Advisory Opinion
on the Exposure Assessment for Substances based on Geo-Referenced Computer Models
FKZ 360 12 007

Sponsor:
Umweltbundesamt
Postfach 33 00 22
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16. **Kurzfassung**

In diesem Gutachten werden die Eigenschaften verschiedener geo-referenzierter Computermodelle (GREAT-ER, MONERIS, RIONET, ATV-DVWK-Gewässergütemodell, BBA-Risk Map Model, ASSESS-Model, DRIP Model, BETR-model, GIS-SoilFug) gegenübergestellt und mit dem generischen Computer- model EUSES verglichen. Es werden Ergebnisse beider Modelltypen analysiert. Für diesen Vergleich wird exemplarisch das Computermodell GREAT-ER verwendet.

Die Analyse zeigt, dass der Einsatz von GREAT-ER in der Chemikalienbewertung einige Vorteile bietet. Es kann ortspezifsche Konzentrationen in Flusssystemen vorhersagen. Die berechneten Konzentrationen können direkt mit gemessenen Werten (z.B. Daten aus Monitoring-Programmen) verglichen werden und anschaulich in Form von Karten mit Hilfe der in GREAT-ER verfügbaren GIS-Module dargestellt werden.

Es wird daher empfohlen, GREAT-ER als ein Bestätigungsmodell (confirmative model) auf einer höheren Stufe der Chemikalienbewertung einzusetzen.

Eine Reihe von Beschränkungen von GREAT-ER werden aufgezählt. Wenn diese Einschränkungen auch nicht wesentlich für seinen Einsatz in der Chemikalienbewertung sind, so wird doch empfohlen, das Modell entsprechend zu verbessern, damit ein reibungsloser Einsatz des Modells in der Behörde sichergestellt ist.

17. **Schlagwörter** GREAT-ER, EUSES, geo-referenzierte Modelle , Expositionsabschätzung, Allgmeinchemikalien, Risikoabschätzung

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16. **Abstract**

In this advisory opinion the properties of different geo-referenced models (GREAT-ER, MONERIS, RIONET, ATV-DVWK-Gewässergütemodell, BBA-Risk Map Model, ASSESS-Model, DRIP Model, BETR-model, GIS-SoilFug) are summarised and compared with the generic computer model EUSES. Results of both model types are analysed. The computer model GREAT-ER is exemplarily used for that comparison.
The analysis shows that the use of GREAT-ER has advantages. The model predicts site-specific concentrations in river systems. The simulated concentrations can directly be compared with measured (monitored) data and can be visualised in maps due to the GIS-tool of GREAT-ER.
It is recommended to consider GREAT-ER as a confirmative model at a higher tier of chemical assessment. If the model is used in the regulatory context, the "level of protection" for GREAT-ER lies in the choice of the "standard scenario" representing a vulnerable river basin.
A couple of limitations are listed and it is recommended to work on the following limitations in order to guarantee an increased functioning of GREAT-ER if it will be used in the regulatory context.

17. Keywords GREAT-ER, EUSES, geo referenced model, exposure assessment, general substances risk assessment

18. Price	19.	20.

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1 Background

Due to different directives on the national and the European level it is necessary to analyse the fate of chemicals in the environment using exposure models. By combining the results of these models with ecotoxicity data the risk assessment is performed. Usually, this analysis is performed based on EUSES (EC (1996),EC (2003a)). It calculates the fate of chemicals based on generic scenarios. Generic scenarios do not represent real local situations, but reflect average situations for a given region, e.g. “the EU” or “Nordrhein-Westfalen”. The aim of the model is to estimate conservative concentrations for the different environmental compartments in the respective region. In the year 2003 a new version of EUSES was released to consider the new version of the Technical Guidance Documents (EC (2003b)).

On the other hand, geo-referenced exposure models are considering detailed input data on the local scale for their predictions. The results of these models can be expressed by thematic maps and directly compared with monitoring data of the respective river system. However, the amount of input data needed to run geo-referenced models is much higher than for generic models like EUSES. A typical geo-referenced model used in Europe is GREAT-ER (Geo-Referenced Regional Exposure Assessment Tool for European Rivers) developed by a group of several European organisations in 1996 to 1999 (Feijtel et al. (1997)).

2 Objectives

The objective of this advisory opinion is to summarise the properties of different geo-referenced models and to compare them with the generic computer model EUSES Additionally, results of both model types will be analysed. The crucial criterion will be the level of protection for the aquatic environment. The computer model GREAT-ER will be exemplarily used for that comparison.

It is the aim of this work to evaluate the fundamental parameters and equations for the calculation of the fate of substances for both approaches in the aquatic environment to assess their respective levels of protection.

3 Description of EUSES

3.1 Introduction

The European Union System for the Evaluation of Substances (EUSES) was developed for quantitative assessment of the risks posed by new and existing chemical substances to man and the environment. EUSES is based on USES 1.0 developed by RIVM (1994) on behalf of the Netherlands' Health Council. As a next step the system EUSES 1.0 was developed in a co-ordinated effort of EU Member States, the European Commission and its European Chemicals Bureau, and the European Chemical Industry (EC (1996)). In 2003 EUSES 2.0 was released (EC (2003a)). Several new or updated modules were programmed into EUSES 2.0 compared to the previous version such as temperature correction for vapour pressure and solubility or the choice of QSAR for estimation of KOC-values.

The risk assessment is attuned to current chemical policies and in accordance with the principles laid down in the "Technical Guidance Documents" for new an existing substances of the European Commission (EC (2003b)).

EUSES is in line with present assessment procedures and is therefore used in the initial (screening) stage as well as the intermediate (refined) stage of environmental risk assessment.

3.1.1 General principles

EUSES is an extensive software package covering the complete assessment of chemicals (e.g. concentrations in soil and groundwater, accumulation in food, risk assessment for the general population and for special sub-groups like workers).

EUSES allows exposure and effect assessments in a stepwise procedure. The EUSES risk assessment is performed by comparing the exposure and the effect assessment (predicted environmental exposure versus predicted no-effect concentration for environmental compartments: PEC/PNEC. A margin of safety (MOS) is considered for human sub-populations. In total following human populations and environmental system are considered within EUSES 2.0:

Human populations

- Workers
- Consumers
- Man exposed via the environment

Ecological systems and populations

- Micro-organisms in sewage treatment systems
- Aquatic ecosystem
- Terrestrial ecosystems
- Sediment ecosystems
- Top predators

Risk assessment with EUSES starts from a screening level in which “generic exposure scenarios” are applied. It is assumed that substances are emitted in a standard environment with predefined environmental characteristics agreed upon by the EU Member States. No measured data is used at this screening level.

3.1.2 The exposure assessment in EUSES

Doses and environmental concentrations of a chemical are predicted in a three-step procedure. Firstly, releases to environmental compartments are predicted based on the volume produced or imported, the use pattern, and physico-chemical properties of the chemical (emission module). In the next step the environmental distribution model does all the necessary calculation to estimate the distribution of a substance in the environment (=surface water, sediment, soil, groundwater, effluent and influent of the model simple

treatment plant). Finally, the exposure assessment is performed considering bioconcentration factors, secondary poisoning, human exposure through environment, consumer products for workers.

Table 1: The structure of EUSES (EC (1996))

Module	Content
Input module	Data entry in HEDSET format: substance identification and physico-chemical properties
Emission module	Use data of the substance Estimation of local emissions to wastewater and air for various life-cycle stages Estimation of regional emissions to wastewater, air and soil for various life-cycle stages Emission tables are used, given in Appendix IV
Distribution module	Local models: STP model: SimpleTreat Air model: OPS Dilution and sorption in surface water One-compartment soil model Regional model: Mackay-type level III multi-media model SimpleBox
Exposure module	Secondary poisoning, estimation of exposure levels for predating birds and mammals Exposure of humans through the environment (including food products) Human exposure through use of consumer products Human exposure in the workplace
Effects module	Toxicological and ecotoxicological data Determination of PNECs for the environmental end-points (water, soil, sediment, STP, predators) by applying assessment factors based on available data For soil and sediment, equilibrium partitioning is used when data are lacking Route-to-route extrapolation for human effects assessment
Risk characterisation module	Determination of RCRs for all end-points of the risk assessment

Abbreviations used: STP = Sewage Treatment Plant; OPS = Operational atmospheric transport model for Priority Substances; PNEC = Predicted No-Effect Concentration; RCR = Risk Characterisation Ratio

In Table 1 (taken from the EUSES user manual) the complete structure is explained in more detail.

3.1.3 Model dimensions

The dimensions of EUSES are determined by three factors:

- Spatial scale
- Time scale
- “Realism scale”

Spatial scale

Three spatial scales are considered within EUSES:

- There is a personal scale were individual workers or consumers are considered.
- The local scale considers the protection goals in the vicinity of one large point source of the substance.
- The regional scale assesses the risks to protection targets due to all releases in a generic, larger region (app. 200 km x 200 km). A fourth spatial scale, the continental scale (sum of all EU Member States) is added to serve as background for the regional system.

Time scale

Local emissions of industrial chemicals can either be continuous or discontinuous.

3.2 Model Description

EUSES considers two scales for its estimation: the local scale (vicinity of a point source) and the regional scale (larger area which includes all point and diffuse sources).
For the calculations EUSES is using so called "primary data" (user input data characterising the chemical) to estimate partition coefficients and degradation constants ("secondary data"). Both types of data use necessary to calculate the fate of substances in the environment.

3.2.1 Partition coefficients

Various partitions coefficients are used within EUSES to describe the distribution of a substance in the environment (incl. organisms). As measured data on fate processes are usually not available, they are extrapolated from the primary input data. Therefore, special equations are built in to extrapolate missing data for all partition coefficients (solid-water, gas-aerosol, air-water) considered in EUSES.

3.2.2 Degradation rates in the environment

Similarly the necessary rate constants of the degradation processes are estimated from the primary data:

- Hydrolysis,
- Photolysis in water,
- Photochemical reaction in the atmosphere,
- Biodegradation in the sewage treatment plant,
- Biodegradation in surface water, sediment and soil.

3.2.3 The sewage treatment plant within EUSES

As most of the wastewater volume is treated in biological treatment plants special modules are implemented within EUSES to consider this entry route. However, dependent on the scale either 100% (for the local scale) or 80% is assumed as default for the waste water passed through a sewage treatment.

The degree of removal in the treatment plant is determined by the physico-chemical and biological properties of the substance and the operating conditions of the plant. However, similar as for missing partition coefficients or degradation rates estimation methods are built in to calculate the necessary input data.

The standard sewage treatment plant is modelled as an average-size treatment plant based on aerobic degradation by activated sludge (SimpleTreat). The model calculates steady-state concentrations in a sewage treatment plant consisting of a primary settler, an aeration tank and a solids-liquid separator. The model itself is of type 'Mackay Level III (Struijs (1996)).

3.2.4 Local environmental distribution

Generally, it is assumed that wastewater will pass through a simple treatment plant before being discharged into environment. However, for the largest local PEC in surface water (additionally) a concentration assuming no sewage treatment is calculated. The concentration in surface water is calculated after complete mixing of the effluent in the receiving water. No degradation processes are considered for the substance. Also volatilisation or sedimentation is **not** taken into account due to the short time between discharge and disposal. The only "removal" processes in the assessment are dilution based on a standard factor and adsorption to suspended matter. Though dilution factors are discussed between 1 (dry riverbeds in summer) up to 100 000 as analysed by Behrend et al. (2000), Behrend et al. (2000) and Matthies and Schröder(2002) an "average" dilution factor of 10 is recommended by the EUSES developers (EC (1996)). The fate processes considered on the local scale are illustrated in Figure 1.

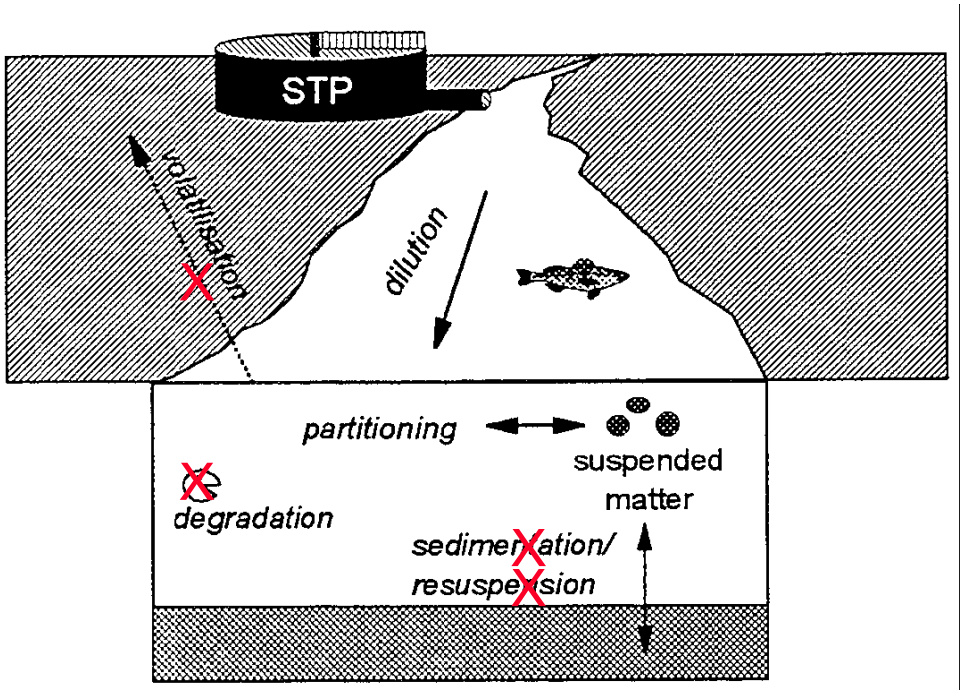

Figure 1: Processes considered an not considered in surface water (local scale) in EUSES

The suspended sediment is taken for the calculation of the $PEC_{sediment}$ in freshly deposited sediment. The respective calculation of the PEC in the bulk sediment the concentration is calculated from the water body concentration assuming thermodynamic equilibrium.

3.2.5 Regional and continental distribution

The fate of chemical at the regional scale differs from the fate at local scale, because more time is available for transport and transformation. Concentrations at the local scale are almost entirely controlled by dilution with the background concentrations (mixing). The models for calculating local PECsw do therefore not consider removal processes.

However, the regional distribution considers inter-media transport and degradation processes. The multi media model SimpleBox model 3.0 by Brandes et al. (1996) and den Hollander and van de Meent (2004) is implemented to calculate regional environmental concentrations on different spatial scales simultaneously. SimpleBox, a level III Mackay model, is able to consider that emissions at the regional scale lead to increased concentrations at larger spatial scales, and that emissions at the continental scale contribute to increased concentrations at the regional scale (see Figure 2)

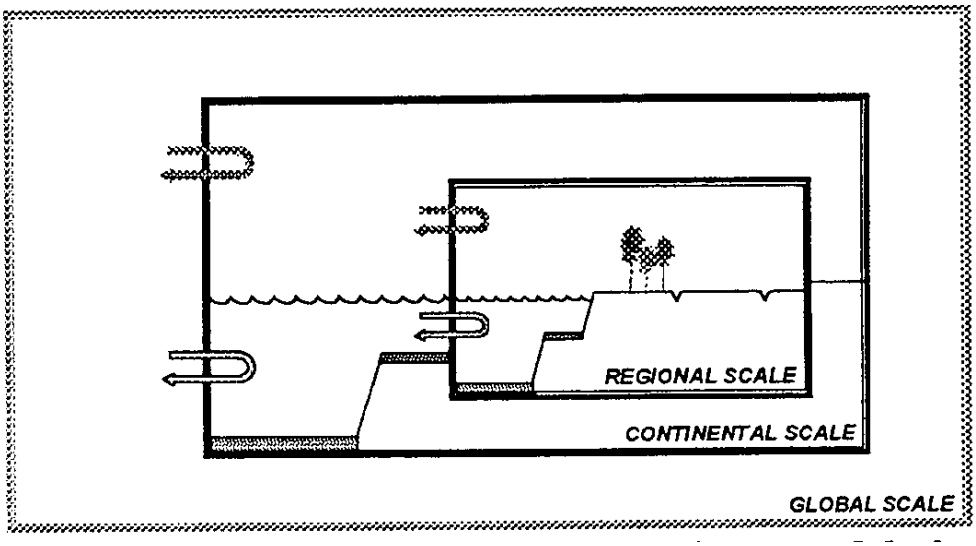

Figure 2: Nested multi-media fate model for regional exposure (EC (1996))

All simulations on the regional and continental are based on following assumptions:

- Similar as for the wastewater simulations (Simple Treat) the regional $PEC_{surfacewater}$ model is of type Mackay level III (non equilibrium steady state).
- Environmental media (air, water, sediment, 3 soil types) are represented by compartments (boxes). Flows of the chemicals are modelled by calculating mass balances for each of the boxes. Concentrations of chemicals in the boxes are calculated by solving the mass-balance equations simultaneously.
- The environmental media are assumed to be homogeneous and totally mixed. Spatial variation within a media is not considered.
- All properties of the environmental media are assumed to be non-variable.
- Emission rates are assumed to be constant in time.
- All degradation processes are assumed to follow first order kinetics.

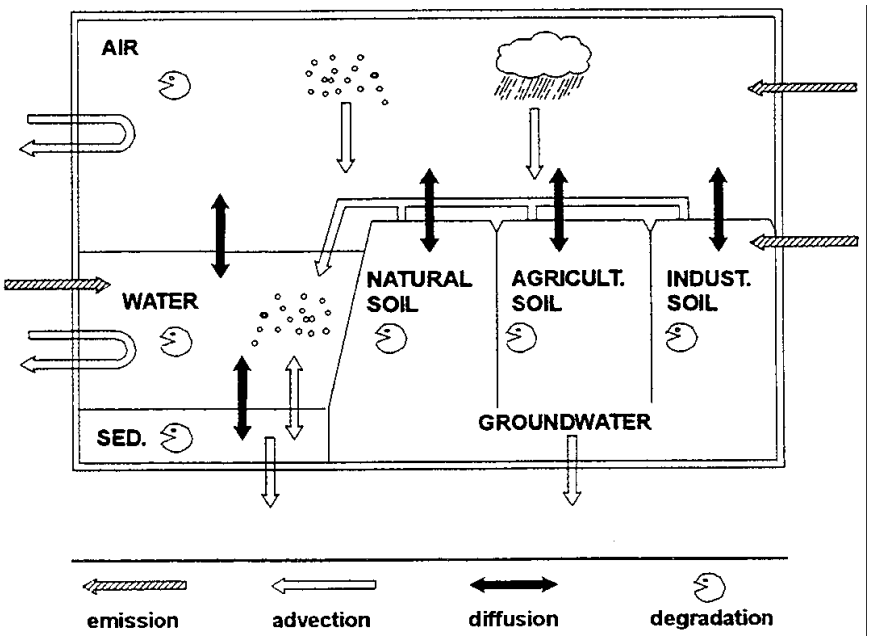

Figure 3: Schematic representations of the model for calculating regional and continental PECs (EC (1996))

As shown in Figure 3, there are four compartments considered for the calculation of regional PECs: atmosphere, surface water, sediment, and soil.

The water compartment contains the chemical in a truly dissolved state and associated with particulate matter (colloidal material, suspended sediment, aquatic biota). All phases in water are assumed to be in thermodynamic equilibrium. Water is defined by a constant resident time so the water boxes are open boxes. The resident time for water is defined by the volume of the water compartment, run-off from soil, incoming river water a direct rainfall into surface water.

Emissions

Emissions are modelled as continuous and diffuse. As the key assumption in EUSES is *steady state under non-equilibrium conditions* the fate of substances is dependent on the emission rate and the entry compartment. The regional and continental models require that the indirect emission to sewage system is specified, the output of the Simple Treat model (annual averaged) is used as input for the PEC models.

Substance environmental import and export

Advective transport with air and water between the continental and regional scales are accounted for in the model. The predicted exposure concentrations at the regional scale are the net result of emissions on both spatial scales, and the modelled rates of advection.

Degradation

First-order kinetics are generally assumed for all degradation processes.

Inter-media transport

There are various processes considered to enable inter-media transport such as dry and wet deposition of aerosol-bound chemicals or sedimentation and re-suspension of particle-bound chemicals. However, not all of these exchange processes are important for the fate in surface water.

Generally, diffusive transfer is two-way (dependent on the concentration in both media), where advective transfer processes are modelled as one-way phenomena.

3.2.6 Limitations

The main limitations of EUSES on the regional scale are:

- The Simple Box model and its assumption of instant mixing within a given box is not in agreement with reality. This assumption does not reflect the variability of concentrations and transport processes within a compartment especially when estimating the regional or continental concentrations.
- Degradation processes are dependent on environmental variables like temperature or pH-values. This was not considered within EUSES 1.0 and is only partly considered within EUSES 2.0.
- EUSES does not consider temporal variability, when estimating concentrations in the media (surface water).

3.3 Conclusions

EUSES is a very complex software system that is designed to make quantitative risk assessments for new and existing chemicals.

EUSES is in line with current assessment procedures of the Technical Guidance Documents and is therefore used in the initial (screening) stage as well as the intermediate (refined) stage for human and environmental risk assessment.

The main advantage of EUSES is that calculation of PECs can be performed without big efforts. However, the choice of the correct input data and the often necessary overwriting of default values make the calculation with EUSES a difficult and time consuming task even if it is not necessary to perform extensive data searches because default values are provided for all parameters.

However, though EUSES principally considers the current Technical Guidelines of the EU the actual estimation of surface water concentrations can only be characterised as a rough and conservative estimation. Especially the “regional” or “continental” concentrations do not have a realistic background. This is mainly the case because the whole estimations is done based on a very small number of compartments using the Simple Box model. It assumes an instant mixing within the whole water of the system (“the region” or the “continent”) resulting in concentrations that would occur after all water within the region or the EU has been well mixed. It is not possible to compare the calculated results with real concentrations as there is no link to locations. Even if the calculated concentrations are compared with statistically processed monitoring data (mean values, percentiles) the measured data are dependent on specific local conditions that cannot be considered within EUSES.

The model assumptions for the degradation and transfer processes between media are more suitable for calculating PECs in surface water. The simulations could be improved, if the important dependency of environmental variables (e.g. pH, temperature) were considered. That was partly realised in the new version EUSES 2.0 that was released in 2003.

