UNIVERSITEIT GENT

BIOMATH
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Dealing with variability in chemical exposure modelling in rivers

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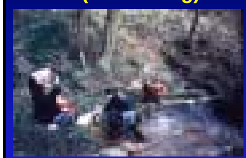
Outline

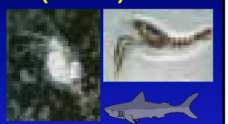
- Introduction
- Screening exposure modelling
- Probabilistic exposure modelling
- Geo-referenced exposure modelling
  - point sources (GREAT-ER)
  - non-point sources
- Dynamic exposure modelling
- Conclusions

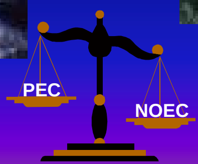
Intro: Ecological risk assessment

Exposure Analysis
Models
(Monitoring)



Effect Analysis
Toxicity tests
(Models)



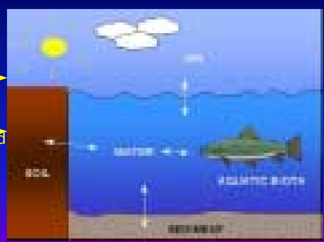


Environmental Concentration

No Effect Concentration

Screening Exposure Modelling

- current methods: multimedia fate models
  = chemical partitioning + decay in generic 'unit world'



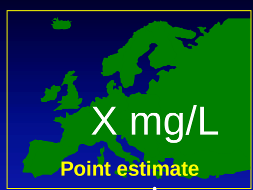
- no uncertainty
- no spatial variability
- no temporal variability
- **low accuracy** (factor 1000)

Problem + goals

When the conservative screening tools indicate a potential risk,
=> a need for **more advanced** risk assessment tools

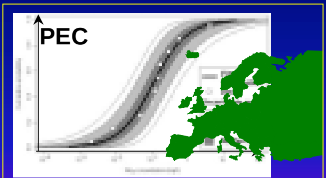
Goal: present 3 higher tier exposure modelling tools:
- probabilistic modelling approach
- geography-referenced modelling approach
  - point sources
  - nonpoint sources
- dynamic modelling approach

Include variability & uncertainty



Make more realistic

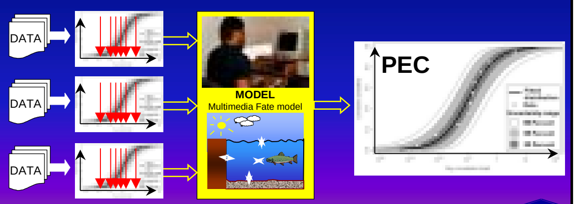
Probabilistic approach



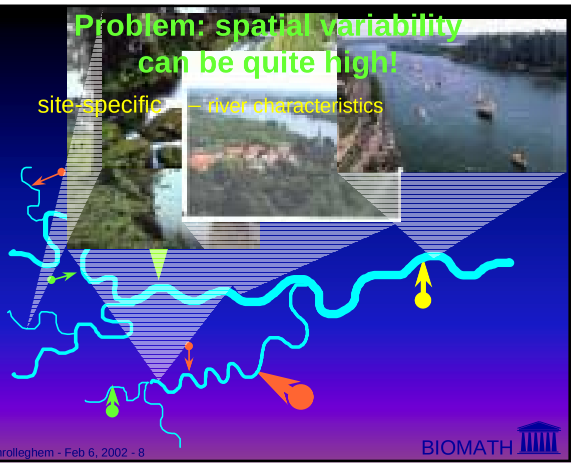
spatial + temporal + other variability & uncertainty

Probabilistic Exposure Modelling

- Variability (spatial & temporal variability, uncertainty) is considered in statistical distributions
- Propagation of variations in Monte Carlo analysis

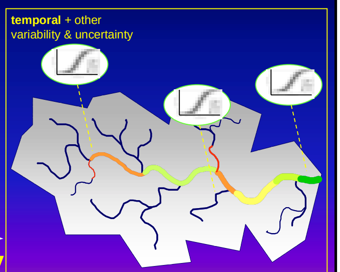


Problem: spatial variability can be quite high!



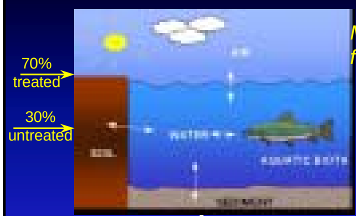
Reduce spatial variability

spatial + temporal + other variability & uncertainty

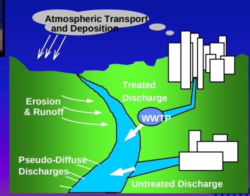


Reduce spatial variability

Reduce spatial variability



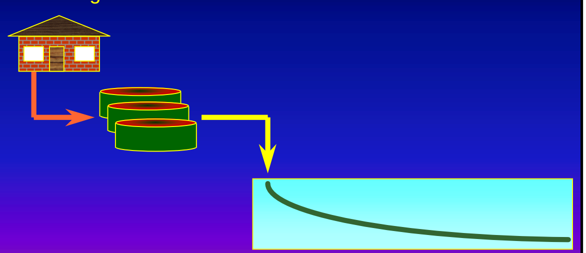
Multimedia fugacity model



Reduce spatial variability → PEC

Aquatic Exposure for point sources GREAT-ER 1.0

- Chemical Emissions
  - Product Consumption
  - Sewage Treatment
- River Fate Processes
  - Dilution + Transport
  - In-stream Removal



