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Dealing with Parameter and Scenario Uncertainty in Pesticide Fate Model Scenarios for Pesticide Registration.

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Background: authorisation of pesticides in the EU

Directive 91/414/EEC concerns the authorization, placing on the market, use and control within the European Community of plant protection products.

Member states shall not authorize a product unless it is included in **Annex I** of the 91/414/EEC directive.

A product can be included in the Annex I list if the residues of the product ‚do not have any harmful effects on human or animal health or on groundwater or any unacceptable influence on the environment.'

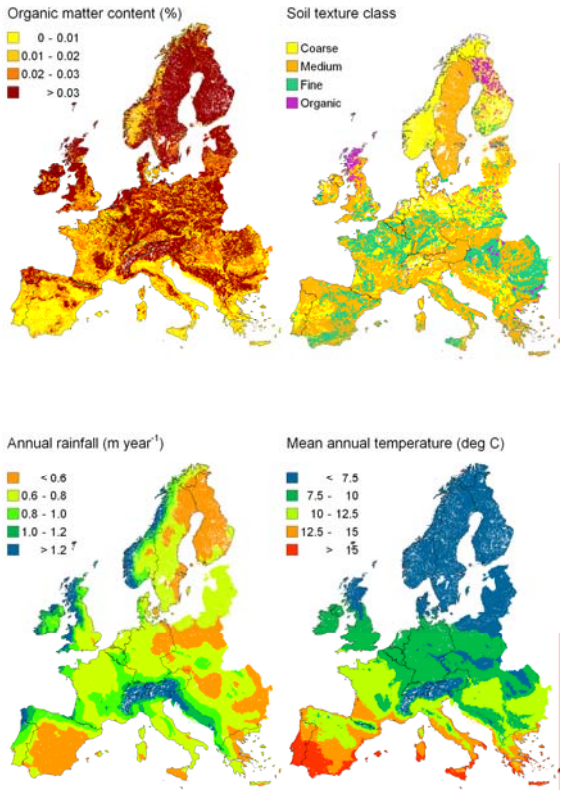
Background: pesticide fate model scenarios

to assess harmful effects on the groundwater and environment:

- pesticide concentrations are predicted in different environmental compartments (surface water, groundwater, air, and soil) for worst case conditions.
- a parameterized pesticide fate model for a worst case condition or a set of environmental conditions (soil, climate, crop type, …) is a pesticide fate model scenario.

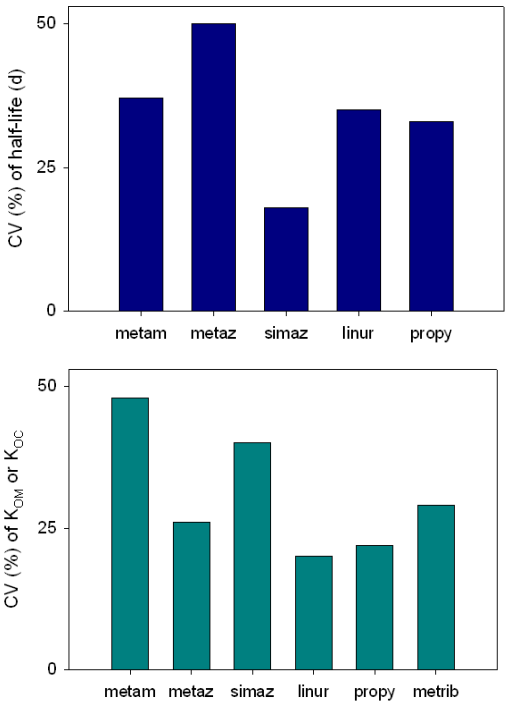
Background: parameterization of scenarios

- Scenario selection has been carried out considering the spatial variability in soil and climate assuming perfectly known pesticide properties.
- A scenario is selected using simulated concentrations of a substance with specific pesticide properties



Background: parameterization of scenarios

Uncertainty in pesticide properties



Allen & Walker (1987) Pestic. Sci. 18: 95-111
Walker & Thompson (1997) Weed Res. 17: 399-405