4 Description of current geo-referenced surface water models

4.1 GREAT-ER

4.1.1 Introduction

GREAT-ER (Geo-Referenced Regional Exposure Assessment Tool for European Rivers) was developed by a group of several European organisations between 1996 and 1999 (Feijtel et al. (1997)). Besides the software, data (especially geographic data) are an essential part of GREAT-ER. Some portions of the data processing have been done at the Institut für Umweltsystemforschung in Osnabrück and information on the processing are a part of this document. Initial data collection and preparation (covering hydrological processing) were done by the Institute of Hydrology, Wallingford, UK.

GREAT-ER 1.0 is set on top of the geographic information system (GIS) ArcView, a product developed and marketed by the Environmental Systems Research Institute, Inc. (ESRI). The development was based on the software package ArcView 3.0 with the patch for version 3.0a, but it is also compatible with the ArcView 3.1. However, as ArcView is not longer supported the new development GREAT-ER 2.0 (GREAT-ER desktop) which gives the same simulation results, is based on an Oracle database without using ARCView 3.0 anylonger.

The objective of the GREAT-ER project was to develop and validate a chemical exposure prediction tool for use within the EU environmental risk assessment scheme. GREAT-ER is able to calculate the distribution of PECs - both in space and time - of down the drain chemicals in European surface waters on a river and catchment area level.

GREAT-ER contains hydrological databases and models to determine river flows in pilot study areas. Within these areas GREAT-ER predicts chemical exposure in aquatic ecosystems and allows the calculation of a realistic distribution of environmental concentrations of down-the-drain chemicals. The aim of the developers was to enable the prediction of the concentrations of chemicals at any location in EU rivers and river basins from site-specific discharges, river and effluent flow data. The methodology delivered is applicable for the entire EU, but not for all European river systems the necessary data were made available, yet.

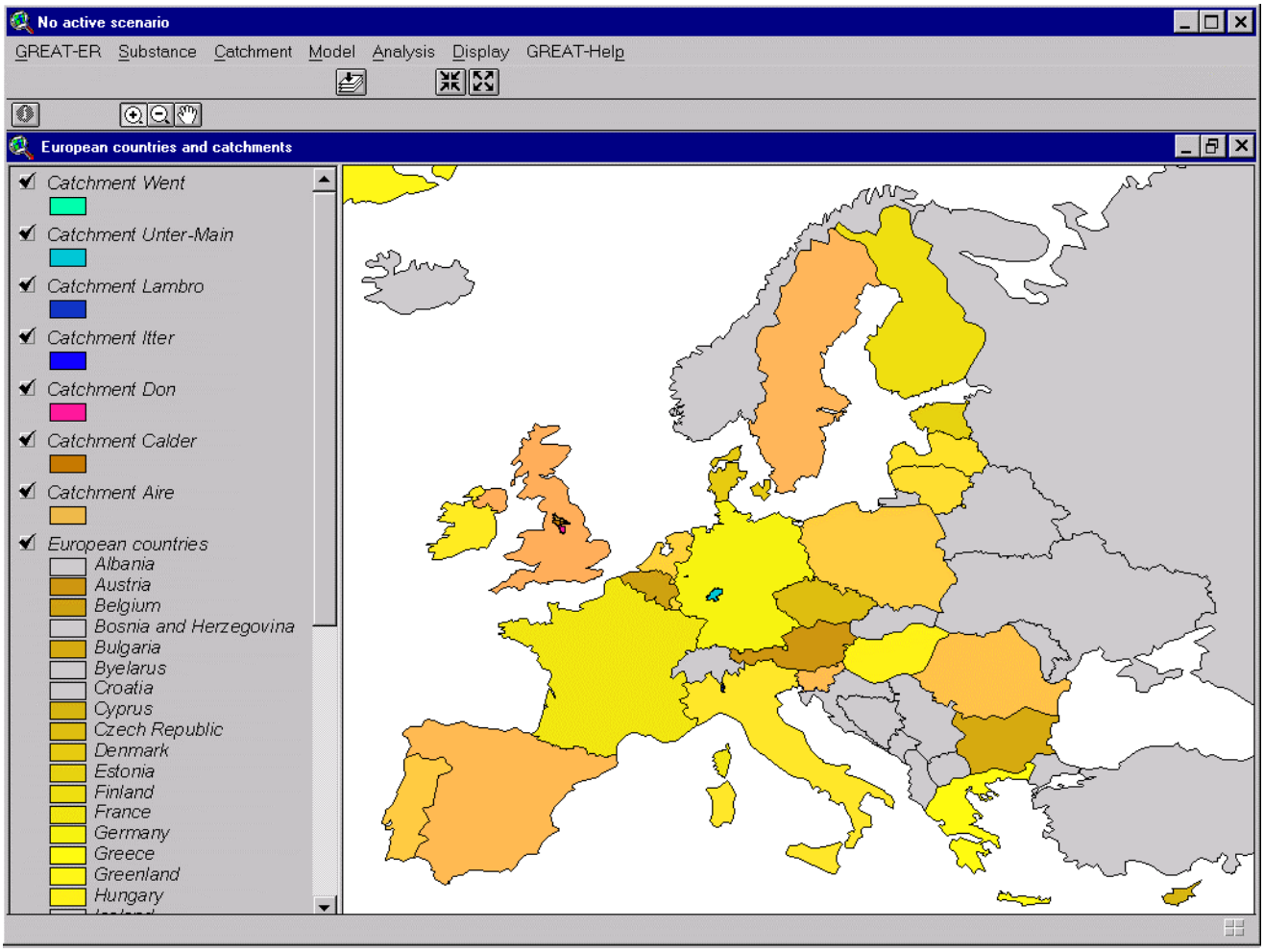

Figure 4: Initial screen of GREAT-ER

4.1.2 General principles

Before doing any simulations a river network has to be parameterised in GREAT-ER. The river system in GREAT-ER consists of lines (or so-called 'polylines'), of which each line is representing a river segment and nodes which represent the point of connection of two segments (see Figure 5). Additionally, for all segments the up- and downstream ends have to be defined.

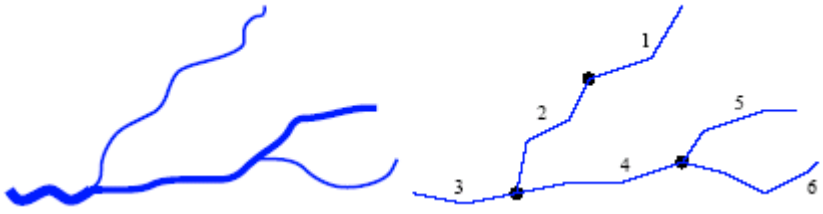

Figure 5 : Real river course (left) and digitised river (right), [GREAT-ER User manual]

All information in the digital river network comes from maps of the corresponding areas. In addition to the geographic information, GREAT-ER needs additional information about the river systems, such as river flow volume (m^3/s) and flow velocity (m/s). Further information is needed like depth and length of a certain river segment.

GREAT-ER was developed to model so called “down-the-drain” chemicals. These type of substances are regularly released into the wastewater system and fractions enter the river-system after having passed treatment-plants. At present, it is not possible to model diffuse emissions via surface runoff or atmospheric deposition.

GREAT-ER is using a special simulation approach to deal with statistically distributed inputs and outputs, involving both stochastic and deterministic techniques. The model core is deterministic. By means of Monte Carlo simulation, a stochastic layer is added on top of this core. A large number of ‘shots’, which are discrete samples from the distributed data set, are generated. For each input parameter, there exists a discrete counterpart in the ‘shot’, which was sampled at random from the input distribution. For each of these ‘shots’, the deterministic model is called, which contains a mechanistic description of the considered processes in the rivers and in the waste water drainage areas. Process rates are derived from knowledge about chemical properties and process specifics. Finally, the (discrete) results from each ‘shot’ are statistically analysed, to obtain distributed results as simulation output.

Generally, only steady-state model simulation can be performed assuming

- constant chemical emissions. Diurnal patterns in product and water consumption are disregarded, as well as variations between different days of the week,
- constant flows within each steady-state model calculation run,
- constant environmental properties.

The **simulation input data** are expressed as statistical frequency distributions in order to include both seasonally effects and parameter variability and/or uncertainty into the simulation input. For river flows and flow velocities, the log-normal distribution is used. For hydrological information this distribution is described by the mean and the 5^{th} percentile.

The **simulation results** are frequency distributions of chemical concentrations, incorporating temporal variability. For risk assessment purposes, these results can be expressed as log-normal distributions, defined by their mean and 95^{th} percentile values. Predicted concentrations are geo-referenced in the same way as the input data set: river concentrations are associated with a river network structure, and waste water drainage area concentrations are associated with discharge points. Within one location, a further differentiation is made between the maximal predicted concentrations (i.e. upon discharge),

the minimal predicted concentrations (i.e. after degradation processes), and an 'internal' average value.

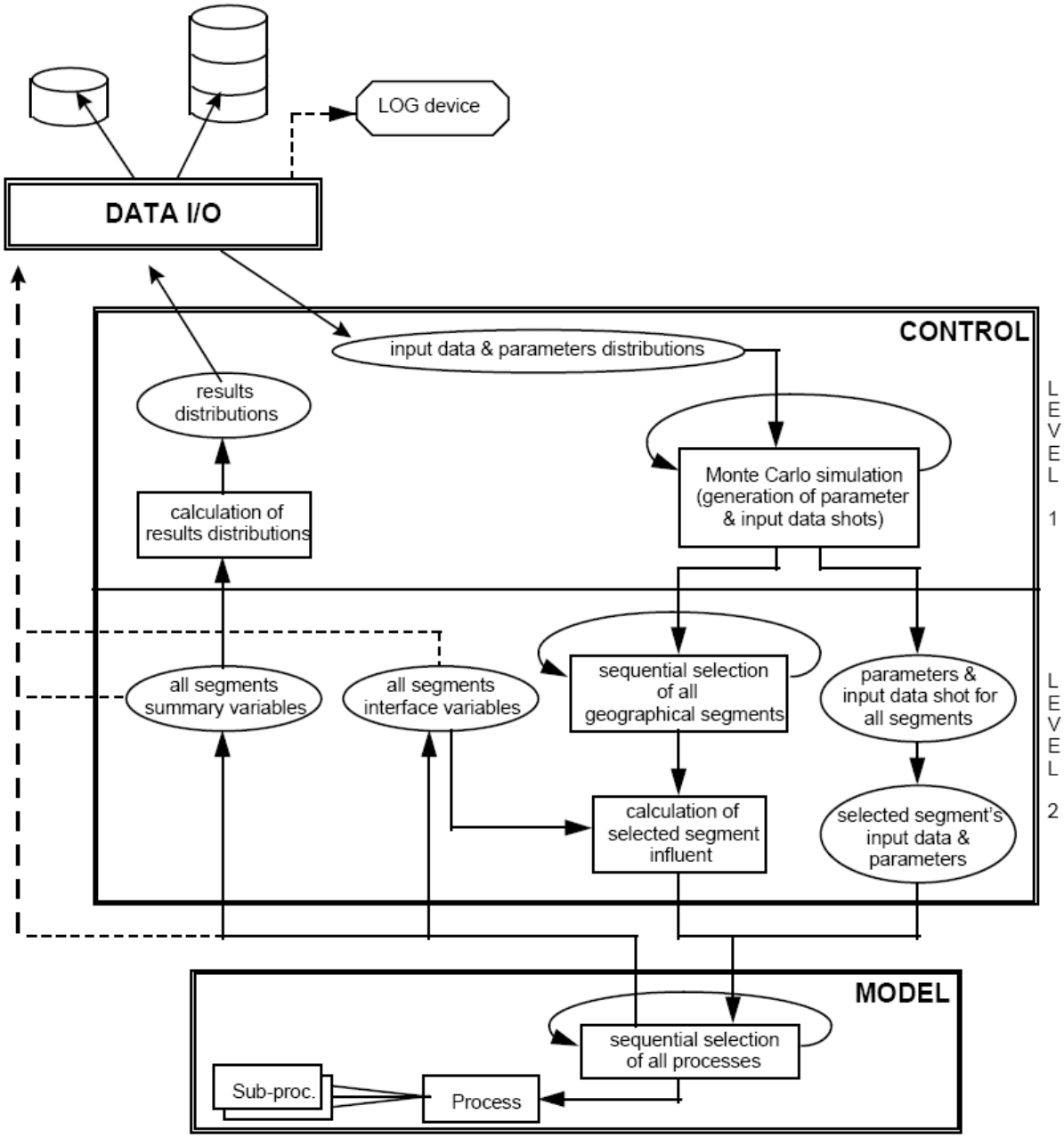

Figure 6: GREAT-ER: General software structure (Technical Documentation)

4.1.3 Model description

4.1.3.1 Simulation levels

GREAT-ER has built in three sub-models: sewer, treatment plant and river. There are three *complexity modes* for each of these sub-models.

- **Complexity Mode 1** allows GREAT-ER simulations with a minimal geographically referenced and chemical input data set.
- **Complexity Mode 2** allows GREAT-ER simulations with a minimal geographically referenced input data set for rivers. However, a detailed set of chemical parameters is needed for waste water treatment plants.
- **Complexity Mode 3** requires detailed parameters for rivers, for waste water treatment plants and for the simulated chemical.

For example, in the simplest mode only first-order elimination rates or percentage removal are considered, whereas higher modes consider elimination processes in more detail.

Because in the simplest model version no physico-chemical properties are required (removal rates belong to the scenario parameters) differences between chemicals can only be simulated, if different use patterns are entered.

A summary of the environmental processes considered for the three sub-models is given in Table 2.

Table 2: Processes considered by GREAT-ER on different simulation levels

submodel	Parameter	mode	
sewer	removal	1	not considered
		2	% removal
		3	same as level 2
wastewater treatment plant	activated sludge	1	% removal
		2	Simpletreat calculation
		3	same as level 2
	trickling filter	1	% removal
		2	same as level 1
		3	same as level 1
river system	removal	1	Lumped 1st order rate
		2	constant volatilisation rate
			constant degradation rate
			constant sedimentation rate
		3	volatilisation rate
			biodegradation rate
			photo-degradation rate
			hydrolysis rate
			sedimentation rate

4.1.3.2 Partition coefficients

Separate partition coefficients can be considered to describe the distribution of a substance in the river, sewage and in mixed liquor. Volatilisation is estimated based on Henry's constant.

4.1.3.3 Degradation rates in the environment

The number of processes considered is increasing when moving to a higher simulation level (Table 2). When GREAT-ER is running in mode 3 the total degradation is calculated as the sum of hydrolysis, photolysis and biodegradation.

The hydrolysis module makes a differentiation between neutral, acid and basic hydrolysis as described in SMPTOX4 mode 3 (Trapp et Matthies (1996)). Also the model for photolysis is

taken from SMPTOX4 mode 3 (Trapp et Matthies (1996)) taking into account the light extinction in the water column, using a 1st order extinction rate and the river depth.
The following processes are taken into account for biodegradation

- different degradation rates in the sorbed and dissolved phase,
- influence of dissolved oxygen on biodegradation,
- temperature correction of the biodegradation rate,
- 1st order kinetics to both chemical's concentration and biomass,
- river's self-purification potential.

However, if not sufficient information is available GREAT-ER can perform a simulation based on a lumped 1st order degradation rate (mode 1).

4.1.3.4 Sedimentation

When running in mode 3 chemical elimination through sedimentation is directly related to suspended solids settling. A suspended solids settling rate can be given as such, as a river-specific property, or it can be derived from the settling velocity and the river's depth. The settling velocity is estimated from annual sediment growth and sediment porosity and density.
In simulation mode 1 sedimentation is not explicitly considered and in mode 2 a constant sedimentation rate has to be given by the user.

4.1.3.5 Volatilisation

Volatilisation is modelled following the approach of Trapp et Matthies (1996). This method is based on the two film theory introduced by Whitman (1923). A complete mixing, due to turbulence, of both the river water column and the atmospheric compartment is assumed. On the other hand, the two boundary layers are considered to be laminar, and are assumed to control the exchange rate between water and air. This exchange rate is calculated from the chemical's Henry's law constant (i.e. the air / water partitioning constant), the conductance of the gaseous and liquid films, and the river's depth. For the estimation of these conductances, two distinct approaches are applied described and compared by Struijs (1996).
In simulation mode 1 volatilisation can only be considered within the overall removal rate. In mode 2 a constant volatilisation rate has to be given by the user.

4.1.3.6 The sewage treatment plant

In the simplest mode (mode 1), GREAT-ER requires a fixed removal efficiency for all treatment plants (to be estimated by the user) during primary, activated sludge or trickling filter treatment. However, for the modes 2 and 3 the model SimpleTreat 3.0 developed by Struijs (1996) was implemented in GREAT-ER. The model calculates steady-state concentrations in a sewage treatment plant consisting of a primary settler, an aeration tank and a solids-liquid separator. The model itself is of type 'Mackay level III.

4.1.3.7 Emission

The emission models are identical on all complexity levels. Based on chemical market (sales) data and the related population the release into the wastewater system is calculated.
If further information is available it is possible to consider industrial sites as an additional input into the treatment plant (via "edit market data", additional input in kg/a). This input reflects discharges resulting from the production processes and can be calculated from the production volume. However, the calculation of the fraction of the production volume, which will be released, is not part of GREAT-ER but must be calculated beforehand. The industrial input is subsequently processed by the treatment plant model, if present, for the selected location as with the loads from domestic inputs.

4.1.3.8 Limitations

The main limitations of GREAT-ER on the regional scale are:

- GREAT-ER strictly couples emissions with the domestic product consumption. It is not possible to simulate any other possible emission (e.g. diffuse entries via surface runoff, atmospheric deposition).
- Compared to other geo-referenced surface water models the river system is modelled on a very simple basis. The geometry of rivers (e.g. width and roughness of the river bed) is not fully covered as river segments are only characterised by lines.
- When a chemical enters the river system instantaneous mixing within the whole river segment is assumed. Especially for slow moving surface waters the resulting concentrations are simulated too low.
- GREAT-ER does not consider real temporal variability, when estimating concentrations in the river system (e.g. flow differences, but also change in river temperatures or during winter and summer). It is questionable, whether these effects can be covered by the Monte Carlo-approach realised in GREAT-ER.

- All emission is based on an annual average basis. For some substances seasonal emissions might be important and would result in more realistic estimations.

4.1.4 Conclusions

The main objective of GREAT-ER is the consideration of spatial variation in the risk assessment. Consequently GREAT-ER provides the user with a couple of evaluation tools to analyse the spatial variability of concentrations in the river network:

- graphical representation of the concentration in the various river stretches,
- calculation of average concentrations over the entire river-system. (comparable with the regional PEC in EUSES)
- calculation of individual mean or percentiles for each river stretch (based on Monte-Carlo simulations),
- calculation of concentration profiles along the river.

The main difference to EUSES is that EUSES is based on a single scenario with a fixed assumption whereas GREAT-ER estimates a local concentration for each stretch in order to consider local characteristics.

When analysing the local environmental situation GREAT-ER provides useful tools such as

- influent and effluent mean concentrations for all discharge sites
- calculation of initial PECs defined as the mean of all individual initial concentrations in the stretches directly receiving a treated or untreated waste water emission.

It is recommended to use EUSES as a conservative screening model, but consider GREAT-ER as a confirmative model at a higher tier of chemical assessment.

4.2 MONERIS (Modelling Nutrient Emissions in River Systems)

4.2.1 Short model description

The nutrient emission Model **MONERIS** (**MO**delling **N**utrient **E**mission in **RI**ver **S**ystems) was developed by Behrend et al. (2000) to estimate nutrient inputs into river basins of Germany by point sources and various diffuse pathways. MONERIS estimates the different pathways using existing approaches as well as new conceptual approaches developed especially for modelling at medium and large spatial scales .

MONERIS considers retention of nutrients (nitrate and phosphate) in rivers basins. Due to the limited and often inconsistent data available for large-scale modelling, MONERIS was designed to work with information collected from standard monitoring programmes or available from federal bureaus.

The model is based on:

- data of river flow (from gauging stations)
- water quality (nutrient concentrations from monitoring stations)
- statistical data about nutrient inputs into the catchment
- geographical data (stored and analysed in a Geographic Information System (GIS)

The model is composed of a series of equations that allow the estimation of point sources and diffuse sources into the river.

MONERIS takes seven pathways into account for emissions into surface waters:

- discharges from point sources,
- emissions via atmospheric deposition,
- emissions via groundwater,
- emissions via tile drainage,
- emissions from paved urban areas,
- emissions by erosion,
- emissions via surface runoff (only dissolved nutrients).

Within the diffuse pathways, various processes of transformation, loss and retention are identified.

In the present stage of MONERIS the quantification and forecast of the nutrient emissions in relation to their causes is not yet possible. Therefore, the authors are planning to implement existing approaches of macro-scale modelling and, if necessary, to derive new applicable

conceptual models using MONERIS for the estimation of nutrient emissions via the individual diffuse pathways (Behrend et al. (2002)).

