Sensitivity and Data Uncertainty Analysis of an Environmental Distribution Model

J. Urbánek, J. Komprda, K. Kubošová

RECETOX, Masaryk University, Brno, Czech Republic

Environmental distribution model for POPs

POPs = Persistent Organic pollutants (persistence, toxicity, bioaccumulation, and long-range transport)

PAHs = Polycyclic Aromatic Hydrocarbons (typical representatives of POPs)

Model – consists of three compartments (air, vegetation, soil)
– soil phase divided into 7 layers

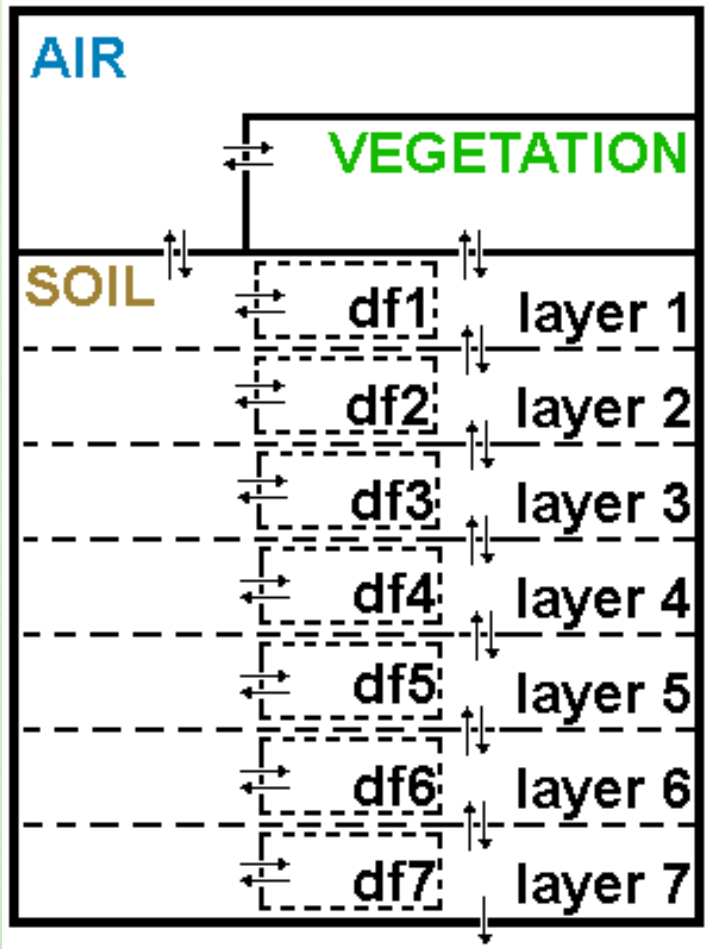
Transport processes (diffusion, degradation, deposition, advection etc.) – occur among the parts of the model

Mathematical description of the model

By expressing mass balance equations we obtain a system of 15 ODEs.

Presumptions:
- constant concentration in air
- no transport processes between the model and surroundings except for leaching from the bottom soil layer
- no production (or rise) of chemicals

Model testing for 3 different PAHs (to include all their characteristics): acenaphtylene, benzo(a)pyrene, pyrene



Model solution

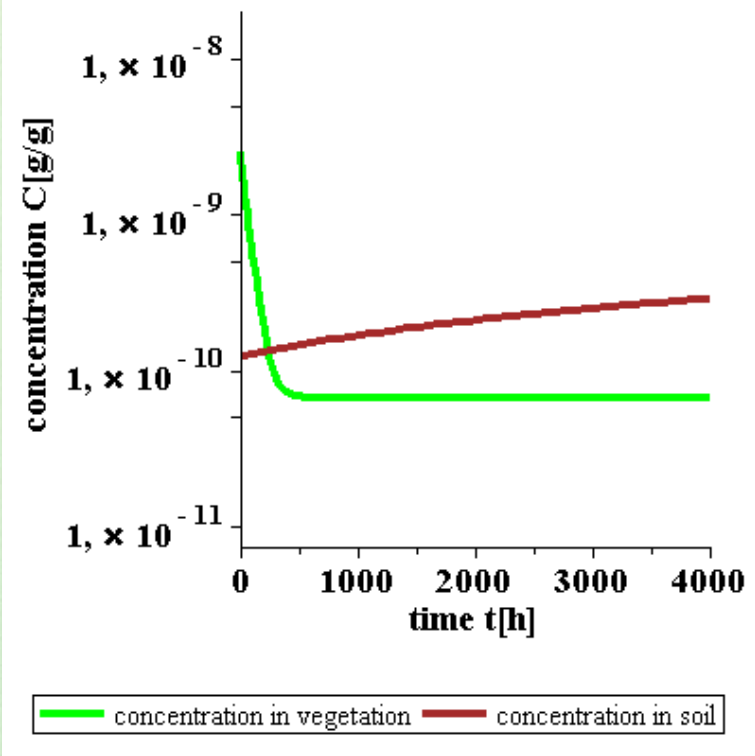
Simply:

$$Y = f(X_1, X_2, ..., X_{39})$$

where

Y …output

X_i …parameters
(chemical properties,
environmental properties)



