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Geography-referenced regional exposure tool for European rivers (GREAT-ER):
A case study for the Rupel basin

GIS/EM4

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Abstract
The GREAT-ER (Geo-referenced Regional Exposure Assessment Tool for European Rivers) project team has developed and validated an accurate aquatic chemical exposure prediction tool for use within environmental risk assessment schemes. The software system GREAT-ER 1.0 calculates the distribution of predicted environmental concentrations (PECs) of consumer chemicals in surface waters, for individual river stretches as well as for entire catchments. The system uses an ARC/INFO - ArcView (® ESRI) based Geographical Information System (GIS) for data storage and visualisation, combined with simple mathematical models for prediction of chemical fate. At present, the system contains information for four catchments in Yorkshire (UK), one catchment in Italy, two in Germany and one in Belgium, while other river basins are being added. GREAT-ER 1.0 has been validated by comparing simulations with the results of an extensive monitoring campaign for two 'down-the-drain' chemicals, i.e. the detergent ingredients boron and Linear Alkylbenzene Sulphonate (LAS). GREAT-ER is currently being expanded with models for the terrestrial (diffuse input), air and estuarine compartments.
The Belgian case study showed the feasibility of implementing a new large catchment on a short term and indicated which efforts are required to apply GREAT-ER on a large, ultimately pan-European scale. It was found that it is possible to simplify the river network without considerable loss of accuracy. This allows gaining time and reducing effort in GREAT-ER studies.

Keywords
Environmental risk assessment, Geographic information systems (GIS), GREAT-ER, Monte Carlo simulation, Model validation, Optimal geographical scale, River basins

Introduction

The assessment of whether a substance presents a risk to organisms in the environment is based on a comparison of the predicted environmental concentration (PEC) of the substance with its predicted no-effect concentration (PNEC) to organisms in ecosystems. This assessment can be performed for different compartments (e.g. air, water and soil) and on different spatial scales (local, regional, and continental). The European Union legislation related to risk assessment is described in a number of EU Commission documents (Technical Guidance Documents supporting the Commission Directive on Risk Assessment of New Chemicals (EEC 1993) and Commission Regulation on Risk Assessment of Existing Substances (1488/94/EEC) in support of Existing Substances Regulation (EEC 1994), and is applied in the computerised calculation model EUSES (European Union System for the Evaluation of Substances 1997).

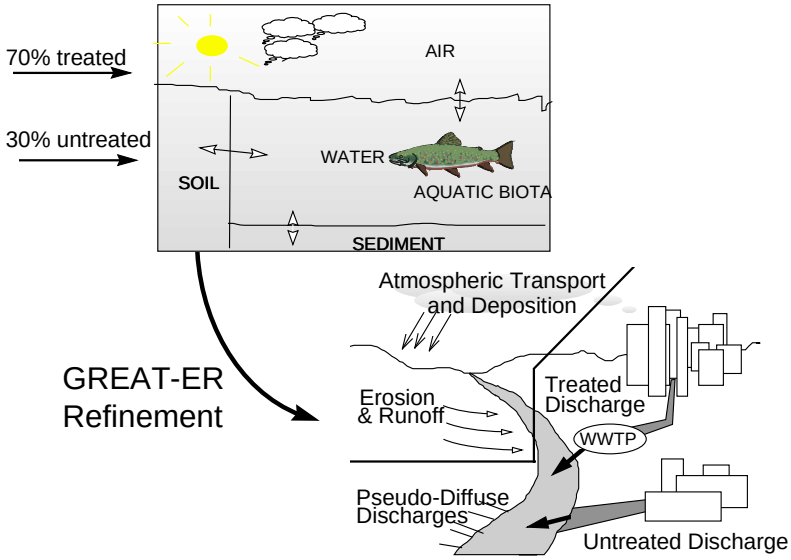

Figure 1. Refinement of generic regional exposure models by taking actual discharge pathway, treatment and river flow data into account.

Problem statement

For environmental exposure assessment, it is essential to define the primary target compartment - i.e. which compartment is being exposed to the substance and for how long- including point source versus diffuse source and intermittent versus continuous exposure. The exposure estimate may describe the exposure of the aquatic compartment close to the source of emission (e.g. wastewater effluent) and assess maximum exposure (i.e. "local" realistic worst-case estimates). Alternatively, the exposure assessment may be developed taking into consideration the fate, transport and distribution of the chemical into different media (air, water, soil and biota) which are far from the source of emission. These are considered to be "regional" background estimates. In order to decrease the complexity inherent to "real" spatial/temporal environments, the use of "generic" or "evaluative" steady state environments with standard properties has been suggested

and developed for chemical assessments. Mathematical distribution and fate models of the "Mackay level III" type (Mackay et al. 1985) are used for this purpose in the screening phases of the assessment (e.g. USES - RIVM, VROM & WVC (1994); HAZCHEM - ECETOC (1994); EUSES (1997)). These techniques to estimate regional PECs do not account for spatial and temporal variability in regional infrastructure, river flows and/or chemical emissions.