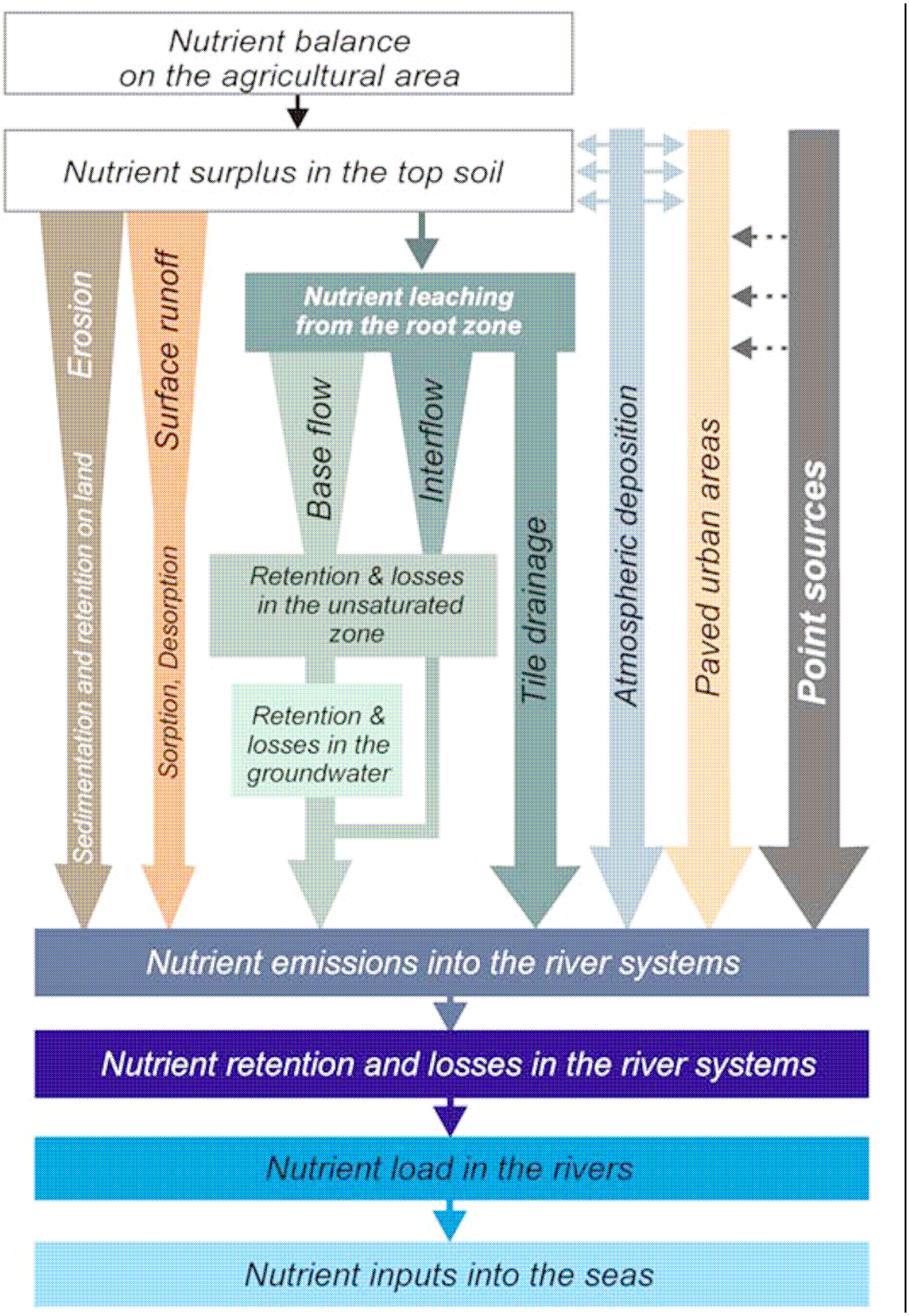

Figure 7: Pathways and Processes in Moneris (Behrend et al. (2002)).

The present MONERIS produces estimates of annual loads through each of the defined point and diffuse pathways. It estimates nutrient retention and loss within the river system itself (i.e., the river's self-purification processes).

The final output is an estimate of annual nutrient loads in the river at the outlet of the study catchment, which is equal to the emissions into the river via point and diffuse sources *minus* the estimated nutrient retention and loss within the river system.

Compared to GREAT-ER MONERIS has a different resolution and calculation strategy. Whereas GREAT-ER is a one-dimensional river model that needs the river network as input together with the detailed location of treatment plants (see Figure 8) MONERIS uses integrated data on individual catchments (Figure 9). Consequently the resolution is quite different. For GREAT-ER it dependent on the size of the individual stretches (app. 1 km). The size of a catchment as considered in MONERIS is above 1000 km².

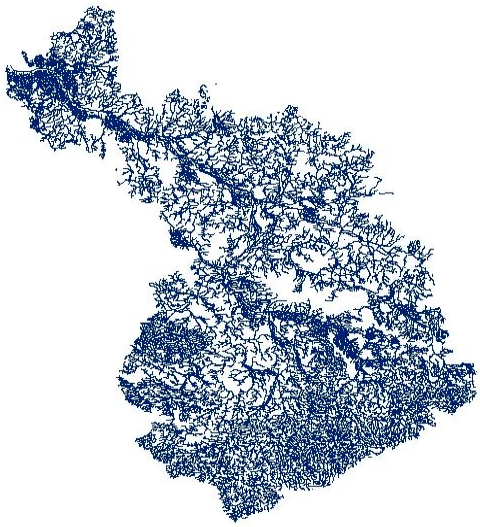

Figure 8: River network as input for GREAT-ER

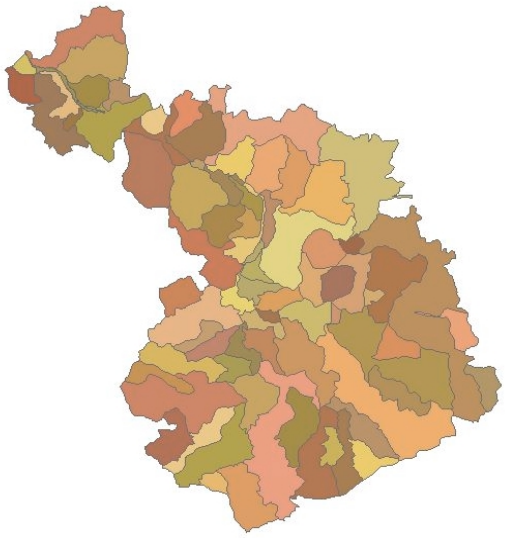

Figure 9: Statistical (mean) data on catchment size in MONERIS

MONERIS is calculating the nutrient input and output level (nutrient balance in mass/time) for a given catchment, where as GREAT-ER is calculating concentrations in rivers within all river segments of a catchment.

An example output is given in Figure 10.

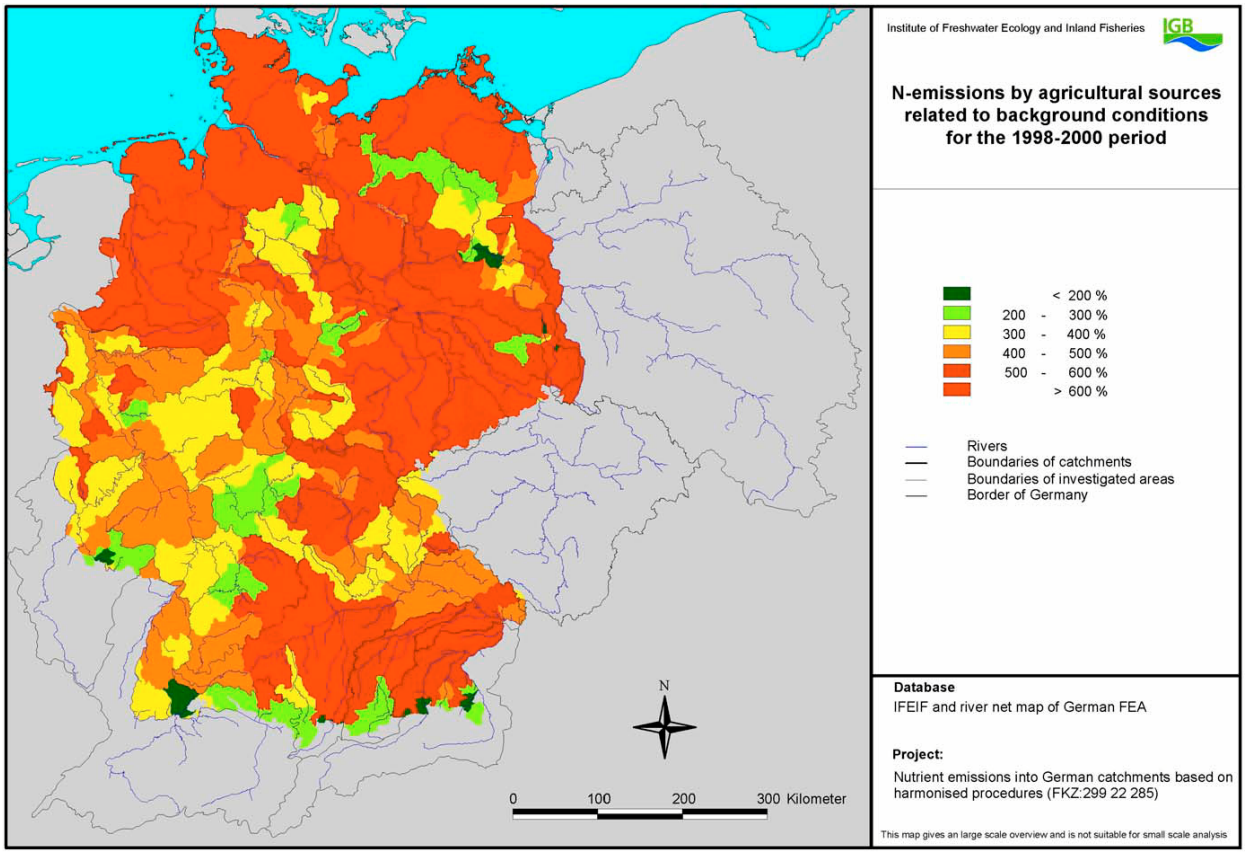

Figure 10: Example output of MONERIS taken from the final report (Behrend et al. (2002))

4.2.2 Conclusions

MONERIS was created for the control of nutrients (phosphate and nitrate) and the reporting of these nutrient inputs ito the North- and the Baltic Sea under international agreements. This model serves a different purpose as compared to EUSES and GREAT-ER.

Therefore, the model is currently only considering nutrients (phosphate and nitrate). The fate of chemical substances in rivers cannot be simulated. Important processes (e.g. transformation and sorption processes) are not covered by MONERIS.

Compared to GREAT-ER the resolution is significantly lower as it only gives one number per catchment where as GREAT-ER is able to calculate distributions of concentrations within a given catchment.

4.3 RIONET

4.3.1 Short model description

The water quality management tool RIONET for river basins was developed with regard to the EU Water Framework Directive (Reuter et al. (2003). The management tool was developed by Harald.Horn (University of Magdeburg-Stendal, department Hydrochemistry) in co-operation with M. Wulkow (Computing in Technology, Rastede) and is able to simulate the water quality in catchment basins not only in a single river but in whole river networks. RIONET is able to simulate complex river-system including artificial arms (millstreams) or weirs based on its net-structure.

A sub-model of the IWA River Water Quality Model No. 1 is used in RIONET. The river model is based on the assumption that self purification processes in the river take place both in the benthic biofilm and the bulk water phase. Laboratory experiments with sediment cores underline the major role of the benthic biofilm. The input parameters of the management tool such as

- volumetric flow rates from waste water treatment plants,
- flow velocities,
- discharge in the main river and its tributaries

can be loaded directly from geographic information systems (GIS). The available substratum at the bottom of the river is mainly dependent on the structure of the river. Intact river morphologies without anthropogenic influence offer larger surface areas for biofilm growth compared to rivers with straightening. The concept of RIONET is to integrate as much river data from monitoring programs as possible. Therefore, the river network must be divided in segments with identical properties with respect to hydraulics, morphology and structure. The data can be loaded directly from the geographical information systems or fed manually by the user.

For a standard simulation following input is required:

- Width of the river
- Depth of the river
- Wetted perimeter.

In order to improve the performance of the model the following data can be used additionally to specify the self purification processes:

- River bed structure
- Line management
- Bank vegetation (shady/sunny).

Beside the biochemical, physical and chemical processes the hydraulic parameters must be entered such as

- the mean flow velocity and the volumetric flow
- pH-value
- water temperature.

At all discharge points the

- concentration of the nitrogen species
- concentration of organic and inorganic carbon species
- phosphorous concentration
- oxygen concentration
- calcium concentration

must be available.

To verify the developed model, data from the basin of the Bode river with a catchment area of 3200 km² and 515 000 inhabitants were used (see Figure 11)

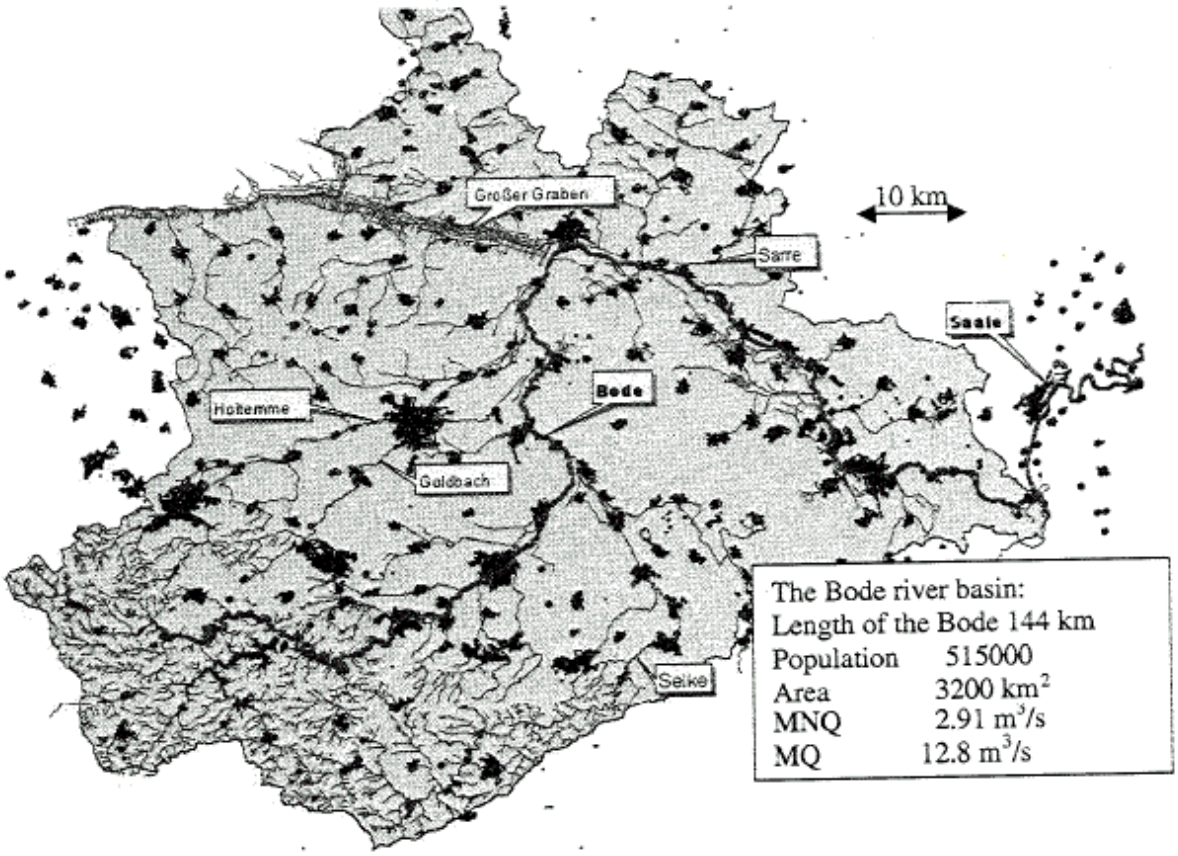

Figure 11: The Bode river basin (Reuter et al. (2003)

The river basin of the Bode was declared a sub-basin which belongs to the river basin of the river Elbe. Unfortunately, the validation focused on ammonium, organic carbon and oxygen. The fate of organic pollutant such as detergents was not analysed so far.

4.3.2 Conclusions and recommendations

RIONET has been developed as a simulation tool for water quality management within the control of the Water Framework Directive. The model is currently only considering nutrients (phosphate and nitrate). The fate of chemical substances in rivers cannot be simulated. Important processes (e.g. transformation and sorption processes) are not covered by RIONET.

4.4 ATV-DVWK-Gewässergütemodell (Water Quality Model)

4.4.1 Short model description

The ATV-DVWK-Water Quality Model (ATV-DVWK = Abwassertechnische Vereinigung – Deutsche Vereinigung für Wasserwirtschaft, Abwasser und Abfall, engl. German Association for Water, Wastewater and Waste) - is a comprehensive tool for the dynamical simulation of the quantitative and qualitative conditions and processes in rivers and streams (Anonym (1998)). It was developed by a working group of the ATV-DVWK in co-operation with the Institute for Applied Mathematics and Statistics of the Technical University of Munich and several other research institutions. It is able to consider point sources as well as diffuse sources.

Background of the development was the need for a water quality simulation model to be used in the practice of water quality protection and watershed management, because several legal and regulatory activities came into force in the last years, especially the Water Framework Directive of the European Commission in December 2000.

The ATV-model is a complex management systems that allows analyses on different levels such as:

- Data analysis (extreme values, longitudinal profiles, time series)
- System analysis (sinks, sources and transformation of substances)
- Cause-effect relations for management planning
  - Comparison of results for different scenarios
  - Cost effect investigations in context with effluent requirements
  - Assessment of advanced requirements with respect to quality objectives or uses
  - Estimation of the fate of priority substances in river systems
  - Development of measures for achieving the aquatic milieu and habitat conditions required for the ecological objectives.

The input of all spatial data at the screen is based on a digitised topographic map, which is geo-referenced by the user at the beginning, whereby all data are attributed with their GK-co-ordinates. The geo-reference is used for some processes in the model, additionally it facilitates the connections to a geographic information system.

The flow simulation is based on the complete St-Venant-Equations, which are solved by the method of characteristics. The algorithm for the solution of the transport equation is nearly free of numerical dispersion and therefore particularly suited in cases of accidental pollution.

The radiation is simulated considering all influences from the upper part of the atmosphere until the water surface and further down to the bottom of the water body. The radiation is the base for the simulation of the temperature in the water body and at the bottom as well as for the photosynthesis and the photolysis.
The conservative substances (chemicals without degradation and sorption, e.g. salts) are influenced by the transport and dispersion only. They are used mainly for the simulation of tracer experiments and thereby for the adjustment of the hydraulic system.
The BOD is simulated together with the COD. Both are closely connected with several other modules, their decay is particularly influencing the oxygen content of the river water.
The nutrients considered in the model (phosphorous, nitrogen and silicate) are mainly influencing the plant growth. The nitrogen cycle is additionally driving the oxygen balance.
Development of the flora and fauna (represented by the phytoplankton, the sessile macrophytes, the phytobenthos, the primary and secondary consumers, and the macrozoobenthos) form an important central part of the model.
The suspended solids are influencing the light intensity in the water body as well as the adsorptive transport as particulate matter, e.g. of heavy metals.
The oxygen balance is essential for the aerobic aquatic life and therefore one of the key elements of the model. The simulation of the pH-Value was included to simulate the fate of heavy metals and the equilibrium of NH_3 and NH_4^+.
The fate of heavy metals can be considered based on pH-dependent sorption constants.
For organic pollutants following processes are considered:

- advection and dispersion
- biodegradation
- oxidation, hydrolysis, photolysis
- volatilisation
- sorption (linear isotherm)
- sedimentation.

Most of the user of the ATV model that is available already for several years, are working in the field of water resources management.
The ATV-model was applied in a number of cases, ranging from large streams on the one side to small rivers and brooks in rural areas on the other. Special attention is focused on the applicability for smaller watercourses, which usually react very sensitive to changes in the morphological and physico-chemical conditions.
Some results of the model are presented.

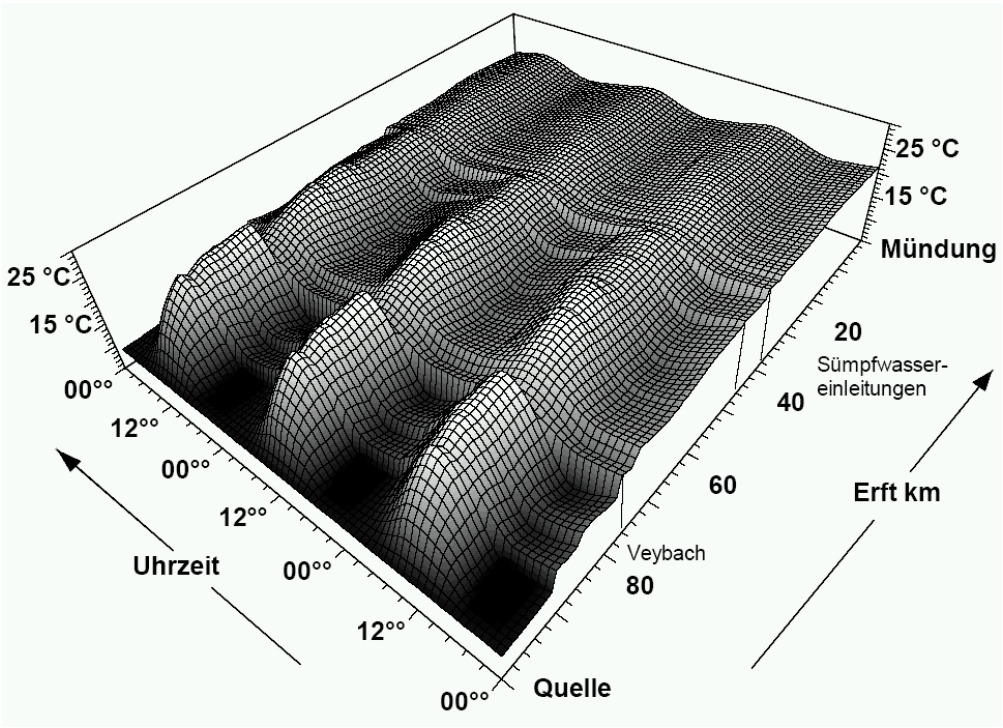

Figure 12: Temperatures in the river Erft calculated by the ATV-model (Christoffels (2001))

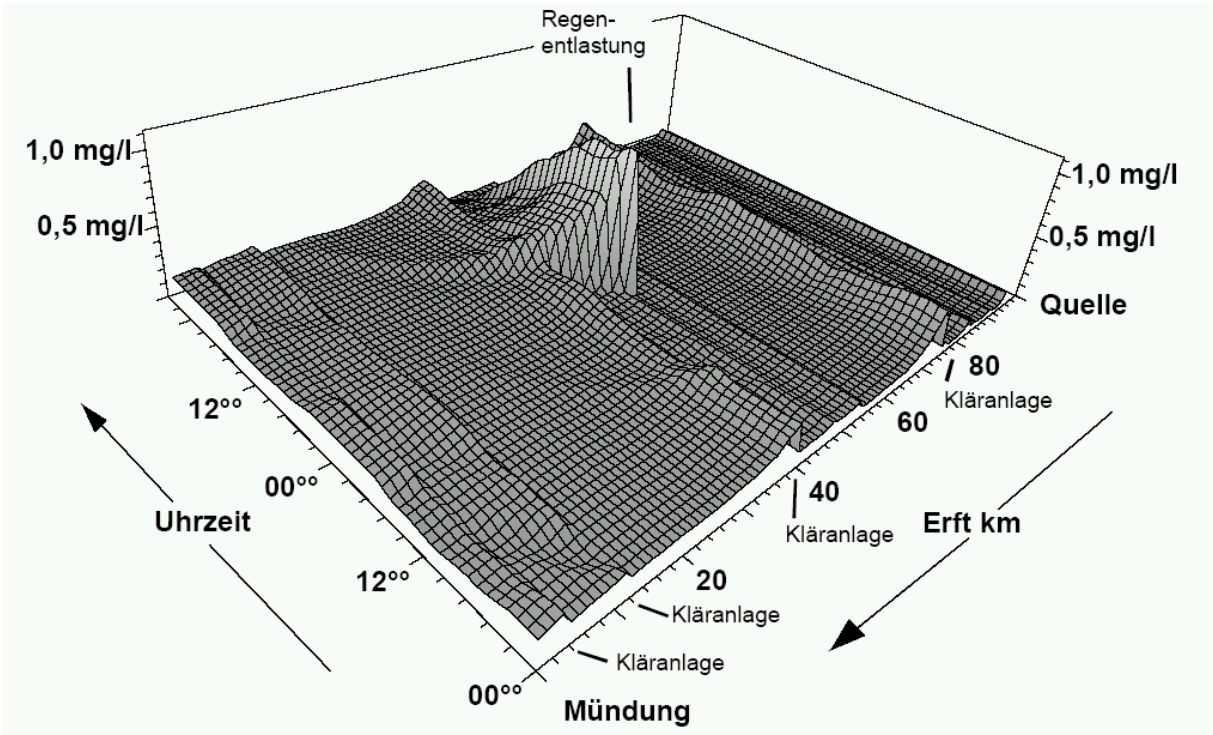

Figure 13: NH_4^{+}-concentrations in the river Erft calc. by the ATV-model (Christoffels (2001))

4.4.2 Conclusions

The ATV-Gewässergütemodell is a complex river model that is simulating many processes in a river system on a very detailed level. For example, in the radiation module the reduction of sunlight because of vegetation close to the riverbanks is included. The time as well as the spatial resolution is high and considers the daily amplitude of important variables in the system (oxygen content, temperatures). It is on one hand analysing current conditions, but is also able to forecast future developments in the river.

