A Geo-Referenced Fate Simulation Methodology for Aquatic Exposure Assessment of ‘Down-the-Drain’ Chemicals

G. Boeije & P. Vanrolleghem
BIOMATH, University of Gent, Coupure 653, B-9000 Gent, Belgium

Abstract

In the GREAT-ER project (Geography-referenced Regional Exposure Assessment Tool for European Rivers) a refined exposure assessment method for ‘down-the-drain’ chemicals was developed. Real-world data are used, including spatial and temporal variability and uncertainty. The results are geo-referenced distributions of predicted environmental concentrations (PEC). A hybrid stochastic-deterministic approach is applied. Geographies are segmented, based on river network properties. In each segment, several processes (emission or transport/conversion) can occur, which further consist of sub-processes (e.g. different treatment types). The system’s core consists of steady-state deterministic models, which describe chemical fate processes in ‘main rivers’ and in the waste water pathway (emission, transport, treatment). The results of these models are discrete PECs in the considered catchments. A stochastic (Monte Carlo) simulation is applied on top of this. Discrete ‘shots’, each of which applies to the entire simulated geography, are sampled from the input distributions. All ‘shots’ are processed in the deterministic model, of which the discrete results are statistically analyzed to obtain the PEC distributions.

Introduction

Background = Environmental Risk Assessment

Regional **predicted environmental concentrations (PEC)** :

	current generic approaches (e.g. RIVM, VROM & WVC, 1994)	GREAT-ER (Feijtel et al., 1997)
applicability	only **screening** (ESF, 1995)	**higher tiers**
spatial variability	average values	**geo-referenced** input data + results
temporal variability	not considered	PEC = **statistical distribution**

Simulation Approach

- **consumer chemicals fate pathway** (Fig. 1)
- Calculations - **steady-state** models
  - hybrid **stochastic / deterministic approach**

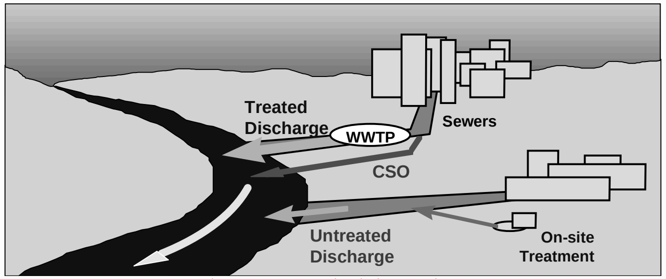

Figure 1. Consumer Chemical Fate Pathway

Predicted Environmental Concentrations (PEC)

- results = **geo-referenced frequency distributions of PECs** (encapsulating temporal variability)
- 2 types: - **river network**
  - **small surface waters** of waste water drainage areas

Segmentation

- river system = set of **interconnected stretches** (Fig. 2)
- **Geographic Unit (GU) = waste water drainage area** of 1 river stretch
- methodology = **scale-independent** (Fig. 3)
- **process segmentation**: segments > processes > sub-processes > input + output terminal

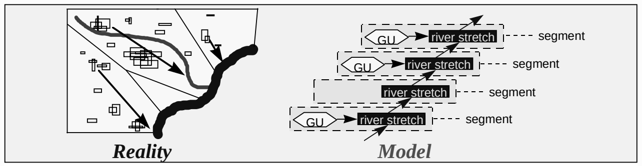

Figure 2. Geographical Segmentation

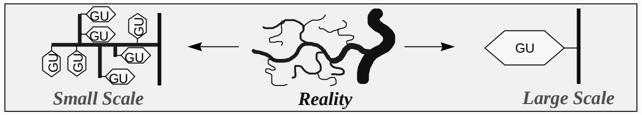

Figure 3. Geographical Scale

Deterministic Fate Model

sequential simulation of all geographical segments:
- influent calculation (from upstream segments)
- waste water pathway and river fate calculations

Segment Selection

recursive tree-walking algorithm (e.g. Fig. 4)