Concentration progression of benzo(a)pyrene

Sensitivity analysis

So far each parameter has had one nominal value, but:
several parameters are varied, values of others are uncertain

Therefore sensitivity analysis:

$$S(X_i) = \frac{\partial Y}{\partial X_i} \cdot \frac{X_i}{Y} \approx \frac{\Delta Y}{\Delta X_i} \cdot \frac{X_i}{Y} \approx \frac{mean(\Delta Y_i^+, \Delta Y_i^-)}{Y} \cdot 10$$

low/no sensitivity: $S < 0.1$

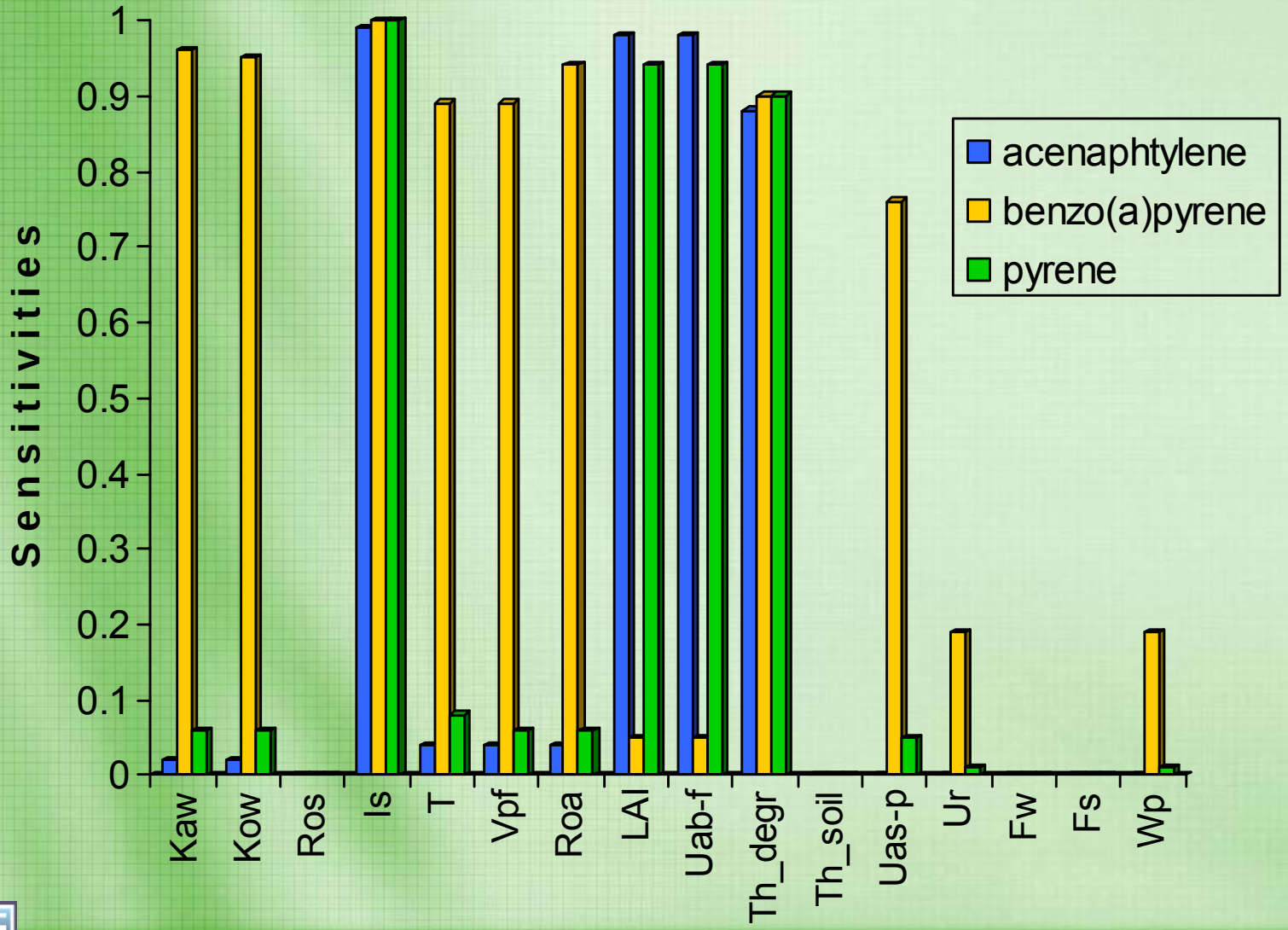
moderate sensitivity: $0.1 \leq S < 0.5$