For simulating the fate of chemicals all relevant processes like degradation, sorption, sedimentation and volatilisation are considered

As the ATV-Gewässergütemodell is not based on the MS-Windows system, input and output processing could be a problem when using this software. Geo-referenced models are based on extended data sets with detailed geographic data. The general windows tools for entering, editing or transferring of this data (e.g. the clipboard) are not available when working with the ATV-Gewässergütemodell. The same problem occurs when evaluating and analysing the results. The standard windows routines for transferring tables or graphs into MS-Windows applications like MS-Word or MS-Excel cannot be used. So, special interfaces have to be made available in order to make the model suitable for regulatory uses.

The level of complexity of this model is far beyond more simple approaches like GREAT-ER. It is is disproportionate to use the model within the standard assessment of new or existing chemicals. However, the model seems to be an excellent tool to support the implementation of the Water Framework Directive, if the above mentioned problems with interfaces to the “MS-Windows world” and the general user friendliness are improved.

4.5 BBA-Risk Map Model

4.5.1 Short model description

The BBA-Risk Map Model was developed by Golla et al. (2002) and can be classified as a decision support system (DSS) for users in the pesticide industry or pesticide registration authorities to examine the effect of pesticide spray drift on adjacent surface water contamination.

The BBA-Risk Map Model is not a river model but a system of GIS-aided procedures that enables to establish risk maps. The system is mainly based on the “Digitales Landschaftsmodell 25 (DLM25: Digital Landscape Model)” from the “Amtliches Topgraphisch-Karthographisches Informationssystem ATKIS” (Authoritative Topographic Cartographic Information System) of the German states. The BBA-Risk Map Model contains a GIS-supporting software. It enables to characterise the agricultural area with respect to minimum distances to water bodies in order to determine the buffer zones around a water body, in which no pesticides must be applied. Furthermore the potential length of a water body affected by pesticide drift is identified. Finally the protective effect of landscape adjacent to a water body is expressed based on attribute data from water body quality mapping (e.g. bank vegetation) and landscape adjacent to natural water courses. All the data is used to derive a summary value called “protective effect of the landscape feature adjacent to a water body”.

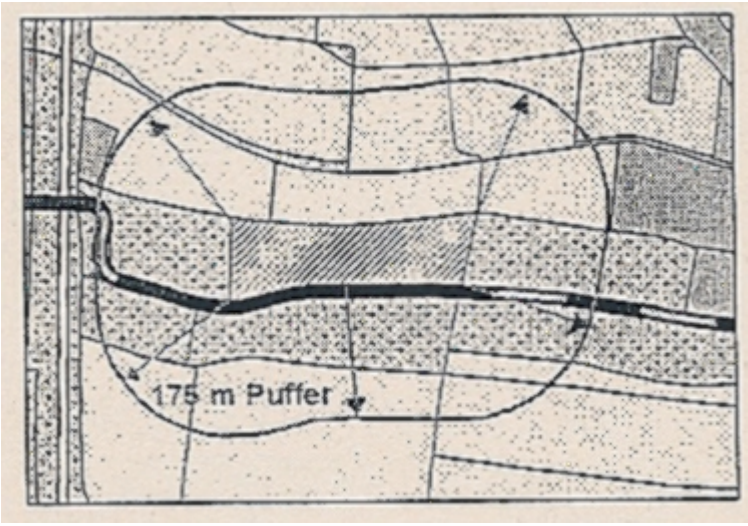

Figure 14: Screen dump of the BBA-Risk model (Golla et al. (2002))

4.5.2 Conclusions

The BBA-Risk Map Model is a decision support system developed to estimate the fate of pesticides only. Aim of the model is to assess the potential risk of exposure on adjacent surface water bodies caused by spray drift during application. The assessment is done on the local field scale and based on the Topographic Cartographic Information System.

It is not suitable to perform exposure assessment for other compounds due to the specific entry routes into the environment of pesticides. The main input route considered by the tool is spray drift during application.

4.6 ASSESS Model

4.6.1 Short model description

The model ASSESS was developed by Knoche et al (1998) within the research and development project “development of criteria and methods for comparison and applicability of regional environmental conditions within the EU member states”. ASSESS is a geo-referenced model that calculates pesticide concentrations in surface and groundwater considering soil, climate and elevation information from maps with a resolution of 1 km². The system is focusing on pesticides only. Additionally especially for surface water concentration special assumptions are made considering the current practise of pesticide registration.

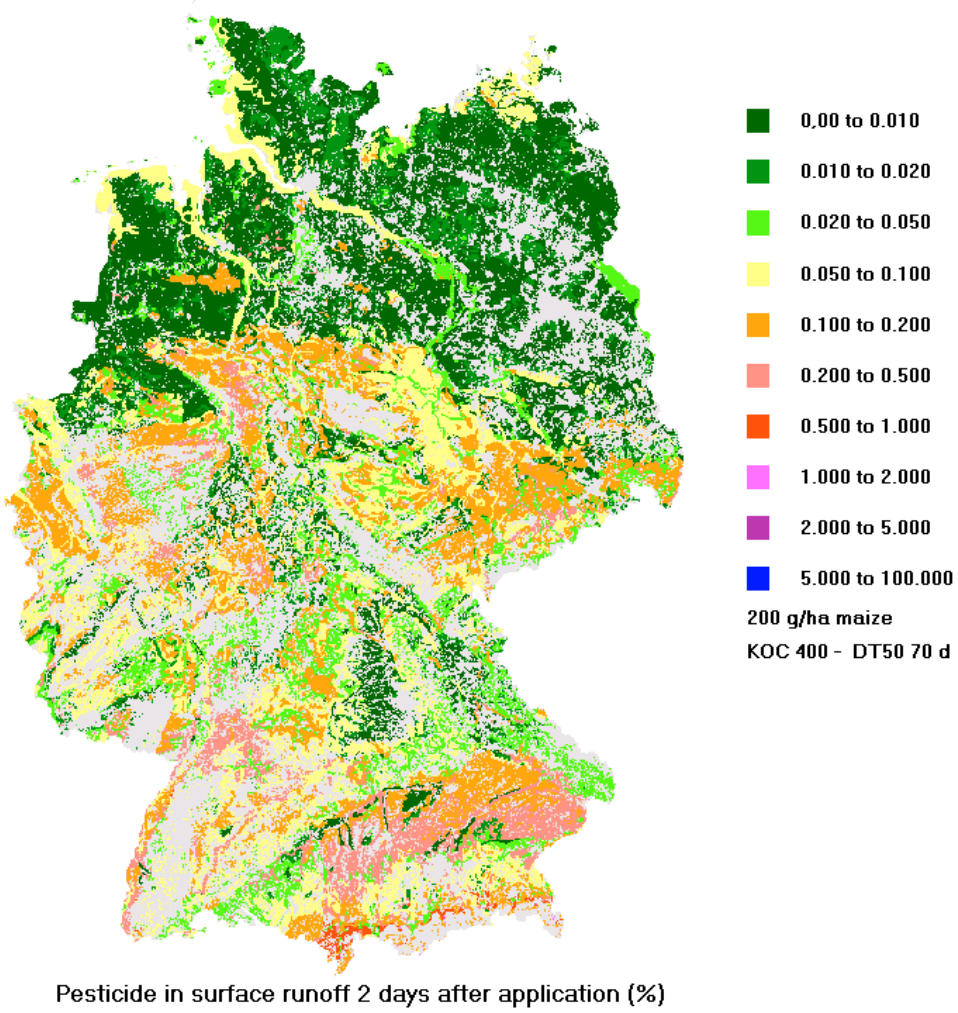

Figure 15: Pesticide losses into surface water calculated by ASSESS (Knoche et al (1998))

For example, the concentrations calculated by ASSESS are not based on the properties of actual rivers, streams or ditches, but all based on the same “standard scenario-surface water” (30 cm deep, 1 m wide) that has been defined by the Umweltbundesamt. In so far

ASSESS estimates the potential of losses into surface water dependent on local climate, soil and relief conditions rather than concentrations in existing surface water bodies. Spray drift during and surface runoff after application are considered as potential input routes.

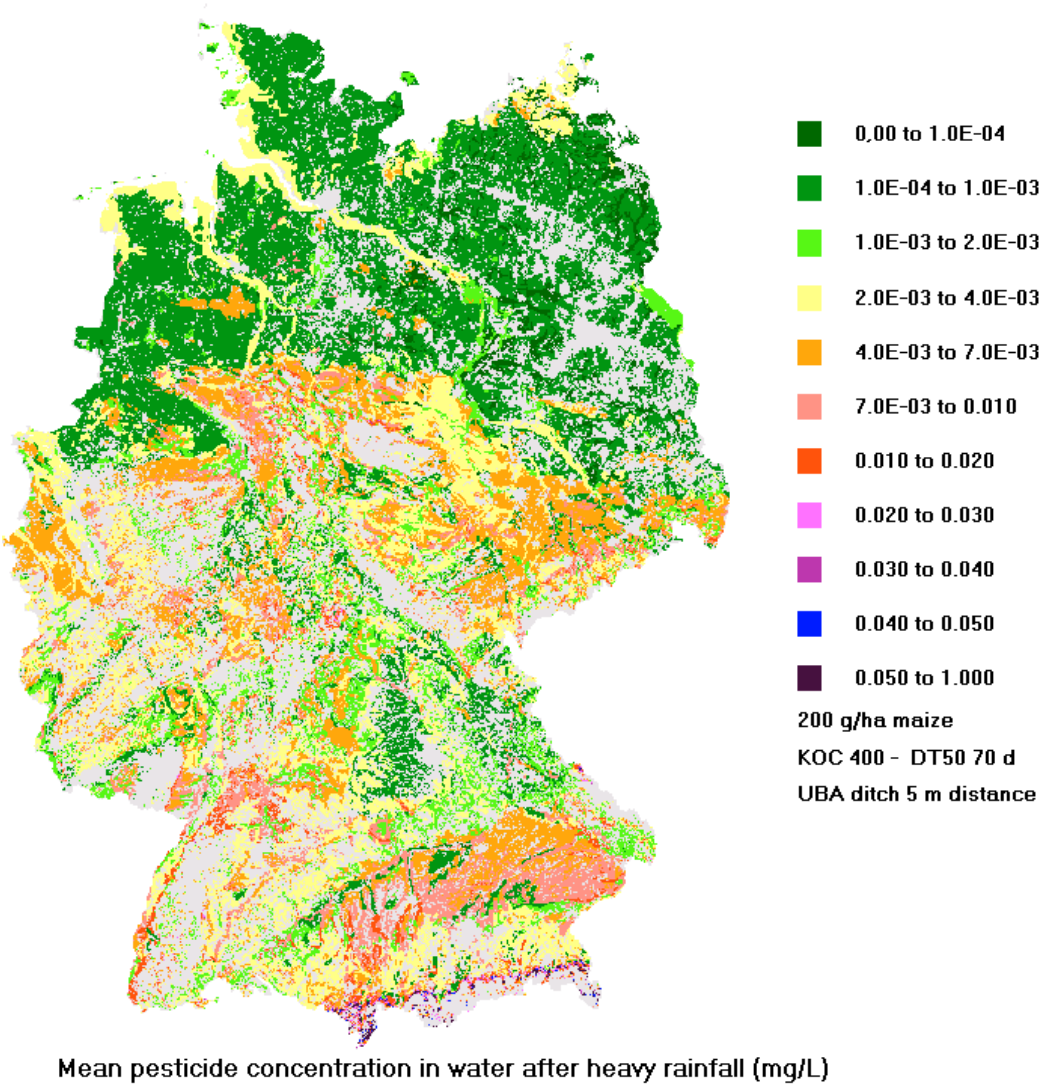

Figure 16: Ditch-concentrations (depth: 30 cm) calculated by ASSESS (Knoche et al (1998)

4.6.2 Conclusions

The ASSESS Model is a decision support system developed to estimate the fate of pesticides. It assesses the potential risk of exposure dependent on the local conditions.

However, it is not suited to perform exposure assessment for other compounds due to the specific entry routes into the environment of pesticides. The main input pathways considered by the model are spray drift and surface runoff after application.

It is also not considering the properties of existing surface water bodies, and can therefore not be used to perform exposure assessments for general substances in the aquatic environment.

4.7 DRIP Model

4.7.1 Short model description

The Drip-model was developed by Bach et al. (1999) to calculate a balance of annual pesticide entries from German surface water bodies into the sea. DRIP considers variables like climate, soil, pesticide properties and application pattern to estimate the most likely amount of pesticides entering the sea on an annual basis. DRIP is a geo-referenced model as digitised raster maps are considered for air temperature, precipitation, soil type and land use. Similar to ASSESS DRIP does not use geo-referenced rivers, ditches or streams. Only the potential entries into surface water bodies are considered. DRIP assumes that potential entry routes are spray drift during application, runoff and drainage after application (diffuse entries) and farmyard discharges (point source). Similar to ASSESS DRIP is focusing on pesticides only.

4.7.2 Conclusions

The DRIP Model is a system developed to balance the diffuse and point inputs of pesticides. It is not suited to perform exposure assessment for other compounds due to the specific entry routes into the environment of pesticides. The main input pathway considered by the tool is spray drift and surface runoff or drainage after application).

It is also not considering the properties of existing surface water bodies, and can therefore not be used to perform exposure assessments for general substances in the aquatic environment.

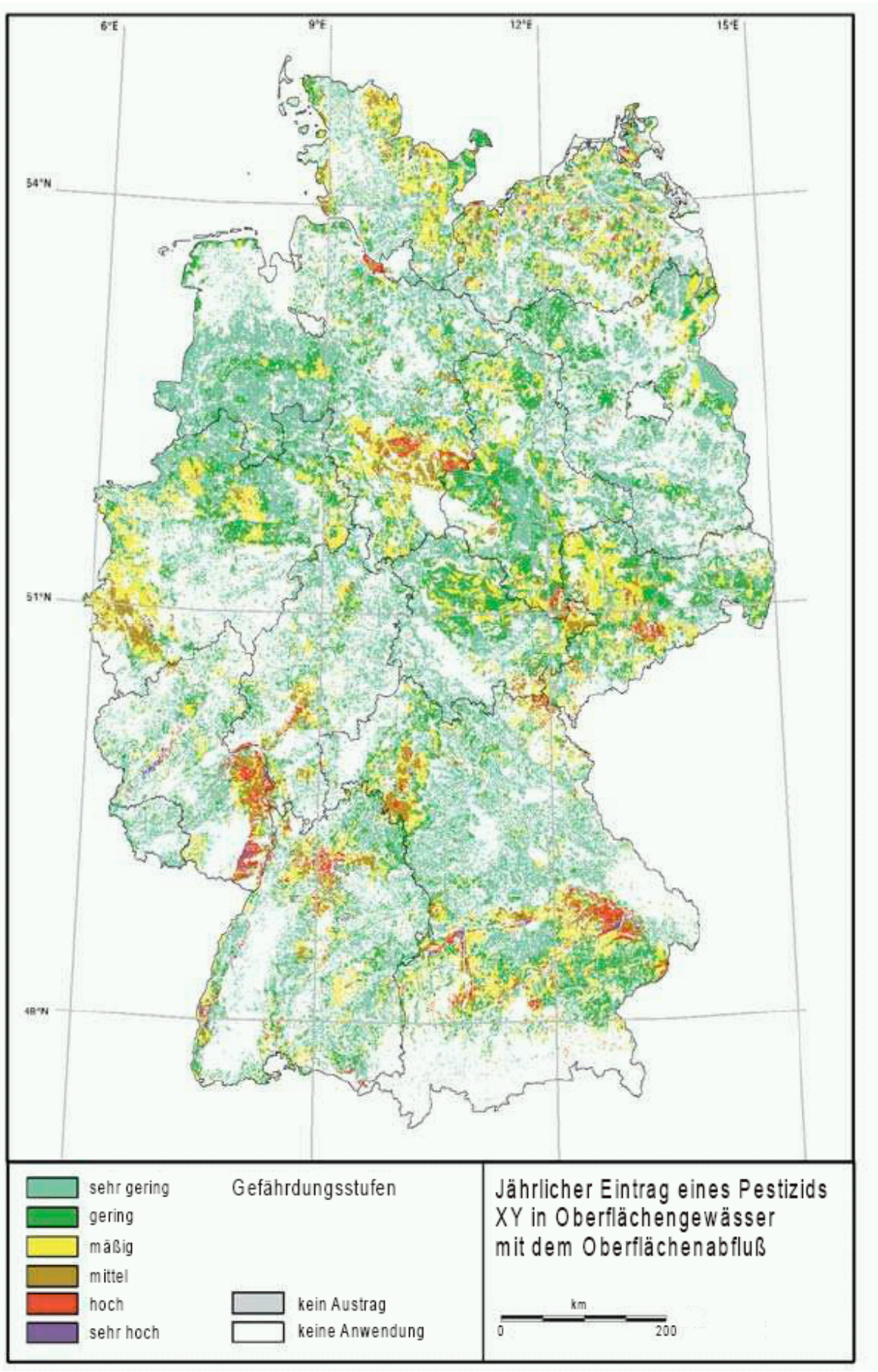

Figure 17: Annual Emission of a pesticide caused by surface runoff (Röpke et al (2002)

4.8 The BETR (Berkeley-Trent)-Model

4.8.1 Short model description

The BETR model was developed by Berkeley Lab and Canada's Trent University to better understand how contaminants such as pesticides travel across the continent (Toose et al. (2004)). The model considers toxic release data, wind and water current patterns, and regional differences such as soil and vegetation. The application area of the model is North America, which is divided into 24 regions by watershed and soil type. Each region is further subdivided into seven compartments: upper atmosphere, lower atmosphere, vegetation, soil, fresh water, coastal water, and freshwater sediment.

The Berkeley-Trent-Model is not a geo-referenced surface water model but simulates the long-range-transport mainly via the atmosphere. So far, the model has been tested using real-world data associated with toxaphene, a banned pesticide, that was used once widely on cotton crops in the Southeast and is now found in high concentrations in the Great Lakes. The team introduced a hypothetical 10,000 kilogram-per-year release in the lower atmosphere compartment of the Mississippi Delta region, and the model determined that although the compound spread throughout North America, the highest concentrations accumulated in the Great Lakes.

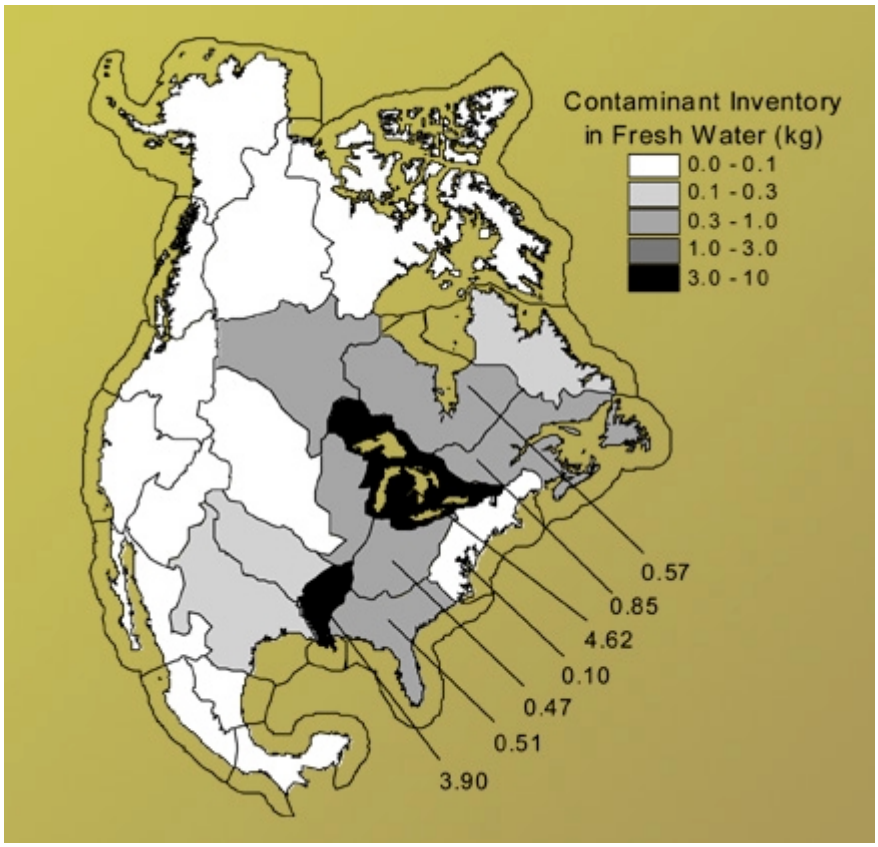

Figure 18: Release of toxaphene calculated by the Berkeley-Trent-Model

4.8.2 Conclusions

The BETR model is a model simulating the long-range-transport of pollutants via the atmosphere. So far, it was parameterised for North America. It does not consider explicit geo-referenced surface water bodies.