Realism can be further increased by incorporating spatial and temporal characteristics of the receiving environment in the models and underlying databases. This is the methodology adopted in GREAT-ER (Fig. 1).

Approach

The GREAT-ER project has been approached in a modular way, as previously described in detail in Feijtel et al. (1997).

GIS Data Manipulation: In the data manipulation module, input data sourced from several databases and from the hydrology module (see below) are transformed into appropriate GIS formats (Wagner et al. 1998). Geographical segmentation is also performed in this module.

Hydrology: The hydrology module combines several hydrological databases with a hydrological model. It provides the GREAT-ER system with the required river flow distributions, flow velocities and river characteristics. The Micro Low Flows model developed by the Institute of Hydrology to predict natural river flows at ungauged sites has been augmented with artificial influence data (abstractions, reservoirs, discharges) to give reliable predictions of flow distributions in the Yorkshire rivers (Young et al. 1998). A rainfall run-off model to provide hydrological data for the northern part of the Lambro catchment (Italy) was also developed. Since the Belgian study area is very large compared to the other study areas, an empirical hydrological model was developed because it was not possible to apply a model which needs a lot of input parameters. The applicability of a power function relating flow to the sum of the lengths of all upstream rivers was demonstrated. A limited validation exercise was made. It appeared that the ratio of the modelled to measured flow varied from 1 to 3 (Verdonck 1999). Because GREAT-ER's aim is to predict chemical concentrations with an accuracy factor 3 to 5 (Feijtel et al. 1997), the accuracy of this hydrological model was considered acceptable.

Waste Pathway and River Modelling: This module is used for the prediction of chemical emission, of chemical removal/transformation during conveyance and treatment, and of chemical fate in rivers (Boeije et al. 1997). Chemical fate in wastewater treatment plants and in rivers is described deterministically, with several levels of complexity being available to reflect the available information concerning both the chemical and the environment. For example, removal during sewage treatment can be either on a simple percentage removal basis, or alternatively it can be predicted using the SimpleTreat model (which is currently also used in EUSES (European Chemicals Bureau 1997)).
On top of this, GREAT-ER applies a stochastic technique (i.e. Monte Carlo simulation), which allows most input parameters to be described in terms of a distribution (normal,

lognormal, or uniform distributions can be specified). The Monte Carlo approach generally requires about 1000 runs for sufficient convergence to be obtained. Thus GREAT-ER can produce a statistical distribution of predicted environmental concentrations, as required for probabilistic risk assessment.

End-User Desktop GIS: In this module, access to and visualisation of the databases and model results is achieved, as well as the linking of the models with the databases. The GIS databases, the waste pathway models and the river models are integrated into one coherent simulation system. Such integration process results in an operational end-user system, which runs on a PC platform. The hydrological models and the ARC/INFO spatial data processing steps are not integrated into the end-user software system.
The user interface (Fig. 2) is the front-end between the user and the software system (ECETOC 1999). It allows the selection of catchments, chemicals as well as the input of model and scenario parameters. The user interface also handles filtering and visualisation of model results by the GIS. Avenue (® ESRI) has been used for the development of this interface in an ArcView (® ESRI) environment.

