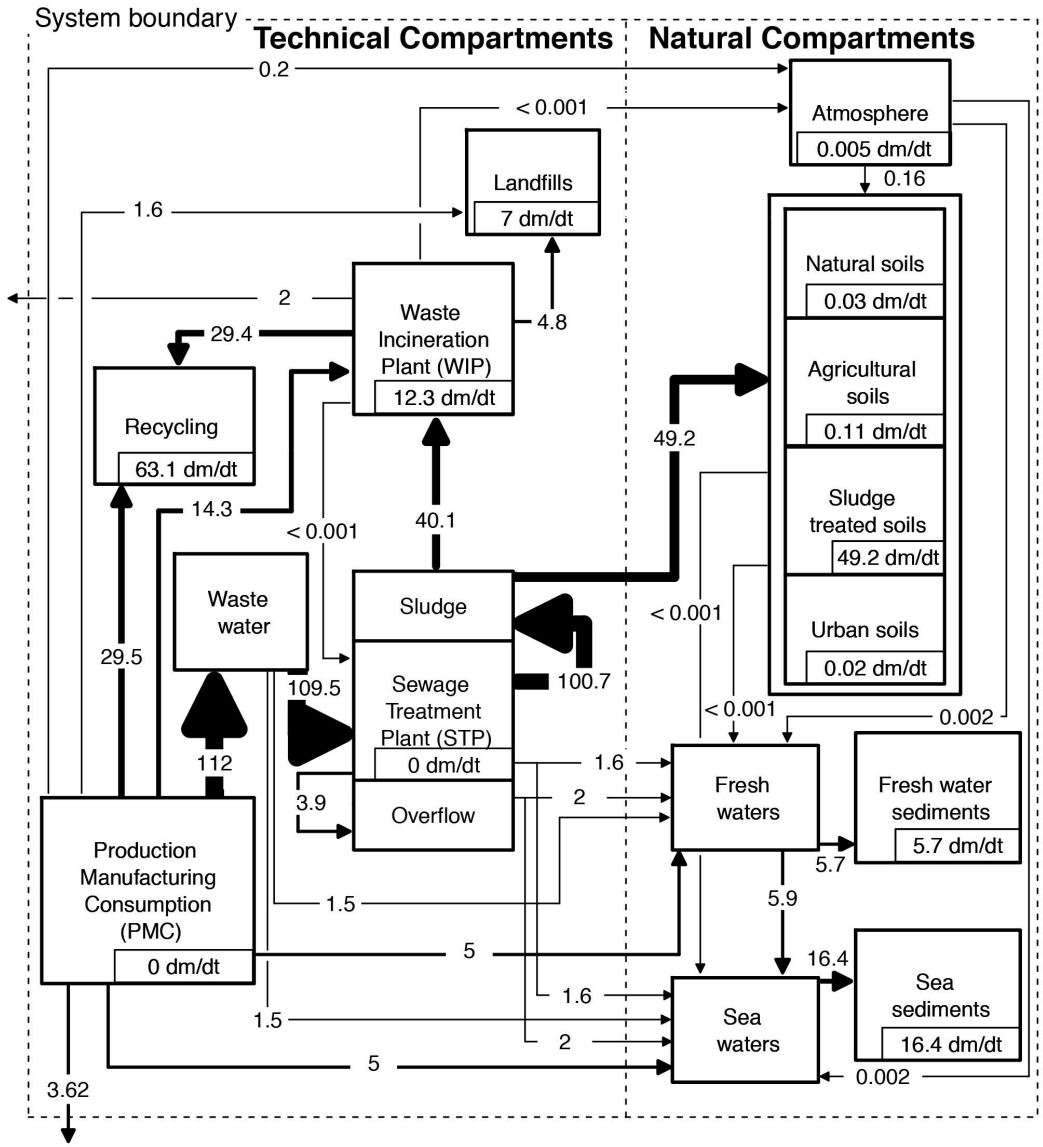
Red: Modal values

Blue: One specific (non-sense) scenario

Typical PMFA simulation outputs

Flow chart based e.g. on modal values (the most frequent value)

Do not take a single Monte Carlo scenario as output for evaluation!



