A GEO-REFERENCED FATE SIMULATION METHODOLOGY FOR AQUATIC EXPOSURE ASSESSMENT OF 'DOWN-THE-DRAIN' CHEMICALS

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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). To calculate these distributions, a hybrid stochastic/deterministic simulation 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

The background of the GREAT-ER project is Environmental Risk Assessment. For such assessments within an EU regulatory context, regional predicted environmental concentrations (PEC) are to be calculated. Currently generic approaches are used for this purpose (e.g. RIVM, VROM & WVC, 1994), which do not include spatial or temporal variability. According to the European Science Foundation (ESF, 1995), these methods are only fit for screening level assessments.

The GREAT-ER project (Feijtel et al., 1997) was launched to develop a refined exposure assessment tool. It is to be applicable at higher assessment tiers. Input data and results are geo-referenced, and PECs are described as frequency distributions. A hybrid stochastic / deterministic simulation approach is used (Boeije et al., 1997).

SEGMENTATION

A river system is represented by a set of interconnected stretches (Fig. 1). A Geographic Unit (GU) is defined as the waste water drainage area associated with one 1 river stretch. This geographical segmentation methodology is scale-independent (Fig. 2).

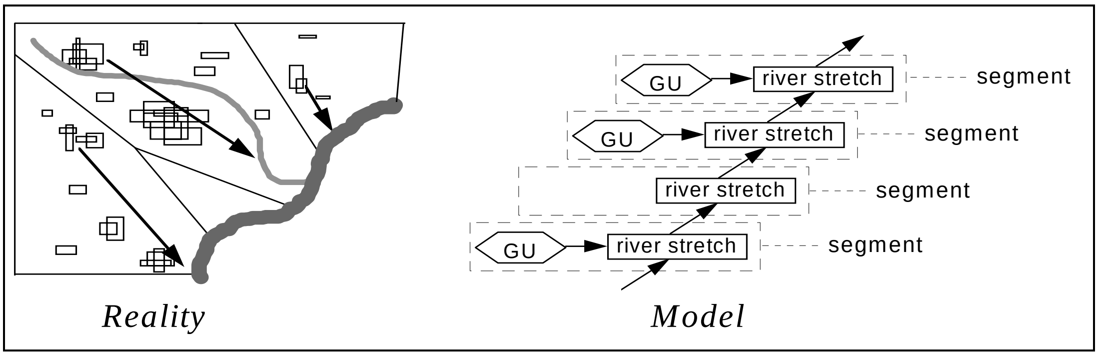

Figure 1. Geographical Segmentation

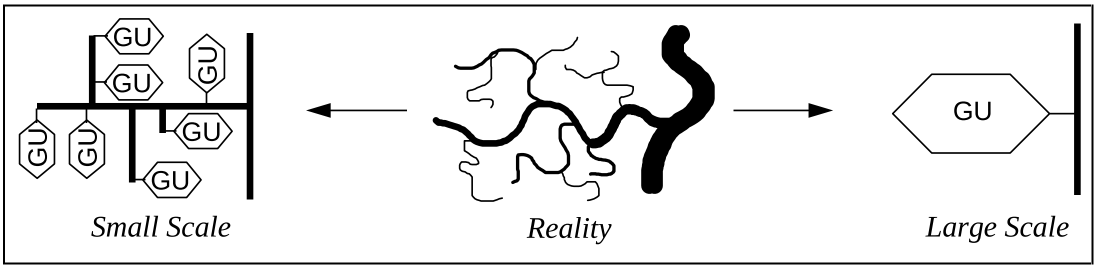

Figure 2. Geographical Scale

A strict process segmentation is also applied. Segments (see above) consist of several processes (e.g. emission, sewer, waste water treatment). The processes are further subdivided into sub-processes (e.g. combined sewer versus separate sewer). Within each sub-process, there is an input and an output terminal.

DETERMINISTIC FATE MODEL

A sequential simulation of all geographical segments is performed. For each segment the influent is calculated (from upstream segments). Next, the waste water pathway and river fate calculations are made. The segment selection algorithm is based on recursive binary tree-walking (e.g. Fig. 3).

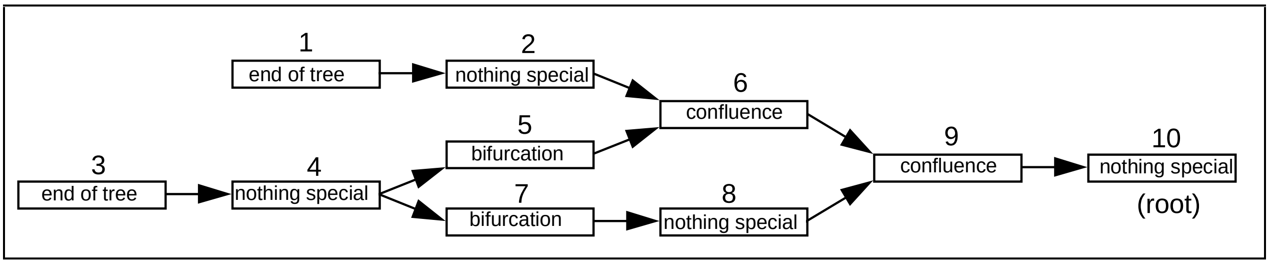

Figure 3. Segment Selection

Calculation Approach

Individual sub-processes are modeled as ‘open boxes’. The actual fate models, which describe the conversions or inputs of chemicals, depend on the implementation. Hence, several models and solution algorithms can be used. To simulate chemical fate in all processes (the complete interconnected waste water pathway and river), a system of steady-state model equations is to be solved. Using matrix notation, this is described as:

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

Matrix-inversion cannot be used to solve this system. A sequential (‘top’ to ‘bottom’) solution is needed, as some elements of A_i may only be obtained as calculations proceed.