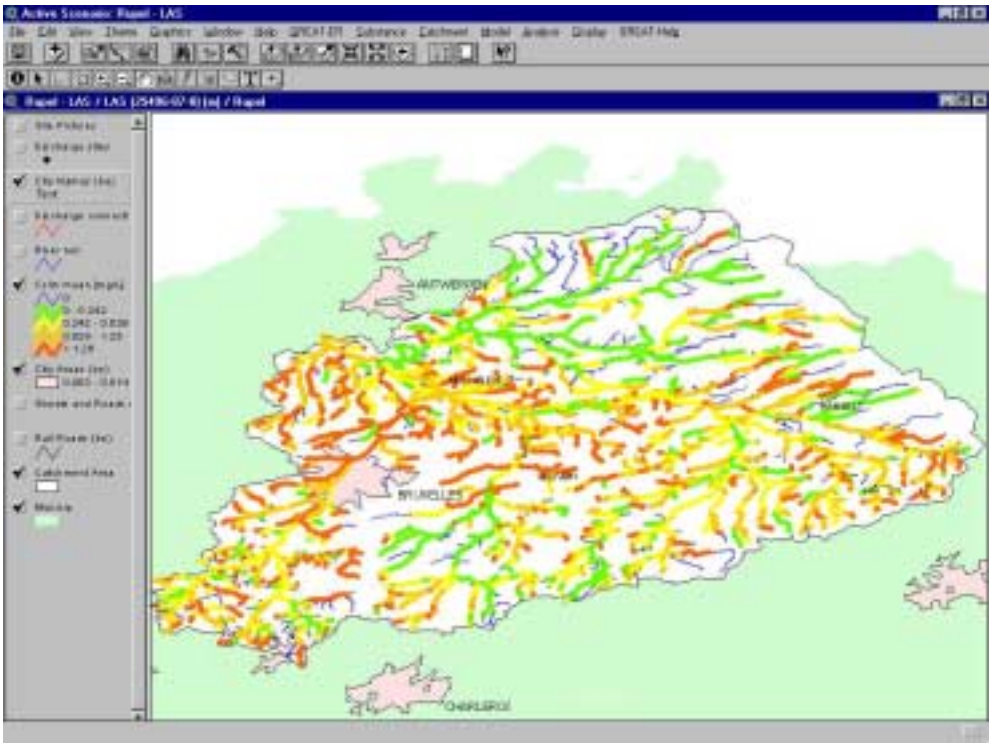

Figure 2. Output screen of GREAT-ER 1.0, showing mean predicted LAS concentrations in the Rupel catchment, Belgium.

Results

Output of GREAT-ER 1.0

GREAT-ER 1.0 offers a set of possibilities for analysis of the simulation results:

Colour-coded River Maps:

GREAT-ER's direct output provides predicted chemical concentrations linked to a river network, which are visualised as colour-coded digital GIS river maps (Fig. 2). To capture the spatial variability, the predicted concentrations are represented as quartiles of the distributions of all concentrations in the catchment. The GIS analysis tools and colour-coded maps allow identification of any locations ('hot spots') within a region where site-specific PEC values may exceed the PNEC. General water quality maps may be overlaid onto the simulation output to compare chemical presence with physico-chemistry- or biology-based water quality indices.

Concentration profiles:

Profiles of predicted concentrations through the studied catchment can be generated and exported. Such simulated profiles clearly illustrate chemical fate from a river's headwater down to its mouth, and can be used to directly compare model predictions with monitoring data, where available (Fig. 3). Results show that wastewater treatment plants have a significant though local improvement on LAS-concentrations in the rivers.

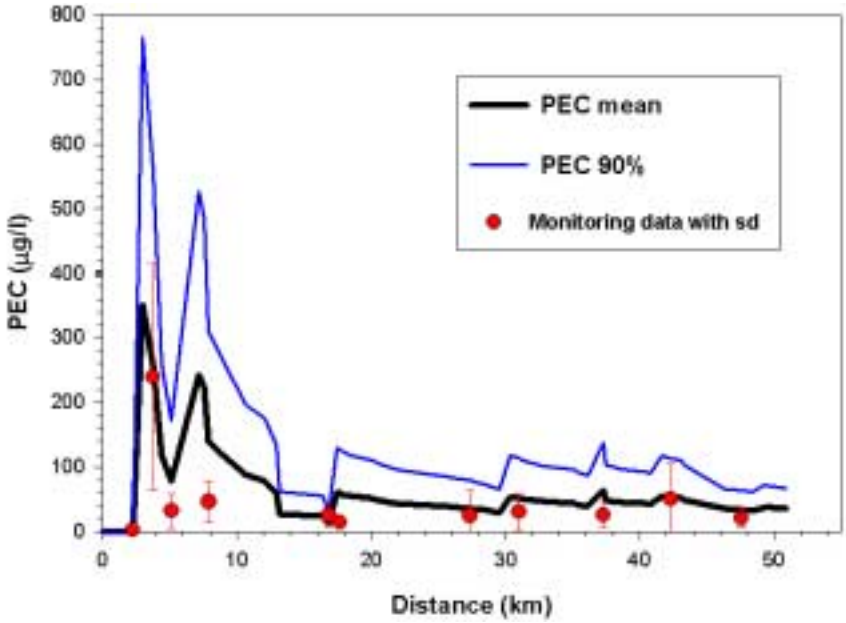

Figure 3. Example of the comparison between measured and simulated Linear Alkylbenzene Sulfonate (LAS) concentrations for the Rother catchment, Yorkshire, UK.