It can therefore not be used to perform exposure assessments for general substances in the aquatic environment.

4.9 GIS-Version of SoilFug

A special version of SoilFug a multimedia fugacity-based model was developed in order to predict pesticide pollution of surface water in a river basin of about 400 km² in northern Italy (Barra et al. (2000)). To account for the heterogeneity of environmental characteristics of the territory, a detailed description of the environmental scenario (hydrological network, land use, rainfall, soil properties) was made by using a Geographical Information System (GIS). Fourteen Uniform Geographic units were defined for applying the SoilFug model on a modular basis. The different units were then combined to predict river concentrations as shown in Figure 19. The system can be used to predict pesticide concentration in rivers, comparisons with monitoring data show a satisfying agreement with the measured data. An advantage of SoilFug (and other fugacity based models) is the small amount of input parameters they need for predictions. However, the application areas of fugacity models are often small and homogeneous and equilibrium conditions can be reached easily. The authors of this SoilFug-GIS combination could demonstrate that meaningful site-specific simulations can be performed also in bigger areas (see Figure 20) assumed the quality of the input data is good and the definition of the necessary spatial compartments within a heterogeneous area is well done.

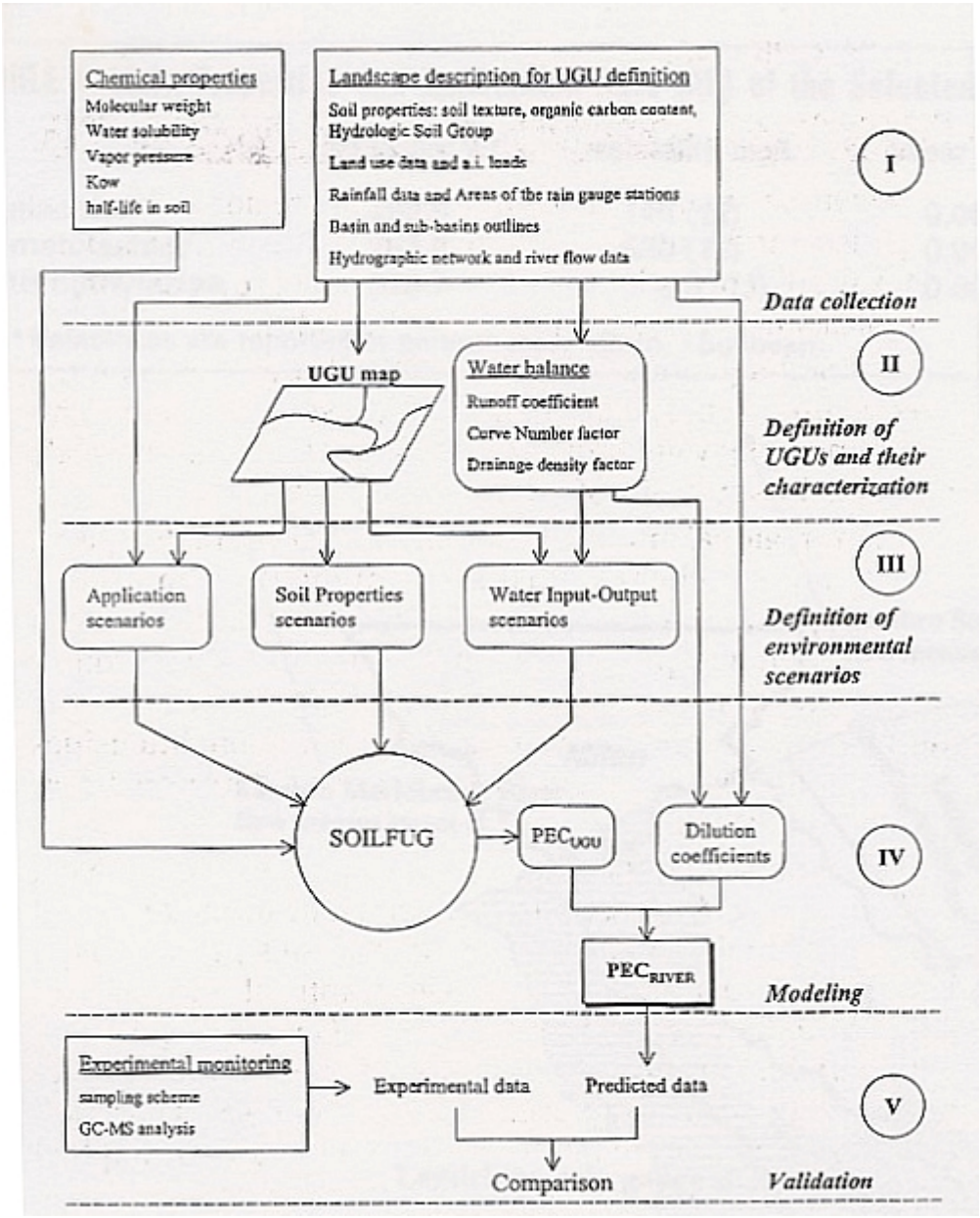

Figure 19: The combination of SoilFug with GIS (Barra et al. (2000))

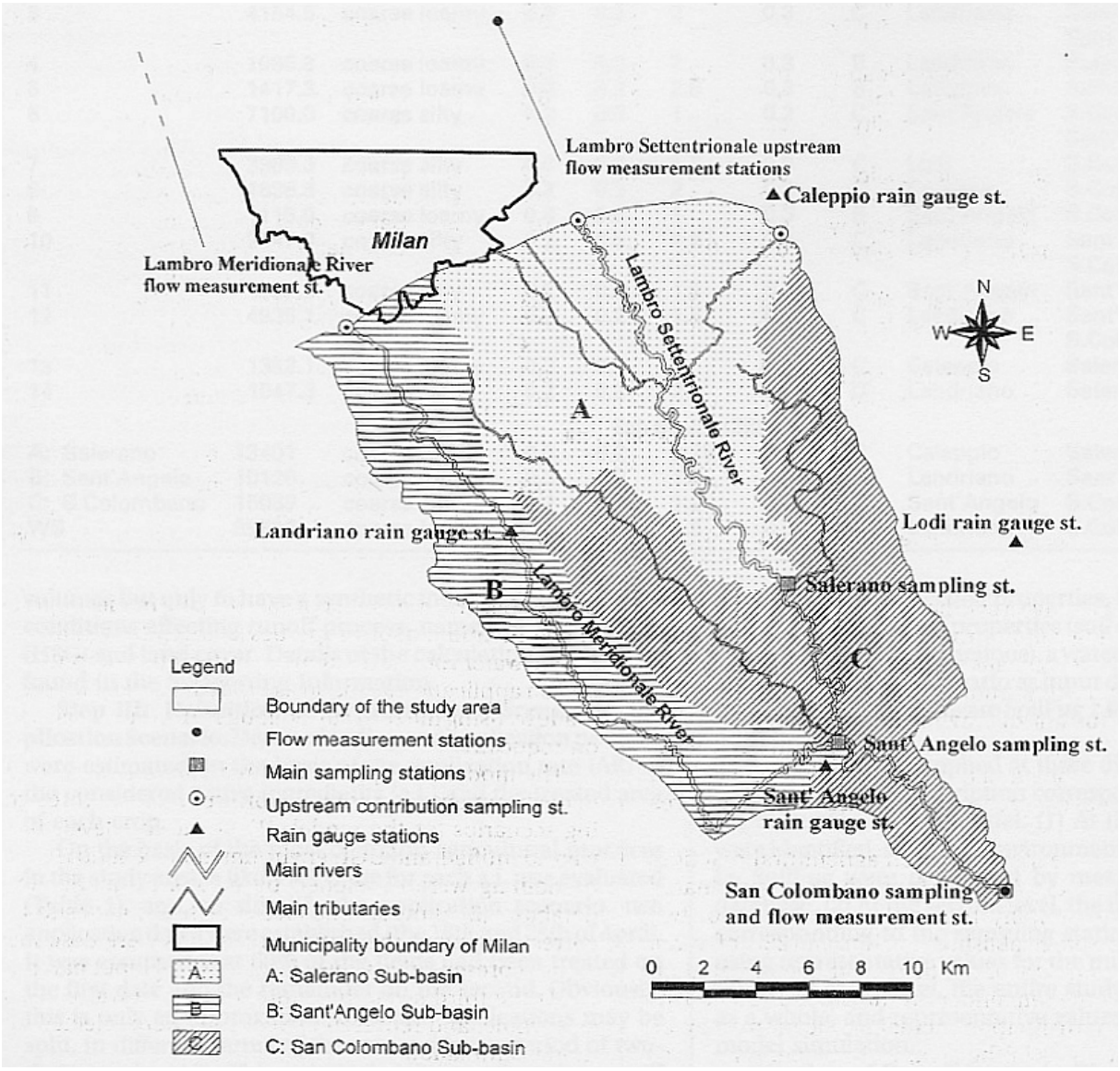

Figure 20: Application area of the SoilFug-GIS-Model (Barra et al. (2000))

4.9.1 Conclusions

The SoilFug-Gis model is a fugacity based model simulating fate of pesticides entering surface water bodies via drainage and surface runoff. Due to these limitation it can not be used to perform exposure assessments for other substances in the aquatic environment.

5 Comparison of EUSES and GREAT-ER

5.1 Principle differences between the two models

There are principle differences between EUSES and GREAT-ER that make it difficult to compare the quality of the results of both models. Especially, if the comparison is aiming at the “level of environmental protection” a clear determination is hardly possible due to the different model approaches.

EUSES is a level III multi-media fate model that works with a high number of default parameters in order to predict a steady state exposure concentration in a fictive unit world based on a minimum set of data required as input parameters. The simulated regional environmental concentrations are based on the assumption of a homogeneous distribution. For example, by definition 80% of the domestic sewage enter the environment via a waste water treatment plant, 20% remain untreated. By default, the local PEC represents the local concentration in a river assuming complete mixing of the effluent and river waters in a certain distance from the point source plus the regional background concentration. Because of the short time between effluent discharge and exposure location, the dilution of treated discharge with the river water will be the main factor for its ultimate predicted concentrations.

Due to its generic character EUSES is able to cover all types of industrial chemicals in 15 industrial and 55 use categories (e.g. plant protection agents, detergents, colouring agents, bleaching agents, cosmetics, fertilisers, fuels, biocides)

GREAT-ER predicts site-specific concentrations in rivers. The results of GREAT-ER can be directly compared with measured (monitoring) data. In contrast to EUSES, GREAT-ER simulates different concentrations at different locations of a river-system. Due to available GIS-tools the concentrations in rivers can be transparently visualised in maps. However, the use of GREAT-ER is limited to so called “down-the-drain”-chemicals in surface water systems.

If the results of GREAT-ER and EUSES are to be compared, it could be performed based on an evaluation of the distribution of concentrations (averages or percentiles) in a river system. A major problem remains, if a comparison is aiming at the “level of protection” of both models: EUSES simulates concentrations in a fictive unit world where as GREAT-ER simulates concentration in specific river stretches.

The background of the problem can be pointed out as follows:

If it were shown by comparisons of GREAT-ER with experimental data that the model estimates realistic concentrations in river-systems fully in line with reality, it does not say anything about the level of protection of the model. The level of protection compared to the

conservative assumptions of EUSES depends mainly on the river system that has been selected for the analysis. The river-system and its suitability of representing average or worst case situations will be responsible for the “level of environmental protection” GREAT-ER will provide:

The “level of environmental protection” is always a function of both, the model and the selected scenario. The following comparison between EUSES and GREAT-ER is not only based on the simple comparison of individual results, but also on processes considered in the model. Finally, results of validation exercises are presented in order to get an impression on the range of confidence.

5.2 Comparison of processes in both models

5.2.1 Release into the river system

Table 3: Removal processes in EUSES and GREAT-ER

Process	EUSES	GREAT-ER
removal in the sewer system	No	Yes (mode 2 or 3): fixed percentage
waste water treatment plant	Yes Simple Treat (Struijs (1996))	Yes (mode 3): Simple Treat Struijs (1996) alternative: fixed percentage (site-specific)

In contrast to EUSES, GREAT-ER is able to consider a removal in the sewer system before entering the waste water treatment plant.

A second removal can be considered by GREAT-ER in the waste water treatment plant. When running in mode 2 or 3 the same model for simulating the fate in a waste water treatment plant can be used as it is done in EUSES. It is questionable whether this option is suited for the geo-referenced model GREAT-ER as site-specific input to characterise the individual treatment plants cannot be considered. The removal rates calculated by the internal Simple Treat model are therefore constant independent on the location of the treatment plant in the river system. Instead of using the Simple Treatmodel the user can enter a site-specific removal rate to cover chemical’s fate in the sewage treatment plant. This option could be useful when calibrating the model with experimental data, but it is questionable whether that option should be used as a standard in the regulatory context.

The method how waste water treatment plants are considered in GREAT-ER demonstrates the limits of this model:

Removal rates in waste water treatment plant always depend on 2 factors:

- site-specific information of the treatment plant (independent on chemical's properties)
- substance related parameters (e.g. degradation rate, Henry's law constant, sorption constant).

A consequent implementation of waste water treatment plants (desirable, when the model is used in regulatory context) would be to parameterise site-specific treatment plants. This work has to be done only once as part of the scenario definition. Based on this information GREAT-ER would be able to estimate site-specific removal rates for any substance based on the properties of the individual waste water treatment plants and the chemical properties. The advantage of the additional parameterisation would be the replacement of a difficult-to-obtain input parameter ("site-specific removal") as well as a non-adequate Simple Treat-calculation by an additional GREAT-ER estimation obtaining a removal rate that would be site as well as substance specific.

5.2.2 Partition in the environment

Generally, similar partition coefficients are used in GREAT-ER and EUSES to describe the distribution in the environment. Both models consider the distribution between solid-water, air-water and sediment-water. As EUSES is a broader surface water model, some additional partition coefficient are used like partitioning between gas and aerosol phase in air or between water and biota.

Partitioning in EUSES and GREAT-ER is not directly comparable, as in EUSES's fictive unit world only a single water compartment is defined for regional PECs. In contrast the strategy of GREAT-ER is to define many stretches each with individual concentrations based on the partition coefficients and degradation rates in order to describe a realistic picture of the fate of the chemical in the river system. Dependent on the properties of a certain stretch individual rates for sedimentation, volatilisation or degradation are calculated that result in different concentrations in the river and the sediment, respectively.

5.2.3 Degradation rates in the environment

Table 4: Comparison of degradation processes considered in EUSES and GREAT-ER

Process	EUSES	GREAT-ER
biodegradation	Yes	Yes (mode 3)
hydrolysis	Yes	Yes (mode 3)
photolysis	Yes	Yes (mode 3)

As summarised in Table 1 there are no differences between both models with respect to degradation processes (supposed the model is used in mode 3).

5.2.4 Local environmental distribution and concentrations

Looking to the processes considered in EUSES and GREAT-ER the estimated local environmental distribution is comparable. Both systems consider similar partition coefficients and waste water treatment plants before entering the water compartment. The local PEC in EUSES is comparable with the initial concentration in GREAT-ER. The main difference is that EUSES is based on a single scenario with a fixed assumption whereas GREAT-ER estimates a local concentration for each stretch in order to consider local characteristics.

When analysing the local environmental situation GREAT-ER provides tools such as

- influent and effluent mean concentrations for all discharge sites
- calculation of initial PECs defined as the mean of all individual initial concentrations in the stretches directly receiving a treated or untreated waste water emission

for the river-system.

5.2.5 Regional distribution and concentrations

As mentioned earlier the estimation of regional concentrations in EUSES is based on the SimpleBox model 3.0. In SimpleBox emissions at the regional scale lead to increased concentrations in larger spatial scales, and emissions at the continental scale contribute to increase concentrations at the regional scale (see Figure 2). Additionally, advective transport with air and water between the continental and regional scales are accounted for in this model. The predicted exposure concentrations at the regional scale are the net result of emissions on both spatial scales and the modelled rates of advection. Some processes are built in EUSES to consider inter-media transport such as dry and wet deposition of aerosol-bound chemicals or sedimentation and re-suspension of particle-bound chemicals in water. As on the local scale the surface water compartment is assumed to be homogeneous and totally mixed. Spatial variation is not considered.

On the other hand spatial variation is the main objective of GREAT-ER. Consequently GREAT-ER provides the user with a couple of evaluation tools to analyse the spatial variability of concentrations in the river network:

- graphical representation of the concentration in the various river stretches,
- calculation of average concentrations over the entire river-system (comparable with the regional PEC in EUSES)
- calculation of individual mean or percentiles for each river stretch (based on Monte-Carlo simulations),
- calculation of concentration profiles along the river.

5.3 Comparisons of GREAT-ER with EUSES or monitoring data

5.3.1 Calder in Yorkshire, UK

The Calder catchment was used to calibrate the catchment parameters during the GREAT-ER project phase for the chemicals boron and LAS that are used in detergents (ECETOC (1999)).

The catchment of River Calder lies in the north of England, east of Manchester and south of Leeds. With an area of about 1000 km² and 790,000 inhabitants it is a predominantly urban region. 5 Activated Sludge and 16 Trickling Filter plants receive and treat all household emissions. The digitised river network has a total length of more than 1000 km of which only 10 percent are downstream of a waste water treatment plant. The Calder is a tributary of the river Aire. At the confluence a mean flow of 17.8 m³ per second is reached.

Figure 21 shows the Calder catchment in Yorkshire, a mostly urban catchment. The main stream is about 80 kilometres, the whole river network consists of about 1600 stretches.

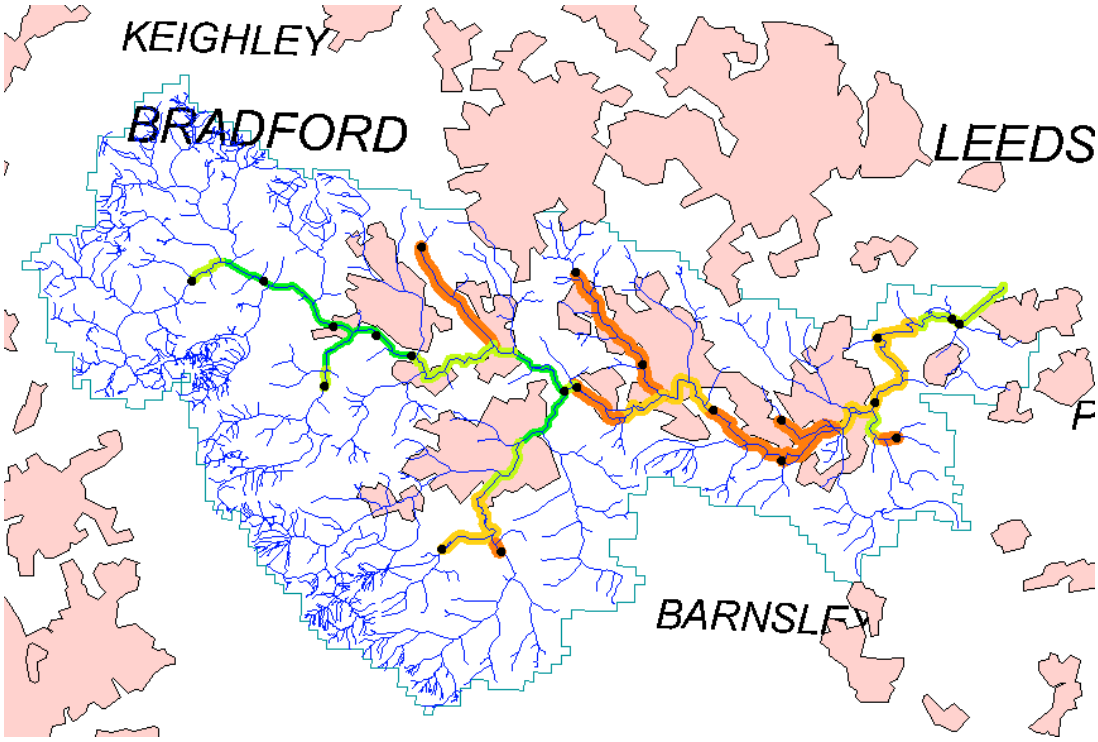

Figure 21: Calder catchment (ECETOC (1999))

The comparison between measured and simulated LAS concentrations is based on a 3 year monitoring programme from 1996 to 1998. In Figure 22 the mean values plus/minus one

standard deviation are displayed. Obviously, the model results fits the monitored concentrations well for the pilot areas.

