# GREAT-ER: a new tool for management and risk assessment of chemicals in river basins
## Contribution to GREAT-ER #10

**D. Schowanek[1]*, K. Fox[2], M. Holt[3], F.R. Schroeder[4], V.Koch[5], G.Cassani[6], M. Matthies[7], G. Boeije[8], P. Vanrolleghem[8], A. Young[9], G. Morris[10], C. Gandolfi[11] and T.C.J. Feijtel[1]**

[1]Procter & Gamble Eurocar, Temselaan 100, B-1853 Strombeek-Bever, Belgium
[2]Unilever Research Port Sunlight Laboratory, Quarry Road East, Bebington, Wirral L63 3JW, UK
[3]ECETOC, Avenue van Nieuwenhuyse 4, Box 6, B-1160, Brussels, Belgium
[4]Henkel, KGaA, D-40191 Düsseldorf; Germany
[5]Clariant AG, ESHA Chemicals, D-65840, Sulzbach, Germany
[6]Condea Augusta S.p.A. Research Center, Via Reali 4, 1-20037 Padermo Dugnano, Italy
[7]University Osnabrück, Institute of Environmental Systems Research, Artilleriestrasse 34, D-49069 Osnabrück, Germany
[8]University Gent, Department of Applied Mathematics, Biometrics and Process Control, Coupure L-653, 9000 Gent, Belgium
[9]Institute of Hydrology, Crowmarsh Gifford, GB-Wallingford, Oxfordshire OX10 8BB, UK
[10]Environment Agency Laboratory Service, Olympia House, Gelderd Lane, Gelderd Road, LS12 6DD Leeds, UK
[11]University of Milan, Istituto di Idraulica Agraria, Via Celoria 2, 20133, Milan, Italy
*corresponding author: schowanek.d@pg.com

**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 visualization, combined with simple mathematical models for prediction of chemical fate. At present, the system contains information for four catchments in Yorkshire, one catchment in Italy, and two in Germany, 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 1.0 is currently being expanded with models for the terrestrial (diffuse input), air and estaurine compartments.

**Keywords** Environmental risk assessment; geographic information systems (GIS); GREAT-ER; river basins; model validation

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## 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, 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 computerized calculation model EUSES (European Union System for the Evaluation of Substances, 1997).

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 – ECOTEC (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 (Figure 1).

## Concepts and system development

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.

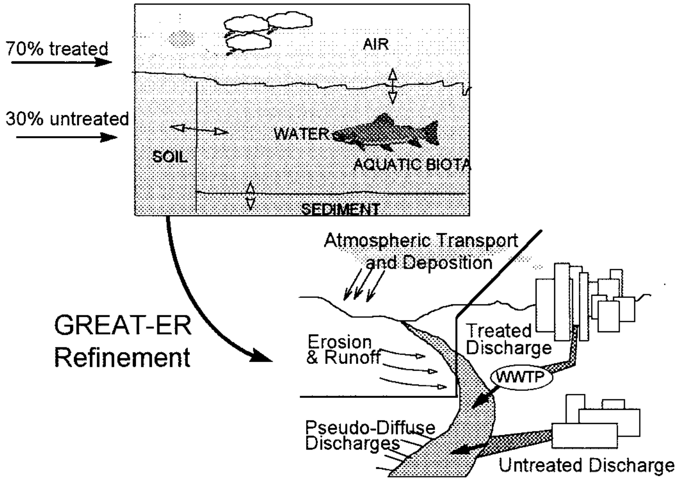


**Figure 1** Refinement of generic regional exposure models by taking actual discharge pathway, treatment and river flow data into account

### 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 unguaged 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.

### 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 deterministic ally, 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 unifier 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 visualization of the databanks and model results is achieved, as well as the linking of the models with the data banks. The GIS databanks, the waste pathway models and the river models are integrated into one coherent simulation system. Such an integration process results in an operational end-user system, which runs on a PLC platform. The hydrological models and the ARC/INFO spatial data processing steps are not integrated in the end-user software system.

The user interface (Figure 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 visualization of model results by the GIS. Avenue (® ESRI) has been used for the development of this interface in an ArcView (® ESRI) environment.

## 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 visualized as colour-coded digital GIS river maps (Figure 2). To capture the spatial variability, the predicted concentrations are represented as quartiles of the distributions of all concentrations in the catchment. PECs can e.g. also be shown as absolute concentration classes pre-defined by the user. The GIS analysis tools and colour-coded maps allow identification of any locations ('hot spots') within a region where