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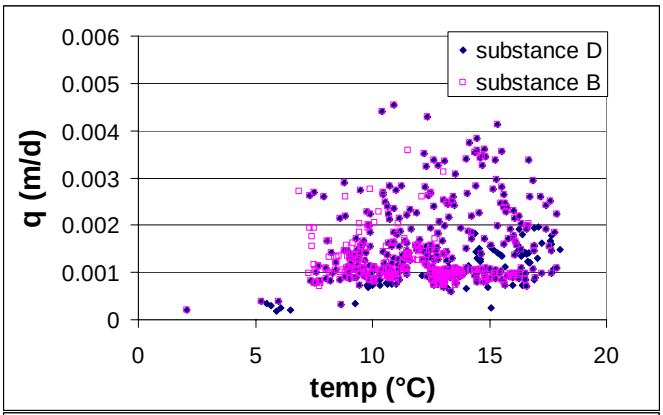
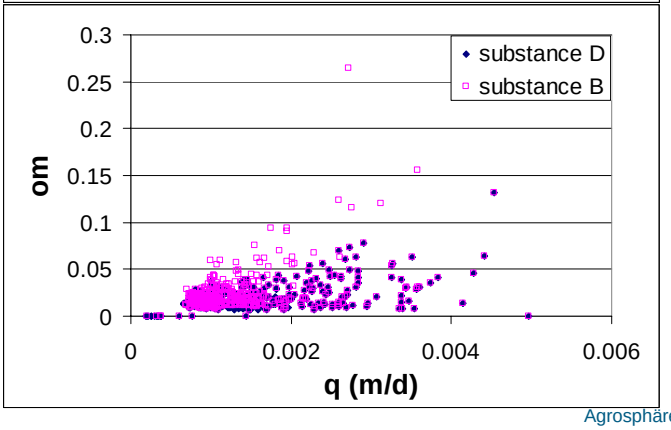
Background: effect of pesticide properties on scenario selection





Conditions or soil and climate parameters that lead to worst-case leaching concentrations depend on pesticide properties.

Parameters (vertical flux at 1m, temperature and organic matter content) of sites where the predicted leached concentration is above the 80th percentile for two different pesticides.

--> Selected scenario may depend on pesticide properties.

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Aim of the study

- What is the effect of pesticide property uncertainty on scenario parameterization?
- What is the effect of the pesticide properties on scenario parameterization?
- What is the uncertainty about the worst-case concentration that is predicted using a scenario that was derived for a different substance?
- Demonstration for concentrations that leach out of a 1 m deep soil profile.

Used model

Metamodel of EuroPEARL (Tiktak et al., 2006, JEQ, 35:1213-1226):
= regression model

$$\ln C_L = \alpha_0 + \alpha_1 X_1 + \alpha_2 X_2$$

Dependent variable: leachate concentration at 1m depth.

Independent variables: $X_1 = \frac{\mu(T)\theta L}{q}$; $X_2 = \frac{\mu(T)\rho f_{om} K_{om} L}{q}$

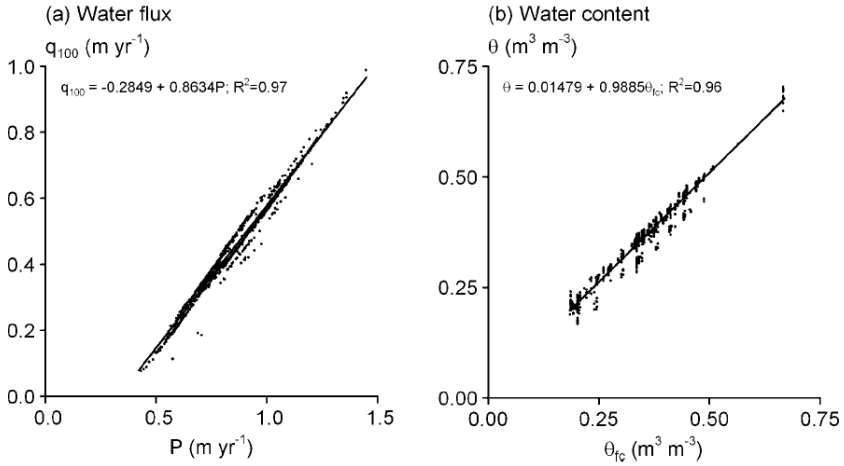
Regression coefficients: estimated from data sets of simulated $\ln C_L$ by the mechanistic transient flow and transport model PEARL that was parameterized for 1062 soil-climate combinations and 56 pesticides