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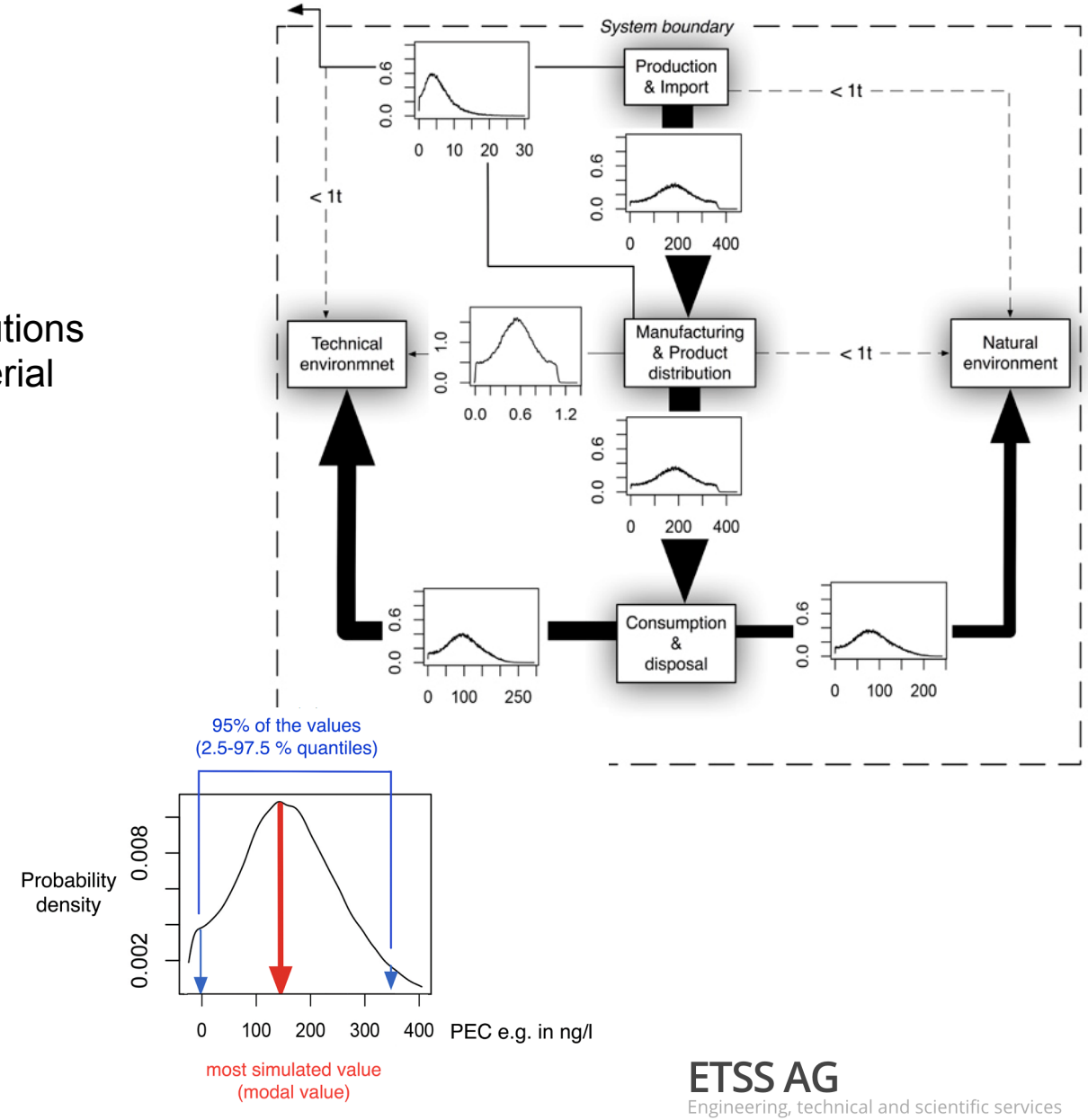
Typical PMFA simulation outputs

Probability distributions for flows and material states!



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Short and simplified demonstration PMFA R-Package

createPSSDModell {PSSD} R Documentation

createPSSDModell

Description

function to create a probabilistic secies sensitivity distribution (PSSD) modell

Usage

```
createPSSDModell(T_data, PSSD_simulations = 1, PSSD_length = 100,
  species_length = 10^2, cv_factor1 = 0.5, cv_factor2 = 0.5,
  cv_factor3 = 0, cv_low_end = 0.5, cv_high_end = 0.5,
  interval_length = 10^2)
```