Models: 3 different complexity levels

Mode 1

lumped decay rate

k

Mode 2

degradation rate k_{deg}

volatilization rate k_{vol}

settling rate k_{sed}

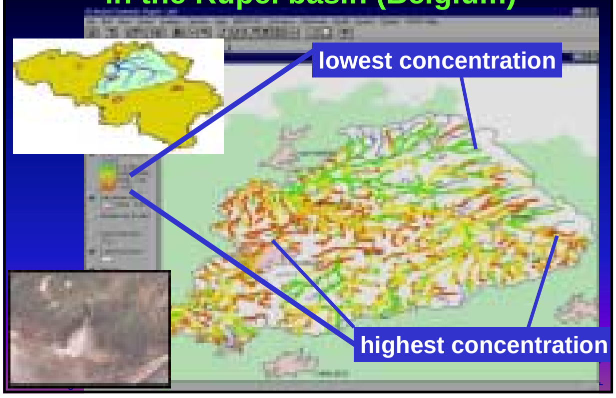
Mode 3

mechanistic and / or empirical process descriptions

- biodeg.
  - sorb/diss
  - DO
- photodeg
  - depth, SS
  - extinction
- hydrolysis
  - pH
- volatilization
  - wind speed
  - flow velocity
  - depth
- settling
  - SS, sorption
  - sediment characteristics
  - depth

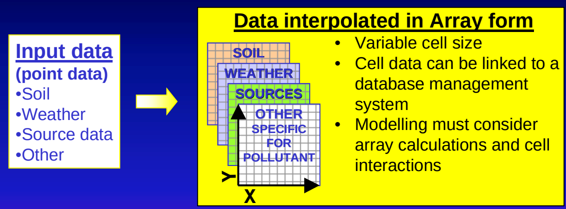
chemical + river properties

Case study on LAS (detergent) in the Rupel basin (Belgium)



Aquatic exposure for non-point sources

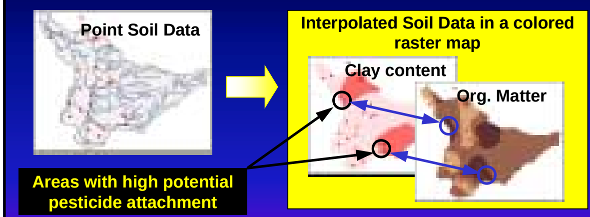
- Point data should be converted to non-point format



- Variable cell size
- Cell data can be linked to a database management system
- Modelling must consider array calculations and cell interactions

more accuracy → *more detailed interpolated data*
→ *more point data is needed*

Case study on Pesticide Usage in Banana Plantations in the Chaguana basin (Ecuador)



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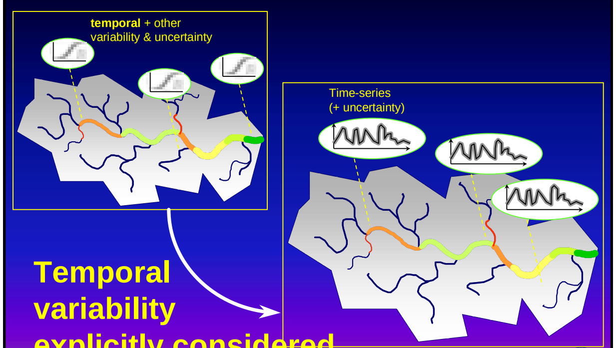
Dynamic river fate modelling

- Why dynamic?

  Currently used steady state models
  - assume uniform emissions, e.g. EXAM, SLSA, TOXIC,...
  - in reality, time variable emissions

- Problem
  - Complex dynamic 3D dynamic river models are seldom used because the required data are seldom available
  - Hence, need for a simplified dynamic model.