Used model

q: vertical flux at 1 m = estimated from rainfall, P

θ: volumetric water content = estimated from water content at field capacity

(Tiktak et al., 2006, JEQ, 35:1213-1226)



μ(T): degradation rate = estimated from DegT50 and temperature

$$\mu(T) = \frac{\ln 2}{DegT50} \exp\left[-\frac{E_a}{R}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right]$$

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Used dataset

- Spatial extent: EU-27, all basic data gridded to 1x1 km^2
- Approximately 2000 points selected from a randomly placed square grid
- Non-agricultural land-use was discarded

- Mean annual temperature and mean annual precipitation from MARS database
- Organic matter from JRC OCTOP map
- Texture from EU soil map

- Water content at field capacity related to soil texture by SPADE pedotransfer function
- Bulk density calculated from organic matter using the GeoPEARL pedotransfer function

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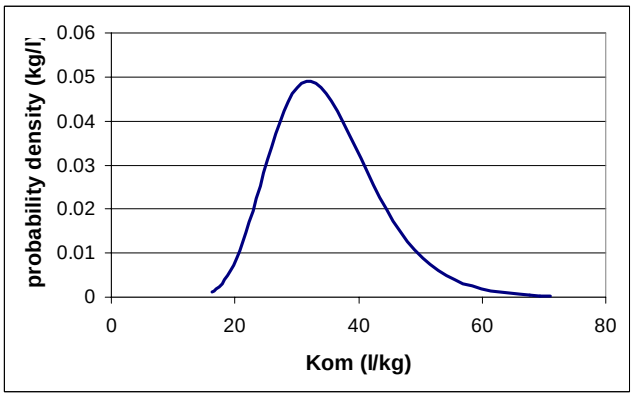
Parameterization of pesticide property uncertainty

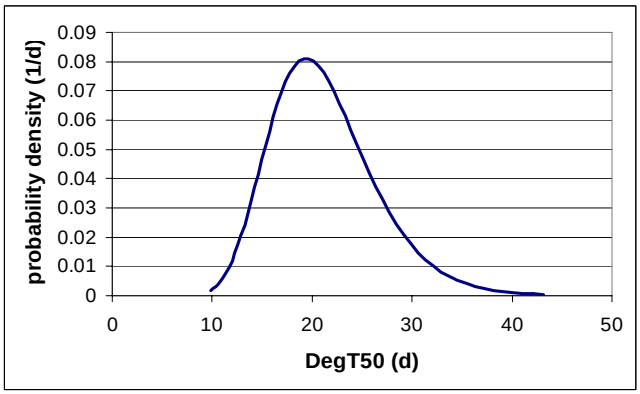
DegT50 or μ and Kom are lognormally distributed with a CV of 25%:

$$\mu = f_{\mu}\mu_{ref}$$

$$Kom = f_{kom}Kom_{ref}$$

Distribution of Kom and DegT50 for pesticide D:
mean Kom = 35 l/kg; mean DegT50 = 20 d