Models

As emissions are assumed constant and continuous, steady-state models are used, for simplicity and calculation speed. An overview of the fate pathway of consumer chemicals is given in Fig. 4. In the Waste Water Pathway Model, a prediction is made of waste water inputs into main rivers. This model consists of emission and transport/conversion processes. The model's architecture is identical for all Geographic Units. For the River Fate Model, the inflow is calculated as the mixture of the segment's influent (from upstream) and the waste water discharge. River fate is calculated at detailed model level (e.g. Trapp and Matthies, 1996).

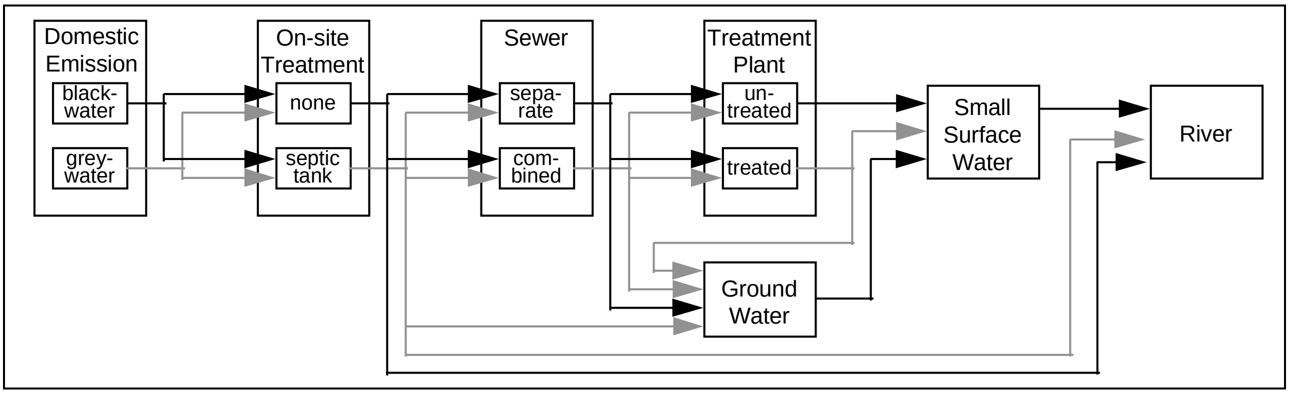

Figure 4. Waste Water Pathway and River Model

STOCHASTIC SIMULATION

The stochastic simulation deals with seasonality (i.e., the environmental variation with time) and parameter uncertainty. Discrete 'shots' of distributed input data set (flows, process parameters, chemical market data,...) are used for the (deterministic) simulation of the entire geography (Fig. 5).

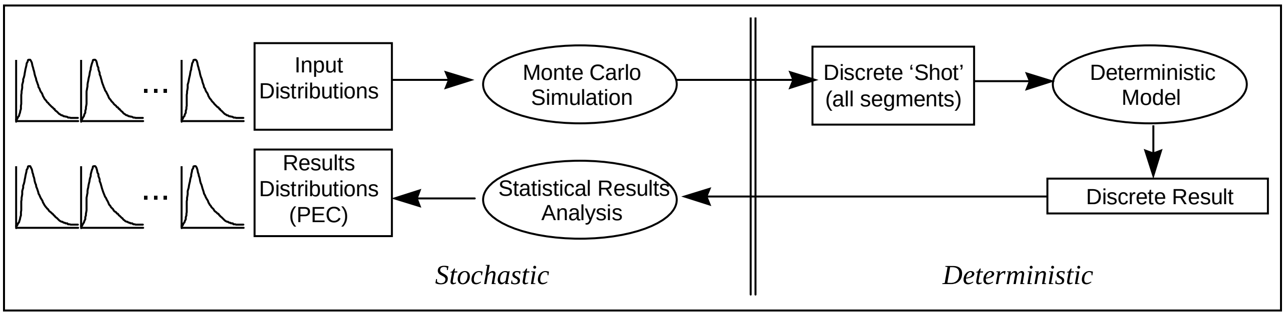

Figure 5. Stochastic and Deterministic Simulation

The probability of different flows in each river stretch is described as a log-normal distribution (e.g. NRA, 1990). A 'Flow Scenario' is defined as a percentile from such a flow distribution. Flow scenarios between segments are assumed fully correlated (i.e., the same flow scenario is assumed to occur simultaneously throughout the river system). The correlation between waste water flows and the river flow within a segment is to be assessed based on the catchment type.

CONCLUDING REMARKS

A geo-referenced simulation method for prediction of aquatic exposure to 'down-the-drain' chemicals was developed. Chemical fate (emission, transport, treatment, river) is predicted by means of deterministic models. Variability and uncertainty are dealt with using Monte Carlo simulation. The results are geo-referenced statistical PEC distributions.

Prototype test results showed that a large sample data set (16,000 segments) could be simulated using 1,000 Monte Carlo 'shots', in less than 1.5 hours on a Windows NT PC (P150). Hence, the approach appears to be feasible for detailed regional or large-scale pan-European simulations.

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