Aggregated PECs:

Geo-referenced model results can be aggregated to obtain a spatially averaged PEC (Fig. 4), which is representative of the river basin under study (Boeije et al. 2000). GREAT-ER can generate a $\mathbf{PEC_{initial}}$ which summarises the distribution of those concentrations found in the river stretches below each emission point source. This can be considered a GIS-analogue of the 'PEC-local' concept used in the EU TGD. GREAT-ER can also generate a $\mathbf{PEC_{catchment}}$ by

incorporating the concentration distributions in each river stretch in the catchment. This involves a weighting procedure, which can be based on stretch flow increment, length or volume. This concept can be considered a GIS analogue of the EU TGD 'PEC regional'.

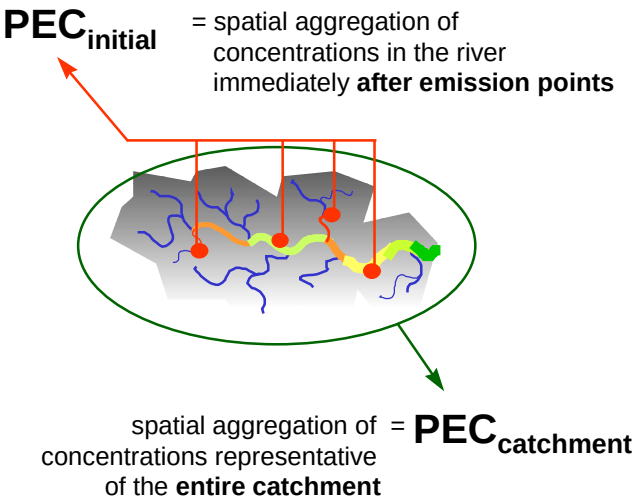

Figure. 4. Schematic illustration of the $PEC_{initial}$ and $PEC_{catchment}$ concepts, as developed within GREAT-ER for GIS-assisted regional risk assessment.

Validation and accuracy aspects

An extensive monitoring programme has been performed in order to provide the specific environmental measurements required for model calibration and validation. The calibration experiments included the determination of Linear Alkylbenzene Sulphonate (LAS) removal in six trickling-filter type sewage treatment works (Holt et al. 1998), and of LAS removal from specific rivers in Yorkshire - UK (Fox et al. 1999a,b), the Lambro - Italy (Whelan et al. in press) and the Itter - Germany (Schulze et al. 1998).

Simulations were performed based on a unique and pre-defined parameter-set:

* LAS removal in trickling filters: 94-98% (uniform distribution)
* LAS removal in activated sludge plants: 98-99.5% (uniform distribution)
* in-stream LAS decay rate: 0.06/h (no distribution)
* no removal for B in sewage treatment or rivers
* LAS usage 1.2 kg/(inhabitant*year), B usage 0.09 kg/(inhabitant*year) (UK)

The results of the validation in the UK catchments show that the predictions of mean values of both LAS and boron agree with the measurements, usually within one standard deviation of the measured values (see example in Fig. 3). The agreement is better for boron than for LAS, which undergoes specific removal processes and is therefore subject to larger environmental variability. The few site-specific deviations can be attributed to processes not included in the model or in the dataset. For example, industrial boron input was not assessed, though provision has been made in GREAT-ER to incorporate geological background boron input. The validation experiments in the Lambro catchment in Italy and the Itter catchment in Germany also indicated good agreement

between the predicted and measured LAS and boron values (not shown). Detailed papers on the accuracy assessment and validation of GREAT-ER 1.0 in the different test regions are in preparation.

Optimal geographical scale

The need to select many or few rivers in a river network (i.e. the level of geographical detail) was investigated. It was found that it is possible to simplify the river network without considerable loss of accuracy. Figure 5 shows 4 possible levels of geographical detail and their effect on an aggregated concentration of the Zuunbeek basin, a subbasin of the Rupel basin (Belgium). Per level, river stretches were selected based on their predicted flow.

