Theoretical Uncertainty Analysis Supporting the Development of a Geo-referenced Regional Exposure Assessment Tool for European Rivers

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Introduction

The **GREAT-ER** system is used to **calculate the PEC** (Predicted Environmental Concentration) of chemicals, **together with its uncertainty and variability**, which arise due to the uncertainty (lack of exact knowledge) and variability (natural changes over space and time) of inputs and parameters.

The **objectives** of this study were:

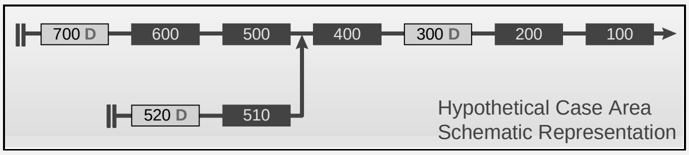
- to check the **applicability of different uncertainty calculation methods**
- to calculate the **overall output uncertainty**
- to calculate the **amount of uncertainty coming forth from each independent variable** (i.e., calculation of model sensitivity to each variable)

To approach these objectives three methods were applied: Monte Carlo simulation, First Order Analysis and Least Square Linearization.

Case Study and Parameter Uncertainties

Study Geography

hypothetical case area (each box = a river stretch, "**D**" = waste water discharge):



Parameter Uncertainties

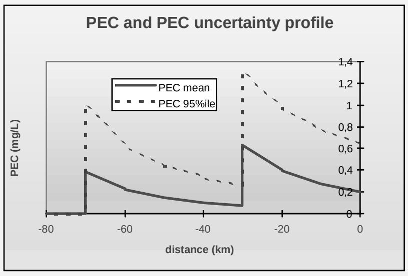
- **fixed uncertainties** for P (population), M (chemical consumption), W (water consumption), R (removal efficiency in WWTP), V (river velocity) predictions (regression parameters a,b,c) → NORMAL distribution

- variability of **Q (river flow)** → LOGNORMAL distribution

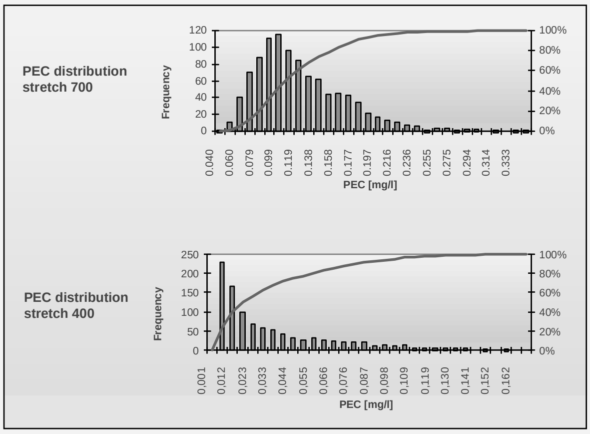
- uncertainty of **in-stream-removal rate K**:
  - series of simulation experiments: different K values, different uncertainties
  - mean values for K: varied from 0.01 to 0.8 h^{-1}
  - range for uncertainty: set from 0 to 0.8 (in terms of standard deviation)
  - distribution types: UNIFORM, NORMAL, LOGNORMAL.

Lumped Uncertainty: Monte Carlo

- Monte Carlo simulation: **lumped predictive uncertainty of the model → probability distribution**
- example of PEC uncertainty + variability profiles along the river:



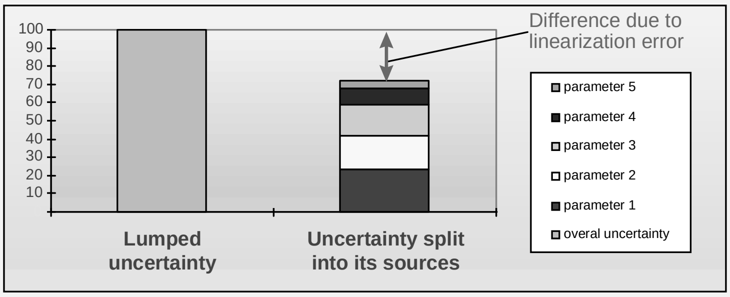
- **coefficient of variation (σ/μ) along river varies strongly** (can go up to 200%)
- simulations with no uncertainty for K → coefficients of variation up to 80% - 90% (distribution width = PEC_{95} divided by PEC_{mean}: 240% - 250%)
- coefficients of variation increase downstream, due to **downstream propagation of the predictive uncertainty**.



Uncertainty Split into its Sources

to obtain the **contribution of each variable to the overall uncertainty** → **two techniques** were used, based on **linearization**.

Compared to Monte Carlo method, sum of uncertainties may be different due to linearization error:



First-Order Analysis

failed
(probably because parameter uncertainties were too big to be properly handled by this method)

Least Square Linearization

= **multilinear regression**, conducted **on results from Monte Carlo** analysis

Sensitivity coefficients (for uniform distribution of K with 0.8 mean and +/- 0.8 deviation):

Segment ID	Q	a	b	M	P	W	f_{bypass}	R_{WWTP}	k	PHI_{up}
100	3.1%	insign.	insign.	-	-	-	-	-	0.2%	96.6%
200	6.2%	insign.	insign.	-	-	-	-	-	2.2%	91.6%
300 D	13.3%	0.2%	0.4%	7.8%	1.0%	insign.	1.0%	0.5%	24.5%	51.3%
400	2.0%	insign.	insign.	-	-	-	-	-	0.3%	97.6%
500	4.5%	insign.	insign.	-	-	-	-	-	0.3%	95.1%
600	8.1%	insign.	insign.	-	-	-	-	-	16.7%	75.2%
700 D	9.0%	0.3%	0.8%	12.0%	1.3%	insign.	11.8%	6.7%	58.1%	-
510	2.7%	0.1%	0.1%	-	-	-	-	-	7.2%	89.9%
520 D	1.8%	insign.	insign.	2.1%	insign.	0.2%	-	-	96.0%	-

most stretches:

- **main uncertainty** due to **downstream propagation** (PHI_{up} = upstream chemical flux)
- most **sensitive** parameters:
  - **river flow** (accounting for natural variability of the system)
  - **degradation parameter** K

'special' stretches:

- **closest to discharge points**: main source of uncertainty is K, and less Q
- **with discharges**: uncertainty also caused by emission parameters (product consumption, WWTP data)

Conclusions

- This study was mainly conducted on a **hypothetical case**, and it should be regarded more as a gross estimation of what the uncertainty of the GREAT-ER model could be. Next, it was also a **test polygon** for the analysis methods.
- **Monte Carlo** proved to be straightforward for calculating the lumped uncertainty.
- In the hypothetical case the **resulting distribution width was rather narrow**: the 95%-ile value did not exceed the mean value more than 3.5 times.
- The **uncertainty strongly propagates downstream**, its main sources are the in-stream removal parameter and the natural system variability.
- To calculate uncertainty split into its sources, **Least Square Linearization** was found to be a very powerful method.

GREAT-ER
Geography-referenced Regional Exposure Assessment Tool for European Rivers

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