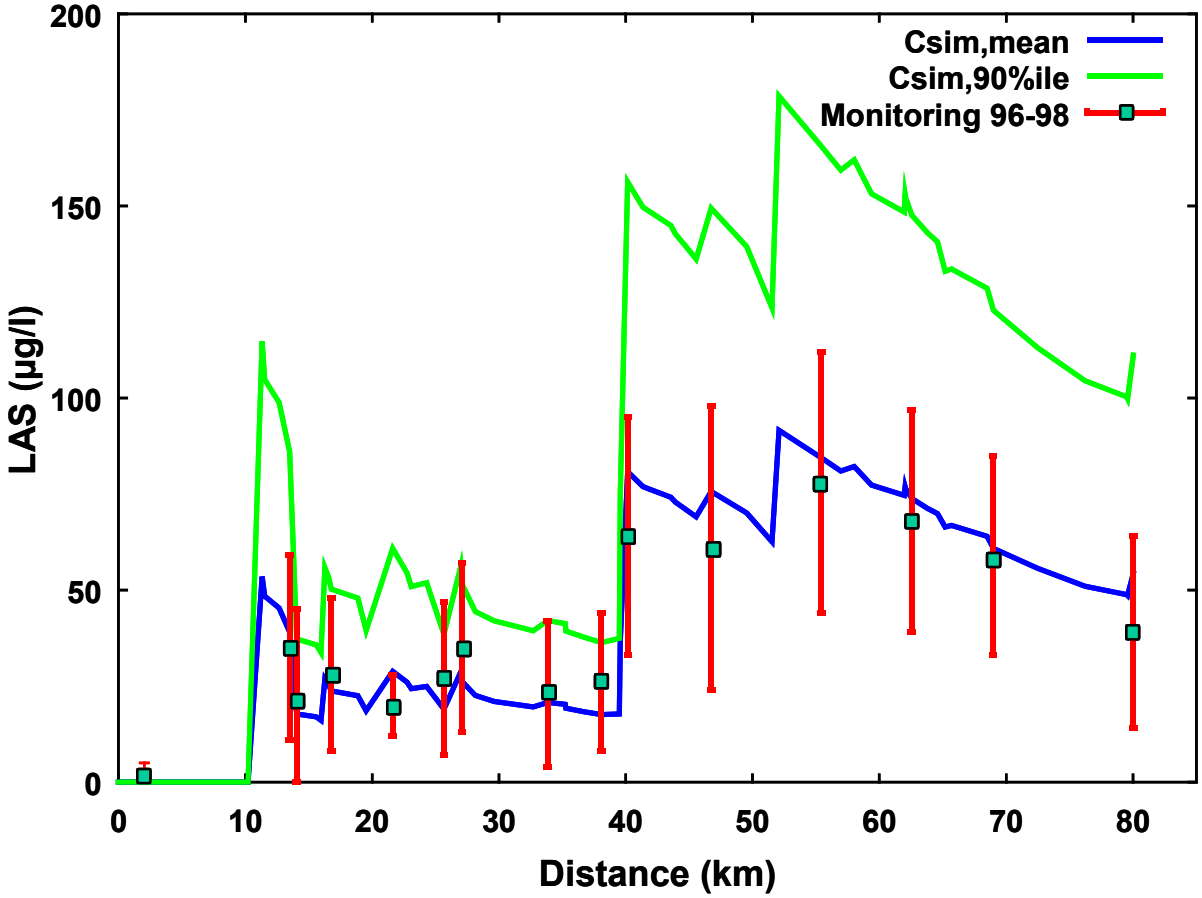

Figure 22: Simulated and measured data of LAS in the river Calder (ECETOC (1999))

5.3.2 Ruhr

In the year 2000 a small comparison of EUSES and GREAT-ER was made within the project "Validation of exposure models and parameters" (Berding et al. (2000)). The authors compared monitoring data of the Ruhr river system in Nordrhein-Westfalen (Germany) with a GREAT-ER simulation and with four different scenarios of EUSES.

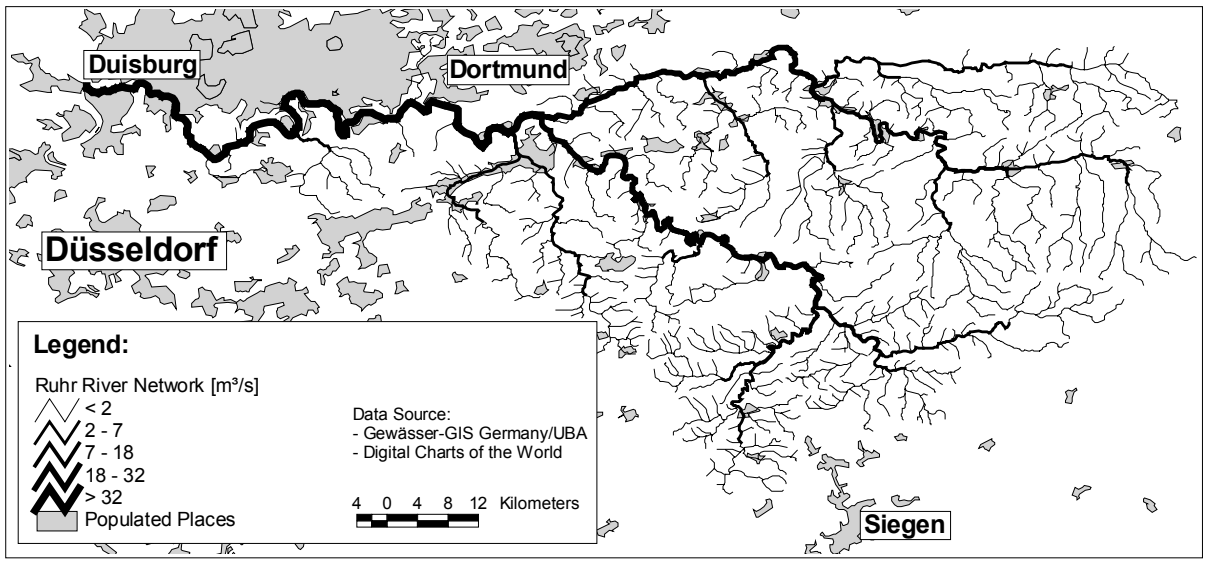

Figure 23: Ruhr river-system (taken from Berding et al. (2000), *figure modified)*

The substance analysed was HHCB with monitoring data dated from 1994 and 1995. Berding et al. (2000) used in total four different EUSES scenarios to describe better the specific characteristics of the river network (see Figure 24). The “EU-Default” is EUSES’s standard European scenario. In the“NRW” scenario the default parameters were replaced by respective parameters adapted to the area of Nordrhein-Westfalen. The “Ruhr 1” scenario is a site-specific adaption of the NRW-scenario (Ruhr catchment area only), whereas in the “Ruhr 2” scenario it was assumed that HHCB was “readily biodegradable”.

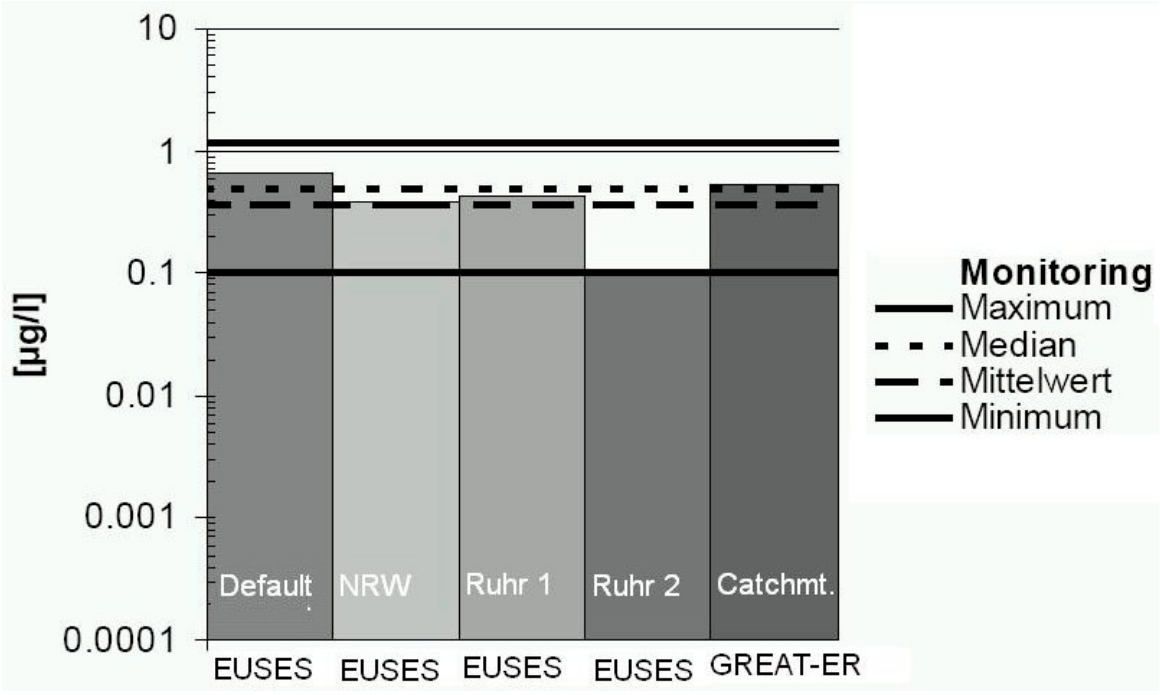

Figure 24: Simulated and measured HHCB-concentrations (Berding et al. (2000), *modified*)

Three of the four EUSES-scenarios (EU-default, NRW and Ruhr1) describe the situation in the Ruhr catchment well, but only if there is no degradation for HHCB considered. . It is interesting that the concentration predicted by GREAT-ER are very well describing the monitoring data though degradation of HHCB has been considered in the simulations.
The comparison also demonstrate the marginal influence of additional site-specific information on the results of EUSES. Only the additional assumption of degradation has a significant effect on the calculated concentration

5.3.3 Itter

In 2004 Thorsten Wind made a comparison of GREAT-ER and EUSES exposure simulations for some consumer-product ingredients (Boron, LAS, EDTA, Triclosan, NTA) in the Itter – river system (Wind (2004)). The aim of his study was to analyse the differences between a generic non-spatial model (EUSES) and a geo-referenced model (GREAT-ER). The river-system he used was the Itter, a small tributary of the Rhine. The consumption data used refer to the use volumes of these consumer-product ingredients for 2000 in Germany.
Wind used in total three different scenarios for EUSES to describe better the situation in Nordrhein-Westfalen (NRW) where the river Itter (close to Düsseldorf, Figure 25) is located (EUSES default scenario, NRW-scenario, Itter catchment-scenario). He compared the three EUSES scenario with respective GREAT-ER simulation of the Itter and with site-specific measurements.

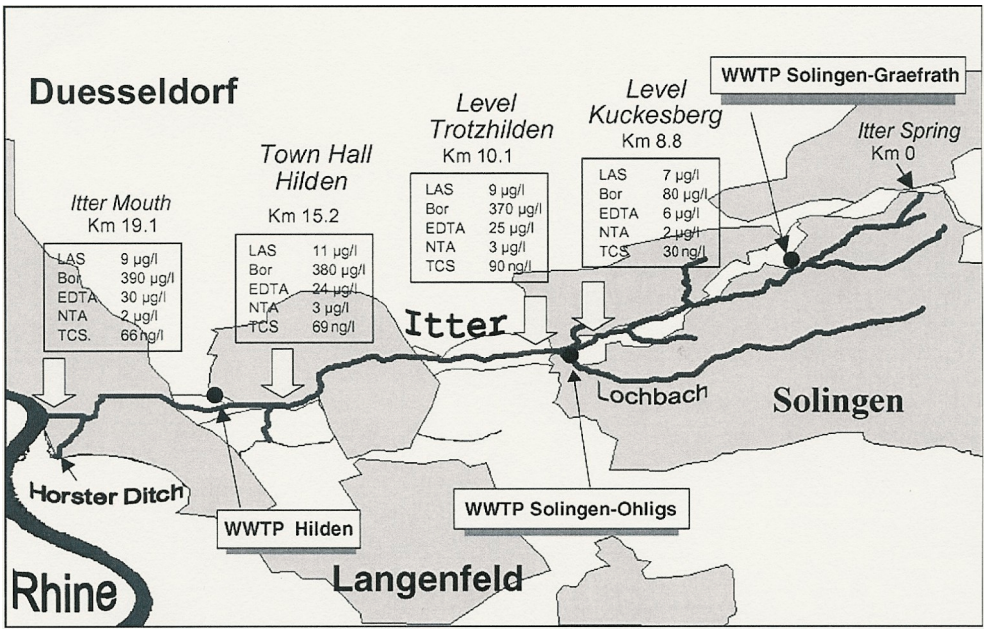

Figure 25: Itter catchment (Wind (2004))

A summary of the results is given in Table 5. The EUSES default scenario is more conservative than GREAT-ER on the local situation, but GREAT-ER seems to be more conservative with respect to regional concentrations. However, when comparing with measured data GREAT-ER clearly produces more realistic concentrations than EUSES. Even if considering more site-specific data (NRW- or Itter-scenario) EUSES is hardly able to reflect the situation in the Itter river-system. Obviously, the assumptions of this generic model are not able to really predict accurate river concentrations, pointing out the limits of the generic approach followed in EUSES.

However, the results demonstrate that both models could be used on different levels of a step-wise approach, where EUSES is used within the initial screening phase whereas GREAT-ER could be used for higher-tier assessment.

Table 5: Comparison of measured and predicted environmental conc. in µg/L (Wind (2004))

scenario	PEC	Boron	LAS	EDTA	NTA	TCS*
EUSES default	*local*	*673*	*498*	*49*	*26.5*	*0.26*
	regional	85.8	4.5	6.2	2.7	0.004
EUSES NRW	*local*	*440*	*264*	*31.9*	*15.2*	*0.14*
	regional	100	5.3	7.2	2.6	0.004
EUSES Itter	*local*	*818*	*554*	*59.3*	*28.1*	*0.28*
	regional	100	3.2	7.2	1.6	0.002
GREAT-ER	*local*	*385*	*15.5*	*28.7*	*2.6*	*0.13*
	regional	336	7.8	25.5	2.5	0.07
Measured c_{lokal}		*370*	*9*	*25*	*3*	*0.009*
Measured Range of *c*		80-390	7-11	6-30	1-3	0.03-0.09

(local PECs in *Italic,* *TCS = Triclosan)

5.3.4 Rhein in Nordrhein-Westfalen

In 2003 a comparison of simulations performed with GREAT-ER and measured concentrations was published for some consumer-products (Boron, EDTA, HHCB, dichlofenac, paracetamol, diuron, ammonium-nitrogen) for the Rhein river-basin in Nordrhein-Westfalen (Heß et al. (2003), Figure 26). The aim of his study was to analyse the differences between GREAT-ER and monitoring data. A comparison with EUSES was not performed.

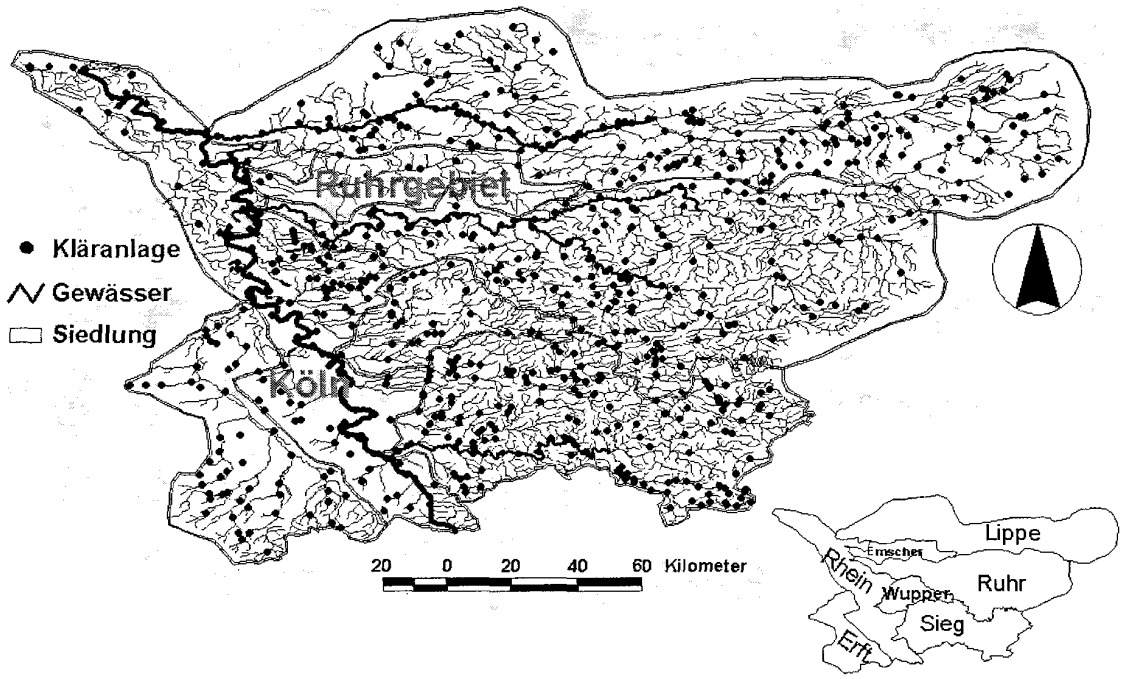

Figure 26: River network and water treatment plants of the Rhein in NRW (Heß et al. (2003))

5.3.4.1 Boron

The comparisons for Boron demonstrated that GREAT-ER was not able to simulate the concentrations close to monitoring data, if only releases from private consumers had been considered. Therefore additional releases from industry were considered. The location of these releases could be found due to the geo-referenced character of GREAT-ER. After considering these inputs the simulation results were well in line with the monitoring data (see Figure 27). B1 is a simulation of boron based on detergents emissions from households only, whereas in B2 additional emissions from mine water and in B3 mine water and waste water from industry were considered.

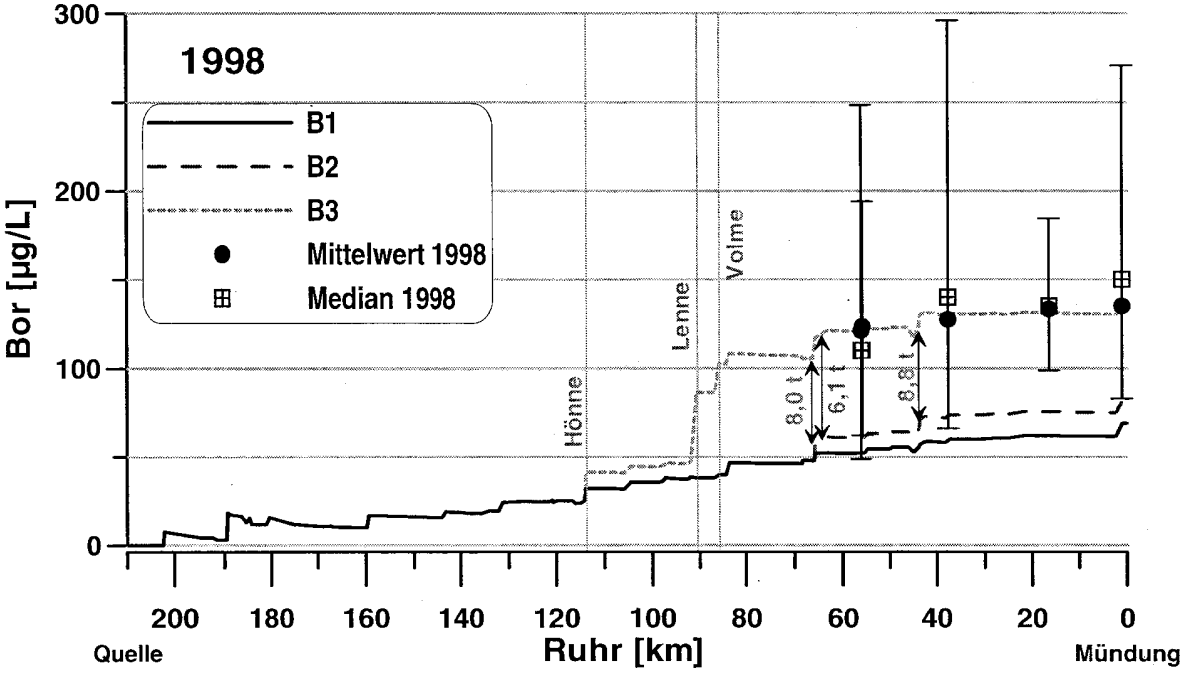

Figure 27: Simulated boron concentrations in the river Ruhr (Heß et al. (2003))

5.3.4.2 HHCB

HHCB (1,3,4,6,7,8-Hexahydro-4,6,6,7,8,8-hexamethylcyclopenta-gamma-2-benzopyran) is a member of a group of substances used in fragrances and known collectively as the polycyclic musks. It is used in shower gels, toilet soaps, or hair spray.

For HHCB deviations were detected between the simulation and the measurements (Figure 28). However, at least the dynamics in the Lippe were modelled rather well.

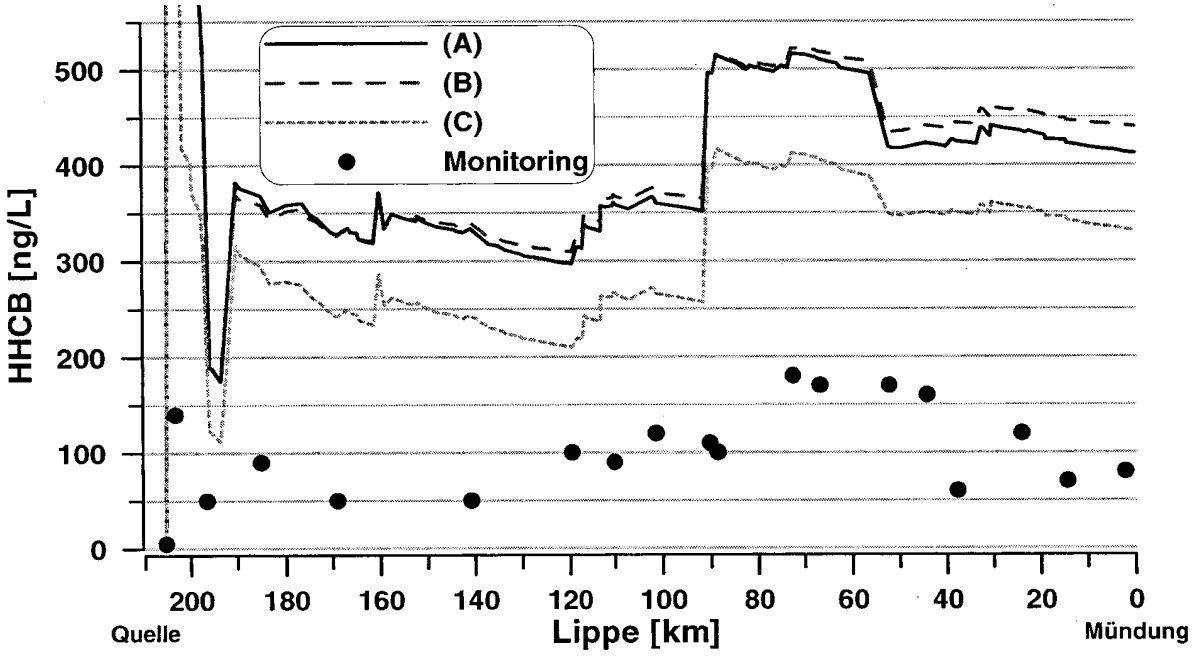

Figure 28: Simulated HHCB concentrations in the river Lippe (Heß et al. (2003))

5.3.4.3 Dichlofenac, Paracetamol and Diuron

For dichlofenac and paracetamol the monitoring data were not sufficient for a meaningful comparison with simulated data. The 3rd compound; diuron; is a herbicides with a special use pattern; as it is sprayed mainly on lanes and places in private gardens and on public areas (e.g. car-parks). Because of these special use pattern its release is comparable with other down-the-drain chemicals. After considering seasonal influences the diuron concentrations in the river system could be simulated well (Figure 29).