high sensitivity: $S \geq 0.5$

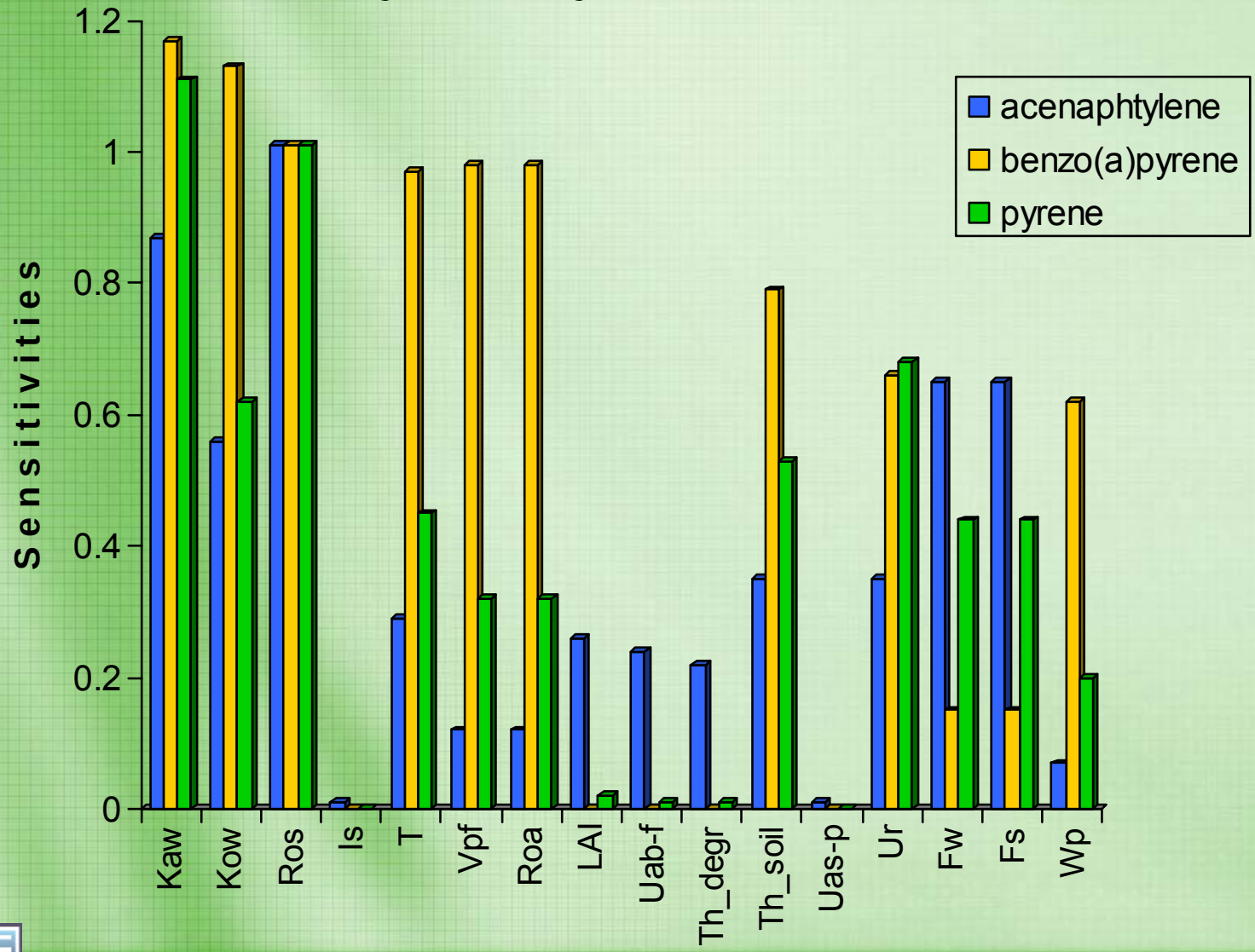
The main parameters

Kaw …… partition coefficient air/water
Kow …….. partition coefficient octanol/water
Ros ..... soil density
Is …… specific biomass
T …… temperature
Vpf ……. volume fraction of particles in air
Roa ……. aerosol density
LAI ……. leaf area index
Uab-f ……. MTC above vegetation
Th_degr … half-time of vegetation degradation
Th_soil ….. chemical half-life in soil
Uas-p …… MTC of dry deposition to vegetation
Ur …….. rain density
Fw ……. water fraction in soil
Fs …….. solids fraction in soil
Wp ……. scavenging ratio