Reducing temporal variability



Temporal variability explicitly considered

Complexity of dynamic River Water Quality Models (RWQM)

- Basic 3D (x,y,z) dynamic RWQM
  - **In bulk water**

Change in concentration over time

$$\frac{\partial C}{\partial t} = -u_x\frac{\partial C}{\partial x} - u_y\frac{\partial C}{\partial y} - u_z\frac{\partial C}{\partial z} + E_x\frac{\partial^2 C}{\partial x^2} + E_y\frac{\partial^2 C}{\partial y^2} + E_z\frac{\partial^2 C}{\partial z^2} + R(c,p)$$

Advection, Dispersion, Reaction

- **In sediment**

$$\frac{\partial C_s}{\partial t} = D_x\frac{\partial^2 C_s}{\partial x^2} + D_y\frac{\partial^2 C_s}{\partial y^2} + D_z\frac{\partial^2 C_s}{\partial z^2} + R_s(C_s, P_s)$$

Simple dynamic river fate model – LAS case study

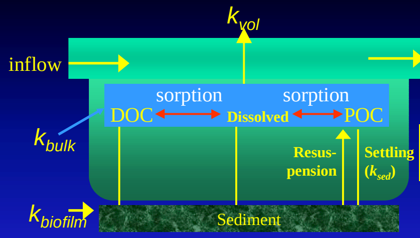
- Basic 3D WQM is reduced to:
  - Series of completely mixed tanks
  - First order kinetics
- General mass balance:
  - In bulk water

e.g resuspension

$$\frac{d(VC)}{dt} = Q_{in}C_{in} - Q_eC - k_{rem}CV + S_{internal}$$

k_{rem} = overall pseudo first order reaction rate constant

LAS removal processes and chemical partitioning

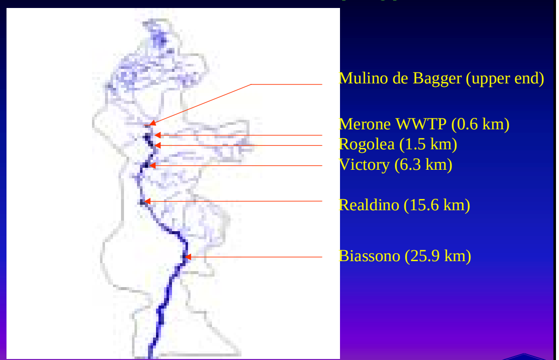


$k_{rem} = k_{deg} + k_{Vol} + k_{sed}$

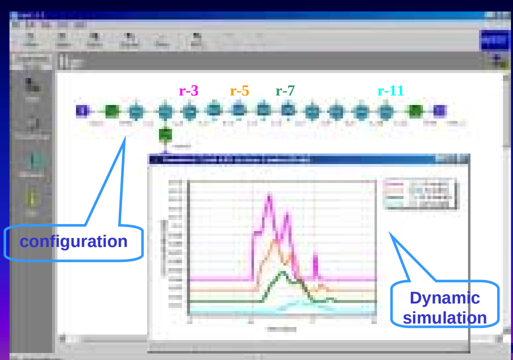
$k_{deg} = k_{bulk} + k_{biofilm}$

- Further considerations
  - dissolved and sorbed phases ➔ bio-available
  - biodegradation ➔ by biomass in the bulk water and biofilm in the benthic sediment

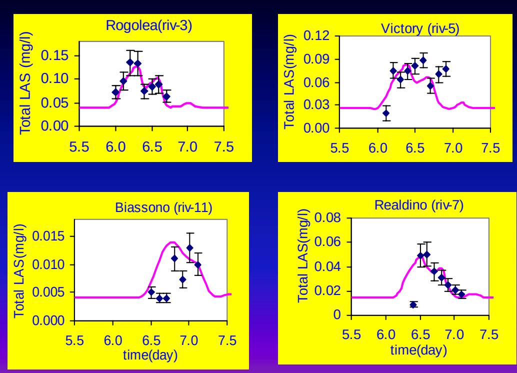
Case study on LAS in the Lambro basin (Italy)



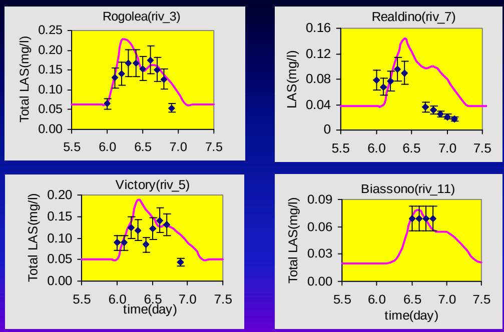
Dynamic river fate model- in WEST® interface



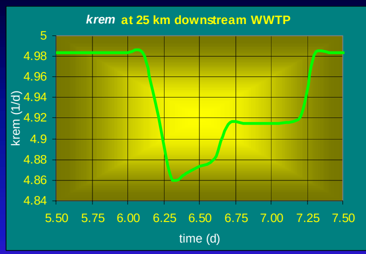
Calibration (Feb. 1998)



Verification (May 1998)



Simulated k_{rem} (Feb. 1998)



k_{rem} varies with time

Conclusions

- Several advanced exposure modelling techniques were presented for a more refined risk assessment
  - Probabilistic techniques (account for uncertainty and spatial/temporal variability)
  - Geo-referencing refines spatial variability
  - Dynamic simulation refines temporal variability
- The case studies show the feasibility and usefulness of the techniques