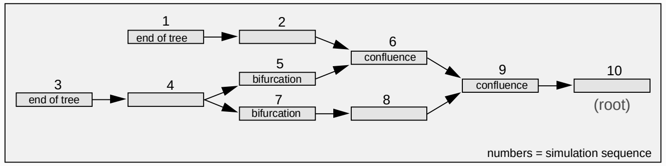

Figure 4 Segment Selection

Calculation Approach

- individual sub-process
  - models for each sub-process = **‘open boxes’**
  - emissions + conversion factors = from **detailed fate model level** (not described - several models and solution algorithms can be used)
- all processes
  - complete **system of model equations** (matrix notation):

$$X_i = A_i \cdot X_i + B_i$$

with X_i = state variables vector
A_i = (square) transport / conversion matrix
B_i = emission vector

- **sequential** (‘top’ to ‘bottom’) **solution is needed** (elements of A_i are only obtained as calculations proceed)

Models

- Waste Water Pathway Model (Fig. 5)
  - prediction of **waste water inputs into main rivers**
  - = **emission** and **transport / conversion** processes
  - identical architecture for all GUs
- River Fate Model
  - **inflow** = mixture of **segment influent** and **waste water discharge**
  - **fate** = calculated at detailed model level (Fig. 6) (e.g. Trapp and Matthies, 1996)

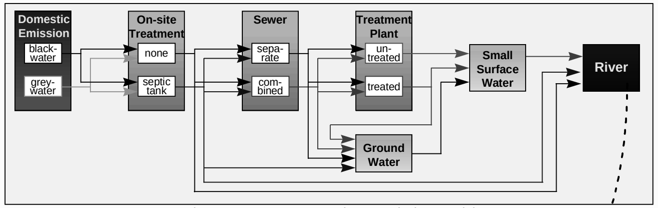

Figure 5. Waste Water Pathway and River Model

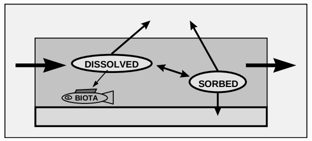

Figure 6. River Model (detailed level)

Stochastic Simulation

- deals with:
  - **seasonality** = environmental variation with time
  - **parameter uncertainty**
- discrete ‘**shots**’ of distributed data set (flows, process parameters, market data,...) = used for deterministic simulation of **entire geography** (Fig. 7)

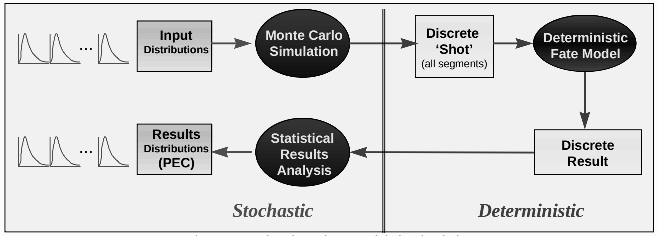

Figure 7 Stochastic and Deterministic Simulation

Flow Scenarios

- **probability of different flows** in river stretch = **log-normal distribution** (e.g. NRA, 1990)
- **flow scenario** = **percentile** from the flow distribution
- **correlations**:
  - flow scenarios **between segments** = full correlation
    → each ‘shot’ = **single flow scenario** for all segments
  - **waste water flow** and **river flow** within a segment = **uncorrelated** (risk assessment: **worst-case scenario**: high chemical mass loads + low river flows)

Concluding Remarks

- **geo-referenced simulation** method for prediction of aquatic exposure to ‘down-the-drain’ chemicals:
  - chemical fate (emission, transport, treatment, river) = **deterministic** models
  - **variability, uncertainty** = Monte Carlo simulation
  - results = statistical **PEC distributions**
- **prototype test** results:
  - large sample data set (16,000 segments) + 1,000 ‘shot’ Monte Carlo simulation
  - calculation time < 1.5 hours on 150 MHz Pentium NT workstation
    → **approach = feasible** for detailed regional or large-scale pan-European simulations

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