Sensitivity analysis – results for vegetation



Sensitivity analysis – results for soil

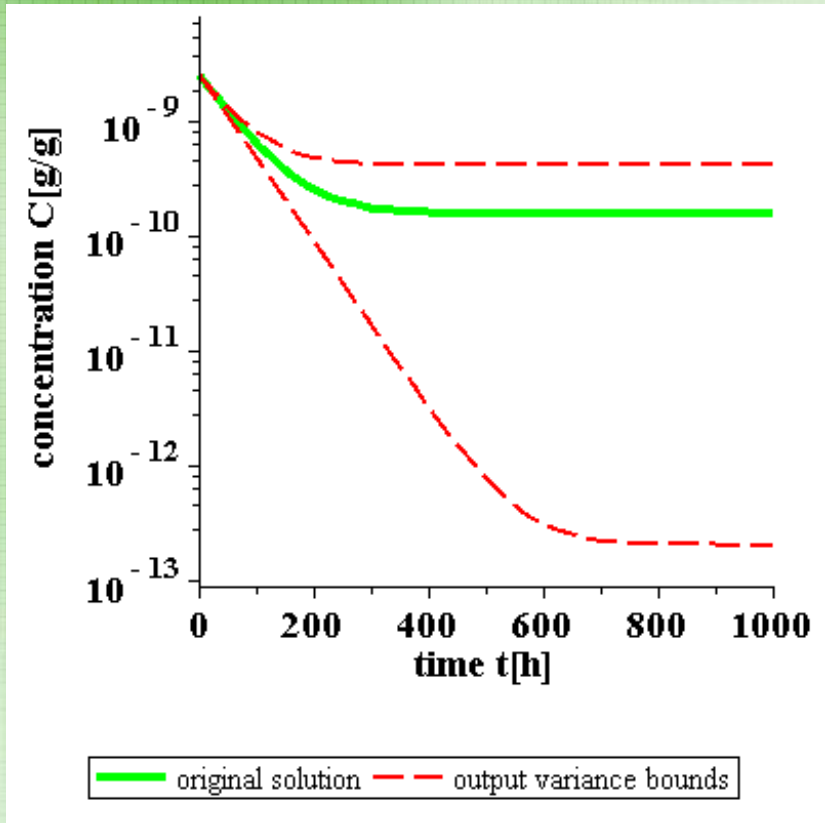


Data uncertainty analysis

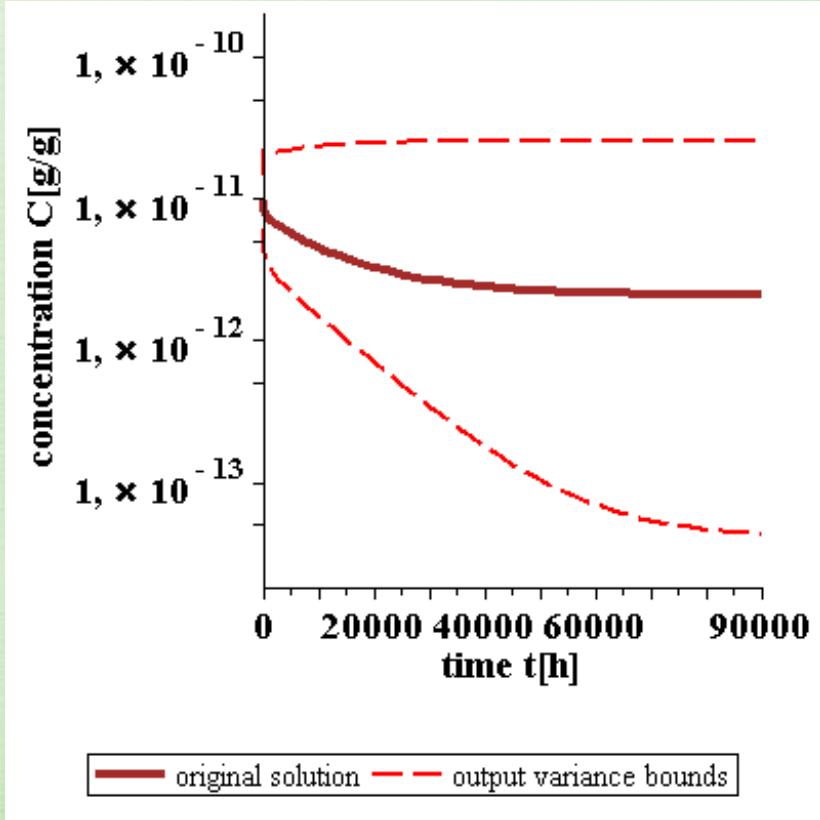
- Previous local sensitivities are only local, one factor at time, and even approximations (finite differences).
- We assigned a probability distribution function (PDF) to each sensitive parameter wherever it was possible.
- We used measured daily values from CHMI, PDFs from previous research and some PDFs were estimated according to several researches.
- Monte Carlo simulation: 4018 samples of values for each parameter
- Spearman rank correlation: parameter contributions to output variance
- (CHMI = Czech Hydrometeorological Institute)