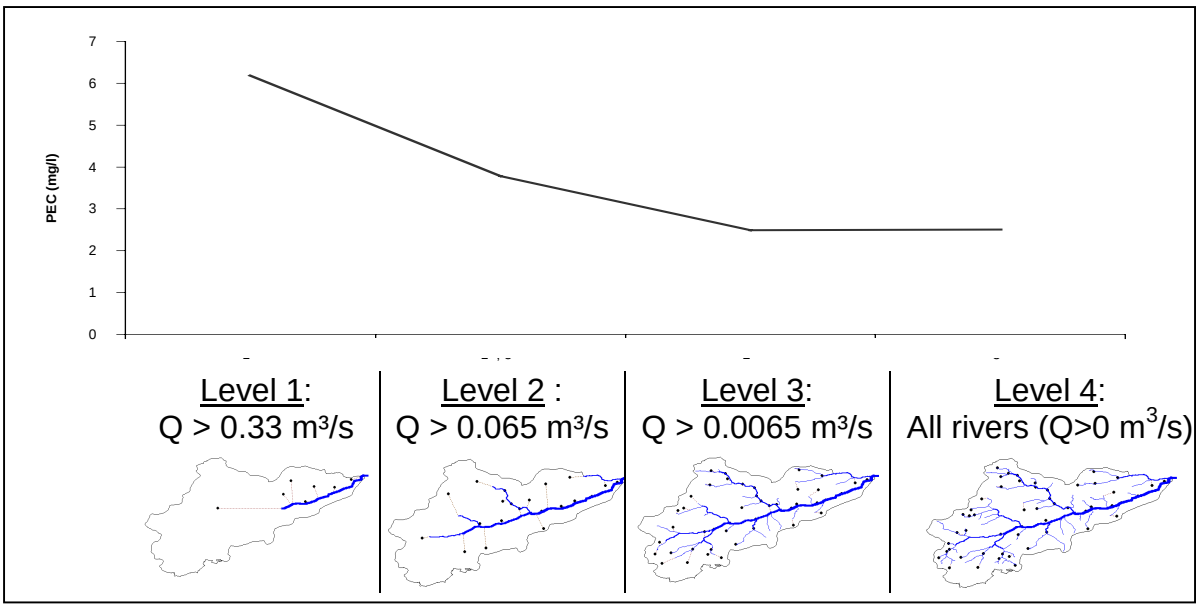

Figure 5: Aggregated $PEC_{catchment,volume}$ for different levels of geographic detail for the Zuunbeek basin, a subbasin of the Rupel basin (Q = flow in m^3/s)

If the level of detail increases, the total river length and residence time will increase (more distance travelled by the chemical in the river). Hence, the simulated impact of biodegradation will increase, and consequently the predicted concentration will decrease. However, the concentrations at level 3 and 4 were found to be practically the same. Hence, simplifying the network to level 3 appeared possible and allows reducing the required effort in terms of data collection (less geographical detail) and calculations (fewer stretches to evaluate). This is an important conclusion in view of the pan-European application of GREAT-ER.

Conclusions

▪ The final deliverable of the first stage of the GREAT-ER project is a CD-ROM which contains the software (GREAT-ER 1.0) for the exposure assessment tool, and complete datasets to run the above-mentioned catchments in Europe. The software runs on a PC, and requires both Microsoft

Windows NT® and ArcView (® ESRI) for operation. A copy of the CD-ROM and user manual can be obtained from ECETOC free of charge (contact martin.holt@ecetoc.org).

▪ The output of GREAT-ER 1.0 is three-fold:

1) a colour-coded GIS map with the distribution of a chemical's predicted aquatic environmental concentration (PEC) in the river basin of interest. These predictions can be overlaid with standard water quality maps.
2) a profile of the chemical concentration as a function of river distance for a selected branch of the river
3) aggregated PECs (i.e. $PEC_{initial}$ and $PEC_{catchment}$) to integrate the results for an entire catchment. These novel PEC definitions can be considered GIS-equivalents of the currently used 'PEC-local' and 'PEC-regional' as defined in the EU TGD.

▪ GREAT-ER 1.0 has been validated for boron and for LAS in six pilot study areas, and market consumption data for these substances are included with the CD-ROM. The results illustrate that GREAT-ER 1.0 can deliver very accurate simulations of chemical concentration in a river basin, provided reliable datasets and accurate hydrological and chemical fate models are used.

▪ This case study also showed the feasibility of implementing a new catchment and indicated which efforts are required to apply GREAT-ER on a large, ultimately pan-European scale. Problems concerning data collection may possibly occur. Fortunately, this was not the case in Belgium. Integrating the data in the GIS was the most time consuming work package. Data incompatibility and inconsistencies could induce some problems, but generally it appeared feasible to collect the necessary data, implement a relatively large catchment in a short period of time (6 man months) using (semi-) automatic procedures.

▪ Several follow-up projects are planned which will a) extend GREAT-ER to other areas in Europe, b) include other environmental compartments and processes (e.g. modelling terrestrial run-off and diffuse inputs), and c) re-design the software to a client-server application with eventual public Internet access.

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