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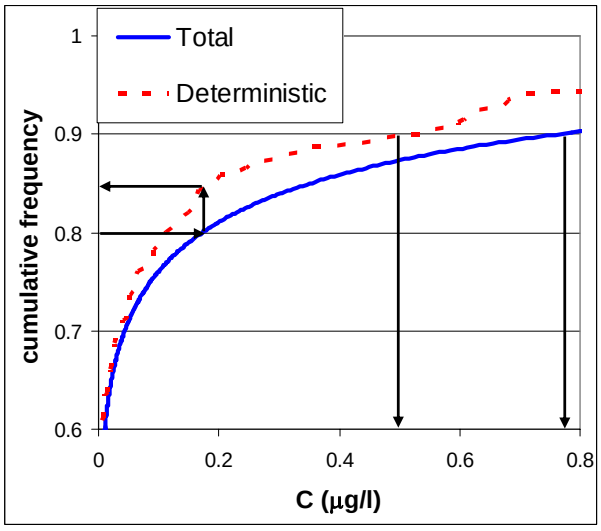
Results: effect of uncertainty

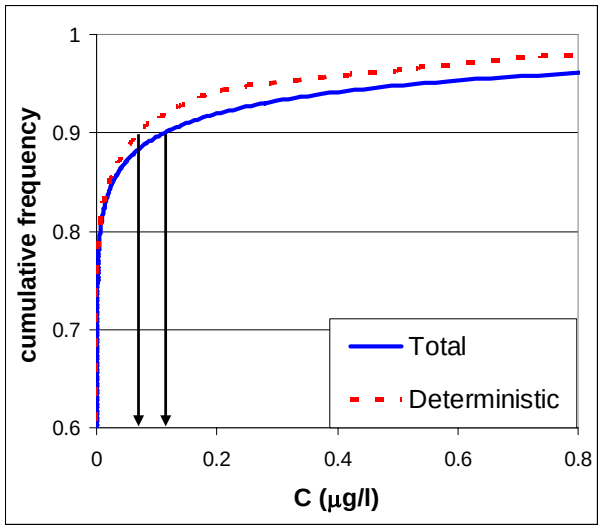
Cumulative distribution of leached concentrations for deterministic versus stochastic (uncertain) pesticide properties.

e.g. pesticide D: Kom 35 l/kg, DegT50= 20 d

temperate-wet climate zone



whole Europe



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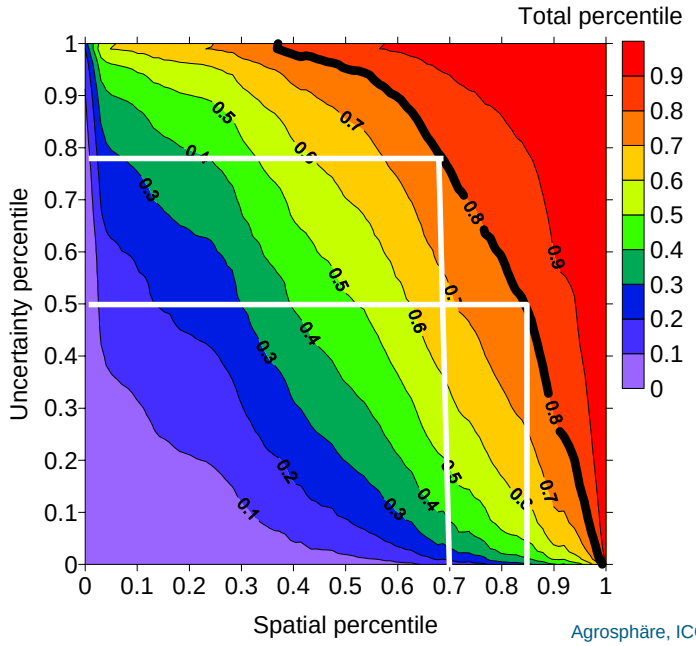
Results: effect of uncertainty

Probability contour plots that unravel the precentile of the concentration distribution into percentiles of distributions that represent:

- deterministic or known variation --> x-axis,
- stochastic or unknown variability--> y-axis



78% highest concentration at the 70% worst location

=

80% highest concentration for all locations and degradation/ sorption parameters of a certain pesticide