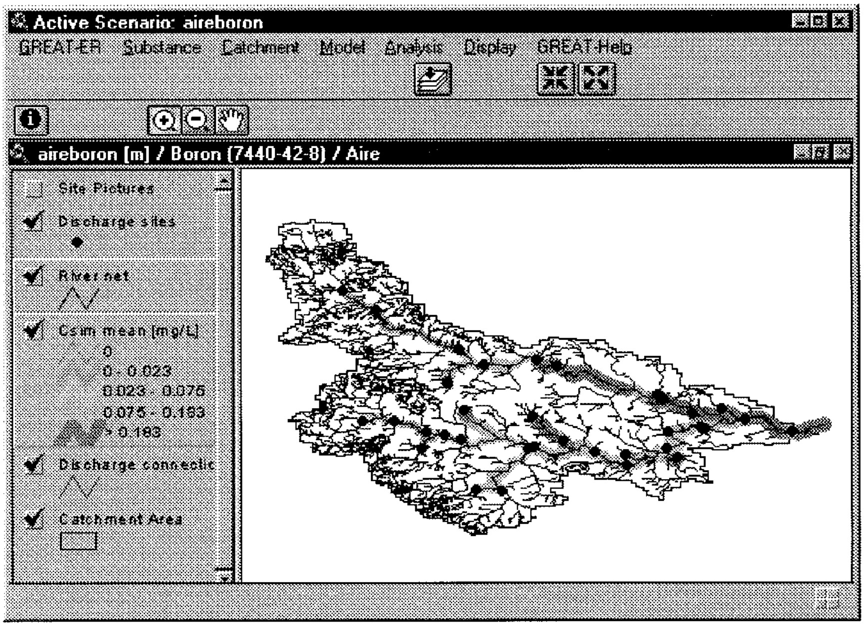


**Figure 2** Output screen of GREAT-ER 1.0, showing mean predicted boron concentrations (Csim mean) in the Aire and Calder rivers, Yorkshire, UK

site-specific PEC values may exceed the PNEC. General water quality maps may be overlain onto the simulation output to compare chemical presence with physico-chemistry- or biology-based water quality indices.

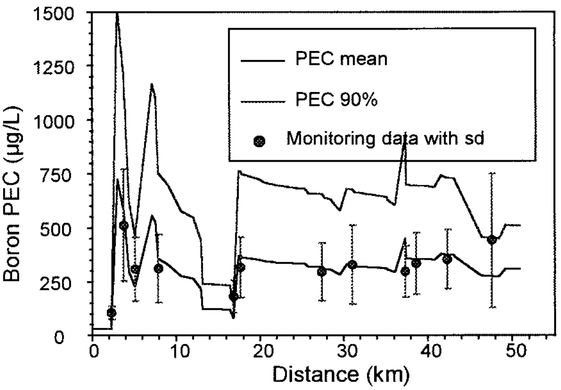
*Concentration profiles* Profiles of predicted concentrations through the studied catchment can be generated and exported. Such simulated profiles clearly illustrate chemical fate from a river's headwater down to its mouth, and can be used to directly compare model predictions with monitoring data, where available (Figure 3).

*Aggregated PECs* Geo-referenced model results can be aggregated to obtain a spatially averaged PEC (Figure 4), which is representative of the river basin under study (Boeije *et al.*, in press). GREAT-ER can generate a $\mathrm{PEC}_{\mathrm{initial}}$ which comes from the distribution of concentrations in the river stretch 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 $\mathrm{PEC}_{\mathrm{catchment}}$ 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'.

### 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 (Fox *et al.*, 1999a,b).

For the validation programme, over 2000 grab samples from sewage treatment plant effluents and from Environment Agency (EA) river monitoring sites in the four Yorkshire



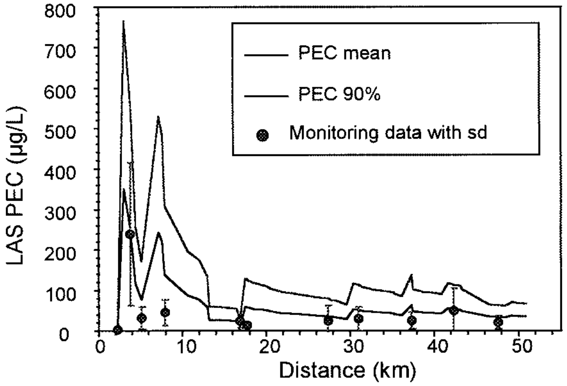


**Figure 3** Example of the comparison between measured and simulated B (top) and Linear Akylbenzene Sulfonate (LAS) concentrations (bottom) for the Rother catchment, Yorkshire, UK

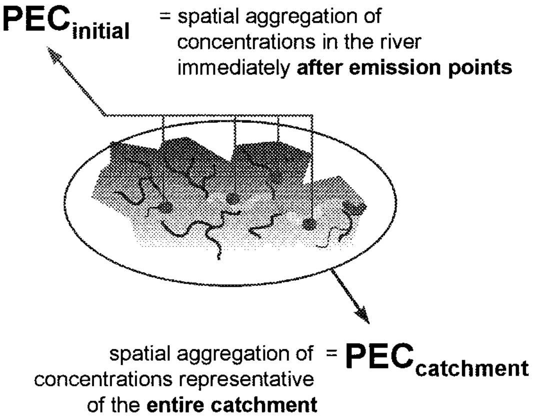


**Figure 4** Schematic illustration of the PEC$_{\text{initial}}$ and PEC$_{\text{catchment}}$ concepts, as developed within GREAT-ER for GIS-assisted regional risk assessment

catchments (Aire, Calder, Went, and Rother) have been collected, over a period spanning almost two years, as part of the EA and Yorkshire Water river sampling and effluent sampling programmes. These have been analysed for the anionic surfactant LAS (which both adsorbs and biodegrades), and boron (a conservative substance), as well as for normal water quality parameters. In the case of the Lambro (Whelan *et al.*, 1999) and the Itter

(Schulze *et al.*, 1998), similar campaigns were executed, with some adjustments in approach as imposed by the local conditions.

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 Figure 3). The agreement is better for boron than for LAS, which undergoes specific removal processes and is therefore subject to greater 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 indicate 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.

## 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 COD-ROM and user manual can be obtained from ECETOC free of charge.
- 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 overlain 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.
- 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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