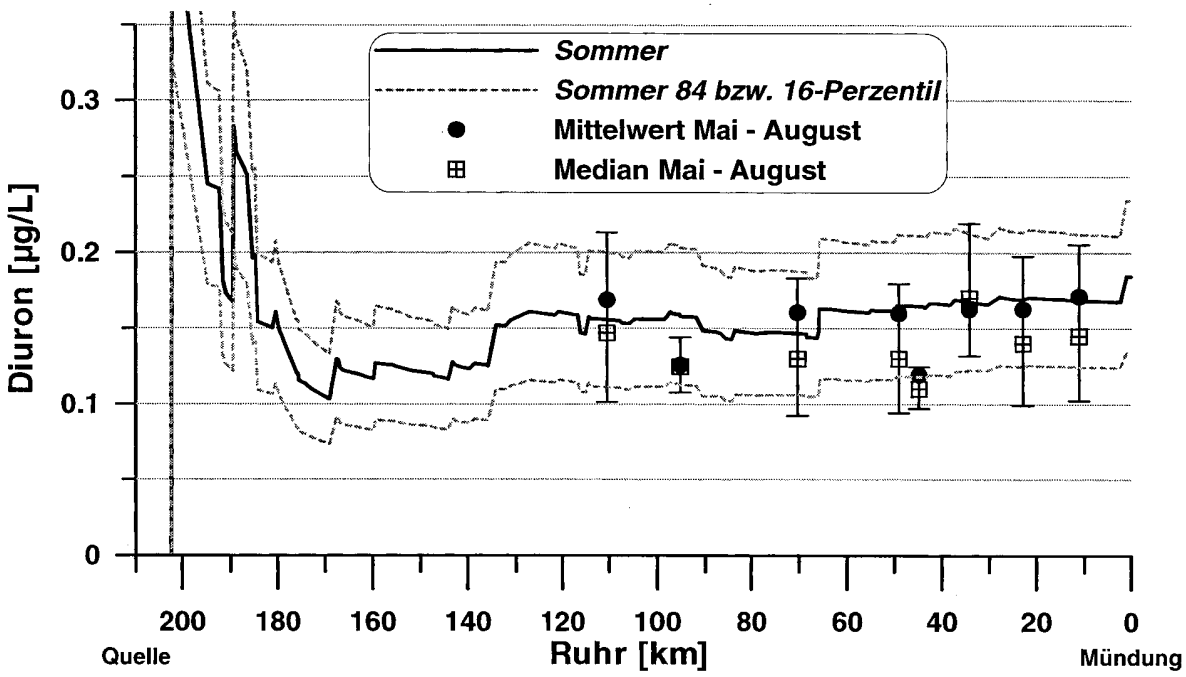

Figure 29: Simulated diuron concentrations in the river Ruhr (Heß et al. (2003))

5.3.5 Elbe in Germany

Parallel to the evaluation of the Rhein river basin the same authors also analysed the situation in the German part of the Elbe river-system using the same consumer-products (Boron, EDTA, HHCB, dichlofenac, paracetamol, ammonium-nitrogen) (Heß et al. (2003), Figure 30).

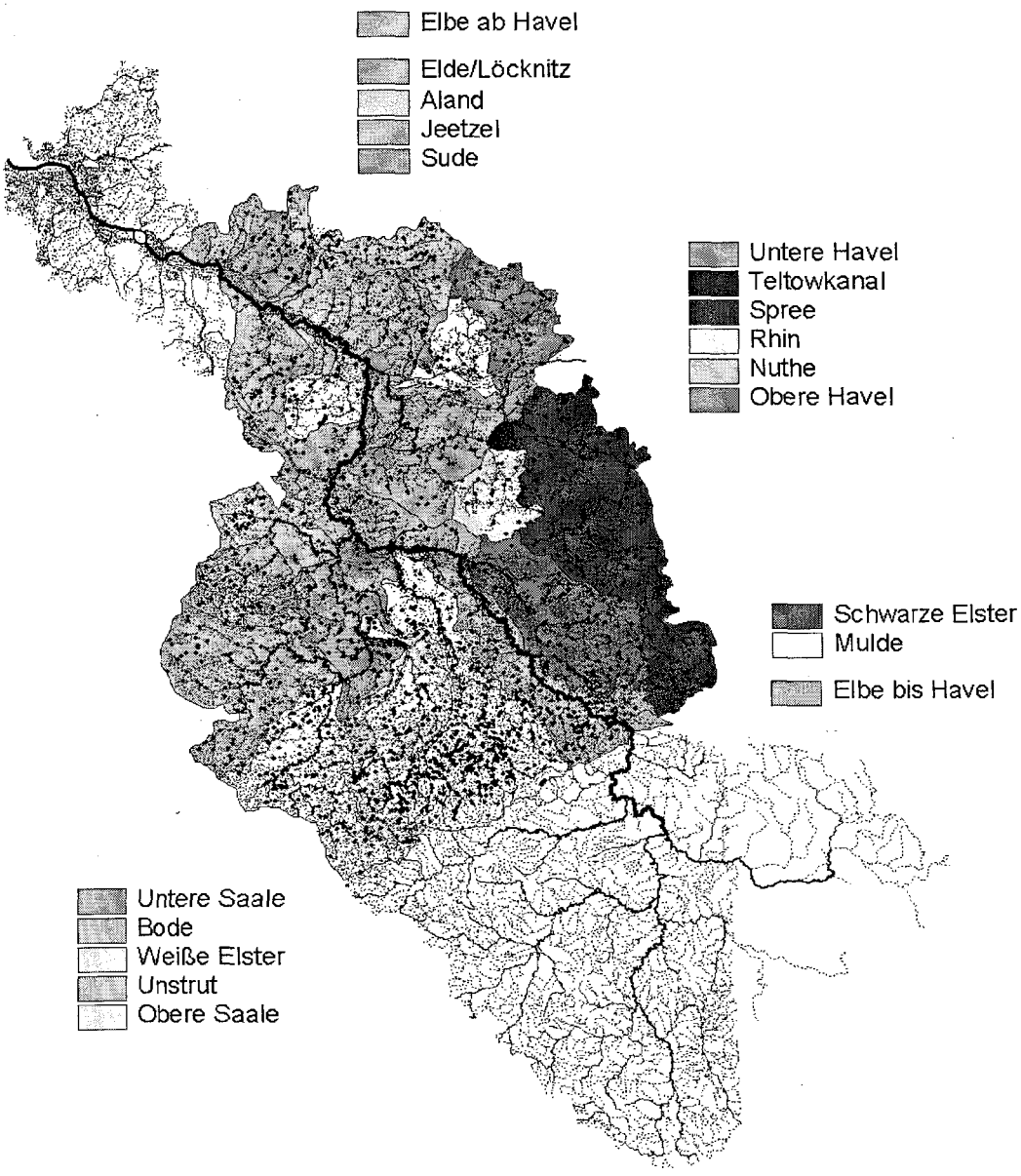

Figure 30: River basin of the Elbe in Germany (Heß et al. (2003))

5.3.5.1 Boron

The overall results were quite similar for both river basins: The comparisons for Boron showed that with one exception the simulation results by GREAT-ER were within a factor of 2 compared to the monitoring.

Also for EDTA the overall comparison between simulated and measured data were also reasonable well assumed that additional emission sources from industry are considered (Leuna and Buna).

5.3.5.2 HHCB

Due to limited information on the fate of HHCB four scenarios were used for the simulation. For HHCB significant deviations were detected between the simulation results and the measurements mainly for one station (Müglitz, Figure 31). Higher deviations than for the previously discussed two chemicals have to be considered for HHCB.

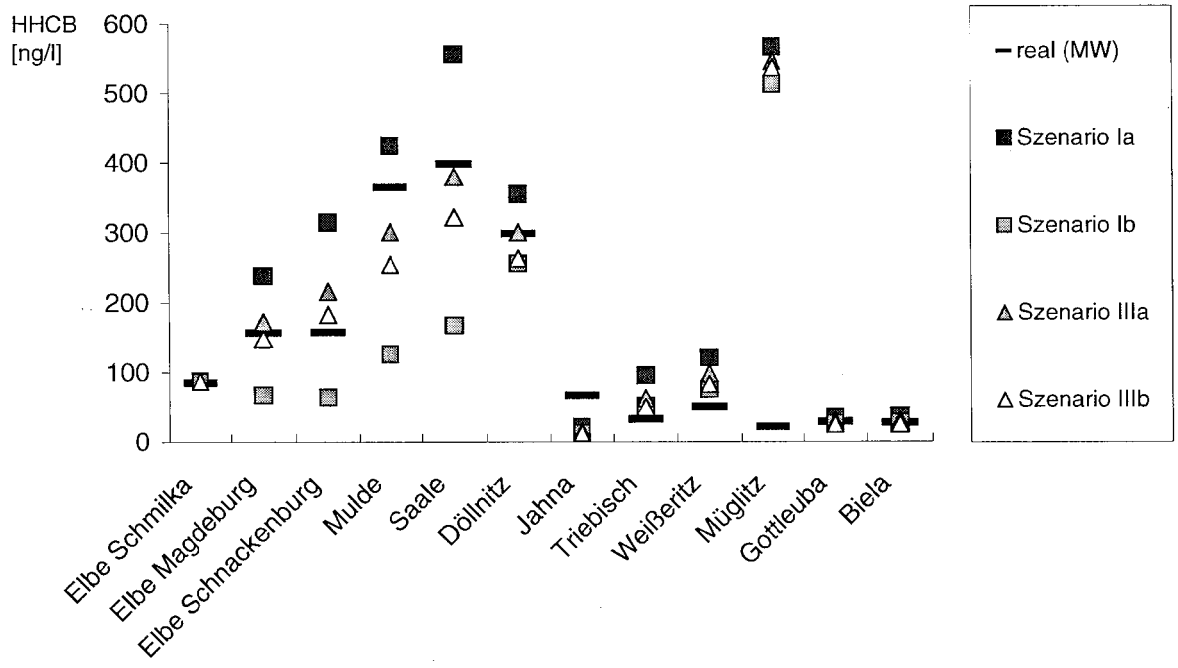

Figure 31: Simulated and measured HHCB concentrations in the Elbe (Heß et al. (2003))

5.3.5.3 Dichlofenac and Paracetamol

For dichlofenac and paracetamol the monitoring data were not sufficient for a meaningful comparison with simulated data.

5.3.5.4 Ammonium ion (NH_4^+)

Due to uncertainties with respect to the ammonium emissions and the fate of this chemical ion in lakes different scenarios were used to model this substance in the Elbe river basin. Generally, the deviations of the simulations were within a factor of 2 compared to the measured numbers (see Figure 32) even for the standard parameterisation.

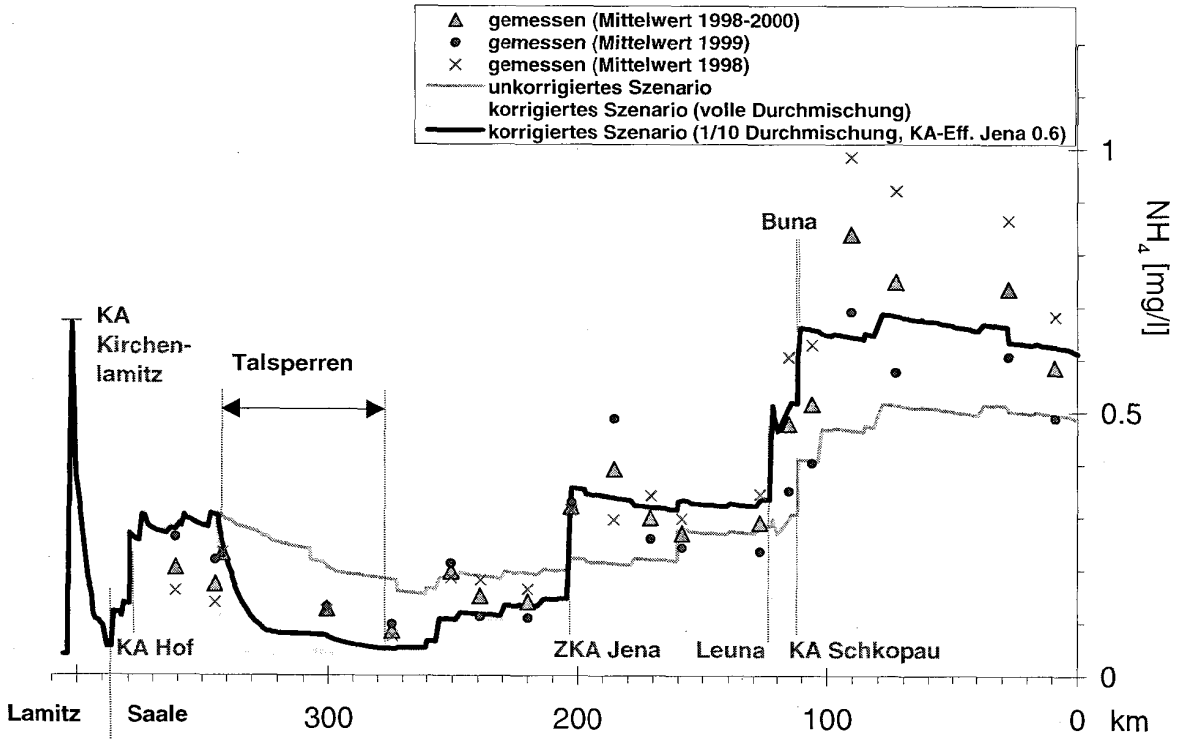

Figure 32: Simulated and measured NH_4^+-concentrations in the Saale (Heß et al. (2003))

5.3.6 Main

The river Main was parameterised in order to simulate the fate of two typical household chemicals (LAS, HHCB) and one drug (diclofenac). Simulated concentrations were compared with monitoring data during a monitoring campaign in May, 1998. The catchment of river *Main* covers a total area of about 27,700 km² with its main part located in Northern-Bavaria. The *Main* has a total length of about 524 km and is roughly divided into three major parts, namely the *upper*, the *middle Main* and the *lower Main*.

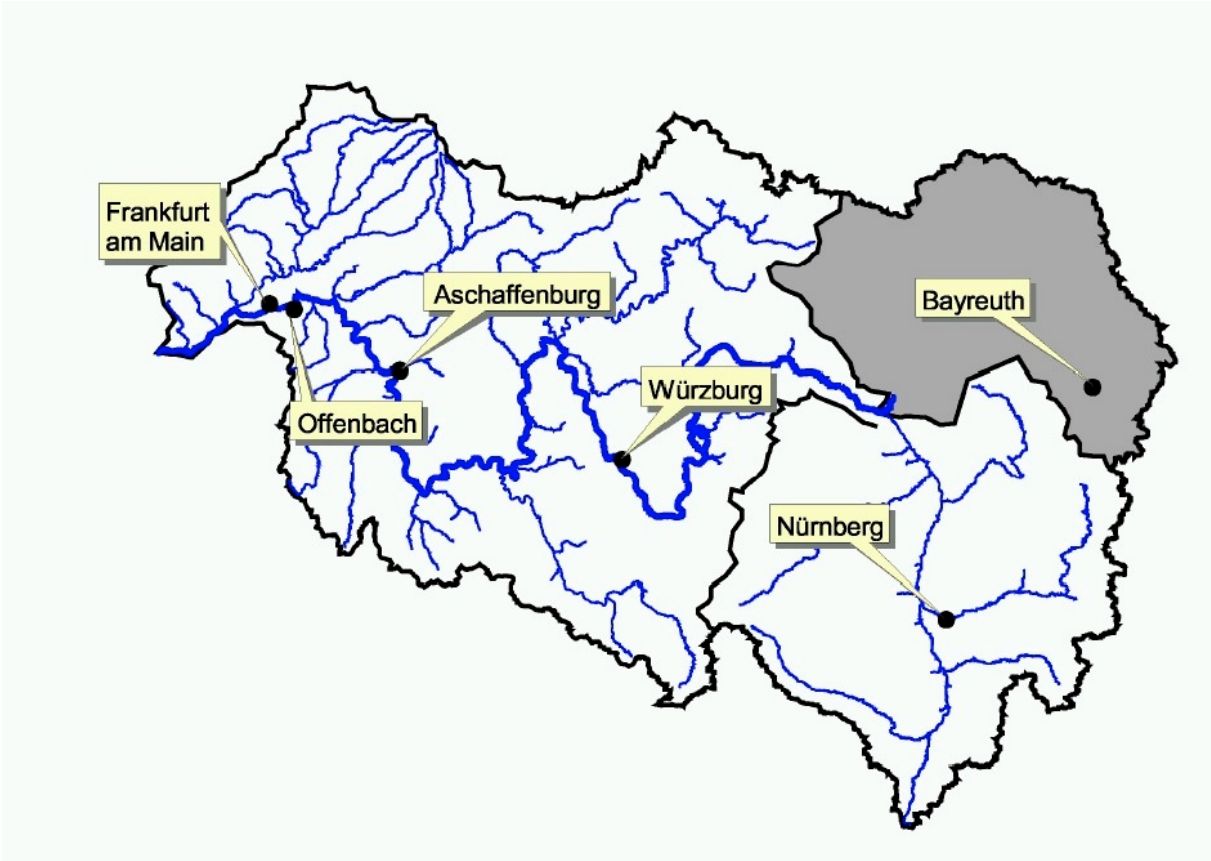

Figure 33: Catchment of the River Main (Klasmeier et Matthies (2001))

The authors showed that a simplistic approach of modelling solely the Main river stretches does not lead to satisfying results. Satisfactory results could only be obtained for the *Main* after considering the river-network in a more detailed way with its major tributaries (as presented in Figure 33).

Two different variations were performed for the degradation of LAS and HHCB.

The in-stream removal rates for LAS were in the range of 0.01 – 0.69 h^{-1} ("standard scenario") and 0.021 – 0.046 h^{-1} ("in-stream removal from Rippen", Rippen (1999)). Many monitoring data points were below the detection limit due to the high limit of 2 µg/L for LAS. Allthough the results of both variations are not totally different, the "Rippen" scenario however fits to the measured concentrations better.

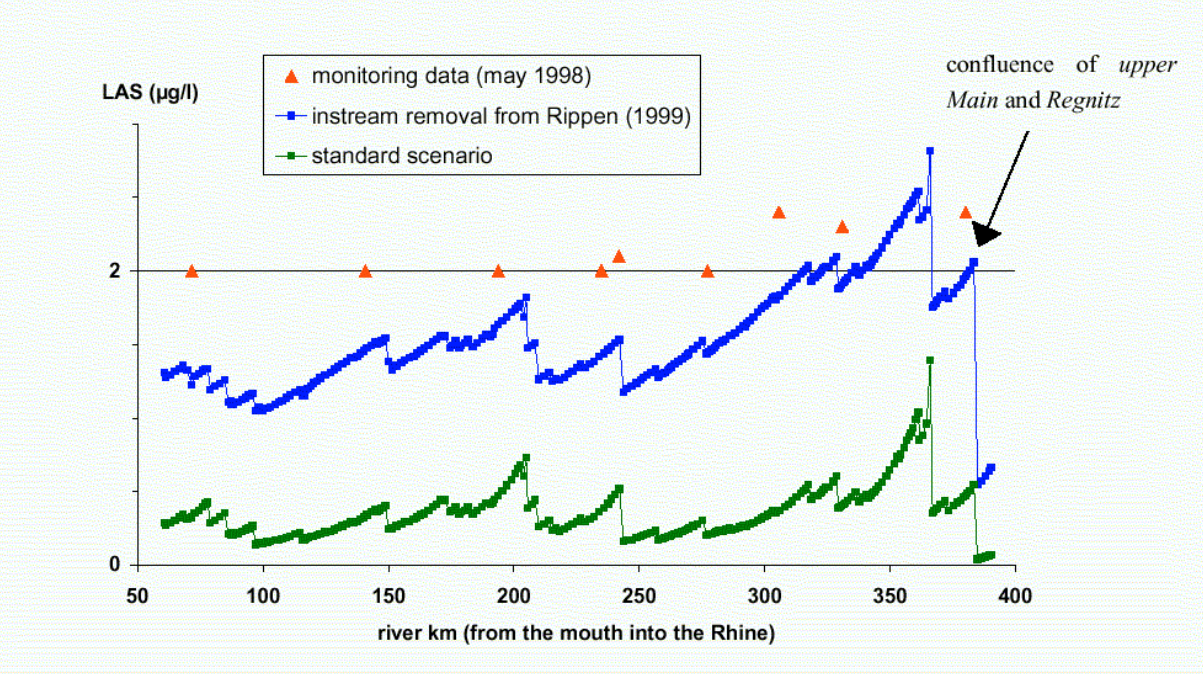

Figure 34: Mean simulated LAS concentration in the Main (Klasmeier et Matthies (2001))

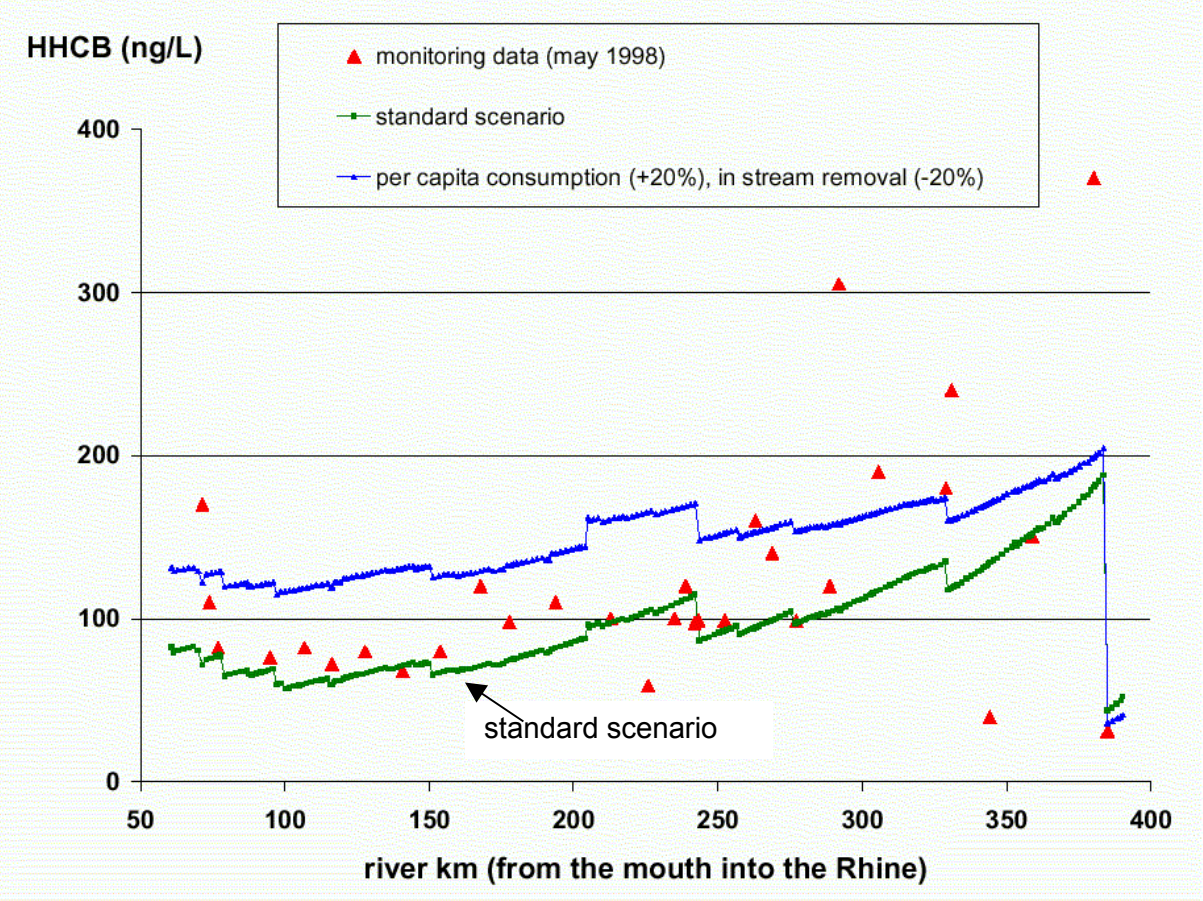

Figure 35: Mean simulated HHCB concentration in the Main (Klasmeier et Matthies (2001))

Two different scenarios were simulated for HHCB: 0.005-0.03 h^{-1} in-stream removal "standard scenario" and an arbitrarily increased per-capita-consumption (+ 20%) and a higher in-stream removal rate (by a factor of two). As shown in Figure 35 the results of the standard scenario are well in line with most of the monitoring data points. However, there are deviations in the region after the confluence of *upper Main* and *Regnitz* (see the arrow in Figure 34). Klasmeier and Mathies explain this deviation by the fact that the measured data are not representing the mean temporal concentration (as it is modelled by GREAT-ER) but the specific situation in May 1998.