Arguments

T_data	A nummeric matrix with nrow = 100 and ncol = 100
PSSD_simulations	A number for the quantity of PSSDs to be computed
PSSD_length	A number for the quantity of the model output values for the PSSD
species_length	A number for the quantity of the model output values of the PSSD of one single species
cv_factor1	A fraction that reflects the uncertainty range (confidence interval) on both sides of the first assessment factor (short to long term toxicity)
cv_factor2	A fraction that reflects the uncertainty range (confidence interval) on both sides of the second assessment factor (extrapolation from the observed effect concentrations into no effect concentrations)
cv_factor3	A fraction that reflects the uncertainty range (confidence interval) on both sides of the third assessment factor (expected differences between lab based experimental conditions and natural conditions)
cv_low_end	A fraction that reflects the uncertainty range (confidence interval) on the left hand side of the lowest toxicological endpoint used for one single species
cv_high_end	A fraction that reflects the uncertainty range (confidence interval) on the right hand side of the highest toxicological endpoint used for one single species
interval_lenth	A number for the quantity of the model output values of the interval distributions that are the distributions between all the toxicological endpoints collected for a particular species

Value

a matrix

[Package *PSSD* version 1.0.0 Index]

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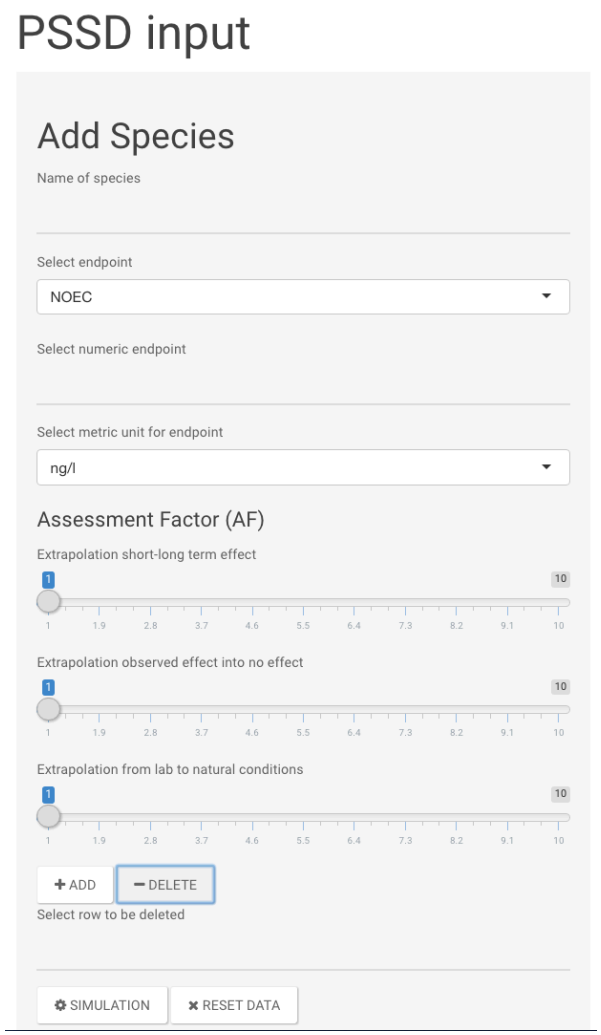
Short and simplified demonstration PMFA GUI



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Conclusions

State of development

- PSSD R-package (incl. version for Excel users) one month finalization
- GUI (graphical user interface) 2-3 months for finalization and
- PMFA R-package (incl. version for Excel users) one month finalization
- GUI 2-4 months for finalization

Improvements needed

- Speed versus e-mail notification
- Package description
- Decision tree distribution selection

Terms of use

- Work for DSS (decision support system) of SUN
- Publish R-packages?
- GUI focused also on commercial stakeholders or internal use

Thanks for questions and attention!

ETSS researches

Specialized in dealing with probabilities, uncertainties and diversity.

UNCERTAINTY RESEARCH

We are solutions-oriented and seek to resolve complex issues in the most pragmatic way possible.

RISK ANALYSIS

We will calculate future scenarios where this is reasonable and quantitatively possible.

DATA MANAGEMENT

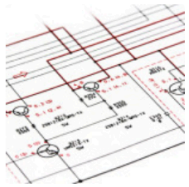
We are happy to assist you in a wide variety of tasks, from simple to difficult works.

DECISION MAKING

We focus our attention on the queries and demands of our clients and customers.

ENVIRONMENTAL IMPACT

Our evaluation is based on professional experience, methodological competence and good sense.



MATERIALFLOW CONSULTING

We develop individual customer-oriented solutions.

FEASIBILITY STUDIES

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QUALITY MANAGEMENT

Early fault avoidance is the best way to avoid late and high compensation costs.

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