=

median (50%) at the 85% worst location

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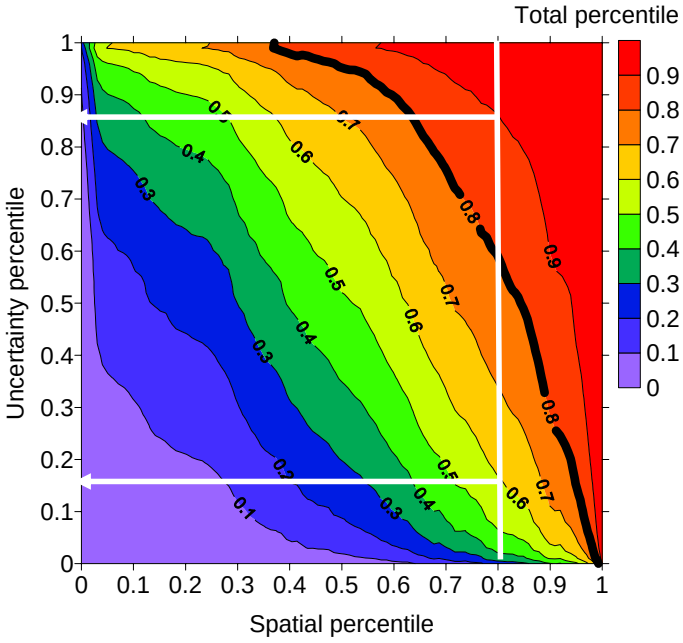
Results: effect of uncertainty

What is the variation of concentrations that can be expected at the 80% worst (in terms of soil and climate) location?



15% probability that a concentration < 60th percentile is observed

15% probability that a concentration > 90th percentile is observed

--> use of experimental data (field, lysimeter) at 80% worst location in terms of soil and climate condtions as an endpoint in registration?

--> uncertainty in maps of leaching concentrations

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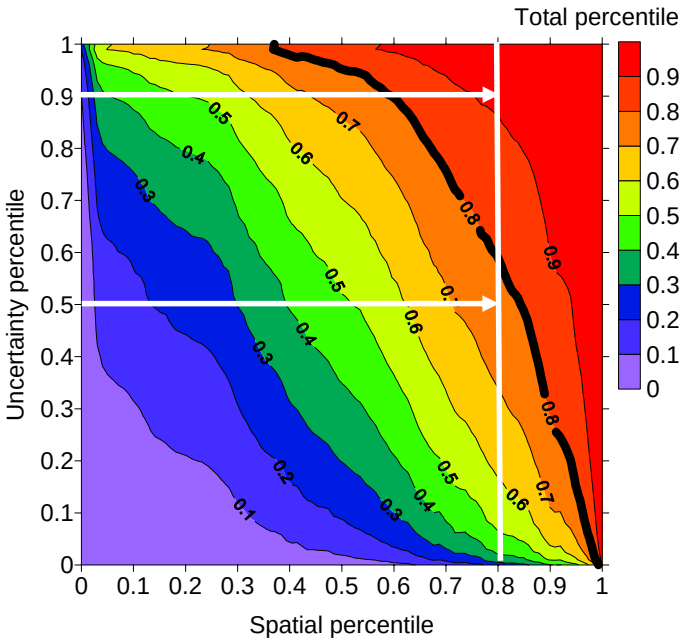
Results: effect of uncertainty

What is the percentile of a prediction at an 80% worst location using 90% worst pesticide parameters or using median pesticide parameters?



80th percentile of determinisitc distribution + 90th percentile of stochastic distribution > 90th overall percentile

80th percentile of deterministic distribution and median pesticide properties --> 75th overall percentile

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Aim of the study

- What is the effect of pesticide property uncertainty on scenario selection and definition?
- **What is the effect of the pesticide properties on the selected scenario?**
- **What is the uncertainty about the P90 concentration that is predicted using a scenario that was derived for a different substance?**
- Demonstration for concentrations that leach out of a 1 m deep soil profile.