5.3.7 Conclusions

The results of six studies were used to analyse the ability of GREAT-ER to simulate concentrations of chemicals in river-systems. Generally, the measured concentations were simulated by the GREAT-ER model by a factor of 2.

GREAT-ER is currently not able to handle chemicals that are released on a seasonal level (summer, winter) without further calibration. Further discrepancies have to be expected, if certain chemicals are released not only by the general public but also by industry. In such cases the measured data were met only after considering additional releases (calibration).

In two studies parallel EUSES and GREAT-ER simulations were performed. They demonstrated that GREAT-ER describes generally describe the fate of chemicals in surface water much better and more comprehensively than EUSES.

Looking at the results of both models it seems reasonable to use both models on different levels of a step-wise approach, where EUSES is used within the initial screening phase and GREAT-ER at the higher-tier assessment.

6 Recommendations for considering GREAT-ER within the assessment of chemicals

6.1 Conclusions

GREAT-ER is a geo-referenced multimedia model for predicting site-specific local and regional concentrations of chemical substances in river systems (catchments). The model focuses on down-the-drain chemicals, i.e. detergents, household chemicals, biocides, human drugs. The release input parameter is the consumption per capita and time [mass per capita per year]. The model was developed by scientific institutions financed by industry and agencies (http://www.great-er.org und http://www.usf.uni-osnabrueck.de/projects/GREAT-ER), among others Umweltbundesamt (Heß et al., 2003, Scharenberg, 2004). Calibration studies with GREAT-ER showed that simulated concentrations lie within a factor of 2 to 3 compared with monitoring concentrations.

EUSES is a generic multimedia model for the prediction of local and regional concentrations of chemical substances in environmental compartments, i.e. surface water, air, soil, sediment, and groundwater. The model does not differentiate between the spatial and temporal scale. The EU Member States introduced this model in the year 1996 as a conservative screening model in chemicals' assessment for new notified and existing chemicals as well as in 2003 also for biocidal products under EU regulations (EC, 2003).

The other geo-referenced models dealt with in this advisory opinion like MONERIS, RIONET, ATV-DVWK-Gewässergütemodell, BBA-Risk Map Model, ASSESS, Drip, BETR, SoilFug are models designed for a special purpose. They should not be compared with GREAT-ER and EUSES, because their objectives are rather different.

It is the advisory opinion that EUSES and GREAT-ER serve two different objectives and should not be replaced one by the other. Both models have their special field of application. It is recommended to rank EUSES as a conservative screening model, but GREAT-ER as a confirmative model at a higher tier of chemical assessment. This statement in mind, there should be no controversy in the field of application of both models.

6.2 Recommended scenarios for GREAT-ER

6.2.1 Introduction

As evaluated in chapter 5.3 the use of GREAT-ER has advantages. The model predicts site-specific concentrations in river systems. The simulated concentrations can directly be compared with measured (monitored) data and can be visualised in maps due to the GIS-tool of GREAT-ER.

A problem remains comparing EUSES with GREAT-ER in a regulatory context. EUSES calculates concentrations in a fictive unit world that is set by policy expert decision by a conservative "level of protection". GREAT-ER simulates realistic concentrations in site-specific river stretches that can vary from stretch to stretch. The "level of protection" in GREAT-ER cannot be set by default. It can only be set in relation of a "standard scenario" that is defined by a policy expert decision as "level of protection". It is not recommended to include any additional algorithms to increase the conservatism of the model itself.

6.2.2 Properties of a suitable "standard scenario" for GREAT-ER

A useful "standard scenario" of GREAT-ER for assessments in the regulatory context should reflect the variability of river systems for a certain area with a focus on vulnerable areas (realistic worst case situation). This means to define a slowly moving river system (typical for Northern Germany) like the river Ems, and also a river system that is characterised by high flow rates, i.e. rivers of the low mountain range mainly in Southern Germany. If a high level of protection is the key parameter, smaller rivers are generally preferred as "standard scenarios" compared with large rivers, e.g. Leine vs. Rhine.

It is not helpful, if the standard river is extremely small or fed mainly by waste-water from treatment plants like the river Itter near Düsseldorf (Wind, 2004). It is expected that high concentrations be simulated for almost all substances under this situation. The relevance of these situations may therefore be questionable, and a meaningful separation between an acceptable and a non-acceptable case is difficult to decide.

As analysed in chapter 5.3 a couple of river systems are already parameterised for GREAT-ER. Some of the medium size rivers, e.g. Saale, Leine, Ruhr, are suited for a "standard

scenario". However, to get more experience with GREAT-ER simulations also large rivers, e.g. Rhine, Elbe, should be considered as "standard scenarios".

6.2.3 Use of the "GREAT-ER standard scenario" in the regulatory context

EUSES produces "local" and "regional" predicted environmental concentrations. GREAT-ER produces "initial" and "catchment" concentrations. The latter two are comparable to the "local" and "regional" concentrations of EUSES.

In the regulatory context, the "level of protection" for GREAT-ER lies in the choice of the "standard scenario" representing a vulnerable river basin. Furthermore, a percentile limit needs to be set, which the PEC/PNEC ratios in that standard scenario must not exceed. Such a limit can be defined as it was done in the EUSES model by an expert policy decision. It is suggested in analogy of the realistic worst case a limit value of 10% for PEC/PNEC >1 ratios that must not be exceeded for the initial concentrations in the standard scenario.

6.2.4 Assessment of costs for the necessary data and GIS-Software

The parameterisation of GREAT-ER is cost intensive due to the huge amount of geo-referenced data. The collection of these data is the main bottleneck for GREAT-ER, especially when suppliers and authorities in different regions and countries present these data in inhomogeneous formats. Furthermore, geo-referenced data are not always free of charge. However, EU Member countries pay an enormous effort to implement the Water Framework Directive, which necessitates the production and maintenance of geo-referenced data for the successful river basin management in the coming years (Müller 2002). In this context, the national authorities are producing river basin geo-referenced data with the location of chemical manufacturers and their industrial waste-water treatment plants as well as the municipal waste-water treatment plants. These data are also necessary geo-referenced data for GREAT-ER.

GREAT-ER itself can be obtained free of charge from ECETOC. It runs on a platform-independent desktop version with the free GIS data viewer THUBAN. The menu items are ordered according to the usual flow of a simulation session, i.e. substance, catchment, environment, and simulation, and allow the most common GIS operations. All currently available river basins are included (November 2003).

The GREAT-ER desktop version is based on the ORACLE database system. The ORACLE software licence can be obtained via TechniData (the developer of the GREAT-ER desktop) for a fee of 300 €.

6.3 Fields of application for GREAT-ER

GREAT-ER can be used in the following fields:

a) For priority setting of substances
   GREAT-ER can be used for priority setting of substances. Based on a default situation GREAT-ER would analyse the environmental fate and behaviour of different substances in the standard scenario. Such a procedure could reveal a ranking of a homogeneous group of substances, e.g. musk fragrances in detergents.

b) In regulatory exposure assessment and risk management
   The most adequate field for regulatory use would be in the exposure assessment of new and existing chemicals, biocides, detergents, and human drugs. The adequate procedure would be to work in a tiered approach and apply EUSES in the screening and GREAT-ER, if necessary and applicable, in the confirmatory stage.

   GREAT-ER would analyse the concentrations in a river basin or in hot spots on a detailed level considering different catchment characteristics: small vs. large river system and urban vs. rural situations.

   Higher tier so-called confirmatory models like GREAT-ER are often used in risk management situations, because they provide a more detailed insight into the actual situation and can influence risk management decisions.

c) Recognise "hot-spots"
   The monitoring community can benefit, when running a GREAT-ER simulation beforehand to figure out concentration hot spots for the "most appropriate" monitoring site.

d) GREAT-ER and the Water Framework Directive

According to current experts' opinion it is questionable whether GREAT-ER is suited for the implementation of the Water Framework Directive 2000/60/EC of 23 October 2000. Compared to the application discussed above the requirements in respect of the simulation quality is rather high in this field. Compared to other geo-referenced models like the ATV-DVWK-Gewässergütemodell GREAT-ER is too simple to predict the fate of Water Framework priority chemicals with the necessary precision. It is therefore recommended to gain more experience in regulatory applications of industrial chemicals first than using GREAT-ER in the context of the Water Framework Directive.

6.4 Recommended extensions and improvements of GREAT-ER

As mentioned in chapter 4.1.3.8 a couple of limitations were listed for GREAT-ER. This does not mean that the model cannot be used within the assessment of chemicals because of these limitations.

It is recommended to work on the following limitations in order to guarantee an increased functioning of GREAT-ER in the regulatory context.

a) Include seasonal and regional/geographical temperature variability

When estimating concentrations in rivers GREAT-ER does not consider temporal variability of the input parameters that depend upon temperature or seasonal changes, i.e. flow rate differences, summer and winter temperatures. It is questionable whether these effects can be covered by the existing Monte Carlo approach. It is therefore recommended to consider a number of scenario input parameters that are seasonally dependent, e.g. flow rates, temperatures etc. Such improvements would allow the model to analyse directly seasonal and regional/geographical temperature influences, even if the chemical emission rate remains constant over the year.

b) Consider seasonal emission rates

Currently, all emissions are based upon the annual average. However, for some emission situations, e.g. medical drugs that are only used in parts of the year, it might be important to use seasonal emission rates. For such emission situations

meaningful simulations can be obtained, if seasonal emission patterns are considered.

c) Standardisation of a set of default scenarios

In the regulatory context a strict disjunction is realised between scenario input parameter and compound dependent input data. Following such a procedure a set of standard default scenarios should be defined that are provided and supported by modelling experts. The "normal" user is only responsible for entering the correct compound dependent input data, when using standard default scenarios.

However, in GREAT-ER this philosophy is currently not strictly realised, as illustrated by the following example:

When running in mode 3 the same properties for the wastewater treatment plant have to be used independent where it is located in the river system. It is questionable whether this option is suited for a geo-referenced model GREAT-ER, while site-specific input data that characterise the individual treatment plant are not build in the model. A consequent implementation would mean the parameterisation of site-specific treatment plants. This work has to be done only once. Based upon this information GREAT-ER would be able to estimate site-specific removal rates for any substance based upon the properties of the individual waste-water treatment plant and the chemical. The advantage of the additional parameterisation would be the replacement of a difficult-to-obtain input parameter "site-specific removal" as well as a non-adequate single SimpleTreat-calculation for all waste-water treatment plants by an additional GREAT-ER estimation.

d) Sensitivity analysis

It is recommended to perform a sensitivity analysis to get an overview about the most sensitive input parameter. Such an analysis would reveal critical input parameters and would result in more confidence in the model. The user will have information on the quality of results, if critical missing input parameters are evaluated by QSAR or by expert estimations.

e) Output formalities

It is recommended to realise a couple of small and formal features are constant in the graphical output, e.g. a combination or sequence in colours to indicate fixed PEC/PNEC ratio ranges. Also the existing report.txt-file could be improved by highlighting the most important results that have to be considered within risk assessment and risk management.

f) Inclusion of diffuse emissions

Presently, GREAT-ER considers releases of consumer chemicals that enter the environment via point sources, the municipal waste-water treatment plants. However, diffuse sources contribute – in some cases – considerably to surface water contamination, e.g. by leaching from products (e.g. polymers, wood preservatives, tire abrasion, pesticides, biocides). It is recognised that such diffuse sources may be difficult to quantify and to localise. The development of GREAT-ER to include diffuse sources is a challenge to modellers. Product environmental emissions become more and more important emission control activities in the future.

7 References

Anonym (1998): Handbuch ATV-Gewässergütemodell, Herausgeber ATV-Fachausschuß 2.2, Hennef.

Bach; M.; Huber; A.; Beisecker; R.; Zullei-Seibert; N.; Klein; Michael (1999): Gewässerbelastung mit Pflanzenschutzmitteln in Deutschland – Kenntnisstand; Schätzung der Einträge und Minderungsmaßnahmen (Water contamination with pesticides in Germany – State of knowledge; estimation of water inputs and reduction measures); Report 295 24 034; Umweltbundesamt Berlin.

Barra; R.; Vighi; M.; Maffioli; G.; Di Guardo; A; P. Ferrario (2000): Coupling SoilFug Model and GIS for Predicting Pesticide Pollution of Surface Water at Watershed Level. Environmental Science & Technology; **34;** 4425-4434.

Behrend; H.; Huber; P.; Kornmilch; M.; Opitz; D.; Schmoll; O.; Scholz; G.; Uebe; R. (2000): Nutrient emissions into river basins of Germany. UBA-Texte 23/00: 1-288; Umweltbundesamt Berlin; Berlin

Behrendt; H.; Bach; M.; Kunkel; R.; Opitz; D.; Pagenkopf; W.; Scholz; G.; Wendland; F. (2002): Nutrient emissions into river basins of Germany on the basis of a harmonised procedure; Report No. 299 222 285; Umweltbundesamt; Berlin.

Berding; V.; Schwarz; S.; Trapp; S. and M. Matthies (2000): Validierung von Umweltexpositionsmodellen und in Modellen verwendeten Parametern; Report 296 67 075; Berichte 9/00 Umweltbundesamt; Berlin; http://www.usf.uos.de/~schwartz/endbericht.pdf.

Brandes; L.J.; D. van de Meent and H. den Hollander (1996): SimpleBox 2.0: a nested multimedia fate model for evaluating the environmental fate of chemicals. Bilthoven National Institute of Public Health and the Environment (RIVM); Report No. 719101029.

Christoffels; E. (2001): Ein Instrument zur Unterstützung wasserwirtschaftlicher Planungsaufgaben am Beispiel der Erft – ATV-Gewässergütemodell. KA-Wasserwirtschaft; Abwasser; Abfall (48) Nr. 7.

De Greef; J.; and A.C.M. De Nijs (1990): Risk assessment of new chemical substances. Dilution of effluents in the Netherlands. Bilthoven; National Institute of Public Health and the Environment (RIVM); Report No. 670208001.

De Nijs T; de Greef J (1992) : Ecotoxicological Risk Evaluation of the Cationic Fabric Softener DTDMAC -- II. Exposure Modelling; Chemosphere 24(5); 611- 627.

Den Hollander; H. A. and D. van de Meent (2004): Model parameters and equations used in Simplebox 3.0. Bilthoven; RIVM; Report No. 601200 003; January 2004.

EC (1996): EUSES; the European Union System for the Evaluation of Substances. National Institute of Public Health and the Environment (RIVM); the Netherlands. Available from the European Chemicals Bureau (EC/JRC); Ispra; Italy.

EC (2003a): EUSES; the European Union System for the Evaluation of Substances. National Institute of Public Health and the Environment (RIVM); the Netherlands. Available from the European Chemicals Bureau (EC/JRC); Ispra; Italy.

EC (2003b): Technical Guidance Document on Risk Assessment European Chemicals Bureau; 2nd edition; document EUR 20418 EN/1; Ispra; Italy; . http://ecb.jrc.it.

ECETOC (1999): GREAT-ER User manual; Special Report No. 16; Brussel; http://www.greater.org.

EPA (1995): SMPTOX version 4.0 (SMPTOX4). User's Manual. United States Environmental Protection Agency. Athens; Georgia; 46p.

Feijtel; T.C.J.; Boeije; G.; Matthies; M.; Young; A.; Morris; G.; Gandolfi; C.; Hansen; B.; Fox; K.; Holt; M.; Koch; V.; Schroder; R.; Cassani; G. ; Schowanek; D.; Rosenblom; J. and Niessen; H. (1997): Development of a Geography-referenced Regional Exposure Assessment Tool for European Rivers - GREAT-ER. Contribution to GREAT-ER # 1. *Chemosphere* **34**; 2351-2373.

Golla; B.; Enzian; S.; Jüttersonke; B.; Gutsche; V. (2002): Entwicklung und Testung eines GIS-gestützten Verfahrens zur Erstellung thematischer Risikokarten als Grundlage für eine Differenzierung von Anwndungsbestimmungen zum Schutz des Naturhaushaltes beim Einsatz von Pflanzenschutzmitteln. Report 201 63 410; Umweltbundesamt Berlin.

Heß; O.; Schröder; A.; Klasmeier; J.; Matthies; M. (2003): Modellierung von Schadstoffflüssen in Flußeinzugsgebieten; Report 298 65 402; Umweltbundesamt Berlin.

Klasmeier J. et M. Mathhies (2001): Application of the Geography-Referenced Environmental Assessment Tool for European Rivers (GREAT-ER) in the Catchment of the River MAIN (Germany). Report. Institute of Environmental Systems Research University of Osnabrück; Osnabrück; Germany.

Knoche; Harald; Klein; Michael; Lepper; Peter; Herrchen Monka; Köhler; Carsten and Storm Ulrike (1998): Development of criteria and methods for comparison and applicability of regional environmental conditions within the EU Member States. Report 126 05 113; Umweltbundesamt Berlin.

Matthies M and Schröder A (2002): Verdünnung von kommunalen Abwässern in Einzugsgebiet der Elbe Wasser&Boden; Heft 6.

Müller; Armin (2002): Nutzung von GIS-Systemen in der Umsetzung der Wasserrahmenrichtlinie; in UBA 2002; p. 50 – 74.

Reuter; H.; Krause; G.; Wulkow; M.; Mönig; A.; Horn; H. (2003) Rionet: A water quality management tool for river basins; Water Science & Technology Vol 48 No 10 pp 47-53.

Rippen G. (1999): Handbuch Umweltchemikalien; Ecomed-Verlag; Landsberg/Lech.

RIVM; VROM; WVC (1994): Uniform System for the Evaluation of Substances (USES); version 1.0 National Institute of Public Health and the Environment (RIVM); Ministry of Housing; Physical Planning and Environment (VROM); Ministry of Welfare; Health and Cultural Affairs (WVC). The Hague; Ministry of Housing; Physical Planning and Environment. Distribution No. 11144/150.

Röpke; B.; Bach; M.; and H.-G. Frede (2002): DSS (Decision Support System) zur Modellierung der Gewässerbelastung mit Pflanzenschutzmittel in Deutschland in Stephan; Bormann; Diekkrüger (eds.) 5. Workshop zur hydrologischen Modellierung: Möglichkeiten und Grenzen für den Einsatz hydrologischer Modelle in Politik; Wirtschaft und Klimafolgeforschung. Kassel.

Scharenberg, B; Schröder, A; Heß, O; Klasmeier, J; Matthies, M (2004): Evaluation of GREAT-ER in two German river catchments. SETAC Europe 14th Annual Meeting, Prague 2004, lecture AM1.

Schowanek D. and S. Webb (2000): Examples of exposure assessment simulation for pharmaceuticals in river basins with the GREAT-ER 1.0 system. Proceedings KVIV Seminar 'Pharmaceuticals in the Environment' March 9, 2000, Brussels

Struijs, J. (1996): SimpleTreat 3.0: A model to predict the distribution and elimination of chemicals by sewage treatment plants. Report no. 719101025. National Institute of Public Health and Environmental Protection (RIVM), Bilthoven, The Netherlands.

Toose, Liisa; Woodfine, David G.; MacLeod, Matthew; Mackay, Don; Gouin, Jenn (2004): BETR-world: A geographically explicit model of chemical fate: Application to transport of a-HCH to the arctic. Environmental Pollution, **128,** 223-240.

Trapp, S. and Harland, B. (1995): Field test of volatilization models. Environmental Science and Pollution Research 2(3), 164-169.

Trapp, S. and Matthies, M. (1996): Dynamik von Schadstoffen - Umweltmodellierung mit CemoS. Eine Einführung. Springer-Verlag; Berlin; 276 p.

UBA (2002): Geo-referenzierte Expositionsabschätzung von Stoffen in Flüssen – UBA-Fachgespräch vom 12. Juni 2002 in Berlin, Umweltbundesamt; UBA-Texte 52/03.

Whitman, W.G. (1923): A preliminary experimental confirmation of the two-film theory of gas-adsorption.Chem. Metall. Eng. 29, 146.

Wind; Thorsten (2004): Prognosis of environmental concentrations by geo-referenced and generic models: A comparison of GREAT-ER and EUSES exposure simulations for some consumer-products ingredients in the Itter. *Chemosphere* **54** 1145-1153.