Output variances for acenaphtylene

vegetation

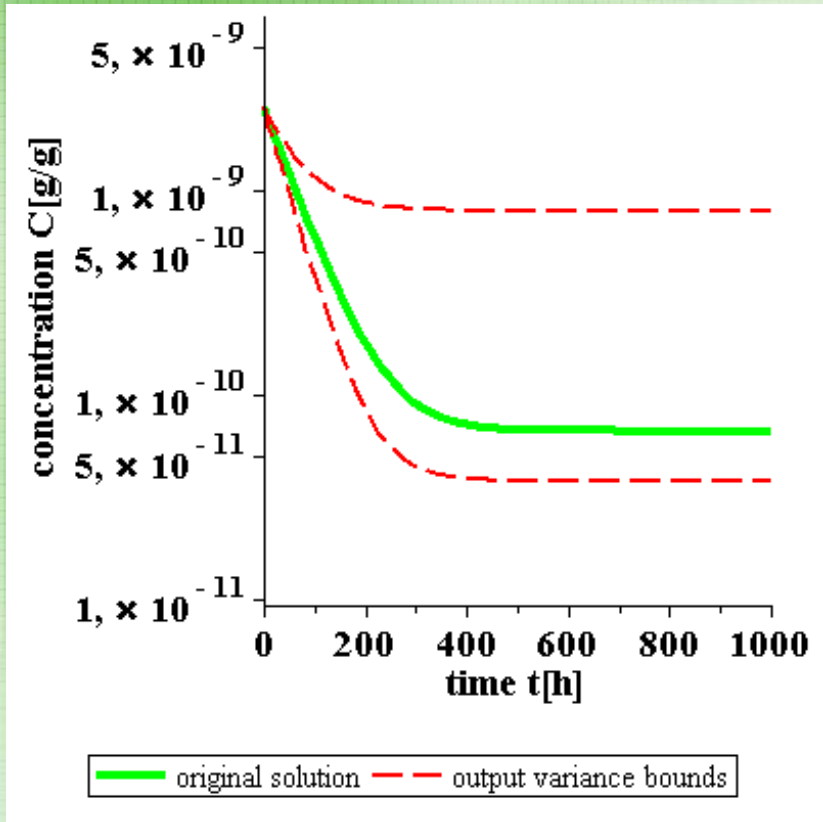


soil

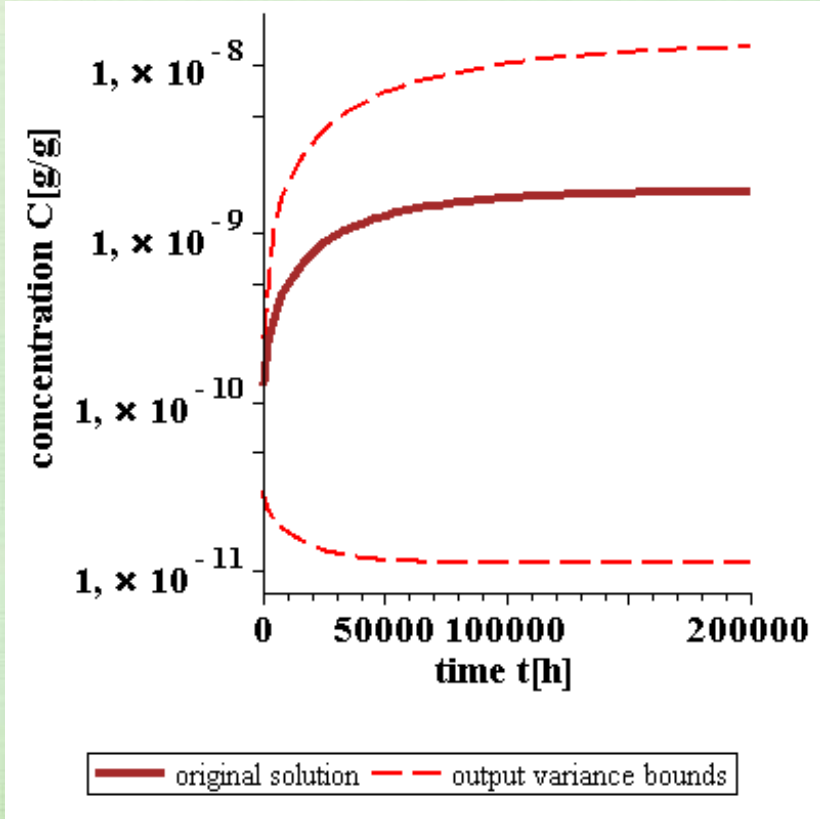


Output variances for benzo(a)pyrene

vegetation

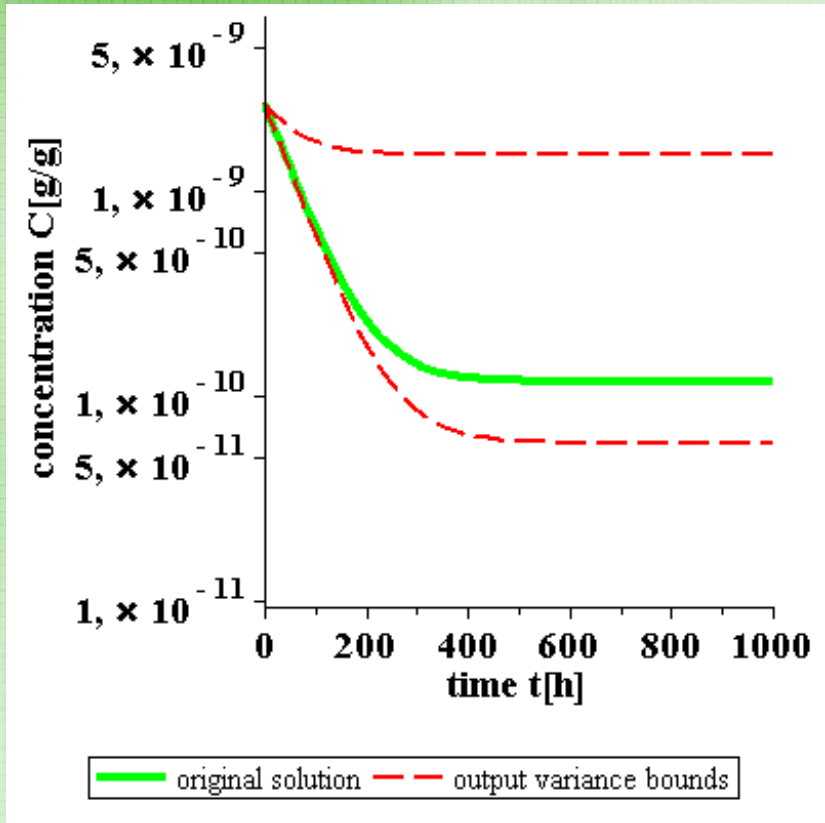


soil

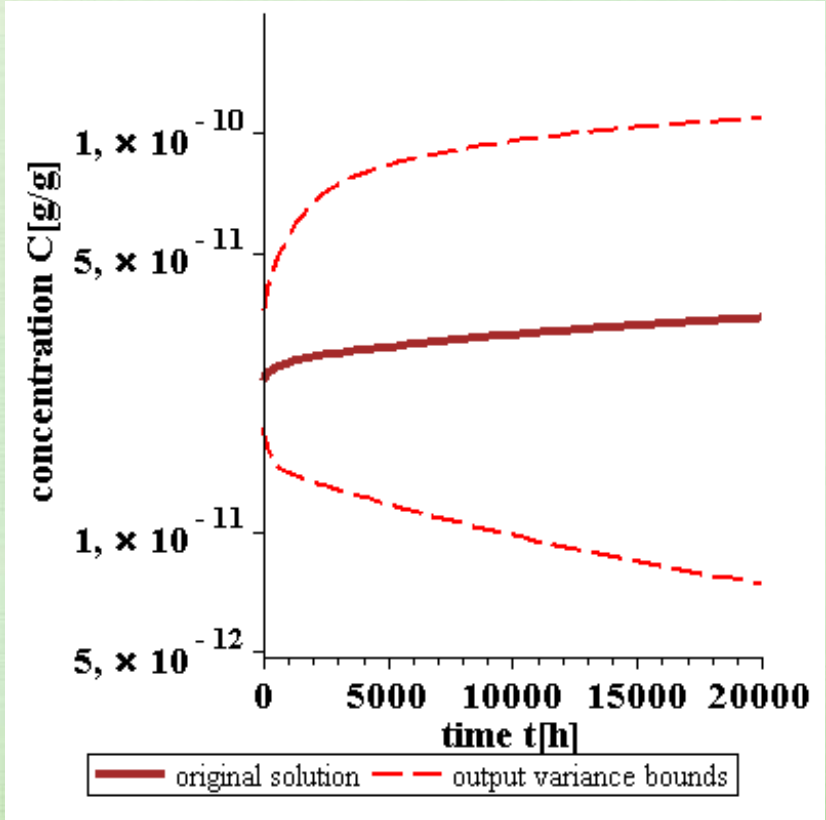


Output variances for pyrene