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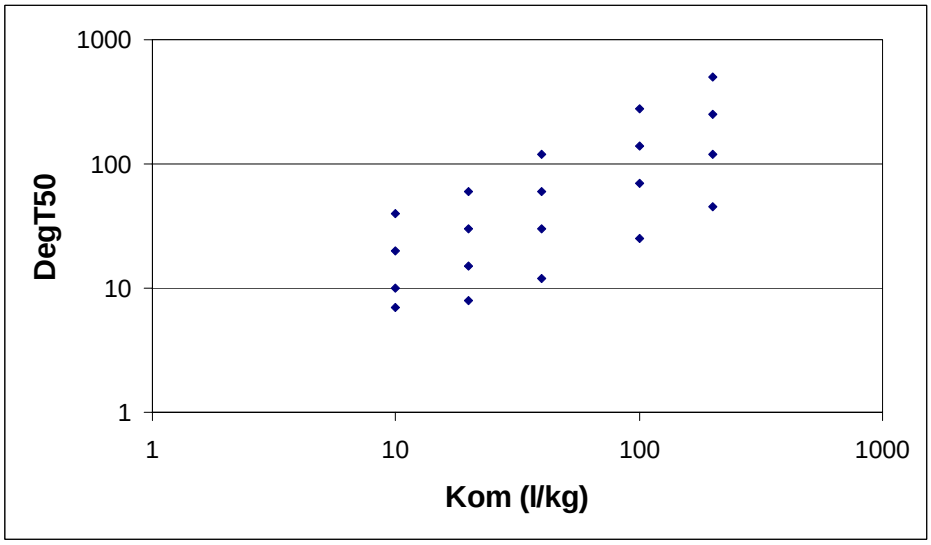
Results: scenario uncertainty

Scenarios (soil/climate conditions, mean pesticide properties), which predict the 80th percentile of the concentration distribution that includes uncertainty, were selected for a set of pesticides:



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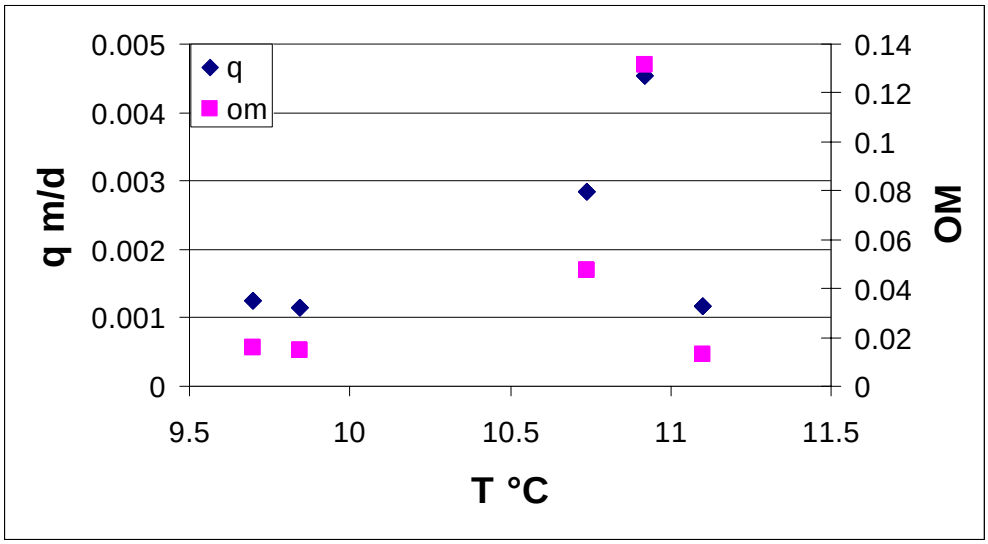
Results: scenario uncertainty

Variation of scenario parameters that are obtained when different pesticides are used to derive a scenarios:



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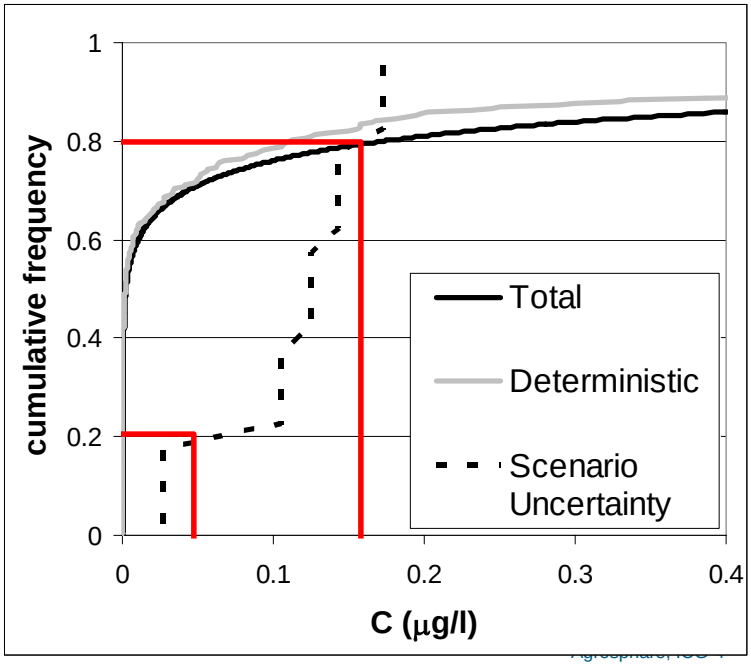
Results: scenario uncertainty

Distribution of leachate concentrations of substance D (Kom = 35 l/d, DegT50 = 20 d) predicted by scenarios that were derived based on other pesticide properties.



20% of the scenarios

-->C < 0.05 µg/l

20% of the scenarios

-->C > 0.15 µg/l

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Summary

Uncertainty of pesticide properties leads to higher concentrations in the higher percentiles of the concentration distribution

- effect of uncertainty is larger for more homogeneous or smaller regulatory zones,
- uncertainty can be accounted for using a higher percentile of a distribution that was derived assuming deterministic pesticide properties.

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Summary

Probability contour plots in which the percentile of the leachate concentration is plotted versus the percentiles of deterministic and stochastic distributions contain information about:

- uncertainty of leachate concentrations at locations/conditions that are selected to represent vulnerable conditions
  --> can experimental data from such experiments be used as an endpoint in pesticide registration?

- uncertainty in maps of leachate concentrations.

Summary

- Selected worst-case conditions (scenario) depend on pesticide properties --> scenario uncertainty

- What is more accurate?
  - *Deriving pesticide specific scenarios and predict leachate concentrations with a simple model and a large dataset of soil/climate conditions?*
  - *Using one scenario for all pesticides and predict leachate concentrations with a detailed pesticide fate model?*

Agrosphäre, ICG-4

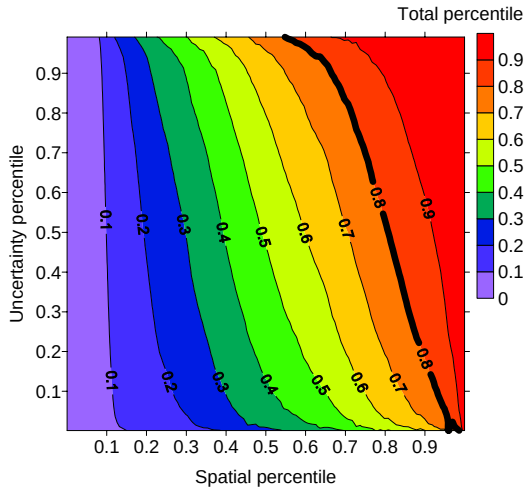
Thank you!

Results: effect of uncertainty

More ‚horizontal' probability contour plots indicate a larger impact of pesticide property uncertainty on the concentration distribution:

e.g. contour plots for larger more heterogeneous zones versus contour plots for smaller more homogeneous zones .

contour plot whole EU



contour plot for temperate wet climate zone