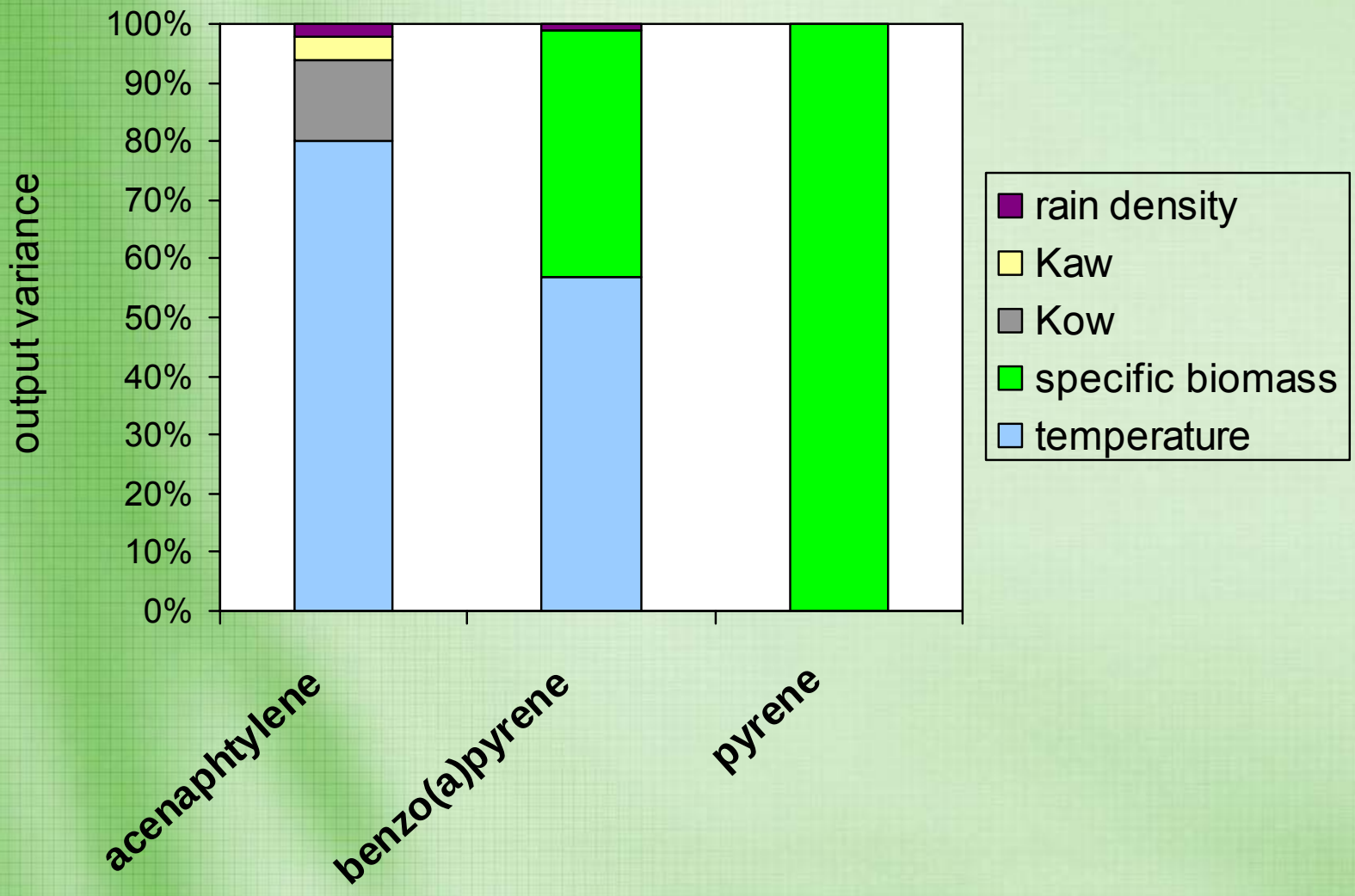
vegetation



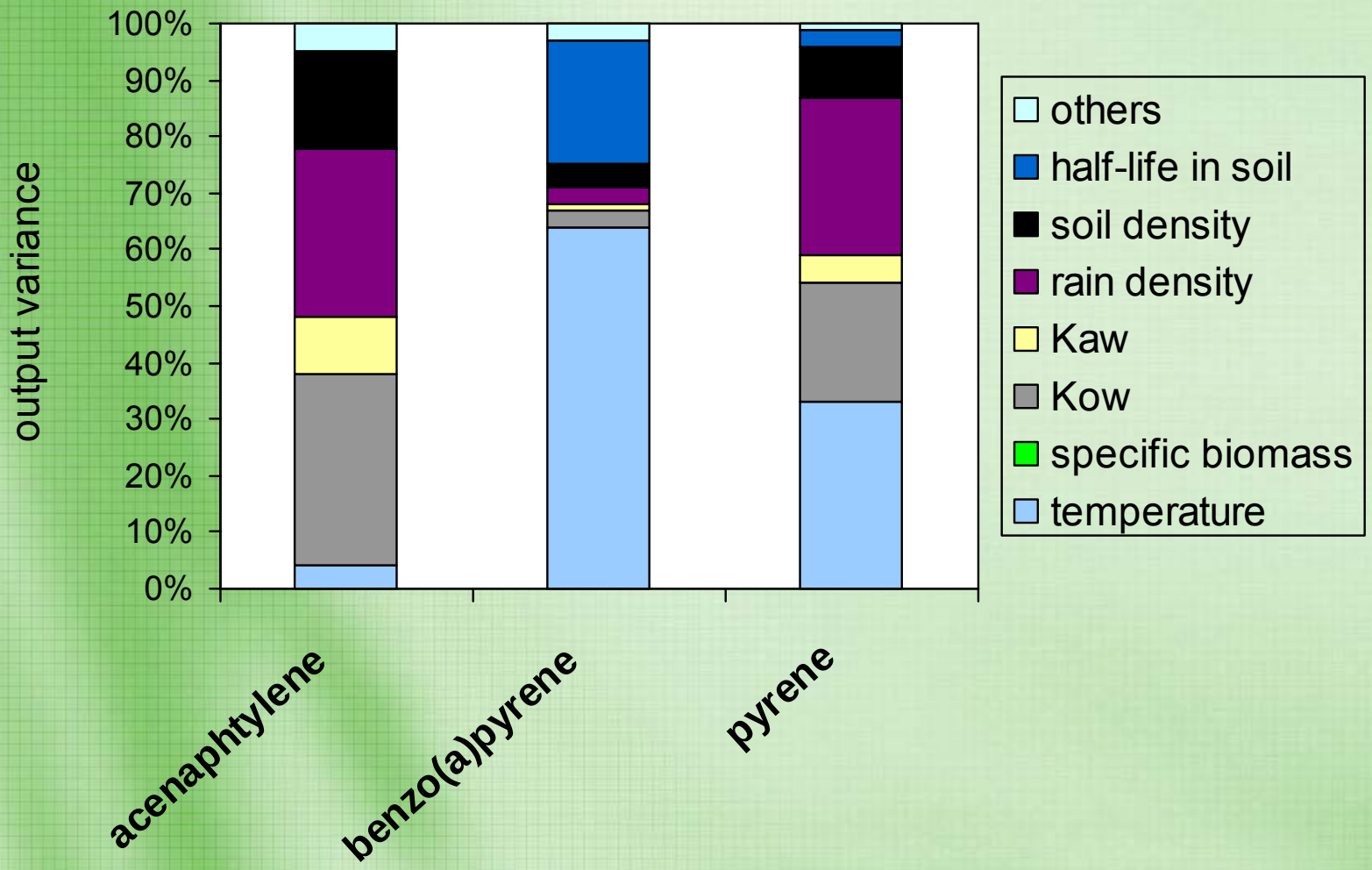
soil



Uncertainty analysis – results for vegetation



Uncertainty analysis – results for soil



Computations – Maple

All the computations were done in computer algebra system Maple.

We used – *Linear Algebra* package (eigenvalues, solving systems of linear equations) and *Statistics* package (Random variables, their distributions, generating samples, rank).

Maple offers three tools for uncertainty handling:
Scientific Error Analysis, *Fuzzy Sets*, *Interval Arithmetic*
(we haven't used them yet).

Problems and plans

- Spearman's method assumes monotonic relationship (it is not model free)
- Finding out the PDFs of parameters
- Complete uncertainty analysis (model uncertainty and uncertainty in model application)

Acknowledgements

- Project INCHEMBIOL
- 7th EU Framework Programme ICT-ENSURE
- Professor Jiří Hřebíček